Entering Link 1 = C:\G09W\l1.exe PID= 4032.

Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009,2011,

Gaussian, Inc. All Rights Reserved.

This is part of the Gaussian(R) 09 program. It is based on

the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),

the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),

the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),

the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),

the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),

the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),

the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon

University), and the Gaussian 82(TM) system (copyright 1983,

Carnegie Mellon University). Gaussian is a federally registered

trademark of Gaussian, Inc.

This software contains proprietary and confidential information,

including trade secrets, belonging to Gaussian, Inc.

This software is provided under written license and may be

used, copied, transmitted, or stored only in accord with that

written license.

The following legend is applicable only to US Government

contracts under FAR:

RESTRICTED RIGHTS LEGEND

Use, reproduction and disclosure by the US Government is

subject to restrictions as set forth in subparagraphs (a)

and (c) of the Commercial Computer Software - Restricted

Rights clause in FAR 52.227-19.

Gaussian, Inc.

340 Quinnipiac St., Bldg. 40, Wallingford CT 06492

---------------------------------------------------------------

Warning -- This program may not be used in any manner that

competes with the business of Gaussian, Inc. or will provide

assistance to any competitor of Gaussian, Inc. The licensee

of this program is prohibited from giving any competitor of

Gaussian, Inc. access to this program. By using this program,

the user acknowledges that Gaussian, Inc. is engaged in the

business of creating and licensing software in the field of

computational chemistry and represents and warrants to the

licensee that it is not a competitor of Gaussian, Inc. and that

it will not use this program in any manner prohibited above.

---------------------------------------------------------------

Cite this work as:

Gaussian 09, Revision C.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,

M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,

G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,

A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,

M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,

Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,

J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,

K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,

K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,

M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,

V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,

O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,

R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,

P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,

O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,

and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Gaussian 09: EM64W-G09RevC.01 23-Sep-2011

07-Feb-2013

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

%chk=\\ic.ac.uk\homes\mc1210\Desktop\module 3\part\_2\exo endo\exo\exo\_opt\_fre.ch

k

----------------------------------------------------

# opt=(calcfc,ts,noeigen) freq am1 geom=connectivity

----------------------------------------------------

1/5=1,10=4,11=1,14=-1,18=20,26=1,38=1,57=2/1,3;

2/9=110,12=2,17=6,18=5,40=1/2;

3/5=2,16=1,25=1,41=700000,71=2/1,2,3;

4/35=1/1;

5/5=2,35=1,38=5/2;

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1,7=6,13=1/2;

6/7=2,8=2,9=2,10=2,28=1/1;

7/10=1,18=20,25=1/1,2,3,16;

1/5=1,10=4,11=1,14=-1,18=20/3(2);

2/9=110/2;

99//99;

2/9=110/2;

3/5=2,16=1,25=1,41=700000,71=1,135=20/1,2,3;

4/5=5,16=3,35=1/1;

5/5=2,35=1,38=5/2;

7//1,2,3,16;

1/5=1,11=1,14=-1,18=20/3(-5);

2/9=110/2;

6/7=2,8=2,9=2,10=2,19=2,28=1/1;

99/9=1/99;

-------------------

Title Card Required

-------------------

Charge = 0 Multiplicity = 1

Symbolic Z-Matrix:

C -1.59136 1.10592 0.17254

C 0.12673 1.32142 0.39439

C -0.93563 3.51406 0.17254

C -2.1091 2.53817 0.17332

H -1.96465 0.55923 -0.73066

H -2.74681 2.72039 -0.72896

C 0.43337 1.83783 -1.07052

H 1.55309 1.83086 -1.08391

H 0.08287 1.29838 -1.98711

C -0.08499 3.26984 -1.0709

H 0.77076 3.99196 -1.08557

H -0.7003 3.45917 -1.98717

H -1.31672 4.56831 0.17258

H 0.50781 0.26717 0.39439

O 3.26422 4.11148 0.96632

C 0.87979 4.06766 1.2851

C 1.28646 2.62406 1.73535

C 2.05768 4.82485 0.68116

O 2.03723 5.875 0.04629

C 2.98194 2.92839 1.71903

O 3.8541 2.14698 2.0865

H 0.57023 4.60714 2.15575

H 0.96687 2.46474 2.744

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

----------------------------

! Initial Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.7457 calculate D2E/DX2 analytically !

! R2 R(1,4) 1.5229 calculate D2E/DX2 analytically !

! R3 R(1,5) 1.1198 calculate D2E/DX2 analytically !

! R4 R(2,7) 1.5832 calculate D2E/DX2 analytically !

! R5 R(2,14) 1.121 calculate D2E/DX2 analytically !

! R6 R(2,17) 2.2 calculate D2E/DX2 analytically !

! R7 R(3,4) 1.5262 calculate D2E/DX2 analytically !

! R8 R(3,10) 1.5262 calculate D2E/DX2 analytically !

! R9 R(3,13) 1.121 calculate D2E/DX2 analytically !

! R10 R(3,16) 2.2 calculate D2E/DX2 analytically !

! R11 R(4,6) 1.1198 calculate D2E/DX2 analytically !

! R12 R(7,8) 1.1198 calculate D2E/DX2 analytically !

! R13 R(7,9) 1.1198 calculate D2E/DX2 analytically !

! R14 R(7,10) 1.5229 calculate D2E/DX2 analytically !

! R15 R(10,11) 1.1198 calculate D2E/DX2 analytically !

! R16 R(10,12) 1.1198 calculate D2E/DX2 analytically !

! R17 R(15,18) 1.4304 calculate D2E/DX2 analytically !

! R18 R(15,20) 1.4304 calculate D2E/DX2 analytically !

! R19 R(16,17) 1.5659 calculate D2E/DX2 analytically !

! R20 R(16,18) 1.525 calculate D2E/DX2 analytically !

! R21 R(16,22) 1.07 calculate D2E/DX2 analytically !

! R22 R(17,20) 1.7227 calculate D2E/DX2 analytically !

! R23 R(17,23) 1.07 calculate D2E/DX2 analytically !

! R24 R(18,19) 1.2273 calculate D2E/DX2 analytically !

! R25 R(20,21) 1.2273 calculate D2E/DX2 analytically !

! A1 A(2,1,4) 102.6163 calculate D2E/DX2 analytically !

! A2 A(2,1,5) 119.3958 calculate D2E/DX2 analytically !

! A3 A(4,1,5) 110.2558 calculate D2E/DX2 analytically !

! A4 A(1,2,7) 96.5054 calculate D2E/DX2 analytically !

! A5 A(1,2,14) 102.6191 calculate D2E/DX2 analytically !

! A6 A(1,2,17) 132.0178 calculate D2E/DX2 analytically !

! A7 A(7,2,14) 103.9401 calculate D2E/DX2 analytically !

! A8 A(7,2,17) 105.5898 calculate D2E/DX2 analytically !

! A9 A(14,2,17) 112.1878 calculate D2E/DX2 analytically !

! A10 A(4,3,10) 109.0642 calculate D2E/DX2 analytically !

! A11 A(4,3,13) 109.8742 calculate D2E/DX2 analytically !

! A12 A(4,3,16) 142.6648 calculate D2E/DX2 analytically !

! A13 A(10,3,13) 109.8752 calculate D2E/DX2 analytically !

! A14 A(10,3,16) 89.562 calculate D2E/DX2 analytically !

! A15 A(13,3,16) 92.5136 calculate D2E/DX2 analytically !

! A16 A(1,4,3) 109.8736 calculate D2E/DX2 analytically !

! A17 A(1,4,6) 110.2561 calculate D2E/DX2 analytically !

! A18 A(3,4,6) 109.4746 calculate D2E/DX2 analytically !

! A19 A(2,7,8) 101.6943 calculate D2E/DX2 analytically !

! A20 A(2,7,9) 122.6558 calculate D2E/DX2 analytically !

! A21 A(2,7,10) 103.9458 calculate D2E/DX2 analytically !

! A22 A(8,7,9) 107.4686 calculate D2E/DX2 analytically !

! A23 A(8,7,10) 110.2543 calculate D2E/DX2 analytically !

! A24 A(9,7,10) 110.2569 calculate D2E/DX2 analytically !

! A25 A(3,10,7) 109.8742 calculate D2E/DX2 analytically !

! A26 A(3,10,11) 109.4759 calculate D2E/DX2 analytically !

! A27 A(3,10,12) 109.4711 calculate D2E/DX2 analytically !

! A28 A(7,10,11) 110.2576 calculate D2E/DX2 analytically !

! A29 A(7,10,12) 110.2551 calculate D2E/DX2 analytically !

! A30 A(11,10,12) 107.4672 calculate D2E/DX2 analytically !

! A31 A(18,15,20) 110.5455 calculate D2E/DX2 analytically !

! A32 A(3,16,17) 97.3384 calculate D2E/DX2 analytically !

! A33 A(3,16,18) 124.198 calculate D2E/DX2 analytically !

! A34 A(3,16,22) 107.4357 calculate D2E/DX2 analytically !

! A35 A(17,16,18) 111.7787 calculate D2E/DX2 analytically !

! A36 A(17,16,22) 107.8169 calculate D2E/DX2 analytically !

! A37 A(18,16,22) 107.1792 calculate D2E/DX2 analytically !

! A38 A(2,17,16) 103.5146 calculate D2E/DX2 analytically !

! A39 A(2,17,20) 128.1456 calculate D2E/DX2 analytically !

! A40 A(2,17,23) 109.2066 calculate D2E/DX2 analytically !

! A41 A(16,17,20) 95.1645 calculate D2E/DX2 analytically !

! A42 A(16,17,23) 109.3136 calculate D2E/DX2 analytically !

! A43 A(20,17,23) 109.2206 calculate D2E/DX2 analytically !

! A44 A(15,18,16) 108.9629 calculate D2E/DX2 analytically !

! A45 A(15,18,19) 122.9503 calculate D2E/DX2 analytically !

! A46 A(16,18,19) 128.0868 calculate D2E/DX2 analytically !

! A47 A(15,20,17) 110.2029 calculate D2E/DX2 analytically !

! A48 A(15,20,21) 122.9521 calculate D2E/DX2 analytically !

! A49 A(17,20,21) 125.7391 calculate D2E/DX2 analytically !

! D1 D(4,1,2,7) -74.1277 calculate D2E/DX2 analytically !

! D2 D(4,1,2,14) 179.9699 calculate D2E/DX2 analytically !

! D3 D(4,1,2,17) 43.7004 calculate D2E/DX2 analytically !

! D4 D(5,1,2,7) 48.1012 calculate D2E/DX2 analytically !

! D5 D(5,1,2,14) -57.8012 calculate D2E/DX2 analytically !

! D6 D(5,1,2,17) 165.9294 calculate D2E/DX2 analytically !

! D7 D(2,1,4,3) 7.5309 calculate D2E/DX2 analytically !

! D8 D(2,1,4,6) 128.2793 calculate D2E/DX2 analytically !

! D9 D(5,1,4,3) -120.6933 calculate D2E/DX2 analytically !

! D10 D(5,1,4,6) 0.0551 calculate D2E/DX2 analytically !

! D11 D(1,2,7,8) -170.2344 calculate D2E/DX2 analytically !

! D12 D(1,2,7,9) -50.4486 calculate D2E/DX2 analytically !

! D13 D(1,2,7,10) 75.2045 calculate D2E/DX2 analytically !

! D14 D(14,2,7,8) -65.4691 calculate D2E/DX2 analytically !

! D15 D(14,2,7,9) 54.3167 calculate D2E/DX2 analytically !

! D16 D(14,2,7,10) 179.9698 calculate D2E/DX2 analytically !

! D17 D(17,2,7,8) 52.7745 calculate D2E/DX2 analytically !

! D18 D(17,2,7,9) 172.5603 calculate D2E/DX2 analytically !

! D19 D(17,2,7,10) -61.7865 calculate D2E/DX2 analytically !

! D20 D(1,2,17,16) -62.3922 calculate D2E/DX2 analytically !

! D21 D(1,2,17,20) -170.2398 calculate D2E/DX2 analytically !

! D22 D(1,2,17,23) 53.9631 calculate D2E/DX2 analytically !

! D23 D(7,2,17,16) 51.7941 calculate D2E/DX2 analytically !

! D24 D(7,2,17,20) -56.0535 calculate D2E/DX2 analytically !

! D25 D(7,2,17,23) 168.1494 calculate D2E/DX2 analytically !

! D26 D(14,2,17,16) 164.3699 calculate D2E/DX2 analytically !

! D27 D(14,2,17,20) 56.5223 calculate D2E/DX2 analytically !

! D28 D(14,2,17,23) -79.2749 calculate D2E/DX2 analytically !

! D29 D(10,3,4,1) 59.4794 calculate D2E/DX2 analytically !

! D30 D(10,3,4,6) -61.7392 calculate D2E/DX2 analytically !

! D31 D(13,3,4,1) 179.9705 calculate D2E/DX2 analytically !

! D32 D(13,3,4,6) 58.7519 calculate D2E/DX2 analytically !

! D33 D(16,3,4,1) -56.6071 calculate D2E/DX2 analytically !

! D34 D(16,3,4,6) -177.8258 calculate D2E/DX2 analytically !

! D35 D(4,3,10,7) -59.5417 calculate D2E/DX2 analytically !

! D36 D(4,3,10,11) 179.2366 calculate D2E/DX2 analytically !

! D37 D(4,3,10,12) 61.6739 calculate D2E/DX2 analytically !

! D38 D(13,3,10,7) 179.9679 calculate D2E/DX2 analytically !

! D39 D(13,3,10,11) 58.7461 calculate D2E/DX2 analytically !

! D40 D(13,3,10,12) -58.8166 calculate D2E/DX2 analytically !

! D41 D(16,3,10,7) 87.4534 calculate D2E/DX2 analytically !

! D42 D(16,3,10,11) -33.7683 calculate D2E/DX2 analytically !

! D43 D(16,3,10,12) -151.3311 calculate D2E/DX2 analytically !

! D44 D(4,3,16,17) 35.2043 calculate D2E/DX2 analytically !

! D45 D(4,3,16,18) 157.8744 calculate D2E/DX2 analytically !

! D46 D(4,3,16,22) -76.1299 calculate D2E/DX2 analytically !

! D47 D(10,3,16,17) -86.7039 calculate D2E/DX2 analytically !

! D48 D(10,3,16,18) 35.9662 calculate D2E/DX2 analytically !

! D49 D(10,3,16,22) 161.9619 calculate D2E/DX2 analytically !

! D50 D(13,3,16,17) 163.4207 calculate D2E/DX2 analytically !

! D51 D(13,3,16,18) -73.9091 calculate D2E/DX2 analytically !

! D52 D(13,3,16,22) 52.0866 calculate D2E/DX2 analytically !

! D53 D(2,7,10,3) -12.3769 calculate D2E/DX2 analytically !

! D54 D(2,7,10,11) 108.3745 calculate D2E/DX2 analytically !

! D55 D(2,7,10,12) -133.1206 calculate D2E/DX2 analytically !

! D56 D(8,7,10,3) -120.6921 calculate D2E/DX2 analytically !

! D57 D(8,7,10,11) 0.0593 calculate D2E/DX2 analytically !

! D58 D(8,7,10,12) 118.5642 calculate D2E/DX2 analytically !

! D59 D(9,7,10,3) 120.8021 calculate D2E/DX2 analytically !

! D60 D(9,7,10,11) -118.4465 calculate D2E/DX2 analytically !

! D61 D(9,7,10,12) 0.0584 calculate D2E/DX2 analytically !

! D62 D(20,15,18,16) 0.0 calculate D2E/DX2 analytically !

! D63 D(20,15,18,19) 179.9979 calculate D2E/DX2 analytically !

! D64 D(18,15,20,17) 11.4095 calculate D2E/DX2 analytically !

! D65 D(18,15,20,21) -179.998 calculate D2E/DX2 analytically !

! D66 D(3,16,17,2) 17.0248 calculate D2E/DX2 analytically !

! D67 D(3,16,17,20) 148.2915 calculate D2E/DX2 analytically !

! D68 D(3,16,17,23) -99.2549 calculate D2E/DX2 analytically !

! D69 D(18,16,17,2) -114.4054 calculate D2E/DX2 analytically !

! D70 D(18,16,17,20) 16.8613 calculate D2E/DX2 analytically !

! D71 D(18,16,17,23) 129.3149 calculate D2E/DX2 analytically !

! D72 D(22,16,17,2) 128.0464 calculate D2E/DX2 analytically !

! D73 D(22,16,17,20) -100.6869 calculate D2E/DX2 analytically !

! D74 D(22,16,17,23) 11.7667 calculate D2E/DX2 analytically !

! D75 D(3,16,18,15) -128.6688 calculate D2E/DX2 analytically !

! D76 D(3,16,18,19) 51.3334 calculate D2E/DX2 analytically !

! D77 D(17,16,18,15) -12.7048 calculate D2E/DX2 analytically !

! D78 D(17,16,18,19) 167.2974 calculate D2E/DX2 analytically !

! D79 D(22,16,18,15) 105.2257 calculate D2E/DX2 analytically !

! D80 D(22,16,18,19) -74.7721 calculate D2E/DX2 analytically !

! D81 D(2,17,20,15) 94.6408 calculate D2E/DX2 analytically !

! D82 D(2,17,20,21) -73.5606 calculate D2E/DX2 analytically !

! D83 D(16,17,20,15) -17.0347 calculate D2E/DX2 analytically !

! D84 D(16,17,20,21) 174.764 calculate D2E/DX2 analytically !

! D85 D(23,17,20,15) -129.5668 calculate D2E/DX2 analytically !

! D86 D(23,17,20,21) 62.2318 calculate D2E/DX2 analytically !

--------------------------------------------------------------------------------

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07

Number of steps in this run= 138 maximum allowed number of steps= 138.

Search for a saddle point of order 1.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.591361 1.105924 0.172543

2 6 0 0.126732 1.321425 0.394386

3 6 0 -0.935634 3.514055 0.172543

4 6 0 -2.109099 2.538166 0.173324

5 1 0 -1.964653 0.559227 -0.730660

6 1 0 -2.746806 2.720388 -0.728960

7 6 0 0.433369 1.837829 -1.070521

8 1 0 1.553089 1.830859 -1.083907

9 1 0 0.082872 1.298376 -1.987108

10 6 0 -0.084995 3.269842 -1.070903

11 1 0 0.770763 3.991955 -1.085571

12 1 0 -0.700299 3.459168 -1.987175

13 1 0 -1.316722 4.568310 0.172575

14 1 0 0.507808 0.267174 0.394388

15 8 0 3.264224 4.111485 0.966319

16 6 0 0.879785 4.067659 1.285098

17 6 0 1.286460 2.624056 1.735350

18 6 0 2.057677 4.824851 0.681163

19 8 0 2.037234 5.875004 0.046288

20 6 0 2.981944 2.928391 1.719026

21 8 0 3.854103 2.146977 2.086501

22 1 0 0.570234 4.607142 2.155750

23 1 0 0.966871 2.464745 2.744004

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.745708 0.000000

3 C 2.495811 2.446520 0.000000

4 C 1.522948 2.555047 1.526231 0.000000

5 H 1.119821 2.494106 3.256634 2.180425 0.000000

6 H 2.180425 3.387657 2.173237 1.119818 2.298344

7 C 2.486046 1.583241 2.495819 2.915779 2.738766

8 H 3.462913 2.116452 3.256618 3.936056 3.757172

9 H 2.739377 2.382009 3.257404 3.318024 2.513436

10 C 2.915105 2.447086 1.526232 2.486051 3.316069

11 H 3.935944 3.120381 2.173253 3.462936 4.403644

12 H 3.316041 3.305413 2.173195 2.738744 3.403980

13 H 3.473261 3.560200 1.121018 2.179300 4.160336

14 H 2.271393 1.121010 3.560193 3.471955 2.732048

15 O 5.765430 4.237381 4.315763 5.654801 6.545183

16 C 4.014500 2.983665 2.200000 3.536780 4.946029

17 C 3.609562 2.200000 2.858699 3.738598 4.573232

18 C 5.234939 4.010584 3.307082 4.780047 6.030583

19 O 5.993894 4.950381 3.798416 5.323787 6.698973

20 C 5.160243 3.534013 4.252296 5.334809 6.006889

21 O 5.865160 4.175894 5.336077 6.274795 6.656971

22 H 4.567726 3.754335 2.719482 3.922945 5.580558

23 H 3.873416 2.744762 3.366450 4.009410 4.929311

6 7 8 9 10

6 H 0.000000

7 C 3.317994 0.000000

8 H 4.405263 1.119822 0.000000

9 H 3.407658 1.119817 1.805782 0.000000

10 C 2.739354 1.522945 2.180404 2.180433 0.000000

11 H 3.757306 2.180440 2.298341 2.922556 1.119814

12 H 2.513383 2.180412 2.923190 2.298343 1.119820

13 H 2.504540 3.473274 4.160313 4.161197 2.179314

14 H 4.227609 2.149059 2.392296 2.629728 3.393303

15 O 6.398562 4.163168 3.511789 5.172747 4.009477

16 C 4.361620 3.274197 3.326980 4.360198 2.667967

17 C 4.727508 3.036252 2.940826 4.130707 3.189511

18 C 5.431415 3.824797 3.511989 4.843093 3.174717

19 O 5.782703 4.485357 4.226919 5.375849 3.541022

20 C 6.233335 3.932700 3.332061 4.979658 4.160096

21 O 7.199140 4.665167 3.930150 5.615745 5.171703

22 H 4.783737 4.254016 4.378256 5.324352 3.553728

23 H 5.090994 3.902338 3.924075 4.952301 4.038330

11 12 13 14 15

11 H 0.000000

12 H 1.805762 0.000000

13 H 2.504538 2.504934 0.000000

14 H 4.016642 4.161753 4.677380 0.000000

15 O 3.231391 4.986590 4.671593 4.764836 0.000000

16 C 2.374381 3.684385 2.512568 3.921150 2.406053

17 C 3.177213 4.301373 3.605404 2.821236 2.591410

18 C 2.339062 4.073272 3.422140 4.822525 1.430371

19 O 2.535927 4.179153 3.601724 5.823064 2.337084

20 C 3.726426 5.251339 4.853800 3.867569 1.430371

21 O 4.793012 6.249740 6.021910 4.194592 2.337104

22 H 3.305273 4.482848 2.737717 4.684188 2.986303

23 H 4.127526 5.113940 4.031380 3.249731 3.339124

16 17 18 19 20

16 C 0.000000

17 C 1.565919 0.000000

18 C 1.524961 2.559215 0.000000

19 O 2.478071 3.739687 1.227317 0.000000

20 C 2.430082 1.722659 2.351167 3.517536 0.000000

21 O 3.630129 2.635091 3.517546 4.621869 1.227317

22 H 1.070000 2.149964 2.105776 2.865205 2.970737

23 H 2.169176 1.070000 3.318926 4.478082 2.307828

21 22 23

21 O 0.000000

22 H 4.103779 0.000000

23 H 2.978154 2.256818 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 3.049064 -1.056745 -0.339287

2 6 0 1.401802 -1.360402 0.152463

3 6 0 1.598845 0.956696 -0.607598

4 6 0 2.976281 0.362119 -0.887828

5 1 0 3.872062 -1.138798 0.415659

6 1 0 3.762865 1.002217 -0.412904

7 6 0 1.430380 -0.449771 1.447293

8 1 0 0.462862 -0.724719 1.939546

9 1 0 2.235316 -0.526106 2.222045

10 6 0 1.358610 0.969452 0.899554

11 1 0 0.354950 1.417472 1.113867

12 1 0 2.127724 1.615451 1.394677

13 1 0 1.545439 2.001294 -1.010892

14 1 0 1.455206 -2.405005 0.555721

15 8 0 -2.536767 0.189003 0.358407

16 6 0 -0.550928 0.618630 -0.930374

17 6 0 -0.526374 -0.943290 -0.821270

18 6 0 -1.653038 1.228588 -0.070834

19 8 0 -1.809020 2.406539 0.236425

20 6 0 -2.107707 -1.076801 -0.151111

21 8 0 -2.702767 -2.125345 0.078599

22 1 0 -0.766259 0.872442 -1.947287

23 1 0 -0.523343 -1.366680 -1.803935

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3034937 0.6159069 0.4941586

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 447.2185372316 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Simple Huckel Guess.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

The electronic state of the initial guess is 1-A.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.310048117241 A.U. after 17 cycles

Convg = 0.4262D-08 -V/T = 1.0067

Range of M.O.s used for correlation: 1 62

NBasis= 62 NAE= 34 NBE= 34 NFC= 0 NFV= 0

NROrb= 62 NOA= 34 NOB= 34 NVA= 28 NVB= 28

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

G2DrvN: will do 24 centers at a time, making 1 passes doing MaxLOS=1.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFDir/FoFCou used for L=0 through L=1.

End of G2Drv Frequency-dependent properties file 721 does not exist.

End of G2Drv Frequency-dependent properties file 722 does not exist.

IDoAtm=11111111111111111111111

Differentiating once with respect to nuclear coordinates.

Electric field/nuclear overlap derivatives assumed to be zero.

Keep J ints in memory in canonical form, NReq=811133.

There are 72 degrees of freedom in the 1st order CPHF. IDoFFX=5.

LinEq1: Iter= 0 NonCon= 69 RMS=1.26D-02 Max=1.11D-01

AX will form 69 AO Fock derivatives at one time.

LinEq1: Iter= 1 NonCon= 69 RMS=2.80D-03 Max=2.17D-02

LinEq1: Iter= 2 NonCon= 69 RMS=7.37D-04 Max=8.09D-03

LinEq1: Iter= 3 NonCon= 69 RMS=1.67D-04 Max=1.78D-03

LinEq1: Iter= 4 NonCon= 69 RMS=4.02D-05 Max=4.75D-04

LinEq1: Iter= 5 NonCon= 53 RMS=8.28D-06 Max=9.47D-05

LinEq1: Iter= 6 NonCon= 16 RMS=1.61D-06 Max=1.84D-05

LinEq1: Iter= 7 NonCon= 0 RMS=3.35D-07 Max=3.63D-06

Linear equations converged to 1.000D-06 1.000D-05 after 7 iterations.

End of Minotr Frequency-dependent properties file 721 does not exist.

End of Minotr Frequency-dependent properties file 722 does not exist.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -1.49907 -1.43880 -1.40234 -1.37371 -1.18869

Alpha occ. eigenvalues -- -1.13219 -1.09160 -0.95423 -0.86745 -0.83114

Alpha occ. eigenvalues -- -0.81680 -0.78511 -0.68134 -0.66206 -0.64866

Alpha occ. eigenvalues -- -0.63444 -0.62295 -0.59246 -0.57663 -0.55871

Alpha occ. eigenvalues -- -0.55220 -0.53798 -0.52048 -0.49962 -0.48119

Alpha occ. eigenvalues -- -0.47147 -0.46411 -0.45698 -0.42856 -0.42834

Alpha occ. eigenvalues -- -0.42046 -0.40433 -0.35886 -0.34692

Alpha virt. eigenvalues -- -0.05624 -0.03709 -0.02788 0.02274 0.03378

Alpha virt. eigenvalues -- 0.04478 0.07964 0.08682 0.09802 0.10861

Alpha virt. eigenvalues -- 0.11907 0.12141 0.12228 0.12941 0.13286

Alpha virt. eigenvalues -- 0.13790 0.14236 0.14473 0.14673 0.15392

Alpha virt. eigenvalues -- 0.15562 0.15697 0.15778 0.16580 0.16785

Alpha virt. eigenvalues -- 0.18763 0.21473 0.22155

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.150971 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 4.012929 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 3.962549 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 4.205229 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.830418 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.849114

7 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 4.203100 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.902607 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.888347 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 4.182198 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.887818 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.912923

13 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.895675 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.901041 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 6.242242 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 4.268006 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 4.063262 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 3.667081

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23

1 C 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 6.256166 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 3.729416 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 6.242419 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.875426 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.871063

Mulliken atomic charges:

1

1 C -0.150971

2 C -0.012929

3 C 0.037451

4 C -0.205229

5 H 0.169582

6 H 0.150886

7 C -0.203100

8 H 0.097393

9 H 0.111653

10 C -0.182198

11 H 0.112182

12 H 0.087077

13 H 0.104325

14 H 0.098959

15 O -0.242242

16 C -0.268006

17 C -0.063262

18 C 0.332919

19 O -0.256166

20 C 0.270584

21 O -0.242419

22 H 0.124574

23 H 0.128937

Sum of Mulliken atomic charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.018612

2 C 0.086030

3 C 0.141776

4 C -0.054343

7 C 0.005947

10 C 0.017061

15 O -0.242242

16 C -0.143432

17 C 0.065675

18 C 0.332919

19 O -0.256166

20 C 0.270584

21 O -0.242419

Sum of Mulliken charges with hydrogens summed into heavy atoms = 0.00000

APT atomic charges:

1

1 C -0.150971

2 C -0.012929

3 C 0.037451

4 C -0.205229

5 H 0.169582

6 H 0.150886

7 C -0.203100

8 H 0.097393

9 H 0.111653

10 C -0.182198

11 H 0.112182

12 H 0.087077

13 H 0.104325

14 H 0.098959

15 O -0.242242

16 C -0.268006

17 C -0.063262

18 C 0.332919

19 O -0.256166

20 C 0.270584

21 O -0.242419

22 H 0.124574

23 H 0.128937

Sum of APT charges= 0.00000

APT Atomic charges with hydrogens summed into heavy atoms:

1

1 C 0.018612

2 C 0.086030

3 C 0.141776

4 C -0.054343

5 H 0.000000

6 H 0.000000

7 C 0.005947

8 H 0.000000

9 H 0.000000

10 C 0.017061

11 H 0.000000

12 H 0.000000

13 H 0.000000

14 H 0.000000

15 O -0.242242

16 C -0.143432

17 C 0.065675

18 C 0.332919

19 O -0.256166

20 C 0.270584

21 O -0.242419

22 H 0.000000

23 H 0.000000

Sum of APT charges= 0.00000

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 4.9494 Y= 0.0003 Z= 0.0441 Tot= 4.9496

N-N= 4.472185372316D+02 E-N=-7.983919806385D+02 KE=-4.596517850927D+01

Exact polarizability: 0.000 0.000 0.000 0.000 0.000 0.000

Approx polarizability: 128.566 1.321 108.017 3.082 -8.055 52.835

Calling FoFJK, ICntrl= 100147 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.040736719 0.187652442 -0.003312660

2 6 -0.032924960 -0.039152784 -0.054371040

3 6 0.000539276 0.049288511 -0.016451131

4 6 0.120483938 -0.127170683 -0.025982654

5 1 0.006202110 -0.015618897 0.034733016

6 1 -0.015762474 0.008754447 0.029239863

7 6 0.010638717 0.022940608 0.053642642

8 1 0.002894324 0.000987277 -0.007402278

9 1 -0.005117710 -0.007581330 0.015835832

10 6 -0.004073016 -0.006637845 0.005926407

11 1 -0.001686319 0.000835389 -0.004522849

12 1 -0.001695467 0.000774987 -0.000626618

13 1 0.006109318 -0.005523764 0.010214357

14 1 0.005248918 0.014380819 0.024433465

15 8 -0.025644328 -0.011875779 0.020561318

16 6 -0.017254939 -0.078804573 -0.010310261

17 6 0.017750446 0.066636782 -0.065244494

18 6 -0.026043017 -0.035988027 0.003943878

19 8 0.019866163 -0.021985225 0.012895680

20 6 -0.054074891 -0.034122988 -0.039862142

21 8 -0.017706777 0.037179960 -0.009270491

22 1 -0.021894021 0.017142736 0.013398263

23 1 -0.006592014 -0.022112063 0.012531896

-------------------------------------------------------------------

Cartesian Forces: Max 0.187652442 RMS 0.040506855

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.121630001 RMS 0.021936277

Search for a saddle point.

Step number 1 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- -0.01861 -0.00969 0.00015 0.00330 0.00408

Eigenvalues --- 0.00567 0.00782 0.00987 0.01260 0.01523

Eigenvalues --- 0.01863 0.01926 0.02143 0.02214 0.02405

Eigenvalues --- 0.02575 0.02854 0.03121 0.03141 0.03432

Eigenvalues --- 0.03573 0.03770 0.03818 0.03946 0.04365

Eigenvalues --- 0.04783 0.04991 0.05397 0.05517 0.06064

Eigenvalues --- 0.06258 0.06726 0.07376 0.07530 0.08772

Eigenvalues --- 0.09661 0.10925 0.13282 0.14191 0.15476

Eigenvalues --- 0.16920 0.20910 0.22778 0.24714 0.25270

Eigenvalues --- 0.27819 0.28207 0.30787 0.31262 0.31477

Eigenvalues --- 0.31882 0.32235 0.32259 0.32872 0.34392

Eigenvalues --- 0.35442 0.37509 0.39574 0.39995 0.42610

Eigenvalues --- 0.44741 1.07860 1.10781

Eigenvectors required to have negative eigenvalues:

R6 R10 A15 A14 D41

1 0.70003 0.57245 -0.10862 -0.09961 0.09842

A8 A12 D43 D3 D42

1 -0.09808 0.08709 0.08442 -0.08381 0.07947

RFO step: Lambda0=9.713945181D-02 Lambda=-1.98367817D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.234

Iteration 1 RMS(Cart)= 0.01862192 RMS(Int)= 0.00056181

Iteration 2 RMS(Cart)= 0.00075886 RMS(Int)= 0.00021442

Iteration 3 RMS(Cart)= 0.00000029 RMS(Int)= 0.00021442

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 3.29891 -0.09264 0.00000 -0.14709 -0.14697 3.15194

R2 2.87795 -0.12163 0.00000 -0.05573 -0.05541 2.82254

R3 2.11616 -0.02246 0.00000 -0.00644 -0.00644 2.10971

R4 2.99189 -0.04044 0.00000 -0.02264 -0.02238 2.96951

R5 2.11840 -0.01174 0.00000 -0.00398 -0.00398 2.11442

R6 4.15740 -0.08152 0.00000 0.20401 0.20383 4.36123

R7 2.88416 -0.05025 0.00000 -0.02607 -0.02601 2.85815

R8 2.88416 -0.01260 0.00000 -0.00662 -0.00703 2.87713

R9 2.11842 -0.00727 0.00000 -0.00477 -0.00477 2.11365

R10 4.15740 -0.08056 0.00000 0.04070 0.04089 4.19829

R11 2.11615 -0.01316 0.00000 -0.00447 -0.00447 2.11168

R12 2.11616 0.00298 0.00000 0.00133 0.00133 2.11748

R13 2.11615 -0.00771 0.00000 -0.00190 -0.00190 2.11425

R14 2.87795 -0.00236 0.00000 0.00430 0.00412 2.88207

R15 2.11614 -0.00069 0.00000 -0.00085 -0.00085 2.11529

R16 2.11615 0.00158 0.00000 0.00141 0.00141 2.11757

R17 2.70301 -0.03788 0.00000 -0.00991 -0.00995 2.69306

R18 2.70301 -0.04975 0.00000 -0.01398 -0.01398 2.68903

R19 2.95916 -0.05680 0.00000 -0.03676 -0.03692 2.92224

R20 2.88176 -0.04167 0.00000 -0.01926 -0.01929 2.86247

R21 2.02201 0.02588 0.00000 0.01065 0.01065 2.03265

R22 3.25535 -0.07586 0.00000 -0.07690 -0.07687 3.17848

R23 2.02201 0.01707 0.00000 0.00682 0.00682 2.02882

R24 2.31929 -0.02581 0.00000 -0.00311 -0.00311 2.31618

R25 2.31929 -0.03903 0.00000 -0.00368 -0.00368 2.31561

A1 1.79099 0.02756 0.00000 0.03201 0.03215 1.82314

A2 2.08385 -0.00195 0.00000 0.00764 0.00732 2.09117

A3 1.92433 -0.00238 0.00000 -0.00035 -0.00100 1.92333

A4 1.68434 0.00793 0.00000 0.02937 0.02901 1.71335

A5 1.79104 0.02379 0.00000 0.03719 0.03674 1.82778

A6 2.30414 -0.03275 0.00000 -0.01583 -0.01590 2.28825

A7 1.81410 0.00800 0.00000 0.02163 0.02044 1.83454

A8 1.84289 0.00927 0.00000 -0.03483 -0.03470 1.80819

A9 1.95805 -0.00668 0.00000 -0.02433 -0.02397 1.93408

A10 1.90353 0.00118 0.00000 0.00704 0.00659 1.91012

A11 1.91767 0.01546 0.00000 0.02237 0.02213 1.93980

A12 2.48997 -0.04109 0.00000 -0.01638 -0.01609 2.47388

A13 1.91768 0.00314 0.00000 0.01051 0.01040 1.92808

A14 1.56315 0.01722 0.00000 -0.00301 -0.00292 1.56023

A15 1.61467 0.00863 0.00000 -0.01860 -0.01870 1.59597

A16 1.91766 0.01330 0.00000 0.00432 0.00454 1.92219

A17 1.92433 0.00489 0.00000 0.01098 0.01078 1.93511

A18 1.91069 0.00470 0.00000 0.00786 0.00759 1.91828

A19 1.77490 0.00690 0.00000 0.00989 0.00996 1.78486

A20 2.14075 -0.01786 0.00000 -0.01641 -0.01651 2.12423

A21 1.81420 0.00923 0.00000 0.00723 0.00732 1.82152

A22 1.87568 0.00149 0.00000 0.00076 0.00080 1.87648

A23 1.92430 0.00032 0.00000 -0.00204 -0.00215 1.92215

A24 1.92435 0.00114 0.00000 0.00150 0.00150 1.92585

A25 1.91767 -0.01657 0.00000 -0.00314 -0.00377 1.91389

A26 1.91071 0.00730 0.00000 0.00404 0.00415 1.91486

A27 1.91063 0.00308 0.00000 -0.00222 -0.00194 1.90869

A28 1.92436 0.00369 0.00000 0.00250 0.00280 1.92716

A29 1.92431 0.00681 0.00000 0.00022 0.00028 1.92459

A30 1.87566 -0.00387 0.00000 -0.00133 -0.00143 1.87423

A31 1.92938 -0.00592 0.00000 -0.00641 -0.00654 1.92284

A32 1.69888 0.00854 0.00000 0.01895 0.01890 1.71778

A33 2.16766 -0.00838 0.00000 -0.00786 -0.00774 2.15993

A34 1.87511 -0.00278 0.00000 -0.02054 -0.02067 1.85444

A35 1.95091 -0.00853 0.00000 -0.00877 -0.00875 1.94216

A36 1.88176 0.00215 0.00000 0.00499 0.00516 1.88692

A37 1.87063 0.00953 0.00000 0.01407 0.01398 1.88461

A38 1.80667 0.00515 0.00000 -0.02056 -0.02085 1.78582

A39 2.23656 -0.01322 0.00000 0.00275 0.00284 2.23940

A40 1.90601 -0.00602 0.00000 -0.02940 -0.02914 1.87688

A41 1.66093 0.00930 0.00000 0.01885 0.01904 1.67998

A42 1.90788 -0.00015 0.00000 0.01527 0.01456 1.92244

A43 1.90626 0.00862 0.00000 0.02047 0.02008 1.92634

A44 1.90176 0.00177 0.00000 -0.00294 -0.00304 1.89872

A45 2.14589 -0.02335 0.00000 -0.01450 -0.01446 2.13143

A46 2.23554 0.02157 0.00000 0.01744 0.01748 2.25302

A47 1.92340 0.00518 0.00000 0.00356 0.00353 1.92694

A48 2.14592 -0.01814 0.00000 -0.01590 -0.01592 2.13000

A49 2.19456 0.01499 0.00000 0.01385 0.01386 2.20842

D1 -1.29377 0.00494 0.00000 0.01270 0.01289 -1.28089

D2 3.14107 -0.00983 0.00000 -0.02439 -0.02478 3.11628

D3 0.76272 0.00738 0.00000 -0.01658 -0.01659 0.74612

D4 0.83953 0.02287 0.00000 0.04282 0.04324 0.88277

D5 -1.00882 0.00810 0.00000 0.00573 0.00557 -1.00325

D6 2.89601 0.02531 0.00000 0.01354 0.01376 2.90977

D7 0.13144 0.00171 0.00000 0.00192 0.00214 0.13358

D8 2.23890 0.01926 0.00000 0.02151 0.02170 2.26060

D9 -2.10650 -0.01236 0.00000 -0.02782 -0.02780 -2.13429

D10 0.00096 0.00518 0.00000 -0.00823 -0.00824 -0.00728

D11 -2.97115 -0.01893 0.00000 -0.01840 -0.01869 -2.98985

D12 -0.88049 -0.02183 0.00000 -0.01884 -0.01919 -0.89968

D13 1.31257 -0.02496 0.00000 -0.02228 -0.02264 1.28992

D14 -1.14265 0.00971 0.00000 0.03292 0.03325 -1.10941

D15 0.94801 0.00681 0.00000 0.03247 0.03276 0.98076

D16 3.14107 0.00368 0.00000 0.02903 0.02930 -3.11282

D17 0.92109 0.00980 0.00000 0.00026 0.00039 0.92148

D18 3.01175 0.00690 0.00000 -0.00019 -0.00010 3.01165

D19 -1.07838 0.00377 0.00000 -0.00363 -0.00356 -1.08193

D20 -1.08895 0.00478 0.00000 0.02089 0.02076 -1.06819

D21 -2.97124 -0.00591 0.00000 0.01227 0.01215 -2.95910

D22 0.94183 0.00458 0.00000 0.01501 0.01500 0.95683

D23 0.90398 0.00391 0.00000 0.01558 0.01574 0.91972

D24 -0.97832 -0.00679 0.00000 0.00696 0.00713 -0.97119

D25 2.93476 0.00371 0.00000 0.00970 0.00997 2.94473

D26 2.86880 0.01536 0.00000 0.01017 0.01035 2.87915

D27 0.98650 0.00466 0.00000 0.00155 0.00174 0.98824

D28 -1.38361 0.01515 0.00000 0.00429 0.00459 -1.37902

D29 1.03811 -0.00363 0.00000 -0.01792 -0.01811 1.02000

D30 -1.07755 -0.02108 0.00000 -0.03925 -0.03941 -1.11696

D31 3.14108 0.01045 0.00000 0.01311 0.01322 -3.12888

D32 1.02541 -0.00700 0.00000 -0.00822 -0.00808 1.01733

D33 -0.98798 0.00319 0.00000 -0.00672 -0.00678 -0.99476

D34 -3.10365 -0.01426 0.00000 -0.02805 -0.02808 -3.13173

D35 -1.03920 0.01766 0.00000 0.03291 0.03300 -1.00619

D36 3.12827 0.01894 0.00000 0.02923 0.02929 -3.12562

D37 1.07641 0.01757 0.00000 0.02978 0.02975 1.10616

D38 3.14103 -0.00398 0.00000 -0.00540 -0.00533 3.13570

D39 1.02531 -0.00271 0.00000 -0.00908 -0.00904 1.01627

D40 -1.02654 -0.00407 0.00000 -0.00853 -0.00859 -1.03513

D41 1.52635 -0.01941 0.00000 0.01538 0.01563 1.54198

D42 -0.58937 -0.01814 0.00000 0.01170 0.01192 -0.57745

D43 -2.64123 -0.01950 0.00000 0.01225 0.01237 -2.62885

D44 0.61443 -0.00132 0.00000 -0.00706 -0.00725 0.60718

D45 2.75543 -0.01013 0.00000 -0.00662 -0.00682 2.74860

D46 -1.32872 -0.00622 0.00000 -0.01444 -0.01445 -1.34317

D47 -1.51327 0.00317 0.00000 -0.00213 -0.00209 -1.51536

D48 0.62773 -0.00564 0.00000 -0.00169 -0.00167 0.62606

D49 2.82677 -0.00173 0.00000 -0.00951 -0.00930 2.81747

D50 2.85223 -0.00080 0.00000 -0.01238 -0.01234 2.83989

D51 -1.28996 -0.00961 0.00000 -0.01193 -0.01192 -1.30188

D52 0.90908 -0.00570 0.00000 -0.01975 -0.01955 0.88953

D53 -0.21602 0.00803 0.00000 0.01462 0.01476 -0.20125

D54 1.89149 0.00878 0.00000 0.01922 0.01927 1.91077

D55 -2.32339 0.01052 0.00000 0.01926 0.01942 -2.30397

D56 -2.10647 -0.00426 0.00000 0.00079 0.00084 -2.10564

D57 0.00104 -0.00351 0.00000 0.00539 0.00535 0.00638

D58 2.06934 -0.00177 0.00000 0.00543 0.00550 2.07483

D59 2.10839 -0.00701 0.00000 0.00019 0.00026 2.10865

D60 -2.06728 -0.00625 0.00000 0.00478 0.00477 -2.06252

D61 0.00102 -0.00452 0.00000 0.00483 0.00491 0.00593

D62 0.00000 0.00427 0.00000 0.00445 0.00439 0.00439

D63 3.14156 0.00524 0.00000 0.01006 0.00994 -3.13169

D64 0.19913 -0.00622 0.00000 -0.01053 -0.01059 0.18854

D65 -3.14156 0.00627 0.00000 -0.00086 -0.00101 3.14061

D66 0.29714 -0.00398 0.00000 -0.01413 -0.01404 0.28310

D67 2.58817 -0.01284 0.00000 -0.01045 -0.01047 2.57771

D68 -1.73232 0.00036 0.00000 0.02336 0.02364 -1.70868

D69 -1.99675 0.00500 0.00000 -0.01237 -0.01235 -2.00910

D70 0.29428 -0.00386 0.00000 -0.00869 -0.00878 0.28551

D71 2.25697 0.00935 0.00000 0.02512 0.02533 2.28230

D72 2.23483 -0.00307 0.00000 -0.02759 -0.02755 2.20728

D73 -1.75732 -0.01193 0.00000 -0.02391 -0.02397 -1.78129

D74 0.20537 0.00127 0.00000 0.00989 0.01014 0.21550

D75 -2.24569 0.00403 0.00000 -0.00510 -0.00512 -2.25081

D76 0.89594 0.00300 0.00000 -0.01108 -0.01117 0.88477

D77 -0.22174 0.00169 0.00000 0.00769 0.00770 -0.21404

D78 2.91989 0.00066 0.00000 0.00171 0.00164 2.92153

D79 1.83653 0.00538 0.00000 0.01749 0.01761 1.85414

D80 -1.30502 0.00434 0.00000 0.01151 0.01155 -1.29347

D81 1.65179 0.01353 0.00000 0.00026 0.00024 1.65204

D82 -1.28387 0.00530 0.00000 -0.00552 -0.00561 -1.28948

D83 -0.29731 0.00386 0.00000 0.00999 0.01013 -0.28718

D84 3.05021 -0.00436 0.00000 0.00421 0.00428 3.05448

D85 -2.26137 -0.00193 0.00000 -0.01939 -0.01942 -2.28079

D86 1.08615 -0.01015 0.00000 -0.02516 -0.02528 1.06088

Item Value Threshold Converged?

Maximum Force 0.121630 0.000450 NO

RMS Force 0.021936 0.000300 NO

Maximum Displacement 0.083021 0.001800 NO

RMS Displacement 0.018987 0.001200 NO

Predicted change in Energy=-2.796189D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.565404 1.123659 0.161965

2 6 0 0.082799 1.291303 0.355165

3 6 0 -0.937574 3.506825 0.161752

4 6 0 -2.086572 2.523357 0.173999

5 1 0 -1.967424 0.570215 -0.720338

6 1 0 -2.754179 2.707197 -0.703042

7 6 0 0.422318 1.830053 -1.081415

8 1 0 1.542712 1.813059 -1.083366

9 1 0 0.075950 1.301580 -2.004717

10 6 0 -0.080791 3.269788 -1.074282

11 1 0 0.780669 3.984516 -1.079299

12 1 0 -0.689657 3.472831 -1.992828

13 1 0 -1.309099 4.561583 0.183789

14 1 0 0.474953 0.243540 0.373974

15 8 0 3.260015 4.118249 0.977210

16 6 0 0.890629 4.067871 1.292497

17 6 0 1.316079 2.653718 1.751259

18 6 0 2.055871 4.823209 0.687387

19 8 0 2.049690 5.864046 0.040174

20 6 0 2.972633 2.944154 1.728054

21 8 0 3.853312 2.174688 2.093914

22 1 0 0.554597 4.612835 2.156838

23 1 0 0.982071 2.474729 2.755766

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.667935 0.000000

3 C 2.464478 2.446857 0.000000

4 C 1.493625 2.501390 1.512466 0.000000

5 H 1.116413 2.424889 3.234555 2.151464 0.000000

6 H 2.160791 3.342605 2.165023 1.117451 2.277274

7 C 2.448679 1.571397 2.491252 2.889856 2.725516

8 H 3.418554 2.114934 3.251305 3.906046 3.741324

9 H 2.724006 2.359914 3.253294 3.303944 2.521885

10 C 2.887603 2.446321 1.522513 2.477604 3.312454

11 H 3.902473 3.130193 2.172731 3.453522 4.397535

12 H 3.305855 3.296790 2.169063 2.747364 3.417177

13 H 3.447534 3.558298 1.118495 2.181496 4.145100

14 H 2.232177 1.118904 3.562205 3.434963 2.696190

15 O 5.737322 4.298054 4.319557 5.636916 6.541890

16 C 3.997322 3.039821 2.221640 3.535575 4.945055

17 C 3.629033 2.307863 2.886742 3.752703 4.607729

18 C 5.203497 4.059279 3.312080 4.765787 6.021341

19 O 5.962802 4.987771 3.807233 5.318531 6.688814

20 C 5.134259 3.601094 4.249661 5.309210 6.002863

21 O 5.848040 4.245042 5.334831 6.252189 6.661480

22 H 4.544037 3.808043 2.725839 3.908112 5.566103

23 H 3.878508 2.823486 3.388092 4.010543 4.940647

6 7 8 9 10

6 H 0.000000

7 C 3.317029 0.000000

8 H 4.405383 1.120525 0.000000

9 H 3.417565 1.118812 1.806070 0.000000

10 C 2.757051 1.525125 2.181262 2.182686 0.000000

11 H 3.777335 2.184062 2.301293 2.924238 1.119363

12 H 2.551861 2.183090 2.926677 2.302308 1.120568

13 H 2.512663 3.472723 4.158472 4.163597 2.181792

14 H 4.202008 2.153591 2.393187 2.633785 3.400659

15 O 6.401941 4.186442 3.536806 5.192666 4.011171

16 C 4.372441 3.295846 3.339777 4.380375 2.679970

17 C 4.753257 3.082414 2.965328 4.180138 3.211615

18 C 5.435750 3.841372 3.529858 4.854830 3.175204

19 O 5.796139 4.492149 4.234367 5.375251 3.537108

20 C 6.225973 3.954546 3.350840 5.002239 4.157225

21 O 7.194822 4.687558 3.945219 5.641769 5.168547

22 H 4.770573 4.271727 4.394774 5.339667 3.556350

23 H 5.096760 3.931016 3.935868 4.985933 4.053524

11 12 13 14 15

11 H 0.000000

12 H 1.805053 0.000000

13 H 2.509089 2.511325 0.000000

14 H 4.024968 4.169700 4.675950 0.000000

15 O 3.224015 4.983734 4.658633 4.809765 0.000000

16 C 2.375807 3.693879 2.512327 3.954994 2.390802

17 C 3.173286 4.325750 3.603952 2.900580 2.553995

18 C 2.334679 4.067555 3.412489 4.854988 1.425107

19 O 2.529085 4.165937 3.605343 5.846479 2.321795

20 C 3.710564 5.247554 4.830533 3.919853 1.422974

21 O 4.773457 6.247016 5.999694 4.254508 2.318718

22 H 3.304312 4.479677 2.714574 4.719713 2.992562

23 H 4.126469 5.132254 4.027342 3.302773 3.324673

16 17 18 19 20

16 C 0.000000

17 C 1.546382 0.000000

18 C 1.514756 2.527016 0.000000

19 O 2.477495 3.711092 1.225669 0.000000

20 C 2.405657 1.681981 2.335442 3.496646 0.000000

21 O 3.606091 2.604694 3.496251 4.591542 1.225368

22 H 1.075634 2.140674 2.111249 2.877690 2.969048

23 H 2.165090 1.073607 3.308564 4.472328 2.288861

21 22 23

21 O 0.000000

22 H 4.102443 0.000000

23 H 2.961772 2.261182 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 3.027681 -1.033624 -0.339443

2 6 0 1.472674 -1.357831 0.169331

3 6 0 1.600996 0.957316 -0.612165

4 6 0 2.956860 0.350415 -0.896521

5 1 0 3.876135 -1.116035 0.381468

6 1 0 3.760627 0.995227 -0.464231

7 6 0 1.459370 -0.440500 1.445111

8 1 0 0.495407 -0.730910 1.937060

9 1 0 2.264061 -0.499409 2.220188

10 6 0 1.359710 0.976896 0.890979

11 1 0 0.350140 1.410054 1.105725

12 1 0 2.119343 1.639439 1.380537

13 1 0 1.524913 1.990397 -1.034051

14 1 0 1.514629 -2.404361 0.562981

15 8 0 -2.535736 0.181560 0.359541

16 6 0 -0.569265 0.606262 -0.932184

17 6 0 -0.567600 -0.936299 -0.823556

18 6 0 -1.656428 1.216703 -0.071996

19 8 0 -1.820124 2.387655 0.251020

20 6 0 -2.102946 -1.074304 -0.150706

21 8 0 -2.703486 -2.115195 0.088928

22 1 0 -0.768990 0.869179 -1.955889

23 1 0 -0.547816 -1.375948 -1.802816

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3147650 0.6140106 0.4948673

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 447.8350851150 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.282361867345 A.U. after 15 cycles

Convg = 0.5243D-08 -V/T = 1.0061

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.041861817 0.169818679 -0.001769682

2 6 -0.034547727 -0.041040507 -0.050083842

3 6 0.004248645 0.054188268 -0.012943211

4 6 0.108901723 -0.113024587 -0.026656150

5 1 0.004924622 -0.018691400 0.032609882

6 1 -0.016678468 0.009378042 0.028428491

7 6 0.013243225 0.023722681 0.048977340

8 1 0.002540246 0.001018907 -0.007122595

9 1 -0.005242017 -0.007324739 0.013915671

10 6 -0.002935106 -0.007657443 0.004951232

11 1 -0.001415875 0.000673496 -0.004491158

12 1 -0.001527810 0.000551171 -0.000371034

13 1 0.005274169 -0.004882873 0.009469522

14 1 0.006784947 0.013285315 0.023685825

15 8 -0.019930473 -0.008709246 0.017530547

16 6 -0.023255291 -0.071516805 -0.006564567

17 6 0.018753882 0.061458892 -0.057464050

18 6 -0.023412783 -0.031866619 0.001867625

19 8 0.017584177 -0.017253082 0.010743993

20 6 -0.054704946 -0.036263946 -0.037351911

21 8 -0.012711024 0.030979163 -0.006533378

22 1 -0.021245992 0.015407722 0.009438494

23 1 -0.006509939 -0.022251089 0.009732955

-------------------------------------------------------------------

Cartesian Forces: Max 0.169818679 RMS 0.037309218

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.102437020 RMS 0.019812916

Search for a saddle point.

Step number 2 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 1 2

ITU= 0 0

Eigenvalues --- -0.02353 -0.00806 0.00154 0.00341 0.00565

Eigenvalues --- 0.00635 0.00783 0.01013 0.01311 0.01521

Eigenvalues --- 0.01862 0.01949 0.02194 0.02215 0.02426

Eigenvalues --- 0.02606 0.02901 0.03134 0.03144 0.03455

Eigenvalues --- 0.03576 0.03769 0.03817 0.03948 0.04385

Eigenvalues --- 0.04785 0.05095 0.05423 0.05523 0.06064

Eigenvalues --- 0.06249 0.06715 0.07381 0.07558 0.08766

Eigenvalues --- 0.09669 0.10955 0.13279 0.14192 0.15481

Eigenvalues --- 0.16916 0.20902 0.22775 0.24770 0.25403

Eigenvalues --- 0.27818 0.28245 0.30786 0.31263 0.31498

Eigenvalues --- 0.31886 0.32250 0.32258 0.32871 0.34437

Eigenvalues --- 0.35499 0.37509 0.39574 0.39997 0.42606

Eigenvalues --- 0.44921 1.07865 1.10783

Eigenvectors required to have negative eigenvalues:

R6 R10 A15 D41 A8

1 0.73954 0.52367 -0.10403 0.09882 -0.09741

A14 A12 D43 D3 D42

1 -0.09035 0.09017 0.08614 -0.08396 0.08133

RFO step: Lambda0=9.214819953D-02 Lambda=-1.75745184D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.243

Iteration 1 RMS(Cart)= 0.02116930 RMS(Int)= 0.00214570

Iteration 2 RMS(Cart)= 0.00335559 RMS(Int)= 0.00024994

Iteration 3 RMS(Cart)= 0.00000217 RMS(Int)= 0.00024994

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00024994

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 3.15194 -0.08516 0.00000 -0.10368 -0.10364 3.04830

R2 2.82254 -0.10244 0.00000 -0.05086 -0.05068 2.77186

R3 2.10971 -0.01828 0.00000 -0.00579 -0.00579 2.10392

R4 2.96951 -0.03350 0.00000 -0.02599 -0.02566 2.94385

R5 2.11442 -0.00966 0.00000 -0.00539 -0.00539 2.10904

R6 4.36123 -0.07641 0.00000 0.22826 0.22806 4.58929

R7 2.85815 -0.04212 0.00000 -0.02057 -0.02051 2.83764

R8 2.87713 -0.00951 0.00000 -0.00519 -0.00561 2.87153

R9 2.11365 -0.00617 0.00000 -0.00370 -0.00370 2.10995

R10 4.19829 -0.07842 0.00000 0.00220 0.00243 4.20072

R11 2.11168 -0.01081 0.00000 -0.00378 -0.00378 2.10790

R12 2.11748 0.00254 0.00000 0.00154 0.00154 2.11903

R13 2.11425 -0.00640 0.00000 -0.00119 -0.00119 2.11306

R14 2.88207 -0.00053 0.00000 0.00472 0.00464 2.88671

R15 2.11529 -0.00064 0.00000 -0.00094 -0.00094 2.11435

R16 2.11757 0.00123 0.00000 0.00112 0.00112 2.11868

R17 2.69306 -0.03122 0.00000 -0.01006 -0.01013 2.68293

R18 2.68903 -0.04050 0.00000 -0.00929 -0.00933 2.67970

R19 2.92224 -0.04758 0.00000 -0.03406 -0.03413 2.88811

R20 2.86247 -0.03470 0.00000 -0.01419 -0.01420 2.84828

R21 2.03265 0.02203 0.00000 0.01017 0.01017 2.04282

R22 3.17848 -0.07053 0.00000 -0.08291 -0.08287 3.09561

R23 2.02882 0.01484 0.00000 0.00637 0.00637 2.03520

R24 2.31618 -0.02041 0.00000 -0.00238 -0.00238 2.31380

R25 2.31561 -0.03054 0.00000 -0.00239 -0.00239 2.31322

A1 1.82314 0.02641 0.00000 0.02254 0.02261 1.84575

A2 2.09117 -0.00238 0.00000 0.00821 0.00797 2.09915

A3 1.92333 -0.00218 0.00000 0.00369 0.00320 1.92654

A4 1.71335 0.00799 0.00000 0.02770 0.02715 1.74050

A5 1.82778 0.02228 0.00000 0.03909 0.03837 1.86615

A6 2.28825 -0.03071 0.00000 -0.02380 -0.02388 2.26437

A7 1.83454 0.00820 0.00000 0.02697 0.02582 1.86035

A8 1.80819 0.00758 0.00000 -0.03415 -0.03409 1.77410

A9 1.93408 -0.00685 0.00000 -0.02244 -0.02187 1.91221

A10 1.91012 0.00023 0.00000 0.00279 0.00241 1.91253

A11 1.93980 0.01451 0.00000 0.01541 0.01518 1.95498

A12 2.47388 -0.03920 0.00000 -0.01425 -0.01391 2.45997

A13 1.92808 0.00399 0.00000 0.00999 0.01010 1.93818

A14 1.56023 0.01646 0.00000 0.00480 0.00489 1.56512

A15 1.59597 0.00811 0.00000 -0.01609 -0.01628 1.57968

A16 1.92219 0.01212 0.00000 0.01361 0.01375 1.93594

A17 1.93511 0.00499 0.00000 0.01182 0.01155 1.94666

A18 1.91828 0.00460 0.00000 0.00594 0.00551 1.92379

A19 1.78486 0.00701 0.00000 0.01105 0.01105 1.79591

A20 2.12423 -0.01717 0.00000 -0.01907 -0.01916 2.10507

A21 1.82152 0.00895 0.00000 0.01063 0.01081 1.83233

A22 1.87648 0.00136 0.00000 0.00055 0.00062 1.87710

A23 1.92215 -0.00003 0.00000 -0.00312 -0.00330 1.91885

A24 1.92585 0.00099 0.00000 0.00093 0.00093 1.92677

A25 1.91389 -0.01424 0.00000 -0.00240 -0.00300 1.91089

A26 1.91486 0.00624 0.00000 0.00495 0.00508 1.91994

A27 1.90869 0.00292 0.00000 -0.00212 -0.00188 1.90680

A28 1.92716 0.00319 0.00000 0.00105 0.00131 1.92847

A29 1.92459 0.00568 0.00000 0.00015 0.00024 1.92483

A30 1.87423 -0.00341 0.00000 -0.00159 -0.00169 1.87254

A31 1.92284 -0.00545 0.00000 -0.00665 -0.00684 1.91601

A32 1.71778 0.00891 0.00000 0.03342 0.03352 1.75130

A33 2.15993 -0.00874 0.00000 -0.01326 -0.01319 2.14673

A34 1.85444 -0.00282 0.00000 -0.02540 -0.02572 1.82872

A35 1.94216 -0.00832 0.00000 -0.01245 -0.01247 1.92969

A36 1.88692 0.00257 0.00000 0.00690 0.00726 1.89418

A37 1.88461 0.00919 0.00000 0.01326 0.01306 1.89767

A38 1.78582 0.00434 0.00000 -0.03185 -0.03220 1.75362

A39 2.23940 -0.01326 0.00000 0.00660 0.00674 2.24614

A40 1.87688 -0.00594 0.00000 -0.03117 -0.03084 1.84604

A41 1.67998 0.01001 0.00000 0.02325 0.02345 1.70343

A42 1.92244 0.00006 0.00000 0.01584 0.01480 1.93724

A43 1.92634 0.00812 0.00000 0.02233 0.02185 1.94819

A44 1.89872 0.00071 0.00000 -0.00226 -0.00235 1.89637

A45 2.13143 -0.02053 0.00000 -0.01366 -0.01361 2.11782

A46 2.25302 0.01981 0.00000 0.01589 0.01593 2.26895

A47 1.92694 0.00490 0.00000 0.00330 0.00329 1.93023

A48 2.13000 -0.01698 0.00000 -0.01809 -0.01813 2.11187

A49 2.20842 0.01398 0.00000 0.01649 0.01650 2.22492

D1 -1.28089 0.00638 0.00000 0.01744 0.01774 -1.26315

D2 3.11628 -0.01018 0.00000 -0.02937 -0.02989 3.08640

D3 0.74612 0.00766 0.00000 -0.01726 -0.01728 0.72884

D4 0.88277 0.02462 0.00000 0.04763 0.04813 0.93090

D5 -1.00325 0.00806 0.00000 0.00081 0.00050 -1.00274

D6 2.90977 0.02590 0.00000 0.01293 0.01311 2.92289

D7 0.13358 0.00155 0.00000 -0.00148 -0.00123 0.13235

D8 2.26060 0.01889 0.00000 0.02314 0.02342 2.28402

D9 -2.13429 -0.01246 0.00000 -0.02976 -0.02975 -2.16404

D10 -0.00728 0.00489 0.00000 -0.00514 -0.00510 -0.01238

D11 -2.98985 -0.01812 0.00000 -0.02105 -0.02136 -3.01121

D12 -0.89968 -0.02082 0.00000 -0.02260 -0.02298 -0.92266

D13 1.28992 -0.02397 0.00000 -0.02568 -0.02605 1.26387

D14 -1.10941 0.01014 0.00000 0.03600 0.03641 -1.07300

D15 0.98076 0.00744 0.00000 0.03445 0.03478 1.01554

D16 -3.11282 0.00429 0.00000 0.03138 0.03171 -3.08111

D17 0.92148 0.00902 0.00000 0.00756 0.00770 0.92918

D18 3.01165 0.00632 0.00000 0.00601 0.00608 3.01772

D19 -1.08193 0.00317 0.00000 0.00294 0.00301 -1.07892

D20 -1.06819 0.00417 0.00000 0.02928 0.02892 -1.03927

D21 -2.95910 -0.00691 0.00000 0.02309 0.02288 -2.93622

D22 0.95683 0.00387 0.00000 0.02006 0.02011 0.97694

D23 0.91972 0.00404 0.00000 0.01847 0.01857 0.93829

D24 -0.97119 -0.00704 0.00000 0.01229 0.01253 -0.95866

D25 2.94473 0.00373 0.00000 0.00925 0.00977 2.95450

D26 2.87915 0.01446 0.00000 0.02267 0.02259 2.90174

D27 0.98824 0.00339 0.00000 0.01649 0.01655 1.00479

D28 -1.37902 0.01416 0.00000 0.01345 0.01379 -1.36523

D29 1.02000 -0.00472 0.00000 -0.01756 -0.01764 1.00236

D30 -1.11696 -0.02206 0.00000 -0.04534 -0.04544 -1.16241

D31 -3.12888 0.01007 0.00000 0.00712 0.00721 -3.12167

D32 1.01733 -0.00726 0.00000 -0.02066 -0.02059 0.99674

D33 -0.99476 0.00266 0.00000 -0.01688 -0.01687 -1.01163

D34 -3.13173 -0.01468 0.00000 -0.04466 -0.04467 3.10679

D35 -1.00619 0.01731 0.00000 0.02846 0.02844 -0.97775

D36 -3.12562 0.01846 0.00000 0.02554 0.02551 -3.10012

D37 1.10616 0.01725 0.00000 0.02582 0.02570 1.13186

D38 3.13570 -0.00368 0.00000 0.00068 0.00075 3.13645

D39 1.01627 -0.00252 0.00000 -0.00224 -0.00219 1.01409

D40 -1.03513 -0.00374 0.00000 -0.00196 -0.00199 -1.03713

D41 1.54198 -0.01847 0.00000 0.01609 0.01634 1.55832

D42 -0.57745 -0.01731 0.00000 0.01316 0.01340 -0.56405

D43 -2.62885 -0.01853 0.00000 0.01345 0.01359 -2.61526

D44 0.60718 -0.00125 0.00000 0.00564 0.00550 0.61268

D45 2.74860 -0.00981 0.00000 0.01058 0.01033 2.75893

D46 -1.34317 -0.00656 0.00000 -0.00725 -0.00714 -1.35031

D47 -1.51536 0.00404 0.00000 0.00449 0.00464 -1.51072

D48 0.62606 -0.00453 0.00000 0.00942 0.00948 0.63554

D49 2.81747 -0.00128 0.00000 -0.00841 -0.00799 2.80948

D50 2.83989 -0.00032 0.00000 -0.00564 -0.00557 2.83432

D51 -1.30188 -0.00888 0.00000 -0.00071 -0.00073 -1.30261

D52 0.88953 -0.00564 0.00000 -0.01854 -0.01820 0.87133

D53 -0.20125 0.00850 0.00000 0.01635 0.01643 -0.18483

D54 1.91077 0.00906 0.00000 0.02162 0.02163 1.93240

D55 -2.30397 0.01038 0.00000 0.02041 0.02052 -2.28345

D56 -2.10564 -0.00373 0.00000 -0.00004 -0.00002 -2.10565

D57 0.00638 -0.00317 0.00000 0.00523 0.00519 0.01157

D58 2.07483 -0.00185 0.00000 0.00402 0.00407 2.07890

D59 2.10865 -0.00601 0.00000 0.00064 0.00070 2.10935

D60 -2.06252 -0.00544 0.00000 0.00592 0.00591 -2.05661

D61 0.00593 -0.00412 0.00000 0.00470 0.00479 0.01072

D62 0.00439 0.00420 0.00000 0.00551 0.00540 0.00979

D63 -3.13169 0.00528 0.00000 0.00960 0.00948 -3.12221

D64 0.18854 -0.00634 0.00000 -0.01321 -0.01327 0.17527

D65 3.14061 0.00556 0.00000 -0.00209 -0.00226 3.13836

D66 0.28310 -0.00425 0.00000 -0.01751 -0.01735 0.26575

D67 2.57771 -0.01319 0.00000 -0.01217 -0.01225 2.56546

D68 -1.70868 0.00032 0.00000 0.02753 0.02785 -1.68083

D69 -2.00910 0.00496 0.00000 -0.01654 -0.01643 -2.02553

D70 0.28551 -0.00398 0.00000 -0.01120 -0.01133 0.27418

D71 2.28230 0.00953 0.00000 0.02850 0.02877 2.31108

D72 2.20728 -0.00301 0.00000 -0.02975 -0.02955 2.17774

D73 -1.78129 -0.01195 0.00000 -0.02441 -0.02444 -1.80573

D74 0.21550 0.00156 0.00000 0.01529 0.01566 0.23116

D75 -2.25081 0.00395 0.00000 -0.01635 -0.01643 -2.26724

D76 0.88477 0.00259 0.00000 -0.02095 -0.02110 0.86367

D77 -0.21404 0.00208 0.00000 0.00942 0.00942 -0.20462

D78 2.92153 0.00073 0.00000 0.00483 0.00475 2.92628

D79 1.85414 0.00608 0.00000 0.01882 0.01903 1.87318

D80 -1.29347 0.00473 0.00000 0.01423 0.01436 -1.27911

D81 1.65204 0.01350 0.00000 -0.00644 -0.00647 1.64556

D82 -1.28948 0.00518 0.00000 -0.01343 -0.01356 -1.30305

D83 -0.28718 0.00438 0.00000 0.01287 0.01305 -0.27413

D84 3.05448 -0.00395 0.00000 0.00588 0.00596 3.06044

D85 -2.28079 -0.00259 0.00000 -0.02166 -0.02165 -2.30244

D86 1.06088 -0.01092 0.00000 -0.02864 -0.02874 1.03213

Item Value Threshold Converged?

Maximum Force 0.102437 0.000450 NO

RMS Force 0.019813 0.000300 NO

Maximum Displacement 0.088819 0.001800 NO

RMS Displacement 0.023365 0.001200 NO

Predicted change in Energy=-2.310200D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.557872 1.139011 0.146770

2 6 0 0.042825 1.252915 0.310645

3 6 0 -0.926349 3.501319 0.154825

4 6 0 -2.060083 2.516885 0.174460

5 1 0 -1.995927 0.583841 -0.713135

6 1 0 -2.757923 2.715449 -0.672784

7 6 0 0.411729 1.815938 -1.094246

8 1 0 1.532620 1.784423 -1.090093

9 1 0 0.063380 1.300785 -2.023549

10 6 0 -0.068783 3.265879 -1.077315

11 1 0 0.802835 3.967410 -1.076758

12 1 0 -0.672974 3.485879 -1.995763

13 1 0 -1.287917 4.556886 0.196053

14 1 0 0.440252 0.210791 0.350716

15 8 0 3.251908 4.138962 0.991382

16 6 0 0.895086 4.059588 1.300301

17 6 0 1.356228 2.680780 1.771471

18 6 0 2.044190 4.823462 0.693805

19 8 0 2.042638 5.854742 0.033773

20 6 0 2.968392 2.969789 1.742035

21 8 0 3.865982 2.221689 2.106879

22 1 0 0.525751 4.608890 2.154964

23 1 0 1.007609 2.477693 2.770021

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.613090 0.000000

3 C 2.445278 2.453345 0.000000

4 C 1.466806 2.457313 1.501615 0.000000

5 H 1.113347 2.377456 3.226303 2.128051 0.000000

6 H 2.144049 3.309128 2.158053 1.115451 2.264070

7 C 2.424392 1.557821 2.488201 2.865449 2.731321

8 H 3.390801 2.112832 3.247165 3.878545 3.746217

9 H 2.713837 2.334775 3.250727 3.289261 2.544001

10 C 2.870425 2.447635 1.519546 2.468442 3.322625

11 H 3.881983 3.141813 2.173502 3.444686 4.406112

12 H 3.298679 3.289076 2.165518 2.751889 3.437610

13 H 3.428873 3.563738 1.116536 2.181355 4.136784

14 H 2.212620 1.116054 3.568410 3.405996 2.684384

15 O 5.731235 4.369312 4.308625 5.613888 6.563843

16 C 3.984647 3.095672 2.222927 3.518590 4.949010

17 C 3.675416 2.428547 2.914959 3.774717 4.669836

18 C 5.181629 4.111093 3.295856 4.736568 6.022991

19 O 5.934186 5.025209 3.790532 5.290879 6.682086

20 C 5.136505 3.681776 4.239194 5.286584 6.030346

21 O 5.867914 4.333764 5.330516 6.240162 6.707981

22 H 4.518228 3.859702 2.708480 3.871100 5.548501

23 H 3.905791 2.911944 3.409876 4.018607 4.973960

6 7 8 9 10

6 H 0.000000

7 C 3.321663 0.000000

8 H 4.410184 1.121342 0.000000

9 H 3.433015 1.118183 1.806630 0.000000

10 C 2.774544 1.527583 2.181597 2.185045 0.000000

11 H 3.795997 2.186802 2.301781 2.924739 1.118867

12 H 2.586668 2.185868 2.929136 2.305998 1.121158

13 H 2.511312 3.473682 4.158864 4.165912 2.185052

14 H 4.189175 2.159913 2.396981 2.639555 3.410565

15 O 6.396398 4.220534 3.582226 5.226066 4.008587

16 C 4.363972 3.316845 3.361073 4.398944 2.685531

17 C 4.785585 3.138848 3.003851 4.240049 3.238608

18 C 5.419556 3.860993 3.560865 4.869998 3.166637

19 O 5.779254 4.499359 4.253315 5.374808 3.520629

20 C 6.219866 3.989034 3.389319 5.040267 4.154616

21 O 7.200448 4.726913 3.982011 5.689313 5.168346

22 H 4.729038 4.286135 4.418347 5.349515 3.550321

23 H 5.107707 3.965546 3.956860 5.025435 4.072082

11 12 13 14 15

11 H 0.000000

12 H 1.804011 0.000000

13 H 2.517691 2.515803 0.000000

14 H 4.035013 4.179885 4.679640 0.000000

15 O 3.210077 4.975365 4.627874 4.873027 0.000000

16 C 2.380633 3.694860 2.496432 3.990216 2.378306

17 C 3.173967 4.354067 3.604611 2.993060 2.515637

18 C 2.325658 4.050419 3.379609 4.895617 1.419745

19 O 2.516429 4.135828 3.578179 5.875566 2.307218

20 C 3.691948 5.243762 4.798449 3.992409 1.418036

21 O 4.750364 6.247558 5.972192 4.343207 2.301598

22 H 3.306402 4.463926 2.670100 4.754566 3.001114

23 H 4.130242 5.153009 4.027133 3.363596 3.310627

16 17 18 19 20

16 C 0.000000

17 C 1.528321 0.000000

18 C 1.507243 2.495143 0.000000

19 O 2.478618 3.683040 1.224412 0.000000

20 C 2.383567 1.638129 2.321431 3.478238 0.000000

21 O 3.585340 2.573349 3.476338 4.563051 1.224104

22 H 1.081013 2.134096 2.118179 2.890077 2.970464

23 H 2.162206 1.076979 3.299668 4.467976 2.267948

21 22 23

21 O 0.000000

22 H 4.105871 0.000000

23 H 2.945436 2.269908 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 3.024981 -1.007194 -0.348786

2 6 0 1.546664 -1.362744 0.189938

3 6 0 1.589486 0.954411 -0.614961

4 6 0 2.930287 0.345337 -0.908440

5 1 0 3.903673 -1.085139 0.330454

6 1 0 3.745149 1.004445 -0.526590

7 6 0 1.494512 -0.439740 1.443792

8 1 0 0.538762 -0.748575 1.942362

9 1 0 2.304419 -0.478924 2.213758

10 6 0 1.357669 0.976016 0.886643

11 1 0 0.342335 1.388928 1.111283

12 1 0 2.107949 1.656871 1.366758

13 1 0 1.490170 1.977542 -1.050841

14 1 0 1.582380 -2.412191 0.568040

15 8 0 -2.536275 0.183839 0.358981

16 6 0 -0.579896 0.587279 -0.931817

17 6 0 -0.619032 -0.936661 -0.823005

18 6 0 -1.651506 1.207113 -0.072028

19 8 0 -1.813633 2.372958 0.265174

20 6 0 -2.107371 -1.067736 -0.151343

21 8 0 -2.723764 -2.095310 0.098821

22 1 0 -0.758642 0.862837 -1.961724

23 1 0 -0.581595 -1.394172 -1.797257

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3261548 0.6106289 0.4947402

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 448.2808210385 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.259590205780 A.U. after 16 cycles

Convg = 0.5604D-08 -V/T = 1.0056

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.041553222 0.149702090 -0.001093428

2 6 -0.033610036 -0.042528614 -0.046787416

3 6 0.007920917 0.057553759 -0.009624955

4 6 0.094763113 -0.097404569 -0.027531943

5 1 0.003565219 -0.021200456 0.030600565

6 1 -0.017208316 0.009810204 0.027882984

7 6 0.016026220 0.024360727 0.044586946

8 1 0.002183294 0.000982734 -0.006844820

9 1 -0.005262781 -0.006953817 0.012064664

10 6 -0.002061698 -0.008806077 0.004222946

11 1 -0.001178844 0.000569717 -0.004409202

12 1 -0.001332016 0.000281797 -0.000177555

13 1 0.004369394 -0.004313181 0.008370353

14 1 0.007684730 0.012141002 0.022781102

15 8 -0.014726624 -0.005666751 0.014436789

16 6 -0.027895228 -0.064286405 -0.002764942

17 6 0.017137754 0.057902679 -0.048285649

18 6 -0.020254011 -0.027429358 -0.000395241

19 8 0.015373873 -0.013032169 0.008918711

20 6 -0.051550488 -0.038218178 -0.034598207

21 8 -0.008674101 0.025430205 -0.004202203

22 1 -0.020621122 0.013439591 0.005776022

23 1 -0.006202471 -0.022334927 0.007074478

-------------------------------------------------------------------

Cartesian Forces: Max 0.149702090 RMS 0.033811040

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.082721060 RMS 0.017525509

Search for a saddle point.

Step number 3 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 2 3

ITU= 0 0 0

Eigenvalues --- -0.03553 -0.00820 0.00172 0.00342 0.00565

Eigenvalues --- 0.00731 0.00832 0.01009 0.01420 0.01519

Eigenvalues --- 0.01817 0.01987 0.02212 0.02328 0.02475

Eigenvalues --- 0.02656 0.03015 0.03129 0.03220 0.03529

Eigenvalues --- 0.03663 0.03779 0.03814 0.03945 0.04450

Eigenvalues --- 0.04784 0.05227 0.05434 0.05646 0.06067

Eigenvalues --- 0.06227 0.06702 0.07387 0.07624 0.08757

Eigenvalues --- 0.09684 0.11053 0.13271 0.14184 0.15495

Eigenvalues --- 0.16902 0.20880 0.22766 0.24820 0.25685

Eigenvalues --- 0.27812 0.28285 0.30783 0.31263 0.31529

Eigenvalues --- 0.31892 0.32257 0.32271 0.32866 0.34500

Eigenvalues --- 0.35596 0.37509 0.39577 0.40006 0.42598

Eigenvalues --- 0.45216 1.07876 1.10787

Eigenvectors required to have negative eigenvalues:

R6 R10 A8 D41 A15

1 0.80234 0.39915 -0.09769 0.09730 -0.08992

D21 D43 A12 D42 R1

1 0.08841 0.08675 0.08576 0.08218 0.07803

RFO step: Lambda0=7.522953574D-02 Lambda=-1.53824139D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.270

Iteration 1 RMS(Cart)= 0.03004523 RMS(Int)= 0.00214115

Iteration 2 RMS(Cart)= 0.00328470 RMS(Int)= 0.00031909

Iteration 3 RMS(Cart)= 0.00000224 RMS(Int)= 0.00031909

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00031909

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 3.04830 -0.07452 0.00000 -0.06428 -0.06420 2.98409

R2 2.77186 -0.08272 0.00000 -0.04399 -0.04384 2.72802

R3 2.10392 -0.01447 0.00000 -0.00577 -0.00577 2.09816

R4 2.94385 -0.02690 0.00000 -0.02894 -0.02862 2.91524

R5 2.10904 -0.00778 0.00000 -0.00700 -0.00700 2.10203

R6 4.58929 -0.06926 0.00000 0.22723 0.22702 4.81631

R7 2.83764 -0.03434 0.00000 -0.01568 -0.01568 2.82196

R8 2.87153 -0.00656 0.00000 -0.00236 -0.00271 2.86882

R9 2.10995 -0.00518 0.00000 -0.00250 -0.00250 2.10745

R10 4.20072 -0.07488 0.00000 -0.06870 -0.06851 4.13221

R11 2.10790 -0.00867 0.00000 -0.00362 -0.00362 2.10428

R12 2.11903 0.00213 0.00000 0.00170 0.00170 2.12073

R13 2.11306 -0.00518 0.00000 -0.00053 -0.00053 2.11253

R14 2.88671 0.00120 0.00000 0.00549 0.00548 2.89220

R15 2.11435 -0.00056 0.00000 -0.00090 -0.00090 2.11345

R16 2.11868 0.00092 0.00000 0.00055 0.00055 2.11924

R17 2.68293 -0.02514 0.00000 -0.01182 -0.01190 2.67103

R18 2.67970 -0.03176 0.00000 -0.00525 -0.00526 2.67444

R19 2.88811 -0.03876 0.00000 -0.03322 -0.03332 2.85479

R20 2.84828 -0.02761 0.00000 -0.00709 -0.00714 2.84114

R21 2.04282 0.01844 0.00000 0.01047 0.01047 2.05329

R22 3.09561 -0.06262 0.00000 -0.06963 -0.06955 3.02606

R23 2.03520 0.01278 0.00000 0.00610 0.00610 2.04130

R24 2.31380 -0.01580 0.00000 -0.00179 -0.00179 2.31201

R25 2.31322 -0.02315 0.00000 -0.00202 -0.00202 2.31120

A1 1.84575 0.02399 0.00000 0.01360 0.01376 1.85952

A2 2.09915 -0.00255 0.00000 0.00846 0.00818 2.10733

A3 1.92654 -0.00152 0.00000 0.00958 0.00921 1.93575

A4 1.74050 0.00794 0.00000 0.02827 0.02736 1.76786

A5 1.86615 0.02036 0.00000 0.04328 0.04206 1.90821

A6 2.26437 -0.02869 0.00000 -0.04112 -0.04116 2.22321

A7 1.86035 0.00828 0.00000 0.03287 0.03169 1.89204

A8 1.77410 0.00579 0.00000 -0.03000 -0.03005 1.74405

A9 1.91221 -0.00665 0.00000 -0.01890 -0.01813 1.89408

A10 1.91253 -0.00035 0.00000 -0.00292 -0.00324 1.90929

A11 1.95498 0.01302 0.00000 0.00709 0.00692 1.96190

A12 2.45997 -0.03646 0.00000 -0.01983 -0.01960 2.44036

A13 1.93818 0.00477 0.00000 0.01000 0.01024 1.94842

A14 1.56512 0.01535 0.00000 0.01950 0.01975 1.58487

A15 1.57968 0.00745 0.00000 -0.00806 -0.00841 1.57127

A16 1.93594 0.01113 0.00000 0.02441 0.02434 1.96028

A17 1.94666 0.00475 0.00000 0.01211 0.01165 1.95832

A18 1.92379 0.00440 0.00000 0.00637 0.00575 1.92954

A19 1.79591 0.00691 0.00000 0.01336 0.01328 1.80919

A20 2.10507 -0.01626 0.00000 -0.02498 -0.02499 2.08008

A21 1.83233 0.00861 0.00000 0.01613 0.01630 1.84863

A22 1.87710 0.00124 0.00000 0.00052 0.00061 1.87771

A23 1.91885 -0.00037 0.00000 -0.00450 -0.00474 1.91411

A24 1.92677 0.00085 0.00000 0.00063 0.00062 1.92740

A25 1.91089 -0.01155 0.00000 -0.00055 -0.00108 1.90981

A26 1.91994 0.00516 0.00000 0.00493 0.00511 1.92505

A27 1.90680 0.00256 0.00000 -0.00115 -0.00101 1.90579

A28 1.92847 0.00244 0.00000 -0.00110 -0.00090 1.92757

A29 1.92483 0.00461 0.00000 -0.00021 -0.00011 1.92473

A30 1.87254 -0.00289 0.00000 -0.00192 -0.00200 1.87054

A31 1.91601 -0.00495 0.00000 -0.00600 -0.00620 1.90981

A32 1.75130 0.00950 0.00000 0.05079 0.05099 1.80229

A33 2.14673 -0.00908 0.00000 -0.02253 -0.02268 2.12405

A34 1.82872 -0.00311 0.00000 -0.03076 -0.03134 1.79738

A35 1.92969 -0.00803 0.00000 -0.01492 -0.01479 1.91490

A36 1.89418 0.00306 0.00000 0.01021 0.01073 1.90491

A37 1.89767 0.00875 0.00000 0.01163 0.01116 1.90883

A38 1.75362 0.00340 0.00000 -0.04130 -0.04169 1.71193

A39 2.24614 -0.01306 0.00000 0.00795 0.00829 2.25443

A40 1.84604 -0.00569 0.00000 -0.02865 -0.02833 1.81772

A41 1.70343 0.01027 0.00000 0.02522 0.02530 1.72873

A42 1.93724 0.00028 0.00000 0.01726 0.01617 1.95340

A43 1.94819 0.00760 0.00000 0.02157 0.02097 1.96916

A44 1.89637 0.00023 0.00000 0.00101 0.00085 1.89721

A45 2.11782 -0.01781 0.00000 -0.01386 -0.01378 2.10404

A46 2.26895 0.01756 0.00000 0.01284 0.01292 2.28188

A47 1.93023 0.00431 0.00000 0.00022 0.00024 1.93046

A48 2.11187 -0.01563 0.00000 -0.01821 -0.01827 2.09360

A49 2.22492 0.01305 0.00000 0.01976 0.01975 2.24467

D1 -1.26315 0.00790 0.00000 0.02655 0.02697 -1.23618

D2 3.08640 -0.01029 0.00000 -0.03315 -0.03403 3.05236

D3 0.72884 0.00786 0.00000 -0.01104 -0.01116 0.71769

D4 0.93090 0.02595 0.00000 0.05888 0.05956 0.99046

D5 -1.00274 0.00776 0.00000 -0.00082 -0.00144 -1.00418

D6 2.92289 0.02591 0.00000 0.02129 0.02144 2.94433

D7 0.13235 0.00112 0.00000 -0.00713 -0.00697 0.12539

D8 2.28402 0.01826 0.00000 0.02742 0.02776 2.31178

D9 -2.16404 -0.01247 0.00000 -0.03489 -0.03502 -2.19907

D10 -0.01238 0.00467 0.00000 -0.00034 -0.00029 -0.01267

D11 -3.01121 -0.01727 0.00000 -0.02663 -0.02700 -3.03820

D12 -0.92266 -0.01980 0.00000 -0.03010 -0.03057 -0.95324

D13 1.26387 -0.02290 0.00000 -0.03314 -0.03366 1.23021

D14 -1.07300 0.01036 0.00000 0.04103 0.04149 -1.03151

D15 1.01554 0.00783 0.00000 0.03756 0.03792 1.05346

D16 -3.08111 0.00473 0.00000 0.03452 0.03483 -3.04628

D17 0.92918 0.00848 0.00000 0.01943 0.01960 0.94878

D18 3.01772 0.00594 0.00000 0.01595 0.01602 3.03374

D19 -1.07892 0.00284 0.00000 0.01292 0.01293 -1.06599

D20 -1.03927 0.00349 0.00000 0.03103 0.03043 -1.00884

D21 -2.93622 -0.00751 0.00000 0.03044 0.03016 -2.90606

D22 0.97694 0.00322 0.00000 0.02360 0.02364 1.00058

D23 0.93829 0.00384 0.00000 0.01753 0.01763 0.95592

D24 -0.95866 -0.00716 0.00000 0.01694 0.01737 -0.94129

D25 2.95450 0.00357 0.00000 0.01010 0.01084 2.96534

D26 2.90174 0.01341 0.00000 0.03338 0.03289 2.93463

D27 1.00479 0.00241 0.00000 0.03279 0.03263 1.03742

D28 -1.36523 0.01314 0.00000 0.02595 0.02610 -1.33913

D29 1.00236 -0.00564 0.00000 -0.01668 -0.01662 0.98574

D30 -1.16241 -0.02268 0.00000 -0.05387 -0.05392 -1.21632

D31 -3.12167 0.00932 0.00000 -0.00100 -0.00092 -3.12260

D32 0.99674 -0.00772 0.00000 -0.03819 -0.03821 0.95853

D33 -1.01163 0.00196 0.00000 -0.02915 -0.02908 -1.04071

D34 3.10679 -0.01507 0.00000 -0.06633 -0.06637 3.04042

D35 -0.97775 0.01620 0.00000 0.02324 0.02316 -0.95459

D36 -3.10012 0.01732 0.00000 0.02180 0.02169 -3.07842

D37 1.13186 0.01630 0.00000 0.02193 0.02174 1.15360

D38 3.13645 -0.00347 0.00000 0.00933 0.00945 -3.13728

D39 1.01409 -0.00235 0.00000 0.00789 0.00799 1.02207

D40 -1.03713 -0.00337 0.00000 0.00802 0.00803 -1.02909

D41 1.55832 -0.01735 0.00000 0.01049 0.01070 1.56902

D42 -0.56405 -0.01623 0.00000 0.00906 0.00923 -0.55482

D43 -2.61526 -0.01725 0.00000 0.00919 0.00928 -2.60598

D44 0.61268 -0.00083 0.00000 0.02153 0.02134 0.63402

D45 2.75893 -0.00901 0.00000 0.03227 0.03178 2.79072

D46 -1.35031 -0.00660 0.00000 0.00162 0.00190 -1.34840

D47 -1.51072 0.00508 0.00000 0.01344 0.01366 -1.49706

D48 0.63554 -0.00310 0.00000 0.02418 0.02410 0.65964

D49 2.80948 -0.00069 0.00000 -0.00647 -0.00578 2.80370

D50 2.83432 0.00022 0.00000 0.00327 0.00334 2.83766

D51 -1.30261 -0.00797 0.00000 0.01401 0.01379 -1.28883

D52 0.87133 -0.00555 0.00000 -0.01664 -0.01610 0.85524

D53 -0.18483 0.00864 0.00000 0.02174 0.02165 -0.16318

D54 1.93240 0.00909 0.00000 0.02682 0.02674 1.95914

D55 -2.28345 0.00992 0.00000 0.02363 0.02364 -2.25981

D56 -2.10565 -0.00328 0.00000 0.00054 0.00049 -2.10517

D57 0.01157 -0.00282 0.00000 0.00562 0.00558 0.01715

D58 2.07890 -0.00199 0.00000 0.00243 0.00248 2.08138

D59 2.10935 -0.00510 0.00000 0.00230 0.00228 2.11163

D60 -2.05661 -0.00464 0.00000 0.00738 0.00737 -2.04924

D61 0.01072 -0.00382 0.00000 0.00419 0.00427 0.01500

D62 0.00979 0.00401 0.00000 0.00700 0.00690 0.01669

D63 -3.12221 0.00509 0.00000 0.00757 0.00755 -3.11466

D64 0.17527 -0.00639 0.00000 -0.01623 -0.01629 0.15898

D65 3.13836 0.00470 0.00000 -0.00420 -0.00438 3.13397

D66 0.26575 -0.00438 0.00000 -0.01867 -0.01873 0.24701

D67 2.56546 -0.01346 0.00000 -0.01508 -0.01529 2.55017

D68 -1.68083 0.00029 0.00000 0.02761 0.02784 -1.65299

D69 -2.02553 0.00496 0.00000 -0.01632 -0.01634 -2.04188

D70 0.27418 -0.00413 0.00000 -0.01273 -0.01290 0.26128

D71 2.31108 0.00962 0.00000 0.02997 0.03023 2.34131

D72 2.17774 -0.00285 0.00000 -0.02796 -0.02771 2.15003

D73 -1.80573 -0.01193 0.00000 -0.02437 -0.02427 -1.83000

D74 0.23116 0.00181 0.00000 0.01832 0.01886 0.25002

D75 -2.26724 0.00337 0.00000 -0.03190 -0.03191 -2.29915

D76 0.86367 0.00189 0.00000 -0.03274 -0.03286 0.83080

D77 -0.20462 0.00232 0.00000 0.00886 0.00887 -0.19576

D78 2.92628 0.00084 0.00000 0.00802 0.00792 2.93420

D79 1.87318 0.00667 0.00000 0.01962 0.01996 1.89313

D80 -1.27911 0.00519 0.00000 0.01878 0.01901 -1.26010

D81 1.64556 0.01302 0.00000 -0.01437 -0.01446 1.63110

D82 -1.30305 0.00480 0.00000 -0.02230 -0.02252 -1.32557

D83 -0.27413 0.00483 0.00000 0.01532 0.01559 -0.25854

D84 3.06044 -0.00339 0.00000 0.00739 0.00753 3.06797

D85 -2.30244 -0.00331 0.00000 -0.02440 -0.02435 -2.32679

D86 1.03213 -0.01153 0.00000 -0.03232 -0.03241 0.99972

Item Value Threshold Converged?

Maximum Force 0.082721 0.000450 NO

RMS Force 0.017526 0.000300 NO

Maximum Displacement 0.127224 0.001800 NO

RMS Displacement 0.031913 0.001200 NO

Predicted change in Energy=-2.470245D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.561581 1.157121 0.134740

2 6 0 0.011798 1.207337 0.259479

3 6 0 -0.893713 3.503350 0.152027

4 6 0 -2.021375 2.524790 0.180292

5 1 0 -2.047676 0.603088 -0.695631

6 1 0 -2.754306 2.749448 -0.627360

7 6 0 0.404767 1.797009 -1.110818

8 1 0 1.525883 1.746815 -1.109251

9 1 0 0.045543 1.295650 -2.043183

10 6 0 -0.045487 3.259504 -1.083173

11 1 0 0.841082 3.941258 -1.085766

12 1 0 -0.649067 3.497722 -1.997829

13 1 0 -1.246260 4.559958 0.206711

14 1 0 0.409463 0.170429 0.322720

15 8 0 3.233485 4.172628 1.008394

16 6 0 0.885374 4.036122 1.306386

17 6 0 1.395509 2.700142 1.793318

18 6 0 2.015599 4.819931 0.699227

19 8 0 2.007761 5.842113 0.026959

20 6 0 2.967468 3.003627 1.760469

21 8 0 3.890505 2.289014 2.125357

22 1 0 0.474526 4.588539 2.147003

23 1 0 1.034301 2.467412 2.784386

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.579115 0.000000

3 C 2.439496 2.470460 0.000000

4 C 1.443608 2.423993 1.493318 0.000000

5 H 1.110296 2.349210 3.234451 2.112077 0.000000

6 H 2.130468 3.288757 2.153513 1.113535 2.260718

7 C 2.414001 1.542678 2.488459 2.843025 2.759041

8 H 3.380487 2.111140 3.245101 3.853726 3.774854

9 H 2.710238 2.304603 3.251936 3.275176 2.584010

10 C 2.863891 2.453036 1.518113 2.457698 3.348954

11 H 3.874771 3.157803 2.175640 3.435542 4.431762

12 H 3.295292 3.282994 2.163738 2.752097 3.468535

13 H 3.418173 3.581279 1.115213 2.177937 4.136823

14 H 2.212219 1.112348 3.582705 3.387075 2.694767

15 O 5.731423 4.442194 4.267911 5.569082 6.598180

16 C 3.955881 3.140250 2.186674 3.464304 4.939289

17 C 3.725075 2.548683 2.929082 3.782552 4.737935

18 C 5.150830 4.154447 3.239894 4.672700 6.019768

19 O 5.890753 5.051641 3.728807 5.221310 6.664539

20 C 5.154112 3.770360 4.212545 5.254979 6.078379

21 O 5.913458 4.438005 5.315768 6.228097 6.786923

22 H 4.468732 3.899921 2.651347 3.789002 5.506895

23 H 3.933966 3.001408 3.423408 4.015190 5.008473

6 7 8 9 10

6 H 0.000000

7 C 3.334758 0.000000

8 H 4.422387 1.122240 0.000000

9 H 3.457924 1.117903 1.807536 0.000000

10 C 2.793855 1.530484 2.181309 2.187836 0.000000

11 H 3.815411 2.188333 2.298931 2.923828 1.118392

12 H 2.621094 2.188556 2.930129 2.309472 1.121451

13 H 2.499564 3.477881 4.162968 4.169710 2.190169

14 H 4.190874 2.168137 2.404564 2.645007 3.424310

15 O 6.368263 4.258670 3.644844 5.268025 3.995010

16 C 4.317658 3.329788 3.389171 4.408528 2.679483

17 C 4.804485 3.198629 3.057897 4.302761 3.265510

18 C 5.366445 3.874158 3.599230 4.880829 3.140057

19 O 5.715766 4.497442 4.277223 5.367132 3.481104

20 C 6.205243 4.033318 3.448628 5.091424 4.150864

21 O 7.207147 4.781765 4.043279 5.757363 5.169966

22 H 4.637316 4.290793 4.447913 5.346476 3.531400

23 H 5.106182 4.002296 3.990153 5.065184 4.092843

11 12 13 14 15

11 H 0.000000

12 H 1.802534 0.000000

13 H 2.531854 2.518925 0.000000

14 H 4.048368 4.192412 4.692850 0.000000

15 O 3.187888 4.956519 4.567366 4.945993 0.000000

16 C 2.394442 3.682692 2.455107 4.017173 2.370877

17 C 3.183848 4.380551 3.599331 3.087782 2.482433

18 C 2.310358 4.015320 3.309061 4.933488 1.413447

19 O 2.492497 4.081013 3.502126 5.900002 2.291897

20 C 3.674469 5.239109 4.753087 4.078912 1.415254

21 O 4.726543 6.250549 5.935044 4.455957 2.286326

22 H 3.317247 4.430798 2.593579 4.780371 3.013514

23 H 4.145797 5.173476 4.027917 3.424376 3.301261

16 17 18 19 20

16 C 0.000000

17 C 1.510690 0.000000

18 C 1.503466 2.464763 0.000000

19 O 2.481590 3.656071 1.223462 0.000000

20 C 2.367986 1.601324 2.308950 3.461661 0.000000

21 O 3.571263 2.550349 3.457552 4.535693 1.223034

22 H 1.086553 2.130575 2.127088 2.901179 2.979281

23 H 2.160444 1.080209 3.293203 4.465382 2.252348

21 22 23

21 O 0.000000

22 H 4.117912 0.000000

23 H 2.936673 2.284467 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 3.028063 -0.980735 -0.371818

2 6 0 1.617578 -1.376725 0.217527

3 6 0 1.555367 0.949042 -0.613202

4 6 0 2.884765 0.344748 -0.925499

5 1 0 3.944124 -1.052962 0.251376

6 1 0 3.707547 1.024607 -0.608036

7 6 0 1.531960 -0.447732 1.446143

8 1 0 0.590015 -0.775198 1.960856

9 1 0 2.354661 -0.467481 2.202767

10 6 0 1.350556 0.966909 0.890926

11 1 0 0.331958 1.356309 1.139172

12 1 0 2.094505 1.665371 1.356054

13 1 0 1.435602 1.965288 -1.056596

14 1 0 1.650223 -2.429594 0.574904

15 8 0 -2.533240 0.199661 0.354676

16 6 0 -0.572897 0.559121 -0.929421

17 6 0 -0.669733 -0.944512 -0.820349

18 6 0 -1.629208 1.198935 -0.071950

19 8 0 -1.778728 2.362364 0.275806

20 6 0 -2.120831 -1.055636 -0.152365

21 8 0 -2.765935 -2.061428 0.108475

22 1 0 -0.723430 0.851687 -1.964961

23 1 0 -0.615710 -1.423300 -1.787145

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3372190 0.6086018 0.4958487

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 448.8279124655 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.234974914653 A.U. after 16 cycles

Convg = 0.6579D-08 -V/T = 1.0051

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.044508885 0.129730832 -0.001412958

2 6 -0.036424168 -0.042703870 -0.044336000

3 6 0.013162348 0.057774491 -0.005401439

4 6 0.079021076 -0.082029440 -0.028430835

5 1 0.002461639 -0.022749042 0.028847510

6 1 -0.017094541 0.010064340 0.027505904

7 6 0.018518604 0.024703742 0.040459262

8 1 0.001796952 0.000870819 -0.006529370

9 1 -0.005103386 -0.006371970 0.010176321

10 6 -0.001763725 -0.010060889 0.003519651

11 1 -0.000981834 0.000488586 -0.004232067

12 1 -0.001091927 -0.000049964 -0.000069644

13 1 0.003153586 -0.003746264 0.006427633

14 1 0.007927880 0.010919912 0.021654164

15 8 -0.010244300 -0.003253454 0.011603127

16 6 -0.031906934 -0.056310592 -0.000065416

17 6 0.014772687 0.054051824 -0.037825035

18 6 -0.017076386 -0.022640460 -0.002460427

19 8 0.013044925 -0.009128329 0.007248967

20 6 -0.046443603 -0.039167136 -0.031544216

21 8 -0.005643146 0.020422838 -0.002247354

22 1 -0.019331385 0.011205095 0.002632354

23 1 -0.005263247 -0.022021069 0.004479868

-------------------------------------------------------------------

Cartesian Forces: Max 0.129730832 RMS 0.030389271

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.070451770 RMS 0.015361056

Search for a saddle point.

Step number 4 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 3 4

ITU= 0 0 0 0

Eigenvalues --- -0.04274 -0.00841 0.00175 0.00342 0.00566

Eigenvalues --- 0.00724 0.00835 0.01047 0.01422 0.01513

Eigenvalues --- 0.01807 0.01986 0.02206 0.02385 0.02499

Eigenvalues --- 0.02654 0.03030 0.03125 0.03239 0.03528

Eigenvalues --- 0.03755 0.03806 0.03810 0.03944 0.04530

Eigenvalues --- 0.04780 0.05226 0.05398 0.05744 0.06071

Eigenvalues --- 0.06213 0.06693 0.07385 0.07619 0.08758

Eigenvalues --- 0.09670 0.11087 0.13250 0.14171 0.15473

Eigenvalues --- 0.16874 0.20851 0.22743 0.24824 0.25841

Eigenvalues --- 0.27806 0.28261 0.30778 0.31261 0.31536

Eigenvalues --- 0.31894 0.32254 0.32277 0.32857 0.34519

Eigenvalues --- 0.35636 0.37507 0.39581 0.40013 0.42591

Eigenvalues --- 0.45339 1.07882 1.10790

Eigenvectors required to have negative eigenvalues:

R6 R10 A8 D41 D21

1 0.82560 0.33795 -0.09962 0.09646 0.09127

D43 A38 D42 A15 A12

1 0.08631 -0.08308 0.08214 -0.08008 0.07947

RFO step: Lambda0=5.881001729D-02 Lambda=-1.37205476D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.285

Iteration 1 RMS(Cart)= 0.03416142 RMS(Int)= 0.00141097

Iteration 2 RMS(Cart)= 0.00206400 RMS(Int)= 0.00036981

Iteration 3 RMS(Cart)= 0.00000113 RMS(Int)= 0.00036980

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00036980

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.98409 -0.06648 0.00000 -0.08822 -0.08801 2.89608

R2 2.72802 -0.06488 0.00000 -0.02658 -0.02622 2.70180

R3 2.09816 -0.01130 0.00000 -0.00457 -0.00457 2.09358

R4 2.91524 -0.02086 0.00000 -0.02201 -0.02172 2.89352

R5 2.10203 -0.00611 0.00000 -0.00551 -0.00551 2.09652

R6 4.81631 -0.06053 0.00000 0.21454 0.21424 5.03055

R7 2.82196 -0.02764 0.00000 -0.01378 -0.01378 2.80818

R8 2.86882 -0.00417 0.00000 -0.00003 -0.00038 2.86844

R9 2.10745 -0.00423 0.00000 -0.00158 -0.00158 2.10586

R10 4.13221 -0.07045 0.00000 -0.10357 -0.10337 4.02884

R11 2.10428 -0.00667 0.00000 -0.00366 -0.00366 2.10061

R12 2.12073 0.00175 0.00000 0.00113 0.00113 2.12186

R13 2.11253 -0.00399 0.00000 0.00006 0.00006 2.11259

R14 2.89220 0.00201 0.00000 0.00442 0.00433 2.89653

R15 2.11345 -0.00047 0.00000 -0.00064 -0.00064 2.11282

R16 2.11924 0.00063 0.00000 0.00007 0.00007 2.11931

R17 2.67103 -0.01946 0.00000 -0.01091 -0.01088 2.66015

R18 2.67444 -0.02374 0.00000 -0.00201 -0.00190 2.67254

R19 2.85479 -0.03002 0.00000 -0.02888 -0.02913 2.82566

R20 2.84114 -0.02119 0.00000 -0.00190 -0.00199 2.83915

R21 2.05329 0.01504 0.00000 0.00994 0.00994 2.06322

R22 3.02606 -0.05412 0.00000 -0.04057 -0.04051 2.98555

R23 2.04130 0.01061 0.00000 0.00485 0.00485 2.04614

R24 2.31201 -0.01169 0.00000 -0.00111 -0.00111 2.31089

R25 2.31120 -0.01686 0.00000 -0.00181 -0.00181 2.30939

A1 1.85952 0.02167 0.00000 0.01721 0.01742 1.87694

A2 2.10733 -0.00298 0.00000 0.00702 0.00655 2.11388

A3 1.93575 -0.00080 0.00000 0.00779 0.00747 1.94321

A4 1.76786 0.00770 0.00000 0.03435 0.03330 1.80116

A5 1.90821 0.01784 0.00000 0.04538 0.04376 1.95197

A6 2.22321 -0.02653 0.00000 -0.05150 -0.05149 2.17172

A7 1.89204 0.00802 0.00000 0.02944 0.02791 1.91995

A8 1.74405 0.00431 0.00000 -0.02863 -0.02849 1.71556

A9 1.89408 -0.00624 0.00000 -0.01839 -0.01760 1.87648

A10 1.90929 -0.00082 0.00000 -0.00489 -0.00525 1.90404

A11 1.96190 0.01130 0.00000 0.00343 0.00339 1.96529

A12 2.44036 -0.03321 0.00000 -0.02702 -0.02698 2.41338

A13 1.94842 0.00510 0.00000 0.00848 0.00862 1.95704

A14 1.58487 0.01449 0.00000 0.02835 0.02890 1.61377

A15 1.57127 0.00663 0.00000 -0.00147 -0.00197 1.56930

A16 1.96028 0.00951 0.00000 0.02143 0.02125 1.98153

A17 1.95832 0.00440 0.00000 0.00933 0.00872 1.96704

A18 1.92954 0.00428 0.00000 0.01120 0.01078 1.94032

A19 1.80919 0.00675 0.00000 0.01499 0.01483 1.82402

A20 2.08008 -0.01508 0.00000 -0.02832 -0.02821 2.05187

A21 1.84863 0.00798 0.00000 0.01710 0.01719 1.86582

A22 1.87771 0.00107 0.00000 0.00065 0.00075 1.87847

A23 1.91411 -0.00068 0.00000 -0.00455 -0.00473 1.90938

A24 1.92740 0.00079 0.00000 0.00139 0.00135 1.92874

A25 1.90981 -0.00908 0.00000 0.00167 0.00110 1.91091

A26 1.92505 0.00404 0.00000 0.00224 0.00251 1.92756

A27 1.90579 0.00237 0.00000 0.00094 0.00101 1.90681

A28 1.92757 0.00187 0.00000 -0.00134 -0.00114 1.92643

A29 1.92473 0.00346 0.00000 -0.00196 -0.00183 1.92290

A30 1.87054 -0.00239 0.00000 -0.00159 -0.00169 1.86885

A31 1.90981 -0.00420 0.00000 -0.00411 -0.00420 1.90561

A32 1.80229 0.00977 0.00000 0.05268 0.05285 1.85514

A33 2.12405 -0.00924 0.00000 -0.02655 -0.02684 2.09720

A34 1.79738 -0.00326 0.00000 -0.02915 -0.02965 1.76773

A35 1.91490 -0.00730 0.00000 -0.01183 -0.01156 1.90335

A36 1.90491 0.00338 0.00000 0.01011 0.01048 1.91539

A37 1.90883 0.00792 0.00000 0.00860 0.00805 1.91688

A38 1.71193 0.00227 0.00000 -0.04097 -0.04141 1.67052

A39 2.25443 -0.01219 0.00000 0.00837 0.00889 2.26333

A40 1.81772 -0.00529 0.00000 -0.02218 -0.02199 1.79573

A41 1.72873 0.00990 0.00000 0.02025 0.02027 1.74900

A42 1.95340 0.00060 0.00000 0.01794 0.01721 1.97062

A43 1.96916 0.00684 0.00000 0.01638 0.01582 1.98498

A44 1.89721 -0.00031 0.00000 0.00305 0.00282 1.90003

A45 2.10404 -0.01477 0.00000 -0.01217 -0.01205 2.09199

A46 2.28188 0.01506 0.00000 0.00914 0.00926 2.29113

A47 1.93046 0.00366 0.00000 -0.00305 -0.00308 1.92738

A48 2.09360 -0.01395 0.00000 -0.01433 -0.01434 2.07927

A49 2.24467 0.01179 0.00000 0.01866 0.01868 2.26334

D1 -1.23618 0.00903 0.00000 0.03350 0.03406 -1.20212

D2 3.05236 -0.01037 0.00000 -0.03305 -0.03428 3.01808

D3 0.71769 0.00800 0.00000 -0.00140 -0.00165 0.71603

D4 0.99046 0.02663 0.00000 0.06734 0.06822 1.05868

D5 -1.00418 0.00722 0.00000 0.00079 -0.00012 -1.00430

D6 2.94433 0.02559 0.00000 0.03244 0.03251 2.97683

D7 0.12539 0.00057 0.00000 -0.01046 -0.01048 0.11491

D8 2.31178 0.01730 0.00000 0.02886 0.02900 2.34078

D9 -2.19907 -0.01229 0.00000 -0.03949 -0.03973 -2.23879

D10 -0.01267 0.00444 0.00000 -0.00016 -0.00025 -0.01292

D11 -3.03820 -0.01617 0.00000 -0.03044 -0.03092 -3.06912

D12 -0.95324 -0.01850 0.00000 -0.03476 -0.03535 -0.98859

D13 1.23021 -0.02155 0.00000 -0.03875 -0.03945 1.19076

D14 -1.03151 0.01034 0.00000 0.04718 0.04760 -0.98390

D15 1.05346 0.00801 0.00000 0.04285 0.04317 1.09662

D16 -3.04628 0.00496 0.00000 0.03886 0.03906 -3.00721

D17 0.94878 0.00802 0.00000 0.02415 0.02438 0.97316

D18 3.03374 0.00569 0.00000 0.01982 0.01994 3.05369

D19 -1.06599 0.00264 0.00000 0.01584 0.01584 -1.05015

D20 -1.00884 0.00255 0.00000 0.01890 0.01835 -0.99050

D21 -2.90606 -0.00777 0.00000 0.02504 0.02486 -2.88120

D22 1.00058 0.00252 0.00000 0.01781 0.01779 1.01837

D23 0.95592 0.00343 0.00000 0.01362 0.01384 0.96976

D24 -0.94129 -0.00689 0.00000 0.01976 0.02035 -0.92094

D25 2.96534 0.00340 0.00000 0.01253 0.01328 2.97863

D26 2.93463 0.01210 0.00000 0.02741 0.02677 2.96140

D27 1.03742 0.00179 0.00000 0.03355 0.03329 1.07071

D28 -1.33913 0.01208 0.00000 0.02632 0.02622 -1.31291

D29 0.98574 -0.00599 0.00000 -0.01654 -0.01649 0.96925

D30 -1.21632 -0.02244 0.00000 -0.05405 -0.05411 -1.27043

D31 -3.12260 0.00805 0.00000 -0.00675 -0.00682 -3.12941

D32 0.95853 -0.00840 0.00000 -0.04426 -0.04444 0.91409

D33 -1.04071 0.00100 0.00000 -0.03485 -0.03489 -1.07560

D34 3.04042 -0.01545 0.00000 -0.07235 -0.07252 2.96790

D35 -0.95459 0.01470 0.00000 0.02293 0.02287 -0.93172

D36 -3.07842 0.01570 0.00000 0.02207 0.02196 -3.05647

D37 1.15360 0.01482 0.00000 0.02213 0.02193 1.17552

D38 -3.13728 -0.00287 0.00000 0.01608 0.01624 -3.12103

D39 1.02207 -0.00187 0.00000 0.01522 0.01533 1.03740

D40 -1.02909 -0.00275 0.00000 0.01528 0.01530 -1.01379

D41 1.56902 -0.01584 0.00000 0.00627 0.00646 1.57548

D42 -0.55482 -0.01484 0.00000 0.00542 0.00555 -0.54927

D43 -2.60598 -0.01572 0.00000 0.00548 0.00552 -2.60046

D44 0.63402 -0.00029 0.00000 0.02585 0.02549 0.65951

D45 2.79072 -0.00787 0.00000 0.03861 0.03785 2.82857

D46 -1.34840 -0.00625 0.00000 0.00662 0.00676 -1.34164

D47 -1.49706 0.00596 0.00000 0.01494 0.01513 -1.48193

D48 0.65964 -0.00163 0.00000 0.02769 0.02749 0.68713

D49 2.80370 -0.00001 0.00000 -0.00429 -0.00360 2.80011

D50 2.83766 0.00067 0.00000 0.00630 0.00625 2.84391

D51 -1.28883 -0.00692 0.00000 0.01906 0.01861 -1.27022

D52 0.85524 -0.00530 0.00000 -0.01293 -0.01248 0.84276

D53 -0.16318 0.00868 0.00000 0.02898 0.02874 -0.13444

D54 1.95914 0.00897 0.00000 0.03200 0.03185 1.99099

D55 -2.25981 0.00933 0.00000 0.02799 0.02794 -2.23187

D56 -2.10517 -0.00274 0.00000 0.00529 0.00515 -2.10002

D57 0.01715 -0.00244 0.00000 0.00831 0.00826 0.02541

D58 2.08138 -0.00208 0.00000 0.00430 0.00435 2.08573

D59 2.11163 -0.00411 0.00000 0.00645 0.00632 2.11795

D60 -2.04924 -0.00382 0.00000 0.00947 0.00943 -2.03980

D61 0.01500 -0.00346 0.00000 0.00546 0.00552 0.02052

D62 0.01669 0.00372 0.00000 0.00727 0.00723 0.02392

D63 -3.11466 0.00476 0.00000 0.00490 0.00500 -3.10966

D64 0.15898 -0.00626 0.00000 -0.01545 -0.01554 0.14344

D65 3.13397 0.00372 0.00000 -0.00605 -0.00619 3.12778

D66 0.24701 -0.00456 0.00000 -0.01633 -0.01675 0.23026

D67 2.55017 -0.01348 0.00000 -0.01465 -0.01488 2.53529

D68 -1.65299 0.00009 0.00000 0.02267 0.02279 -1.63020

D69 -2.04188 0.00474 0.00000 -0.01211 -0.01249 -2.05436

D70 0.26128 -0.00418 0.00000 -0.01042 -0.01061 0.25067

D71 2.34131 0.00940 0.00000 0.02689 0.02706 2.36836

D72 2.15003 -0.00258 0.00000 -0.02165 -0.02168 2.12835

D73 -1.83000 -0.01150 0.00000 -0.01997 -0.01980 -1.84981

D74 0.25002 0.00207 0.00000 0.01735 0.01787 0.26789

D75 -2.29915 0.00262 0.00000 -0.03734 -0.03721 -2.33636

D76 0.83080 0.00118 0.00000 -0.03481 -0.03481 0.79599

D77 -0.19576 0.00242 0.00000 0.00528 0.00534 -0.19041

D78 2.93420 0.00098 0.00000 0.00781 0.00774 2.94194

D79 1.89313 0.00697 0.00000 0.01573 0.01601 1.90914

D80 -1.26010 0.00552 0.00000 0.01826 0.01841 -1.24169

D81 1.63110 0.01196 0.00000 -0.01981 -0.01999 1.61111

D82 -1.32557 0.00412 0.00000 -0.02594 -0.02623 -1.35180

D83 -0.25854 0.00518 0.00000 0.01389 0.01417 -0.24437

D84 3.06797 -0.00266 0.00000 0.00776 0.00793 3.07590

D85 -2.32679 -0.00392 0.00000 -0.02509 -0.02499 -2.35178

D86 0.99972 -0.01176 0.00000 -0.03122 -0.03123 0.96850

Item Value Threshold Converged?

Maximum Force 0.070452 0.000450 NO

RMS Force 0.015361 0.000300 NO

Maximum Displacement 0.133284 0.001800 NO

RMS Displacement 0.035232 0.001200 NO

Predicted change in Energy=-2.638461D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.552742 1.175617 0.130446

2 6 0 -0.022030 1.161521 0.203958

3 6 0 -0.850594 3.511346 0.150711

4 6 0 -1.974610 2.540242 0.193398

5 1 0 -2.092922 0.622886 -0.663333

6 1 0 -2.746732 2.786141 -0.567529

7 6 0 0.397886 1.779294 -1.132664

8 1 0 1.518481 1.708400 -1.135626

9 1 0 0.025370 1.292224 -2.067421

10 6 0 -0.018860 3.253786 -1.092646

11 1 0 0.883556 3.913786 -1.102400

12 1 0 -0.623775 3.509543 -2.001715

13 1 0 -1.195799 4.569062 0.213181

14 1 0 0.377671 0.129976 0.287550

15 8 0 3.210857 4.208080 1.026858

16 6 0 0.868625 4.007341 1.309838

17 6 0 1.421837 2.713131 1.814633

18 6 0 1.981849 4.812933 0.702386

19 8 0 1.963830 5.826439 0.018357

20 6 0 2.967632 3.038037 1.783127

21 8 0 3.915238 2.359545 2.150767

22 1 0 0.417303 4.562280 2.134704

23 1 0 1.051528 2.451398 2.797874

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.532542 0.000000

3 C 2.439067 2.492193 0.000000

4 C 1.429733 2.390304 1.486027 0.000000

5 H 1.107877 2.308878 3.247961 2.103388 0.000000

6 H 2.122868 3.264749 2.153400 1.111597 2.261928

7 C 2.401005 1.531186 2.491136 2.822449 2.785979

8 H 3.364403 2.113465 3.243114 3.828831 3.800478

9 H 2.708257 2.275630 3.257595 3.266309 2.628049

10 C 2.857890 2.461456 1.517911 2.447042 3.377526

11 H 3.866914 3.178304 2.177044 3.425613 4.458949

12 H 3.294890 3.277239 2.164345 2.753692 3.504632

13 H 3.413168 3.604046 1.114375 2.173257 4.140702

14 H 2.201033 1.109430 3.600142 3.369195 2.692763

15 O 5.717628 4.517770 4.212892 5.510482 6.621211

16 C 3.908023 3.180397 2.131971 3.388629 4.911080

17 C 3.748141 2.662052 2.927409 3.767513 4.781525

18 C 5.103971 4.194850 3.165629 4.591053 6.002120

19 O 5.831722 5.073415 3.646663 5.132352 6.633167

20 C 5.160789 3.866932 4.179431 5.215438 6.117788

21 O 5.948292 4.552735 5.295282 6.209207 6.858070

22 H 4.400865 3.935220 2.578420 3.684909 5.445096

23 H 3.940179 3.089451 3.427686 3.993583 5.021053

6 7 8 9 10

6 H 0.000000

7 C 3.349887 0.000000

8 H 4.435797 1.122838 0.000000

9 H 3.487982 1.117934 1.808542 0.000000

10 C 2.817042 1.532778 2.180248 2.190861 0.000000

11 H 3.838836 2.189257 2.295204 2.922385 1.118055

12 H 2.662169 2.189247 2.929758 2.311322 1.121490

13 H 2.488716 3.483380 4.167731 4.174933 2.195522

14 H 4.189066 2.176618 2.412115 2.649684 3.438077

15 O 6.329048 4.298295 3.713337 5.312636 3.979201

16 C 4.252839 3.339402 3.418733 4.414614 2.669720

17 C 4.801770 3.256853 3.118149 4.363421 3.289405

18 C 5.299061 3.883209 3.637461 4.888255 3.107397

19 O 5.637026 4.489589 4.299797 5.354176 3.432772

20 C 6.184092 4.085323 3.519530 5.150872 4.151596

21 O 7.207840 4.846583 4.119321 5.836381 5.176535

22 H 4.524141 4.291978 4.477977 5.338982 3.509726

23 H 5.085742 4.040804 4.030200 5.105662 4.114086

11 12 13 14 15

11 H 0.000000

12 H 1.801173 0.000000

13 H 2.546342 2.521023 0.000000

14 H 4.062647 4.202987 4.710289 0.000000

15 O 3.168072 4.936052 4.495664 5.020404 0.000000

16 C 2.414098 3.666257 2.404170 4.039811 2.367790

17 C 3.200063 4.402649 3.586244 3.177256 2.460905

18 C 2.296076 3.974955 3.224321 4.967450 1.407689

19 O 2.466035 4.018009 3.406201 5.919295 2.278429

20 C 3.665593 5.238850 4.705627 4.171506 1.414250

21 O 4.710611 6.258453 5.895668 4.577874 2.275172

22 H 3.334183 4.393411 2.508863 4.801965 3.026008

23 H 4.168805 5.192530 4.026862 3.484940 3.299263

16 17 18 19 20

16 C 0.000000

17 C 1.495273 0.000000

18 C 1.502413 2.441285 0.000000

19 O 2.485260 3.634976 1.222872 0.000000

20 C 2.359954 1.579885 2.300005 3.449234 0.000000

21 O 3.564301 2.540680 3.443096 4.513815 1.222075

22 H 1.091811 2.128588 2.135923 2.910115 2.991839

23 H 2.160710 1.082772 3.291416 4.466421 2.246177

21 22 23

21 O 0.000000

22 H 4.133745 0.000000

23 H 2.937349 2.301708 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 3.016167 -0.962246 -0.396587

2 6 0 1.692710 -1.388559 0.247929

3 6 0 1.509330 0.943639 -0.611287

4 6 0 2.825806 0.342671 -0.948937

5 1 0 3.971711 -1.028901 0.160085

6 1 0 3.658637 1.037392 -0.705211

7 6 0 1.572186 -0.450596 1.452185

8 1 0 0.646908 -0.796049 1.986309

9 1 0 2.409823 -0.449038 2.192548

10 6 0 1.343192 0.959795 0.897419

11 1 0 0.323749 1.326176 1.174094

12 1 0 2.082606 1.675527 1.343217

13 1 0 1.372421 1.954653 -1.059548

14 1 0 1.721178 -2.443577 0.589924

15 8 0 -2.527995 0.219388 0.349923

16 6 0 -0.557709 0.527434 -0.926599

17 6 0 -0.708273 -0.956225 -0.817382

18 6 0 -1.600192 1.190473 -0.071700

19 8 0 -1.732957 2.353525 0.281994

20 6 0 -2.138132 -1.044325 -0.151214

21 8 0 -2.813356 -2.026097 0.120198

22 1 0 -0.681319 0.835116 -1.966841

23 1 0 -0.641771 -1.458198 -1.774460

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3458501 0.6081774 0.4980788

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 449.4518921073 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.208870697669 A.U. after 16 cycles

Convg = 0.7554D-08 -V/T = 1.0045

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.037263325 0.113899823 -0.002896640

2 6 -0.031483685 -0.043184845 -0.042148198

3 6 0.018074904 0.055441427 -0.001139261

4 6 0.065316420 -0.069228255 -0.029341850

5 1 0.000903588 -0.023665919 0.027459965

6 1 -0.016443035 0.010150634 0.027429824

7 6 0.021060503 0.024959042 0.036786220

8 1 0.001427291 0.000632493 -0.006017153

9 1 -0.004816288 -0.005683361 0.008464075

10 6 -0.001519314 -0.011179426 0.002859831

11 1 -0.000718018 0.000344265 -0.004048497

12 1 -0.001013513 -0.000203649 0.000099477

13 1 0.001717952 -0.003135103 0.004111005

14 1 0.008446786 0.009680394 0.020313773

15 8 -0.007018261 -0.001820509 0.009515947

16 6 -0.034943929 -0.048925994 0.001464920

17 6 0.015981734 0.051265696 -0.027836945

18 6 -0.014322547 -0.018601300 -0.003675252

19 8 0.010858102 -0.006056260 0.005872725

20 6 -0.043425514 -0.039153606 -0.028925694

21 8 -0.003725448 0.016601419 -0.000819882

22 1 -0.017544139 0.009208030 0.000311842

23 1 -0.004076914 -0.021344994 0.002159769

-------------------------------------------------------------------

Cartesian Forces: Max 0.113899823 RMS 0.027372614

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.065068035 RMS 0.013337814

Search for a saddle point.

Step number 5 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 4 5

ITU= 0 0 0 0 0

Eigenvalues --- -0.05089 -0.00898 0.00213 0.00344 0.00565

Eigenvalues --- 0.00805 0.00874 0.01222 0.01419 0.01520

Eigenvalues --- 0.01772 0.01987 0.02201 0.02354 0.02469

Eigenvalues --- 0.02664 0.03049 0.03122 0.03349 0.03522

Eigenvalues --- 0.03746 0.03795 0.03882 0.03938 0.04498

Eigenvalues --- 0.04781 0.05253 0.05481 0.06035 0.06171

Eigenvalues --- 0.06219 0.06708 0.07390 0.07972 0.08743

Eigenvalues --- 0.09661 0.11079 0.13222 0.14208 0.15426

Eigenvalues --- 0.16839 0.20807 0.22691 0.24818 0.25848

Eigenvalues --- 0.27793 0.28240 0.30778 0.31258 0.31536

Eigenvalues --- 0.31899 0.32251 0.32294 0.32846 0.34517

Eigenvalues --- 0.35666 0.37507 0.39576 0.40005 0.42575

Eigenvalues --- 0.45385 1.07880 1.10791

Eigenvectors required to have negative eigenvalues:

R6 R10 R1 D34 A38

1 0.82132 0.27074 0.15364 -0.10698 -0.09783

D21 A8 D41 D68 D43

1 0.09448 -0.09131 0.09070 0.08398 0.08236

RFO step: Lambda0=3.873788977D-02 Lambda=-1.23746901D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.312

Iteration 1 RMS(Cart)= 0.03844121 RMS(Int)= 0.00105819

Iteration 2 RMS(Cart)= 0.00123316 RMS(Int)= 0.00039096

Iteration 3 RMS(Cart)= 0.00000076 RMS(Int)= 0.00039096

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.89608 -0.05091 0.00000 0.01498 0.01521 2.91129

R2 2.70180 -0.05148 0.00000 -0.04040 -0.04047 2.66133

R3 2.09358 -0.00831 0.00000 -0.00517 -0.00517 2.08842

R4 2.89352 -0.01570 0.00000 -0.02919 -0.02914 2.86438

R5 2.09652 -0.00443 0.00000 -0.00789 -0.00789 2.08863

R6 5.03055 -0.05178 0.00000 0.16856 0.16855 5.19910

R7 2.80818 -0.02128 0.00000 -0.01055 -0.01084 2.79735

R8 2.86844 -0.00190 0.00000 0.00279 0.00270 2.87114

R9 2.10586 -0.00328 0.00000 -0.00013 -0.00013 2.10573

R10 4.02884 -0.06507 0.00000 -0.14902 -0.14900 3.87984

R11 2.10061 -0.00511 0.00000 -0.00233 -0.00233 2.09828

R12 2.12186 0.00140 0.00000 0.00168 0.00168 2.12354

R13 2.11259 -0.00300 0.00000 0.00077 0.00077 2.11336

R14 2.89653 0.00233 0.00000 0.00462 0.00459 2.90112

R15 2.11282 -0.00034 0.00000 -0.00044 -0.00044 2.11238

R16 2.11931 0.00042 0.00000 -0.00019 -0.00019 2.11912

R17 2.66015 -0.01514 0.00000 -0.01133 -0.01155 2.64860

R18 2.67254 -0.01782 0.00000 0.00368 0.00366 2.67621

R19 2.82566 -0.02276 0.00000 -0.01560 -0.01527 2.81039

R20 2.83915 -0.01646 0.00000 0.00046 0.00033 2.83948

R21 2.06322 0.01217 0.00000 0.00945 0.00945 2.07267

R22 2.98555 -0.04908 0.00000 -0.09617 -0.09597 2.88958

R23 2.04614 0.00852 0.00000 0.00554 0.00554 2.05169

R24 2.31089 -0.00846 0.00000 -0.00074 -0.00074 2.31015

R25 2.30939 -0.01235 0.00000 0.00034 0.00034 2.30973

A1 1.87694 0.01820 0.00000 0.00404 0.00428 1.88122

A2 2.11388 -0.00272 0.00000 0.00213 0.00164 2.11552

A3 1.94321 0.00012 0.00000 0.02323 0.02316 1.96637

A4 1.80116 0.00750 0.00000 0.02456 0.02346 1.82462

A5 1.95197 0.01567 0.00000 0.03947 0.03727 1.98924

A6 2.17172 -0.02493 0.00000 -0.06427 -0.06416 2.10756

A7 1.91995 0.00731 0.00000 0.03728 0.03629 1.95624

A8 1.71556 0.00317 0.00000 -0.01666 -0.01691 1.69865

A9 1.87648 -0.00577 0.00000 -0.01183 -0.01116 1.86532

A10 1.90404 -0.00053 0.00000 -0.00602 -0.00586 1.89817

A11 1.96529 0.00917 0.00000 -0.00559 -0.00575 1.95954

A12 2.41338 -0.02957 0.00000 -0.02900 -0.02927 2.38411

A13 1.95704 0.00503 0.00000 0.00746 0.00732 1.96436

A14 1.61377 0.01305 0.00000 0.03617 0.03651 1.65028

A15 1.56930 0.00595 0.00000 0.00539 0.00502 1.57432

A16 1.98153 0.00890 0.00000 0.03337 0.03265 2.01417

A17 1.96704 0.00343 0.00000 0.01127 0.01058 1.97762

A18 1.94032 0.00422 0.00000 0.00887 0.00813 1.94845

A19 1.82402 0.00627 0.00000 0.01552 0.01546 1.83947

A20 2.05187 -0.01344 0.00000 -0.02993 -0.02973 2.02214

A21 1.86582 0.00691 0.00000 0.01971 0.01944 1.88527

A22 1.87847 0.00087 0.00000 0.00016 0.00021 1.87868

A23 1.90938 -0.00052 0.00000 -0.00435 -0.00461 1.90477

A24 1.92874 0.00061 0.00000 0.00020 0.00041 1.92915

A25 1.91091 -0.00667 0.00000 0.00393 0.00359 1.91450

A26 1.92756 0.00325 0.00000 0.00352 0.00369 1.93126

A27 1.90681 0.00180 0.00000 -0.00035 -0.00032 1.90649

A28 1.92643 0.00105 0.00000 -0.00475 -0.00471 1.92172

A29 1.92290 0.00266 0.00000 -0.00106 -0.00092 1.92197

A30 1.86885 -0.00188 0.00000 -0.00138 -0.00144 1.86741

A31 1.90561 -0.00360 0.00000 -0.00582 -0.00607 1.89954

A32 1.85514 0.01017 0.00000 0.06399 0.06408 1.91923

A33 2.09720 -0.00914 0.00000 -0.03092 -0.03118 2.06603

A34 1.76773 -0.00347 0.00000 -0.02863 -0.02930 1.73843

A35 1.90335 -0.00680 0.00000 -0.02174 -0.02126 1.88209

A36 1.91539 0.00355 0.00000 0.01254 0.01293 1.92831

A37 1.91688 0.00700 0.00000 0.00904 0.00844 1.92532

A38 1.67052 0.00096 0.00000 -0.04650 -0.04668 1.62383

A39 2.26333 -0.01124 0.00000 -0.00121 -0.00063 2.26270

A40 1.79573 -0.00462 0.00000 -0.02012 -0.02004 1.77569

A41 1.74900 0.00951 0.00000 0.03138 0.03100 1.78000

A42 1.97062 0.00091 0.00000 0.01222 0.01126 1.98188

A43 1.98498 0.00595 0.00000 0.02042 0.01978 2.00476

A44 1.90003 -0.00093 0.00000 -0.00147 -0.00174 1.89829

A45 2.09199 -0.01188 0.00000 -0.00902 -0.00888 2.08310

A46 2.29113 0.01279 0.00000 0.01050 0.01064 2.30177

A47 1.92738 0.00346 0.00000 0.00366 0.00386 1.93125

A48 2.07927 -0.01240 0.00000 -0.02455 -0.02474 2.05453

A49 2.26334 0.01023 0.00000 0.02300 0.02289 2.28623

D1 -1.20212 0.01024 0.00000 0.04040 0.04075 -1.16137

D2 3.01808 -0.01027 0.00000 -0.03682 -0.03805 2.98003

D3 0.71603 0.00809 0.00000 0.00656 0.00610 0.72214

D4 1.05868 0.02695 0.00000 0.08091 0.08162 1.14030

D5 -1.00430 0.00644 0.00000 0.00369 0.00282 -1.00148

D6 2.97683 0.02480 0.00000 0.04708 0.04697 3.02381

D7 0.11491 -0.00042 0.00000 -0.01709 -0.01712 0.09779

D8 2.34078 0.01610 0.00000 0.03382 0.03422 2.37500

D9 -2.23879 -0.01259 0.00000 -0.04287 -0.04335 -2.28214

D10 -0.01292 0.00394 0.00000 0.00804 0.00799 -0.00493

D11 -3.06912 -0.01550 0.00000 -0.03691 -0.03721 -3.10633

D12 -0.98859 -0.01765 0.00000 -0.04278 -0.04314 -1.03173

D13 1.19076 -0.02083 0.00000 -0.04776 -0.04821 1.14255

D14 -0.98390 0.01035 0.00000 0.04033 0.04069 -0.94321

D15 1.09662 0.00821 0.00000 0.03446 0.03476 1.13138

D16 -3.00721 0.00503 0.00000 0.02948 0.02969 -2.97752

D17 0.97316 0.00763 0.00000 0.03108 0.03128 1.00444

D18 3.05369 0.00549 0.00000 0.02521 0.02535 3.07904

D19 -1.05015 0.00230 0.00000 0.02023 0.02029 -1.02986

D20 -0.99050 0.00182 0.00000 0.02216 0.02156 -0.96893

D21 -2.88120 -0.00766 0.00000 0.02231 0.02199 -2.85921

D22 1.01837 0.00205 0.00000 0.01667 0.01665 1.03502

D23 0.96976 0.00308 0.00000 0.01227 0.01229 0.98205

D24 -0.92094 -0.00640 0.00000 0.01242 0.01272 -0.90822

D25 2.97863 0.00332 0.00000 0.00678 0.00738 2.98601

D26 2.96140 0.01061 0.00000 0.04252 0.04161 3.00301

D27 1.07071 0.00114 0.00000 0.04267 0.04204 1.11274

D28 -1.31291 0.01085 0.00000 0.03704 0.03670 -1.27621

D29 0.96925 -0.00619 0.00000 -0.01284 -0.01252 0.95673

D30 -1.27043 -0.02200 0.00000 -0.06395 -0.06399 -1.33443

D31 -3.12941 0.00651 0.00000 -0.01170 -0.01152 -3.14093

D32 0.91409 -0.00930 0.00000 -0.06280 -0.06299 0.85110

D33 -1.07560 -0.00021 0.00000 -0.04079 -0.04043 -1.11603

D34 2.96790 -0.01602 0.00000 -0.09189 -0.09190 2.87600

D35 -0.93172 0.01274 0.00000 0.01159 0.01143 -0.92028

D36 -3.05647 0.01372 0.00000 0.01266 0.01255 -3.04392

D37 1.17552 0.01301 0.00000 0.01249 0.01232 1.18785

D38 -3.12103 -0.00233 0.00000 0.01799 0.01805 -3.10299

D39 1.03740 -0.00136 0.00000 0.01906 0.01916 1.05656

D40 -1.01379 -0.00206 0.00000 0.01889 0.01894 -0.99486

D41 1.57548 -0.01432 0.00000 -0.00294 -0.00299 1.57250

D42 -0.54927 -0.01335 0.00000 -0.00186 -0.00187 -0.55114

D43 -2.60046 -0.01406 0.00000 -0.00204 -0.00210 -2.60256

D44 0.65951 0.00062 0.00000 0.04132 0.04121 0.70072

D45 2.82857 -0.00641 0.00000 0.04591 0.04530 2.87386

D46 -1.34164 -0.00544 0.00000 0.01672 0.01699 -1.32466

D47 -1.48193 0.00656 0.00000 0.02465 0.02504 -1.45689

D48 0.68713 -0.00048 0.00000 0.02924 0.02912 0.71625

D49 2.80011 0.00050 0.00000 0.00005 0.00081 2.80092

D50 2.84391 0.00105 0.00000 0.01636 0.01640 2.86032

D51 -1.27022 -0.00599 0.00000 0.02095 0.02049 -1.24973

D52 0.84276 -0.00501 0.00000 -0.00823 -0.00782 0.83494

D53 -0.13444 0.00819 0.00000 0.02454 0.02436 -0.11007

D54 1.99099 0.00854 0.00000 0.02843 0.02827 2.01927

D55 -2.23187 0.00851 0.00000 0.02315 0.02306 -2.20881

D56 -2.10002 -0.00236 0.00000 -0.00144 -0.00147 -2.10149

D57 0.02541 -0.00200 0.00000 0.00245 0.00244 0.02785

D58 2.08573 -0.00204 0.00000 -0.00283 -0.00277 2.08296

D59 2.11795 -0.00348 0.00000 0.00091 0.00085 2.11881

D60 -2.03980 -0.00312 0.00000 0.00480 0.00476 -2.03504

D61 0.02052 -0.00316 0.00000 -0.00048 -0.00045 0.02007

D62 0.02392 0.00343 0.00000 0.00919 0.00893 0.03285

D63 -3.10966 0.00444 0.00000 0.00739 0.00721 -3.10245

D64 0.14344 -0.00602 0.00000 -0.01942 -0.01949 0.12395

D65 3.12778 0.00283 0.00000 -0.00440 -0.00473 3.12306

D66 0.23026 -0.00443 0.00000 -0.01685 -0.01739 0.21287

D67 2.53529 -0.01319 0.00000 -0.02427 -0.02492 2.51037

D68 -1.63020 0.00003 0.00000 0.02456 0.02433 -1.60587

D69 -2.05436 0.00453 0.00000 -0.00838 -0.00855 -2.06292

D70 0.25067 -0.00423 0.00000 -0.01581 -0.01608 0.23459

D71 2.36836 0.00899 0.00000 0.03302 0.03317 2.40153

D72 2.12835 -0.00202 0.00000 -0.01367 -0.01346 2.11489

D73 -1.84981 -0.01077 0.00000 -0.02110 -0.02099 -1.87079

D74 0.26789 0.00244 0.00000 0.02773 0.02826 0.29615

D75 -2.33636 0.00178 0.00000 -0.03421 -0.03433 -2.37069

D76 0.79599 0.00045 0.00000 -0.03226 -0.03246 0.76353

D77 -0.19041 0.00259 0.00000 0.01105 0.01099 -0.17942

D78 2.94194 0.00126 0.00000 0.01299 0.01287 2.95481

D79 1.90914 0.00701 0.00000 0.01848 0.01870 1.92784

D80 -1.24169 0.00567 0.00000 0.02042 0.02057 -1.22112

D81 1.61111 0.01057 0.00000 -0.01579 -0.01585 1.59526

D82 -1.35180 0.00328 0.00000 -0.02698 -0.02720 -1.37900

D83 -0.24437 0.00537 0.00000 0.01959 0.01999 -0.22438

D84 3.07590 -0.00193 0.00000 0.00840 0.00864 3.08454

D85 -2.35178 -0.00441 0.00000 -0.02398 -0.02412 -2.37590

D86 0.96850 -0.01170 0.00000 -0.03517 -0.03548 0.93302

Item Value Threshold Converged?

Maximum Force 0.065068 0.000450 NO

RMS Force 0.013338 0.000300 NO

Maximum Displacement 0.139542 0.001800 NO

RMS Displacement 0.038781 0.001200 NO

Predicted change in Energy=-3.150048D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.561465 1.202574 0.133581

2 6 0 -0.023097 1.121642 0.150566

3 6 0 -0.795761 3.521328 0.152426

4 6 0 -1.921603 2.561928 0.209829

5 1 0 -2.156002 0.645761 -0.613296

6 1 0 -2.733938 2.841365 -0.493686

7 6 0 0.406276 1.764261 -1.153362

8 1 0 1.526579 1.678862 -1.173305

9 1 0 0.013345 1.286703 -2.085152

10 6 0 0.015503 3.248039 -1.102789

11 1 0 0.931837 3.887786 -1.127060

12 1 0 -0.595871 3.516860 -2.003605

13 1 0 -1.138856 4.579499 0.217524

14 1 0 0.371458 0.094761 0.257461

15 8 0 3.171624 4.235596 1.043044

16 6 0 0.839759 3.972885 1.308491

17 6 0 1.451463 2.722941 1.833081

18 6 0 1.935991 4.802340 0.701816

19 8 0 1.909357 5.808443 0.007909

20 6 0 2.942385 3.060876 1.800057

21 8 0 3.917510 2.422430 2.168059

22 1 0 0.345737 4.526735 2.116074

23 1 0 1.071370 2.429393 2.806794

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.540589 0.000000

3 C 2.441983 2.521013 0.000000

4 C 1.408317 2.383750 1.480292 0.000000

5 H 1.105142 2.315002 3.271922 2.098612 0.000000

6 H 2.110401 3.274319 2.153217 1.110364 2.273541

7 C 2.417379 1.515766 2.497451 2.813110 2.847453

8 H 3.386860 2.112966 3.247385 3.818747 3.865529

9 H 2.722110 2.242099 3.264193 3.261466 2.698747

10 C 2.863454 2.468593 1.519342 2.438462 3.424454

11 H 3.875066 3.193083 2.180819 3.418668 4.506598

12 H 3.294823 3.271940 2.165283 2.751137 3.551081

13 H 3.404302 3.634031 1.114306 2.164104 4.147185

14 H 2.231320 1.105254 3.621436 3.368578 2.729446

15 O 5.694601 4.549667 4.128380 5.425530 6.634303

16 C 3.849794 3.196075 2.053123 3.289829 4.872125

17 C 3.778565 2.751244 2.917540 3.746792 4.828379

18 C 5.051080 4.205881 3.066804 4.488043 5.979220

19 O 5.768573 5.071571 3.545341 5.025623 6.600479

20 C 5.149281 3.908393 4.111015 5.141610 6.136009

21 O 5.970454 4.614186 5.242640 6.160306 6.912310

22 H 4.314829 3.948914 2.483903 3.554584 5.363778

23 H 3.947528 3.156520 3.424058 3.964806 5.029343

6 7 8 9 10

6 H 0.000000

7 C 3.384712 0.000000

8 H 4.468255 1.123730 0.000000

9 H 3.535152 1.118343 1.809733 0.000000

10 C 2.845315 1.535206 2.179596 2.193600 0.000000

11 H 3.864462 2.187753 2.288057 2.920137 1.117825

12 H 2.703236 2.190620 2.927871 2.313307 1.121389

13 H 2.463984 3.491751 4.177637 4.179998 2.201944

14 H 4.213258 2.186061 2.427091 2.652698 3.452556

15 O 6.259480 4.310318 3.762349 5.334445 3.942203

16 C 4.159266 3.335662 3.448707 4.406285 2.649352

17 C 4.790142 3.306104 3.183411 4.414014 3.310142

18 C 5.204122 3.874484 3.666035 4.880928 3.059530

19 O 5.533113 4.468021 4.312219 5.331219 3.372833

20 C 6.126181 4.103137 3.571463 5.178978 4.126522

21 O 7.176500 4.877887 4.175423 5.884062 5.158074

22 H 4.374440 4.280670 4.508302 5.315881 3.479252

23 H 5.054035 4.070330 4.075746 5.133838 4.131570

11 12 13 14 15

11 H 0.000000

12 H 1.799947 0.000000

13 H 2.564009 2.521398 0.000000

14 H 4.076513 4.214132 4.732391 0.000000

15 O 3.137988 4.898232 4.402271 5.060098 0.000000

16 C 2.438776 3.638540 2.339467 4.045222 2.361583

17 C 3.223246 4.420639 3.573037 3.249049 2.423064

18 C 2.278052 3.922000 3.120718 4.980614 1.401579

19 O 2.435698 3.946354 3.293303 5.922295 2.266864

20 C 3.646107 5.214885 4.633267 4.217476 1.416187

21 O 4.681807 6.242689 5.833041 4.652194 2.260437

22 H 3.357035 4.344909 2.410663 4.805986 3.036740

23 H 4.197807 5.205979 4.026460 3.526966 3.283938

16 17 18 19 20

16 C 0.000000

17 C 1.487192 0.000000

18 C 1.502589 2.416284 0.000000

19 O 2.490949 3.614035 1.222481 0.000000

20 C 2.344022 1.529097 2.291650 3.439196 0.000000

21 O 3.551805 2.506771 3.426406 4.490436 1.222255

22 H 1.096812 2.134570 2.145924 2.920966 2.998531

23 H 2.163545 1.085706 3.287762 4.466985 2.216526

21 22 23

21 O 0.000000

22 H 4.145885 0.000000

23 H 2.916940 2.324324 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 3.009199 -0.935013 -0.437084

2 6 0 1.733851 -1.404534 0.288486

3 6 0 1.448860 0.936047 -0.603685

4 6 0 2.754828 0.343374 -0.970358

5 1 0 4.001191 -1.005714 0.044884

6 1 0 3.588453 1.059468 -0.811657

7 6 0 1.594039 -0.457522 1.463717

8 1 0 0.687372 -0.811162 2.025557

9 1 0 2.451861 -0.440297 2.181028

10 6 0 1.326295 0.949348 0.910648

11 1 0 0.310328 1.297301 1.220928

12 1 0 2.065916 1.677780 1.334748

13 1 0 1.301818 1.945013 -1.053178

14 1 0 1.762585 -2.462149 0.608190

15 8 0 -2.508915 0.237328 0.340420

16 6 0 -0.531081 0.496978 -0.923633

17 6 0 -0.750753 -0.969510 -0.810078

18 6 0 -1.561421 1.183948 -0.072604

19 8 0 -1.679592 2.346365 0.286954

20 6 0 -2.131458 -1.034101 -0.156150

21 8 0 -2.840398 -1.988505 0.127437

22 1 0 -0.623551 0.819211 -1.967957

23 1 0 -0.668880 -1.495037 -1.756585

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3524562 0.6135071 0.5043917

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 450.6260615154 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.178905580815 A.U. after 16 cycles

Convg = 0.4472D-08 -V/T = 1.0039

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.053828657 0.092027028 -0.005445874

2 6 -0.046846019 -0.037836478 -0.037456218

3 6 0.027963471 0.052149206 0.004895002

4 6 0.049525619 -0.054400469 -0.029331917

5 1 0.001191960 -0.023187472 0.026277181

6 1 -0.015163075 0.010119385 0.026931180

7 6 0.021289182 0.024244135 0.033155154

8 1 0.001060636 0.000503275 -0.005583206

9 1 -0.004295480 -0.004921981 0.006634055

10 6 -0.002599054 -0.011866060 0.001747048

11 1 -0.000616712 0.000340332 -0.003683532

12 1 -0.000775492 -0.000502277 0.000029737

13 1 0.000057246 -0.002229688 0.001087469

14 1 0.007596532 0.008564206 0.018995949

15 8 -0.003449119 0.000519381 0.006603272

16 6 -0.042001745 -0.041183366 -0.000649859

17 6 0.000965215 0.041722065 -0.019174565

18 6 -0.011675437 -0.014304754 -0.004272683

19 8 0.008558899 -0.003212405 0.004467684

20 6 -0.026551829 -0.035973759 -0.025977854

21 8 -0.000604700 0.012410312 0.000735790

22 1 -0.014037963 0.007231416 -0.000258832

23 1 -0.003420794 -0.020212032 0.000275019

-------------------------------------------------------------------

Cartesian Forces: Max 0.092027028 RMS 0.024382413

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.062302034 RMS 0.011774562

Search for a saddle point.

Step number 6 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 5 6

ITU= 0 0 0 0 0 0

Eigenvalues --- -0.04737 -0.01970 0.00227 0.00344 0.00563

Eigenvalues --- 0.00807 0.00860 0.01269 0.01413 0.01675

Eigenvalues --- 0.01980 0.02111 0.02187 0.02434 0.02649

Eigenvalues --- 0.02996 0.03105 0.03213 0.03385 0.03525

Eigenvalues --- 0.03774 0.03781 0.03879 0.03980 0.04591

Eigenvalues --- 0.04859 0.05247 0.05619 0.06031 0.06183

Eigenvalues --- 0.06377 0.06879 0.07388 0.08575 0.09415

Eigenvalues --- 0.09625 0.11317 0.13270 0.14232 0.15326

Eigenvalues --- 0.16777 0.20791 0.22753 0.24806 0.25966

Eigenvalues --- 0.27765 0.28157 0.30767 0.31255 0.31529

Eigenvalues --- 0.31896 0.32252 0.32291 0.32829 0.34516

Eigenvalues --- 0.35656 0.37499 0.39581 0.40027 0.42638

Eigenvalues --- 0.45405 1.07913 1.10800

Eigenvectors required to have negative eigenvalues:

R6 R10 R22 D34 A8

1 -0.82149 -0.22060 -0.16740 0.11113 0.10124

D21 D41 D4 A38 D43

1 -0.09563 -0.09477 -0.09184 0.08512 -0.08450

RFO step: Lambda0=2.740459492D-02 Lambda=-1.23169464D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.296

Iteration 1 RMS(Cart)= 0.04010961 RMS(Int)= 0.00130581

Iteration 2 RMS(Cart)= 0.00135338 RMS(Int)= 0.00051017

Iteration 3 RMS(Cart)= 0.00000173 RMS(Int)= 0.00051016

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00051016

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.91129 -0.05800 0.00000 -0.14046 -0.14001 2.77128

R2 2.66133 -0.03593 0.00000 -0.00439 -0.00365 2.65768

R3 2.08842 -0.00672 0.00000 -0.00264 -0.00264 2.08577

R4 2.86438 -0.01097 0.00000 -0.00685 -0.00676 2.85763

R5 2.08863 -0.00341 0.00000 -0.00196 -0.00196 2.08667

R6 5.19910 -0.04575 0.00000 0.12414 0.12359 5.32269

R7 2.79735 -0.01676 0.00000 -0.00858 -0.00853 2.78882

R8 2.87114 -0.00119 0.00000 0.00422 0.00396 2.87510

R9 2.10573 -0.00207 0.00000 0.00141 0.00141 2.10714

R10 3.87984 -0.06230 0.00000 -0.17377 -0.17346 3.70638

R11 2.09828 -0.00342 0.00000 -0.00369 -0.00369 2.09459

R12 2.12354 0.00112 0.00000 0.00007 0.00007 2.12361

R13 2.11336 -0.00192 0.00000 0.00132 0.00132 2.11468

R14 2.90112 0.00202 0.00000 0.00123 0.00095 2.90207

R15 2.11238 -0.00023 0.00000 0.00007 0.00007 2.11245

R16 2.11912 0.00028 0.00000 -0.00070 -0.00070 2.11842

R17 2.64860 -0.00950 0.00000 -0.00669 -0.00651 2.64209

R18 2.67621 -0.01105 0.00000 0.00103 0.00132 2.67752

R19 2.81039 -0.01502 0.00000 -0.01782 -0.01820 2.79219

R20 2.83948 -0.01067 0.00000 0.00486 0.00469 2.84417

R21 2.07267 0.00978 0.00000 0.00920 0.00920 2.08187

R22 2.88958 -0.02988 0.00000 0.03464 0.03467 2.92425

R23 2.05169 0.00691 0.00000 0.00152 0.00152 2.05321

R24 2.31015 -0.00537 0.00000 0.00029 0.00029 2.31045

R25 2.30973 -0.00674 0.00000 -0.00153 -0.00153 2.30819

A1 1.88122 0.01804 0.00000 0.02952 0.02968 1.91090

A2 2.11552 -0.00446 0.00000 -0.00248 -0.00361 2.11191

A3 1.96637 0.00047 0.00000 0.01055 0.01041 1.97678

A4 1.82462 0.00680 0.00000 0.03925 0.03826 1.86288

A5 1.98924 0.01200 0.00000 0.04059 0.03819 2.02744

A6 2.10756 -0.02195 0.00000 -0.06671 -0.06673 2.04083

A7 1.95624 0.00674 0.00000 0.02189 0.02013 1.97637

A8 1.69865 0.00262 0.00000 -0.01857 -0.01811 1.68053

A9 1.86532 -0.00535 0.00000 -0.01732 -0.01666 1.84866

A10 1.89817 -0.00171 0.00000 -0.00844 -0.00867 1.88950

A11 1.95954 0.00811 0.00000 -0.00078 -0.00061 1.95893

A12 2.38411 -0.02706 0.00000 -0.04601 -0.04624 2.33787

A13 1.96436 0.00454 0.00000 0.00455 0.00416 1.96852

A14 1.65028 0.01386 0.00000 0.04779 0.04880 1.69908

A15 1.57432 0.00525 0.00000 0.01113 0.01035 1.58467

A16 2.01417 0.00514 0.00000 0.01000 0.00962 2.02379

A17 1.97762 0.00396 0.00000 0.01081 0.00995 1.98757

A18 1.94845 0.00431 0.00000 0.01978 0.01972 1.96817

A19 1.83947 0.00617 0.00000 0.01773 0.01749 1.85696

A20 2.02214 -0.01240 0.00000 -0.03101 -0.03058 1.99156

A21 1.88527 0.00646 0.00000 0.01609 0.01579 1.90105

A22 1.87868 0.00072 0.00000 -0.00003 0.00005 1.87873

A23 1.90477 -0.00131 0.00000 -0.00468 -0.00467 1.90011

A24 1.92915 0.00084 0.00000 0.00303 0.00296 1.93211

A25 1.91450 -0.00554 0.00000 0.00315 0.00254 1.91704

A26 1.93126 0.00204 0.00000 -0.00267 -0.00221 1.92905

A27 1.90649 0.00243 0.00000 0.00548 0.00539 1.91189

A28 1.92172 0.00126 0.00000 -0.00061 -0.00049 1.92124

A29 1.92197 0.00158 0.00000 -0.00445 -0.00422 1.91775

A30 1.86741 -0.00160 0.00000 -0.00102 -0.00112 1.86629

A31 1.89954 -0.00241 0.00000 0.00153 0.00164 1.90118

A32 1.91923 0.00864 0.00000 0.04403 0.04419 1.96341

A33 2.06603 -0.00867 0.00000 -0.03230 -0.03280 2.03323

A34 1.73843 -0.00217 0.00000 -0.01265 -0.01276 1.72568

A35 1.88209 -0.00507 0.00000 -0.00290 -0.00246 1.87964

A36 1.92831 0.00310 0.00000 0.00599 0.00574 1.93406

A37 1.92532 0.00532 0.00000 -0.00089 -0.00126 1.92406

A38 1.62383 0.00101 0.00000 -0.02809 -0.02878 1.59505

A39 2.26270 -0.00977 0.00000 0.00188 0.00284 2.26554

A40 1.77569 -0.00471 0.00000 -0.01475 -0.01491 1.76079

A41 1.78000 0.00736 0.00000 0.00624 0.00609 1.78609

A42 1.98188 0.00137 0.00000 0.02159 0.02149 2.00336

A43 2.00476 0.00561 0.00000 0.01252 0.01209 2.01686

A44 1.89829 0.00027 0.00000 0.00947 0.00913 1.90742

A45 2.08310 -0.00985 0.00000 -0.01101 -0.01084 2.07226

A46 2.30177 0.00957 0.00000 0.00157 0.00173 2.30350

A47 1.93125 0.00132 0.00000 -0.01117 -0.01126 1.91998

A48 2.05453 -0.01004 0.00000 -0.00363 -0.00360 2.05093

A49 2.28623 0.00978 0.00000 0.01561 0.01566 2.30189

D1 -1.16137 0.01001 0.00000 0.04167 0.04235 -1.11903

D2 2.98003 -0.01025 0.00000 -0.03699 -0.03862 2.94141

D3 0.72214 0.00791 0.00000 0.01520 0.01449 0.73663

D4 1.14030 0.02625 0.00000 0.08782 0.08882 1.22911

D5 -1.00148 0.00600 0.00000 0.00917 0.00784 -0.99364

D6 3.02381 0.02415 0.00000 0.06136 0.06096 3.08477

D7 0.09779 -0.00051 0.00000 -0.01451 -0.01495 0.08284

D8 2.37500 0.01475 0.00000 0.03507 0.03488 2.40988

D9 -2.28214 -0.01163 0.00000 -0.04833 -0.04911 -2.33125

D10 -0.00493 0.00363 0.00000 0.00124 0.00072 -0.00421

D11 -3.10633 -0.01333 0.00000 -0.03535 -0.03592 3.14093

D12 -1.03173 -0.01528 0.00000 -0.04091 -0.04158 -1.07331

D13 1.14255 -0.01796 0.00000 -0.04642 -0.04729 1.09527

D14 -0.94321 0.00987 0.00000 0.05336 0.05356 -0.88966

D15 1.13138 0.00792 0.00000 0.04780 0.04790 1.17928

D16 -2.97752 0.00524 0.00000 0.04229 0.04219 -2.93532

D17 1.00444 0.00717 0.00000 0.03146 0.03174 1.03618

D18 3.07904 0.00522 0.00000 0.02590 0.02609 3.10512

D19 -1.02986 0.00254 0.00000 0.02039 0.02038 -1.00948

D20 -0.96893 0.00018 0.00000 -0.00302 -0.00330 -0.97224

D21 -2.85921 -0.00735 0.00000 0.01301 0.01316 -2.84605

D22 1.03502 0.00112 0.00000 0.00988 0.00988 1.04490

D23 0.98205 0.00206 0.00000 0.00702 0.00728 0.98933

D24 -0.90822 -0.00548 0.00000 0.02305 0.02374 -0.88448

D25 2.98601 0.00300 0.00000 0.01992 0.02046 3.00647

D26 3.00301 0.00887 0.00000 0.01833 0.01738 3.02039

D27 1.11274 0.00133 0.00000 0.03436 0.03384 1.14659

D28 -1.27621 0.00981 0.00000 0.03123 0.03056 -1.24565

D29 0.95673 -0.00537 0.00000 -0.01493 -0.01488 0.94185

D30 -1.33443 -0.02020 0.00000 -0.05950 -0.05955 -1.39398

D31 -3.14093 0.00493 0.00000 -0.01587 -0.01634 3.12591

D32 0.85110 -0.00990 0.00000 -0.06044 -0.06102 0.79009

D33 -1.11603 -0.00102 0.00000 -0.04218 -0.04252 -1.15856

D34 2.87600 -0.01585 0.00000 -0.08675 -0.08720 2.78880

D35 -0.92028 0.01149 0.00000 0.02311 0.02297 -0.89731

D36 -3.04392 0.01225 0.00000 0.02353 0.02334 -3.02058

D37 1.18785 0.01152 0.00000 0.02302 0.02274 1.21059

D38 -3.10299 -0.00092 0.00000 0.02720 0.02729 -3.07570

D39 1.05656 -0.00016 0.00000 0.02762 0.02766 1.08423

D40 -0.99486 -0.00089 0.00000 0.02711 0.02706 -0.96779

D41 1.57250 -0.01285 0.00000 -0.00533 -0.00522 1.56727

D42 -0.55114 -0.01210 0.00000 -0.00491 -0.00485 -0.55599

D43 -2.60256 -0.01282 0.00000 -0.00542 -0.00545 -2.60801

D44 0.70072 0.00078 0.00000 0.03230 0.03162 0.73234

D45 2.87386 -0.00552 0.00000 0.04187 0.04069 2.91455

D46 -1.32466 -0.00481 0.00000 0.01560 0.01506 -1.30959

D47 -1.45689 0.00691 0.00000 0.01984 0.02021 -1.43668

D48 0.71625 0.00060 0.00000 0.02942 0.02928 0.74553

D49 2.80092 0.00132 0.00000 0.00315 0.00365 2.80457

D50 2.86032 0.00138 0.00000 0.01253 0.01220 2.87252

D51 -1.24973 -0.00493 0.00000 0.02210 0.02127 -1.22846

D52 0.83494 -0.00421 0.00000 -0.00417 -0.00436 0.83058

D53 -0.11007 0.00858 0.00000 0.03775 0.03717 -0.07291

D54 2.01927 0.00833 0.00000 0.03608 0.03575 2.05502

D55 -2.20881 0.00809 0.00000 0.03177 0.03155 -2.17726

D56 -2.10149 -0.00140 0.00000 0.01083 0.01052 -2.09097

D57 0.02785 -0.00166 0.00000 0.00917 0.00911 0.03696

D58 2.08296 -0.00189 0.00000 0.00485 0.00491 2.08786

D59 2.11881 -0.00199 0.00000 0.01193 0.01156 2.13037

D60 -2.03504 -0.00225 0.00000 0.01026 0.01015 -2.02489

D61 0.02007 -0.00248 0.00000 0.00594 0.00594 0.02601

D62 0.03285 0.00266 0.00000 0.00451 0.00456 0.03741

D63 -3.10245 0.00360 0.00000 -0.00037 -0.00019 -3.10264

D64 0.12395 -0.00560 0.00000 -0.01302 -0.01313 0.11082

D65 3.12306 0.00210 0.00000 -0.00651 -0.00664 3.11641

D66 0.21287 -0.00496 0.00000 -0.01609 -0.01740 0.19547

D67 2.51037 -0.01302 0.00000 -0.02178 -0.02220 2.48817

D68 -1.60587 -0.00046 0.00000 0.00963 0.00948 -1.59639

D69 -2.06292 0.00372 0.00000 -0.00442 -0.00557 -2.06849

D70 0.23459 -0.00433 0.00000 -0.01012 -0.01038 0.22421

D71 2.40153 0.00822 0.00000 0.02130 0.02130 2.42283

D72 2.11489 -0.00146 0.00000 -0.00509 -0.00591 2.10898

D73 -1.87079 -0.00951 0.00000 -0.01079 -0.01071 -1.88151

D74 0.29615 0.00304 0.00000 0.02063 0.02096 0.31711

D75 -2.37069 0.00177 0.00000 -0.03015 -0.02982 -2.40051

D76 0.76353 0.00056 0.00000 -0.02449 -0.02427 0.73926

D77 -0.17942 0.00237 0.00000 0.00275 0.00297 -0.17645

D78 2.95481 0.00117 0.00000 0.00842 0.00851 2.96332

D79 1.92784 0.00617 0.00000 0.00774 0.00770 1.93554

D80 -1.22112 0.00496 0.00000 0.01340 0.01325 -1.20787

D81 1.59526 0.00938 0.00000 -0.01867 -0.01902 1.57625

D82 -1.37900 0.00265 0.00000 -0.02373 -0.02410 -1.40310

D83 -0.22438 0.00552 0.00000 0.01328 0.01359 -0.21079

D84 3.08454 -0.00122 0.00000 0.00822 0.00851 3.09305

D85 -2.37590 -0.00441 0.00000 -0.02471 -0.02469 -2.40059

D86 0.93302 -0.01115 0.00000 -0.02976 -0.02977 0.90325

Item Value Threshold Converged?

Maximum Force 0.062302 0.000450 NO

RMS Force 0.011775 0.000300 NO

Maximum Displacement 0.171393 0.001800 NO

RMS Displacement 0.040516 0.001200 NO

Predicted change in Energy=-3.616226D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.515784 1.226250 0.146380

2 6 0 -0.056493 1.088931 0.099152

3 6 0 -0.732963 3.541362 0.151341

4 6 0 -1.856233 2.587891 0.235503

5 1 0 -2.162831 0.659523 -0.545283

6 1 0 -2.714375 2.878563 -0.402989

7 6 0 0.402178 1.752863 -1.179730

8 1 0 1.520356 1.645018 -1.209762

9 1 0 -0.008710 1.285901 -2.109985

10 6 0 0.048686 3.246148 -1.120132

11 1 0 0.980167 3.862906 -1.159717

12 1 0 -0.567607 3.527919 -2.013144

13 1 0 -1.073666 4.601320 0.212575

14 1 0 0.340686 0.066446 0.225915

15 8 0 3.136690 4.264196 1.056981

16 6 0 0.803399 3.940007 1.303515

17 6 0 1.435453 2.719329 1.845400

18 6 0 1.890549 4.789986 0.702782

19 8 0 1.852763 5.792626 0.004120

20 6 0 2.938779 3.085125 1.817364

21 8 0 3.932565 2.479339 2.187959

22 1 0 0.280316 4.495704 2.098048

23 1 0 1.049674 2.395651 2.808165

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.466498 0.000000

3 C 2.443886 2.544554 0.000000

4 C 1.406384 2.346175 1.475779 0.000000

5 H 1.103743 2.244181 3.291627 2.102911 0.000000

6 H 2.113899 3.243342 2.161615 1.108409 2.290980

7 C 2.390495 1.512192 2.501804 2.792950 2.859578

8 H 3.351512 2.123426 3.244405 3.791984 3.870219

9 H 2.714039 2.218415 3.274941 3.257273 2.735119

10 C 2.851598 2.480182 1.521437 2.428943 3.451361

11 H 3.858448 3.217818 2.181073 3.408440 4.529639

12 H 3.295491 3.266756 2.170833 2.756922 3.595421

13 H 3.404548 3.658468 1.115052 2.160285 4.159134

14 H 2.190423 1.104217 3.637764 3.344284 2.685905

15 O 5.630615 4.603929 4.039417 5.330488 6.606500

16 C 3.752605 3.212249 1.961334 3.168991 4.793553

17 C 3.718300 2.816644 2.871864 3.666639 4.786002

18 C 4.961139 4.225299 2.957358 4.371035 5.920159

19 O 5.676190 5.077305 3.431594 4.907189 6.540304

20 C 5.107909 3.988571 4.057768 5.073625 6.123077

21 O 5.951704 4.712635 5.200274 6.110159 6.923597

22 H 4.210025 3.964231 2.393151 3.416675 5.260462

23 H 3.877392 3.204664 3.398406 3.885851 4.957816

6 7 8 9 10

6 H 0.000000

7 C 3.403444 0.000000

8 H 4.483911 1.123768 0.000000

9 H 3.573658 1.119043 1.810362 0.000000

10 C 2.878180 1.535711 2.176571 2.196741 0.000000

11 H 3.897591 2.187865 2.283273 2.919220 1.117861

12 H 2.760955 2.187666 2.924094 2.312659 1.121018

13 H 2.457384 3.497190 4.182309 4.185740 2.207323

14 H 4.199634 2.196275 2.438171 2.658115 3.465201

15 O 6.187605 4.334424 3.822402 5.365954 3.913057

16 C 4.051364 3.333329 3.478155 4.399521 2.631558

17 C 4.722466 3.339630 3.239656 4.448078 3.315878

18 C 5.107014 3.870816 3.699418 4.878264 3.016440

19 O 5.432885 4.452570 4.334357 5.314611 3.317104

20 C 6.077071 4.146305 3.639962 5.229625 4.124010

21 O 7.145222 4.932821 4.249630 5.952332 5.159067

22 H 4.223566 4.275728 4.539352 5.300369 3.460019

23 H 4.971195 4.090933 4.114453 5.151691 4.142082

11 12 13 14 15

11 H 0.000000

12 H 1.798933 0.000000

13 H 2.578114 2.522322 0.000000

14 H 4.091702 4.221395 4.750333 0.000000

15 O 3.118554 4.867195 4.307409 5.111694 0.000000

16 C 2.470770 3.612437 2.269550 4.047197 2.368570

17 C 3.247427 4.422039 3.536055 3.295305 2.429491

18 C 2.270942 3.874480 3.010393 4.994128 1.398134

19 O 2.416559 3.880263 3.166488 5.926610 2.256785

20 C 3.647482 5.211872 4.579729 4.288965 1.416884

21 O 4.673098 6.245024 5.785092 4.751132 2.257929

22 H 3.391646 4.307840 2.323668 4.809039 3.048981

23 H 4.231047 5.209860 4.013805 3.549067 3.303595

16 17 18 19 20

16 C 0.000000

17 C 1.477561 0.000000

18 C 1.505071 2.408383 0.000000

19 O 2.494351 3.606883 1.222637 0.000000

20 C 2.356844 1.547444 2.290772 3.434800 0.000000

21 O 3.564754 2.531898 3.422670 4.480245 1.221444

22 H 1.101679 2.133935 2.150865 2.922179 3.022572

23 H 2.170175 1.086512 3.297355 4.477393 2.241825

21 22 23

21 O 0.000000

22 H 4.172856 0.000000

23 H 2.950037 2.346571 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.954858 -0.927368 -0.460441

2 6 0 1.801904 -1.404939 0.309779

3 6 0 1.379293 0.936096 -0.593386

4 6 0 2.668321 0.341026 -0.996155

5 1 0 3.979928 -1.009813 -0.059589

6 1 0 3.511310 1.057525 -0.928554

7 6 0 1.630259 -0.453011 1.472145

8 1 0 0.745557 -0.823586 2.057663

9 1 0 2.506446 -0.417820 2.167352

10 6 0 1.313542 0.947156 0.926589

11 1 0 0.302215 1.274217 1.272801

12 1 0 2.051828 1.688840 1.328486

13 1 0 1.222801 1.945831 -1.039801

14 1 0 1.826147 -2.465758 0.615347

15 8 0 -2.492280 0.255019 0.336099

16 6 0 -0.497192 0.469796 -0.922321

17 6 0 -0.746211 -0.982574 -0.813699

18 6 0 -1.522566 1.174357 -0.075301

19 8 0 -1.627658 2.338904 0.281949

20 6 0 -2.142474 -1.029735 -0.148262

21 8 0 -2.874797 -1.962100 0.145550

22 1 0 -0.574009 0.802883 -1.969626

23 1 0 -0.652752 -1.531732 -1.746544

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3552971 0.6202268 0.5112636

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 451.7874802932 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.146992766634 A.U. after 16 cycles

Convg = 0.8694D-08 -V/T = 1.0032

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.017874231 0.085210719 -0.006163172

2 6 -0.012415428 -0.038125961 -0.032800827

3 6 0.034497938 0.047508919 0.011573708

4 6 0.038605036 -0.045864351 -0.029723955

5 1 -0.001858604 -0.022446301 0.025501485

6 1 -0.013133002 0.009541639 0.026747787

7 6 0.024146520 0.023411035 0.028967949

8 1 0.000656184 -0.000045484 -0.004623399

9 1 -0.003680125 -0.003959688 0.005407590

10 6 -0.002288725 -0.012653226 0.000809335

11 1 -0.000247217 0.000072677 -0.003395403

12 1 -0.001064089 -0.000191570 0.000444121

13 1 -0.002187027 -0.001531464 -0.002073752

14 1 0.008717080 0.007145481 0.016217439

15 8 -0.003279960 -0.001314305 0.006838295

16 6 -0.045835678 -0.035970502 -0.005026632

17 6 0.016784130 0.039488859 -0.015051601

18 6 -0.009458726 -0.012208445 -0.003302745

19 8 0.006889511 -0.002001926 0.003813518

20 6 -0.038149332 -0.035244957 -0.023868846

21 8 -0.002448421 0.011126902 0.000755176

22 1 -0.010822092 0.006329219 0.000247497

23 1 -0.001302202 -0.018277268 -0.001293568

-------------------------------------------------------------------

Cartesian Forces: Max 0.085210719 RMS 0.021830305

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.058627139 RMS 0.010271198

Search for a saddle point.

Step number 7 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 6 7

ITU= 0 0 0 0 0 0 0

Eigenvalues --- -0.04770 -0.02338 0.00227 0.00342 0.00561

Eigenvalues --- 0.00816 0.00884 0.01198 0.01415 0.01686

Eigenvalues --- 0.01974 0.02160 0.02227 0.02429 0.02650

Eigenvalues --- 0.03006 0.03095 0.03167 0.03466 0.03688

Eigenvalues --- 0.03702 0.03772 0.03886 0.04017 0.04502

Eigenvalues --- 0.04811 0.05243 0.05835 0.06069 0.06184

Eigenvalues --- 0.06433 0.06908 0.07391 0.08685 0.09589

Eigenvalues --- 0.10974 0.12662 0.13612 0.15197 0.16636

Eigenvalues --- 0.18387 0.20846 0.23217 0.24797 0.25888

Eigenvalues --- 0.27747 0.28346 0.30811 0.31249 0.31530

Eigenvalues --- 0.31915 0.32251 0.32447 0.32832 0.34515

Eigenvalues --- 0.35744 0.37501 0.39576 0.40063 0.42919

Eigenvalues --- 0.45398 1.07950 1.10800

Eigenvectors required to have negative eigenvalues:

R6 R10 D34 R1 D4

1 -0.81999 -0.18150 0.13571 -0.11671 -0.10594

A38 D21 D41 A8 D45

1 0.09821 -0.09673 -0.09373 0.09252 -0.09211

RFO step: Lambda0=2.171166657D-02 Lambda=-1.11638623D-01.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.332

Iteration 1 RMS(Cart)= 0.04431451 RMS(Int)= 0.00148508

Iteration 2 RMS(Cart)= 0.00190368 RMS(Int)= 0.00051588

Iteration 3 RMS(Cart)= 0.00000153 RMS(Int)= 0.00051588

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00051588

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.77128 -0.01860 0.00000 0.03707 0.03764 2.80892

R2 2.65768 -0.03031 0.00000 -0.02668 -0.02668 2.63100

R3 2.08577 -0.00337 0.00000 -0.00251 -0.00251 2.08326

R4 2.85763 -0.00724 0.00000 -0.02017 -0.02032 2.83731

R5 2.08667 -0.00162 0.00000 -0.00567 -0.00567 2.08100

R6 5.32269 -0.04273 0.00000 0.11293 0.11307 5.43575

R7 2.78882 -0.00998 0.00000 -0.00309 -0.00365 2.78517

R8 2.87510 0.00186 0.00000 0.00758 0.00758 2.88268

R9 2.10714 -0.00090 0.00000 0.00416 0.00416 2.11131

R10 3.70638 -0.05863 0.00000 -0.20450 -0.20463 3.50175

R11 2.09459 -0.00274 0.00000 -0.00204 -0.00204 2.09255

R12 2.12361 0.00078 0.00000 0.00088 0.00088 2.12449

R13 2.11468 -0.00149 0.00000 0.00173 0.00173 2.11642

R14 2.90207 0.00264 0.00000 0.00167 0.00144 2.90352

R15 2.11245 -0.00005 0.00000 0.00032 0.00032 2.11277

R16 2.11842 0.00018 0.00000 -0.00033 -0.00033 2.11808

R17 2.64209 -0.00939 0.00000 -0.00838 -0.00855 2.63355

R18 2.67752 -0.01080 0.00000 0.00257 0.00266 2.68018

R19 2.79219 -0.00971 0.00000 0.00026 0.00062 2.79280

R20 2.84417 -0.01059 0.00000 0.00189 0.00169 2.84586

R21 2.08187 0.00851 0.00000 0.01109 0.01109 2.09296

R22 2.92425 -0.04255 0.00000 -0.07231 -0.07210 2.85214

R23 2.05321 0.00476 0.00000 0.00201 0.00201 2.05522

R24 2.31045 -0.00403 0.00000 0.00035 0.00035 2.31079

R25 2.30819 -0.00728 0.00000 0.00087 0.00087 2.30906

A1 1.91090 0.01113 0.00000 0.00435 0.00464 1.91553

A2 2.11191 -0.00179 0.00000 0.00489 0.00391 2.11582

A3 1.97678 0.00179 0.00000 0.02781 0.02762 2.00440

A4 1.86288 0.00641 0.00000 0.02704 0.02574 1.88862

A5 2.02744 0.01093 0.00000 0.04146 0.03822 2.06565

A6 2.04083 -0.02179 0.00000 -0.08211 -0.08170 1.95913

A7 1.97637 0.00519 0.00000 0.02898 0.02757 2.00393

A8 1.68053 0.00216 0.00000 -0.01002 -0.01023 1.67031

A9 1.84866 -0.00440 0.00000 -0.01348 -0.01274 1.83592

A10 1.88950 0.00069 0.00000 -0.00428 -0.00383 1.88567

A11 1.95893 0.00453 0.00000 -0.01452 -0.01458 1.94435

A12 2.33787 -0.02260 0.00000 -0.03908 -0.03985 2.29802

A13 1.96852 0.00380 0.00000 0.00300 0.00231 1.97083

A14 1.69908 0.01021 0.00000 0.04802 0.04863 1.74771

A15 1.58467 0.00563 0.00000 0.01457 0.01411 1.59878

A16 2.02379 0.00701 0.00000 0.02903 0.02776 2.05155

A17 1.98757 0.00150 0.00000 0.00954 0.00882 1.99638

A18 1.96817 0.00391 0.00000 0.01260 0.01209 1.98026

A19 1.85696 0.00479 0.00000 0.01402 0.01391 1.87087

A20 1.99156 -0.00953 0.00000 -0.02769 -0.02731 1.96424

A21 1.90105 0.00433 0.00000 0.01662 0.01609 1.91714

A22 1.87873 0.00045 0.00000 -0.00009 -0.00008 1.87865

A23 1.90011 0.00006 0.00000 -0.00199 -0.00208 1.89802

A24 1.93211 0.00030 0.00000 0.00011 0.00032 1.93243

A25 1.91704 -0.00247 0.00000 0.01040 0.01010 1.92714

A26 1.92905 0.00188 0.00000 0.00145 0.00173 1.93078

A27 1.91189 0.00050 0.00000 -0.00283 -0.00292 1.90896

A28 1.92124 -0.00066 0.00000 -0.00852 -0.00858 1.91266

A29 1.91775 0.00178 0.00000 -0.00054 -0.00032 1.91743

A30 1.86629 -0.00094 0.00000 -0.00032 -0.00038 1.86591

A31 1.90118 -0.00246 0.00000 -0.00345 -0.00355 1.89763

A32 1.96341 0.00982 0.00000 0.05841 0.05820 2.02161

A33 2.03323 -0.00779 0.00000 -0.03124 -0.03152 2.00172

A34 1.72568 -0.00222 0.00000 -0.01115 -0.01140 1.71428

A35 1.87964 -0.00598 0.00000 -0.01786 -0.01720 1.86244

A36 1.93406 0.00279 0.00000 0.00453 0.00425 1.93830

A37 1.92406 0.00444 0.00000 -0.00112 -0.00150 1.92256

A38 1.59505 -0.00012 0.00000 -0.03851 -0.03862 1.55643

A39 2.26554 -0.00957 0.00000 -0.00872 -0.00789 2.25764

A40 1.76079 -0.00282 0.00000 -0.01384 -0.01387 1.74692

A41 1.78609 0.00761 0.00000 0.02265 0.02193 1.80802

A42 2.00336 0.00142 0.00000 0.01976 0.01933 2.02269

A43 2.01686 0.00393 0.00000 0.01500 0.01427 2.03113

A44 1.90742 -0.00186 0.00000 -0.00035 -0.00068 1.90674

A45 2.07226 -0.00688 0.00000 -0.00691 -0.00674 2.06552

A46 2.30350 0.00874 0.00000 0.00726 0.00742 2.31093

A47 1.91998 0.00406 0.00000 0.00442 0.00470 1.92468

A48 2.05093 -0.00940 0.00000 -0.01798 -0.01817 2.03276

A49 2.30189 0.00624 0.00000 0.01513 0.01497 2.31686

D1 -1.11903 0.01132 0.00000 0.05009 0.05054 -1.06848

D2 2.94141 -0.00932 0.00000 -0.04303 -0.04474 2.89667

D3 0.73663 0.00783 0.00000 0.01670 0.01587 0.75250

D4 1.22911 0.02549 0.00000 0.10495 0.10589 1.33500

D5 -0.99364 0.00485 0.00000 0.01183 0.01061 -0.98303

D6 3.08477 0.02200 0.00000 0.07156 0.07122 -3.12720

D7 0.08284 -0.00220 0.00000 -0.02215 -0.02228 0.06057

D8 2.40988 0.01294 0.00000 0.03865 0.03895 2.44883

D9 -2.33125 -0.01298 0.00000 -0.06219 -0.06296 -2.39421

D10 -0.00421 0.00217 0.00000 -0.00140 -0.00174 -0.00595

D11 3.14093 -0.01377 0.00000 -0.04551 -0.04576 3.09517

D12 -1.07331 -0.01551 0.00000 -0.05224 -0.05251 -1.12582

D13 1.09527 -0.01861 0.00000 -0.05913 -0.05945 1.03581

D14 -0.88966 0.00952 0.00000 0.05183 0.05196 -0.83770

D15 1.17928 0.00778 0.00000 0.04510 0.04521 1.22450

D16 -2.93532 0.00468 0.00000 0.03821 0.03827 -2.89706

D17 1.03618 0.00709 0.00000 0.03971 0.03989 1.07607

D18 3.10512 0.00534 0.00000 0.03298 0.03314 3.13827

D19 -1.00948 0.00224 0.00000 0.02609 0.02620 -0.98329

D20 -0.97224 0.00027 0.00000 0.00444 0.00401 -0.96823

D21 -2.84605 -0.00704 0.00000 0.01066 0.01052 -2.83552

D22 1.04490 0.00136 0.00000 0.01439 0.01440 1.05930

D23 0.98933 0.00189 0.00000 0.00312 0.00321 0.99254

D24 -0.88448 -0.00542 0.00000 0.00934 0.00973 -0.87475

D25 3.00647 0.00298 0.00000 0.01308 0.01361 3.02008

D26 3.02039 0.00710 0.00000 0.02691 0.02566 3.04605

D27 1.14659 -0.00021 0.00000 0.03313 0.03218 1.17876

D28 -1.24565 0.00819 0.00000 0.03687 0.03605 -1.20960

D29 0.94185 -0.00573 0.00000 -0.01438 -0.01398 0.92787

D30 -1.39398 -0.01960 0.00000 -0.07301 -0.07307 -1.46705

D31 3.12591 0.00277 0.00000 -0.02370 -0.02367 3.10224

D32 0.79009 -0.01109 0.00000 -0.08233 -0.08277 0.70731

D33 -1.15856 -0.00240 0.00000 -0.05250 -0.05199 -1.21055

D34 2.78880 -0.01626 0.00000 -0.11113 -0.11109 2.67771

D35 -0.89731 0.00803 0.00000 0.00723 0.00703 -0.89028

D36 -3.02058 0.00926 0.00000 0.01006 0.00994 -3.01064

D37 1.21059 0.00899 0.00000 0.01131 0.01114 1.22173

D38 -3.07570 -0.00094 0.00000 0.02701 0.02697 -3.04873

D39 1.08423 0.00029 0.00000 0.02984 0.02987 1.11410

D40 -0.96779 0.00001 0.00000 0.03109 0.03108 -0.93672

D41 1.56727 -0.01211 0.00000 -0.01009 -0.01028 1.55700

D42 -0.55599 -0.01088 0.00000 -0.00726 -0.00737 -0.56336

D43 -2.60801 -0.01115 0.00000 -0.00602 -0.00617 -2.61418

D44 0.73234 0.00299 0.00000 0.04936 0.04915 0.78150

D45 2.91455 -0.00326 0.00000 0.05003 0.04927 2.96382

D46 -1.30959 -0.00280 0.00000 0.02767 0.02732 -1.28227

D47 -1.43668 0.00746 0.00000 0.02778 0.02835 -1.40833

D48 0.74553 0.00121 0.00000 0.02844 0.02846 0.77399

D49 2.80457 0.00166 0.00000 0.00608 0.00651 2.81108

D50 2.87252 0.00208 0.00000 0.01925 0.01916 2.89168

D51 -1.22846 -0.00417 0.00000 0.01992 0.01928 -1.20918

D52 0.83058 -0.00372 0.00000 -0.00244 -0.00267 0.82791

D53 -0.07291 0.00661 0.00000 0.02930 0.02897 -0.04394

D54 2.05502 0.00691 0.00000 0.03237 0.03211 2.08713

D55 -2.17726 0.00644 0.00000 0.02657 0.02637 -2.15090

D56 -2.09097 -0.00147 0.00000 0.00468 0.00459 -2.08638

D57 0.03696 -0.00118 0.00000 0.00775 0.00773 0.04469

D58 2.08786 -0.00165 0.00000 0.00195 0.00199 2.08985

D59 2.13037 -0.00224 0.00000 0.00594 0.00577 2.13614

D60 -2.02489 -0.00194 0.00000 0.00900 0.00891 -2.01598

D61 0.02601 -0.00241 0.00000 0.00320 0.00317 0.02918

D62 0.03741 0.00245 0.00000 0.00503 0.00479 0.04220

D63 -3.10264 0.00329 0.00000 0.00248 0.00230 -3.10034

D64 0.11082 -0.00488 0.00000 -0.01624 -0.01630 0.09452

D65 3.11641 0.00159 0.00000 -0.00459 -0.00479 3.11162

D66 0.19547 -0.00360 0.00000 -0.01332 -0.01449 0.18098

D67 2.48817 -0.01195 0.00000 -0.02941 -0.03017 2.45800

D68 -1.59639 -0.00060 0.00000 0.01792 0.01765 -1.57874

D69 -2.06849 0.00405 0.00000 -0.00200 -0.00268 -2.07117

D70 0.22421 -0.00430 0.00000 -0.01809 -0.01836 0.20585

D71 2.42283 0.00705 0.00000 0.02924 0.02946 2.45229

D72 2.10898 0.00073 0.00000 0.00794 0.00742 2.11639

D73 -1.88151 -0.00762 0.00000 -0.00815 -0.00826 -1.88977

D74 0.31711 0.00373 0.00000 0.03918 0.03956 0.35667

D75 -2.40051 0.00094 0.00000 -0.02649 -0.02641 -2.42692

D76 0.73926 -0.00007 0.00000 -0.02350 -0.02346 0.71581

D77 -0.17645 0.00303 0.00000 0.01317 0.01312 -0.16333

D78 2.96332 0.00202 0.00000 0.01616 0.01608 2.97940

D79 1.93554 0.00535 0.00000 0.00692 0.00686 1.94240

D80 -1.20787 0.00433 0.00000 0.00991 0.00981 -1.19806

D81 1.57625 0.00805 0.00000 -0.01554 -0.01561 1.56064

D82 -1.40310 0.00203 0.00000 -0.02572 -0.02591 -1.42901

D83 -0.21079 0.00524 0.00000 0.02012 0.02050 -0.19029

D84 3.09305 -0.00078 0.00000 0.00994 0.01019 3.10325

D85 -2.40059 -0.00460 0.00000 -0.03084 -0.03095 -2.43154

D86 0.90325 -0.01062 0.00000 -0.04102 -0.04125 0.86200

Item Value Threshold Converged?

Maximum Force 0.058627 0.000450 NO

RMS Force 0.010271 0.000300 NO

Maximum Displacement 0.200539 0.001800 NO

RMS Displacement 0.045117 0.001200 NO

Predicted change in Energy=-3.663057D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.513566 1.256085 0.163320

2 6 0 -0.046001 1.053678 0.042027

3 6 0 -0.663551 3.555194 0.155618

4 6 0 -1.794225 2.616034 0.264163

5 1 0 -2.222784 0.681377 -0.454767

6 1 0 -2.692131 2.940363 -0.296869

7 6 0 0.420850 1.742010 -1.208000

8 1 0 1.537426 1.620553 -1.257012

9 1 0 -0.011068 1.286839 -2.135673

10 6 0 0.089912 3.240541 -1.132899

11 1 0 1.034081 3.836341 -1.192542

12 1 0 -0.538344 3.536321 -2.012725

13 1 0 -1.008422 4.616502 0.209908

14 1 0 0.355837 0.038910 0.188481

15 8 0 3.084835 4.282637 1.070416

16 6 0 0.760236 3.905298 1.288772

17 6 0 1.437118 2.720877 1.857218

18 6 0 1.836452 4.776202 0.696135

19 8 0 1.794363 5.774724 -0.008471

20 6 0 2.897614 3.100688 1.831659

21 8 0 3.909955 2.528974 2.207634

22 1 0 0.207158 4.461144 2.070949

23 1 0 1.047853 2.361718 2.807114

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.486414 0.000000

3 C 2.451221 2.579119 0.000000

4 C 1.392264 2.355120 1.473848 0.000000

5 H 1.102412 2.263581 3.326050 2.107943 0.000000

6 H 2.106557 3.267482 2.167464 1.107331 2.312626

7 C 2.420456 1.501438 2.514561 2.799597 2.946372

8 H 3.385075 2.125109 3.253100 3.795373 3.957883

9 H 2.746600 2.190424 3.289557 3.271945 2.843188

10 C 2.861711 2.486221 1.525447 2.427295 3.515359

11 H 3.871251 3.230163 2.185986 3.407412 4.594049

12 H 3.299349 3.260050 2.172037 2.758330 3.662688

13 H 3.398491 3.694341 1.117255 2.149954 4.171532

14 H 2.230878 1.101216 3.661214 3.357092 2.734195

15 O 5.579259 4.613664 3.926376 5.218509 6.592881

16 C 3.668126 3.214985 1.853046 3.039292 4.725676

17 C 3.704246 2.876476 2.829194 3.604219 4.785366

18 C 4.888530 4.222401 2.834260 4.246732 5.879589

19 O 5.602678 5.067324 3.315808 4.788488 6.502218

20 C 5.064031 4.007231 3.962017 4.970441 6.107314

21 O 5.934142 4.745097 5.116723 6.026801 6.936317

22 H 4.107595 3.973844 2.290714 3.267176 5.154658

23 H 3.843557 3.248567 3.373976 3.822130 4.915331

6 7 8 9 10

6 H 0.000000

7 C 3.457870 0.000000

8 H 4.533534 1.124231 0.000000

9 H 3.647389 1.119960 1.811421 0.000000

10 C 2.920414 1.536475 2.176020 2.198341 0.000000

11 H 3.935692 2.182318 2.273153 2.912352 1.118030

12 H 2.817469 2.187965 2.924054 2.313721 1.120841

13 H 2.429227 3.509414 4.196297 4.193223 2.214212

14 H 4.236049 2.203392 2.446875 2.663388 3.473788

15 O 6.086420 4.329293 3.859803 5.370142 3.861363

16 C 3.919719 3.320974 3.507862 4.379276 2.599178

17 C 4.662507 3.374395 3.304421 4.482955 3.320514

18 C 4.986424 3.851750 3.723213 4.858818 2.958719

19 O 5.314641 4.425855 4.345343 5.284476 3.254470

20 C 5.983443 4.149685 3.685213 5.243109 4.085505

21 O 7.073141 4.945677 4.296265 5.981776 5.124278

22 H 4.040447 4.265074 4.573171 5.274419 3.430490

23 H 4.894591 4.110755 4.160063 5.167960 4.148937

11 12 13 14 15

11 H 0.000000

12 H 1.798675 0.000000

13 H 2.597564 2.515524 0.000000

14 H 4.097282 4.228091 4.776611 0.000000

15 O 3.086382 4.815617 4.196033 5.121959 0.000000

16 C 2.497332 3.566838 2.190413 4.040191 2.365127

17 C 3.272268 4.420844 3.505380 3.338683 2.402732

18 C 2.257042 3.809840 2.890541 4.989175 1.393612

19 O 2.395284 3.803814 3.040521 5.916732 2.248475

20 C 3.627634 5.174444 4.492759 4.305247 1.418290

21 O 4.641235 6.213980 5.704307 4.786351 2.247092

22 H 3.424114 4.252936 2.228283 4.808528 3.051878

23 H 4.262857 5.208316 4.007218 3.568131 3.294745

16 17 18 19 20

16 C 0.000000

17 C 1.477889 0.000000

18 C 1.505965 2.394147 0.000000

19 O 2.499402 3.596443 1.222820 0.000000

20 C 2.347447 1.509290 2.285351 3.428369 0.000000

21 O 3.557992 2.504903 3.410877 4.463379 1.221904

22 H 1.107547 2.141731 2.154988 2.927235 3.024343

23 H 2.184199 1.087577 3.302704 4.487026 2.217928

21 22 23

21 O 0.000000

22 H 4.178836 0.000000

23 H 2.928990 2.378297 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.928897 -0.901061 -0.507663

2 6 0 1.834448 -1.413106 0.358027

3 6 0 1.298941 0.928209 -0.581830

4 6 0 2.577041 0.342866 -1.024619

5 1 0 3.985837 -0.996454 -0.209182

6 1 0 3.407653 1.074247 -1.061318

7 6 0 1.644280 -0.449198 1.493383

8 1 0 0.782028 -0.826163 2.108456

9 1 0 2.539989 -0.392795 2.163335

10 6 0 1.288323 0.940663 0.943530

11 1 0 0.285078 1.250123 1.327880

12 1 0 2.027162 1.697554 1.314363

13 1 0 1.138426 1.940579 -1.026352

14 1 0 1.852434 -2.474504 0.650922

15 8 0 -2.463028 0.265160 0.326125

16 6 0 -0.458586 0.445473 -0.916262

17 6 0 -0.761901 -0.996906 -0.808105

18 6 0 -1.479714 1.166821 -0.076687

19 8 0 -1.578391 2.331817 0.281550

20 6 0 -2.121147 -1.025351 -0.152670

21 8 0 -2.877110 -1.936408 0.149896

22 1 0 -0.519251 0.787090 -1.968059

23 1 0 -0.654610 -1.574697 -1.723240

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3553188 0.6312951 0.5218113

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 453.3645039269 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.113584612259 A.U. after 16 cycles

Convg = 0.3482D-08 -V/T = 1.0024

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.039895313 0.066882630 -0.011285369

2 6 -0.032041276 -0.027157638 -0.024429299

3 6 0.047530524 0.042308023 0.020343638

4 6 0.026876142 -0.037264512 -0.028957578

5 1 0.000307041 -0.020098534 0.024547694

6 1 -0.010780747 0.009122018 0.025640865

7 6 0.020521095 0.020814175 0.026747312

8 1 0.000412012 -0.000172352 -0.003996304

9 1 -0.003003218 -0.003146851 0.003792499

10 6 -0.004029475 -0.012421047 -0.000489953

11 1 -0.000257112 0.000236753 -0.002979705

12 1 -0.000863553 -0.000414733 0.000344859

13 1 -0.004350233 -0.000483226 -0.006105926

14 1 0.006272923 0.006248897 0.014475831

15 8 -0.000615913 0.000848808 0.004257677

16 6 -0.057244785 -0.031860941 -0.012066376

17 6 0.003579968 0.029904761 -0.011743482

18 6 -0.006368366 -0.008512049 -0.002367758

19 8 0.004974658 -0.000440739 0.002888102

20 6 -0.024045936 -0.031460306 -0.020722226

21 8 0.000507748 0.008048290 0.001880737

22 1 -0.005863573 0.005254429 0.002596457

23 1 -0.001413237 -0.016235855 -0.002371696

-------------------------------------------------------------------

Cartesian Forces: Max 0.066882630 RMS 0.020156425

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.059188542 RMS 0.009385396

Search for a saddle point.

Step number 8 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 7 8

ITU= 0 0 0 0 0 0 0 0

Eigenvalues --- -0.04194 -0.01475 0.00223 0.00340 0.00564

Eigenvalues --- 0.00812 0.00879 0.01211 0.01485 0.01879

Eigenvalues --- 0.01974 0.02149 0.02242 0.02407 0.02636

Eigenvalues --- 0.03005 0.03092 0.03288 0.03413 0.03683

Eigenvalues --- 0.03721 0.03804 0.03862 0.03990 0.04503

Eigenvalues --- 0.04783 0.05218 0.05905 0.06064 0.06173

Eigenvalues --- 0.06395 0.06842 0.07387 0.08666 0.09545

Eigenvalues --- 0.10930 0.12712 0.13715 0.15079 0.16579

Eigenvalues --- 0.19649 0.21097 0.24262 0.24791 0.25888

Eigenvalues --- 0.27710 0.28428 0.30825 0.31247 0.31521

Eigenvalues --- 0.31917 0.32245 0.32616 0.32828 0.34503

Eigenvalues --- 0.35737 0.37487 0.39583 0.40084 0.43206

Eigenvalues --- 0.45301 1.07987 1.10807

Eigenvectors required to have negative eigenvalues:

R6 R10 D41 R22 A8

1 0.79387 0.42408 0.10786 0.10578 -0.10445

A12 D43 D42 A15 D68

1 0.09567 0.09401 0.08996 -0.08874 0.08326

RFO step: Lambda0=4.706669656D-02 Lambda=-8.22652488D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.325

Iteration 1 RMS(Cart)= 0.02997004 RMS(Int)= 0.00424380

Iteration 2 RMS(Cart)= 0.00672707 RMS(Int)= 0.00041571

Iteration 3 RMS(Cart)= 0.00000875 RMS(Int)= 0.00041566

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00041566

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.80892 -0.03617 0.00000 -0.05848 -0.05813 2.75079

R2 2.63100 -0.02198 0.00000 -0.00263 -0.00218 2.62882

R3 2.08326 -0.00348 0.00000 -0.00126 -0.00126 2.08200

R4 2.83731 -0.00567 0.00000 -0.01232 -0.01199 2.82532

R5 2.08100 -0.00154 0.00000 -0.00265 -0.00265 2.07835

R6 5.43575 -0.04045 0.00000 0.25598 0.25556 5.69132

R7 2.78517 -0.00797 0.00000 -0.00396 -0.00395 2.78122

R8 2.88268 0.00097 0.00000 0.00024 -0.00005 2.88263

R9 2.11131 0.00059 0.00000 0.00464 0.00464 2.11594

R10 3.50175 -0.05919 0.00000 -0.06464 -0.06442 3.43733

R11 2.09255 -0.00158 0.00000 -0.00157 -0.00157 2.09098

R12 2.12449 0.00060 0.00000 0.00061 0.00061 2.12510

R13 2.11642 -0.00070 0.00000 0.00277 0.00277 2.11919

R14 2.90352 0.00123 0.00000 0.00063 0.00068 2.90420

R15 2.11277 0.00007 0.00000 0.00044 0.00044 2.11321

R16 2.11808 0.00010 0.00000 0.00087 0.00087 2.11895

R17 2.63355 -0.00521 0.00000 -0.00212 -0.00214 2.63141

R18 2.68018 -0.00560 0.00000 0.00188 0.00191 2.68209

R19 2.79280 -0.00510 0.00000 -0.01096 -0.01125 2.78155

R20 2.84586 -0.00575 0.00000 0.00311 0.00307 2.84893

R21 2.09296 0.00740 0.00000 0.01163 0.01163 2.10460

R22 2.85214 -0.02609 0.00000 -0.01465 -0.01461 2.83754

R23 2.05522 0.00380 0.00000 -0.00041 -0.00041 2.05482

R24 2.31079 -0.00220 0.00000 0.00130 0.00130 2.31209

R25 2.30906 -0.00277 0.00000 0.00134 0.00134 2.31040

A1 1.91553 0.01281 0.00000 0.02041 0.02066 1.93619

A2 2.11582 -0.00453 0.00000 0.00315 0.00223 2.11805

A3 2.00440 0.00155 0.00000 0.01369 0.01293 2.01733

A4 1.88862 0.00531 0.00000 0.02894 0.02686 1.91549

A5 2.06565 0.00690 0.00000 0.03220 0.03013 2.09578

A6 1.95913 -0.01855 0.00000 -0.05559 -0.05512 1.90401

A7 2.00393 0.00448 0.00000 0.02325 0.02147 2.02541

A8 1.67031 0.00253 0.00000 -0.03862 -0.03823 1.63207

A9 1.83592 -0.00359 0.00000 -0.01164 -0.01100 1.82492

A10 1.88567 -0.00145 0.00000 -0.00328 -0.00406 1.88160

A11 1.94435 0.00431 0.00000 -0.00054 -0.00044 1.94391

A12 2.29802 -0.02079 0.00000 -0.01293 -0.01261 2.28542

A13 1.97083 0.00231 0.00000 0.00769 0.00796 1.97879

A14 1.74771 0.01246 0.00000 0.02145 0.02203 1.76974

A15 1.59878 0.00525 0.00000 -0.00954 -0.01006 1.58872

A16 2.05155 0.00297 0.00000 0.01482 0.01469 2.06623

A17 1.99638 0.00260 0.00000 0.00905 0.00831 2.00469

A18 1.98026 0.00384 0.00000 0.01188 0.01130 1.99156

A19 1.87087 0.00467 0.00000 0.01349 0.01323 1.88410

A20 1.96424 -0.00863 0.00000 -0.02427 -0.02416 1.94008

A21 1.91714 0.00406 0.00000 0.01612 0.01635 1.93349

A22 1.87865 0.00035 0.00000 -0.00013 -0.00002 1.87862

A23 1.89802 -0.00077 0.00000 -0.00374 -0.00390 1.89413

A24 1.93243 0.00057 0.00000 -0.00091 -0.00107 1.93136

A25 1.92714 -0.00307 0.00000 0.00936 0.00897 1.93611

A26 1.93078 0.00093 0.00000 -0.00083 -0.00060 1.93018

A27 1.90896 0.00177 0.00000 -0.00280 -0.00280 1.90617

A28 1.91266 0.00059 0.00000 -0.00069 -0.00053 1.91213

A29 1.91743 0.00085 0.00000 -0.00587 -0.00582 1.91162

A30 1.86591 -0.00096 0.00000 0.00042 0.00035 1.86627

A31 1.89763 -0.00175 0.00000 -0.00287 -0.00298 1.89465

A32 2.02161 0.00755 0.00000 0.03709 0.03699 2.05860

A33 2.00172 -0.00666 0.00000 -0.01405 -0.01405 1.98767

A34 1.71428 0.00055 0.00000 -0.00795 -0.00799 1.70629

A35 1.86244 -0.00449 0.00000 -0.01111 -0.01099 1.85144

A36 1.93830 0.00114 0.00000 -0.00230 -0.00239 1.93591

A37 1.92256 0.00265 0.00000 -0.00214 -0.00229 1.92027

A38 1.55643 0.00015 0.00000 -0.03526 -0.03574 1.52069

A39 2.25764 -0.00765 0.00000 -0.00122 -0.00081 2.25683

A40 1.74692 -0.00335 0.00000 -0.02688 -0.02635 1.72057

A41 1.80802 0.00573 0.00000 0.01705 0.01696 1.82498

A42 2.02269 0.00140 0.00000 0.02087 0.01983 2.04252

A43 2.03113 0.00364 0.00000 0.01980 0.01893 2.05006

A44 1.90674 -0.00050 0.00000 0.00659 0.00645 1.91320

A45 2.06552 -0.00545 0.00000 -0.00893 -0.00887 2.05665

A46 2.31093 0.00595 0.00000 0.00235 0.00241 2.31334

A47 1.92468 0.00224 0.00000 -0.00433 -0.00436 1.92032

A48 2.03276 -0.00751 0.00000 -0.00744 -0.00745 2.02531

A49 2.31686 0.00603 0.00000 0.01275 0.01277 2.32963

D1 -1.06848 0.00956 0.00000 0.04783 0.04840 -1.02008

D2 2.89667 -0.00915 0.00000 -0.04724 -0.04808 2.84860

D3 0.75250 0.00696 0.00000 -0.00732 -0.00745 0.74505

D4 1.33500 0.02332 0.00000 0.10099 0.10173 1.43673

D5 -0.98303 0.00461 0.00000 0.00593 0.00525 -0.97778

D6 -3.12720 0.02072 0.00000 0.04584 0.04588 -3.08132

D7 0.06057 -0.00193 0.00000 -0.01401 -0.01378 0.04678

D8 2.44883 0.01130 0.00000 0.03505 0.03528 2.48411

D9 -2.39421 -0.01150 0.00000 -0.05830 -0.05854 -2.45274

D10 -0.00595 0.00173 0.00000 -0.00924 -0.00947 -0.01542

D11 3.09517 -0.01093 0.00000 -0.04062 -0.04099 3.05418

D12 -1.12582 -0.01248 0.00000 -0.04610 -0.04660 -1.17242

D13 1.03581 -0.01488 0.00000 -0.05263 -0.05327 0.98255

D14 -0.83770 0.00828 0.00000 0.05520 0.05552 -0.78217

D15 1.22450 0.00673 0.00000 0.04971 0.04991 1.27441

D16 -2.89706 0.00433 0.00000 0.04319 0.04324 -2.85381

D17 1.07607 0.00676 0.00000 0.02796 0.02809 1.10416

D18 3.13827 0.00521 0.00000 0.02247 0.02248 -3.12244

D19 -0.98329 0.00281 0.00000 0.01595 0.01581 -0.96748

D20 -0.96823 -0.00089 0.00000 0.00896 0.00838 -0.95985

D21 -2.83552 -0.00674 0.00000 0.01691 0.01657 -2.81896

D22 1.05930 0.00033 0.00000 0.02156 0.02130 1.08060

D23 0.99254 0.00114 0.00000 0.00722 0.00764 1.00018

D24 -0.87475 -0.00472 0.00000 0.01517 0.01583 -0.85892

D25 3.02008 0.00236 0.00000 0.01981 0.02056 3.04063

D26 3.04605 0.00592 0.00000 0.01520 0.01475 3.06081

D27 1.17876 0.00006 0.00000 0.02315 0.02294 1.20170

D28 -1.20960 0.00714 0.00000 0.02780 0.02767 -1.18193

D29 0.92787 -0.00395 0.00000 -0.02297 -0.02299 0.90488

D30 -1.46705 -0.01656 0.00000 -0.07040 -0.07044 -1.53750

D31 3.10224 0.00083 0.00000 -0.01590 -0.01607 3.08616

D32 0.70731 -0.01178 0.00000 -0.06334 -0.06353 0.64378

D33 -1.21055 -0.00277 0.00000 -0.04176 -0.04193 -1.25248

D34 2.67771 -0.01537 0.00000 -0.08919 -0.08938 2.58833

D35 -0.89028 0.00738 0.00000 0.02265 0.02260 -0.86768

D36 -3.01064 0.00808 0.00000 0.01781 0.01763 -2.99301

D37 1.22173 0.00763 0.00000 0.01949 0.01925 1.24098

D38 -3.04873 0.00137 0.00000 0.02053 0.02076 -3.02797

D39 1.11410 0.00206 0.00000 0.01569 0.01579 1.12989

D40 -0.93672 0.00161 0.00000 0.01737 0.01741 -0.91931

D41 1.55700 -0.01051 0.00000 0.01985 0.02015 1.57715

D42 -0.56336 -0.00981 0.00000 0.01501 0.01518 -0.54818

D43 -2.61418 -0.01026 0.00000 0.01669 0.01679 -2.59738

D44 0.78150 0.00235 0.00000 0.02181 0.02154 0.80304

D45 2.96382 -0.00335 0.00000 0.02650 0.02613 2.98995

D46 -1.28227 -0.00255 0.00000 0.01381 0.01355 -1.26872

D47 -1.40833 0.00719 0.00000 0.01188 0.01205 -1.39628

D48 0.77399 0.00149 0.00000 0.01657 0.01664 0.79063

D49 2.81108 0.00229 0.00000 0.00387 0.00407 2.81515

D50 2.89168 0.00239 0.00000 0.00366 0.00369 2.89538

D51 -1.20918 -0.00331 0.00000 0.00835 0.00828 -1.20090

D52 0.82791 -0.00251 0.00000 -0.00434 -0.00430 0.82362

D53 -0.04394 0.00706 0.00000 0.02721 0.02690 -0.01703

D54 2.08713 0.00661 0.00000 0.03183 0.03170 2.11883

D55 -2.15090 0.00628 0.00000 0.02850 0.02843 -2.12246

D56 -2.08638 -0.00040 0.00000 0.00402 0.00379 -2.08259

D57 0.04469 -0.00086 0.00000 0.00864 0.00859 0.05327

D58 2.08985 -0.00118 0.00000 0.00530 0.00532 2.09517

D59 2.13614 -0.00069 0.00000 0.00700 0.00680 2.14294

D60 -2.01598 -0.00115 0.00000 0.01162 0.01160 -2.00438

D61 0.02918 -0.00147 0.00000 0.00828 0.00833 0.03751

D62 0.04220 0.00145 0.00000 -0.00062 -0.00064 0.04156

D63 -3.10034 0.00230 0.00000 0.00180 0.00182 -3.09853

D64 0.09452 -0.00430 0.00000 -0.01387 -0.01394 0.08058

D65 3.11162 0.00150 0.00000 -0.00590 -0.00605 3.10558

D66 0.18098 -0.00476 0.00000 -0.01191 -0.01229 0.16869

D67 2.45800 -0.01164 0.00000 -0.02077 -0.02102 2.43698

D68 -1.57874 -0.00120 0.00000 0.03373 0.03402 -1.54472

D69 -2.07117 0.00229 0.00000 -0.01212 -0.01244 -2.08361

D70 0.20585 -0.00459 0.00000 -0.02098 -0.02117 0.18468

D71 2.45229 0.00584 0.00000 0.03353 0.03387 2.48616

D72 2.11639 0.00120 0.00000 -0.00134 -0.00164 2.11476

D73 -1.88977 -0.00568 0.00000 -0.01019 -0.01037 -1.90014

D74 0.35667 0.00475 0.00000 0.04431 0.04467 0.40134

D75 -2.42692 0.00194 0.00000 -0.01405 -0.01391 -2.44083

D76 0.71581 0.00093 0.00000 -0.01693 -0.01686 0.69895

D77 -0.16333 0.00315 0.00000 0.01556 0.01558 -0.14775

D78 2.97940 0.00214 0.00000 0.01268 0.01264 2.99204

D79 1.94240 0.00331 0.00000 0.00486 0.00488 1.94728

D80 -1.19806 0.00230 0.00000 0.00197 0.00194 -1.19612

D81 1.56064 0.00745 0.00000 -0.01251 -0.01279 1.54785

D82 -1.42901 0.00177 0.00000 -0.01989 -0.02019 -1.44920

D83 -0.19029 0.00524 0.00000 0.02068 0.02099 -0.16930

D84 3.10325 -0.00044 0.00000 0.01330 0.01359 3.11684

D85 -2.43154 -0.00389 0.00000 -0.03480 -0.03489 -2.46643

D86 0.86200 -0.00957 0.00000 -0.04218 -0.04229 0.81971

Item Value Threshold Converged?

Maximum Force 0.059189 0.000450 NO

RMS Force 0.009385 0.000300 NO

Maximum Displacement 0.130341 0.001800 NO

RMS Displacement 0.033692 0.001200 NO

Predicted change in Energy=-1.434071D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.512738 1.257695 0.144477

2 6 0 -0.089348 1.003147 -0.023129

3 6 0 -0.629646 3.552908 0.155352

4 6 0 -1.762762 2.620526 0.268432

5 1 0 -2.267646 0.684641 -0.417278

6 1 0 -2.687575 2.970837 -0.227895

7 6 0 0.413609 1.723214 -1.233023

8 1 0 1.528268 1.582526 -1.281672

9 1 0 -0.024451 1.292928 -2.171401

10 6 0 0.115116 3.227629 -1.135549

11 1 0 1.071884 3.803609 -1.193432

12 1 0 -0.509559 3.543329 -2.011579

13 1 0 -0.969878 4.617969 0.215662

14 1 0 0.312756 -0.007558 0.139290

15 8 0 3.074048 4.319784 1.087477

16 6 0 0.750219 3.895173 1.289999

17 6 0 1.454791 2.748014 1.885142

18 6 0 1.818306 4.781990 0.702146

19 8 0 1.769113 5.774330 -0.011863

20 6 0 2.904324 3.138777 1.856129

21 8 0 3.930571 2.592644 2.234725

22 1 0 0.174438 4.452882 2.063156

23 1 0 1.059760 2.356011 2.819293

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.455653 0.000000

3 C 2.459263 2.612482 0.000000

4 C 1.391110 2.345472 1.471759 0.000000

5 H 1.101747 2.236467 3.352299 2.114890 0.000000

6 H 2.110393 3.265658 2.172730 1.106498 2.332145

7 C 2.413508 1.495093 2.522647 2.792154 2.988846

8 H 3.374482 2.129857 3.256384 3.783007 3.995289

9 H 2.753094 2.168699 3.299629 3.276740 2.911852

10 C 2.858149 2.495517 1.525420 2.422016 3.558126

11 H 3.866775 3.249716 2.185698 3.401757 4.634958

12 H 3.298343 3.253158 2.170277 2.760531 3.715477

13 H 3.404586 3.728175 1.119709 2.149703 4.189974

14 H 2.221107 1.099814 3.683110 3.351310 2.728989

15 O 5.595019 4.715994 3.895421 5.191631 6.634173

16 C 3.659165 3.285269 1.818955 2.997232 4.725445

17 C 3.749292 3.011714 2.825757 3.603144 4.838924

18 C 4.881342 4.294743 2.793223 4.205244 5.893758

19 O 5.585246 5.120370 3.273640 4.743330 6.508819

20 C 5.096926 4.129721 3.943741 4.956920 6.159582

21 O 5.981708 4.876900 5.103085 6.023381 7.006532

22 H 4.091102 4.040154 2.257481 3.214235 5.129910

23 H 3.870231 3.351127 3.373906 3.813593 4.933610

6 7 8 9 10

6 H 0.000000

7 C 3.490585 0.000000

8 H 4.561927 1.124555 0.000000

9 H 3.699300 1.121426 1.812848 0.000000

10 C 2.957170 1.536835 2.173640 2.198985 0.000000

11 H 3.969799 2.182415 2.269202 2.908933 1.118261

12 H 2.872808 2.184310 2.920659 2.307635 1.121300

13 H 2.420799 3.520274 4.206739 4.200928 2.221718

14 H 4.243542 2.211106 2.454582 2.672876 3.482917

15 O 6.061861 4.382332 3.936354 5.420594 3.858746

16 C 3.869991 3.346095 3.545023 4.399214 2.594659

17 C 4.655510 3.443432 3.375273 4.556421 3.339062

18 C 4.944513 3.882546 3.775741 4.881247 2.948562

19 O 5.269565 4.442990 4.386529 5.288047 3.237910

20 C 5.969983 4.213116 3.763143 5.310921 4.091175

21 O 7.071590 5.014998 4.376808 6.061799 5.130268

22 H 3.954300 4.286384 4.610822 5.287376 3.425855

23 H 4.868869 4.152013 4.199487 5.216578 4.158467

11 12 13 14 15

11 H 0.000000

12 H 1.799465 0.000000

13 H 2.611039 2.515422 0.000000

14 H 4.108213 4.232168 4.800675 0.000000

15 O 3.078578 4.800965 4.147567 5.220123 0.000000

16 C 2.505849 3.551232 2.152991 4.092287 2.370968

17 C 3.276967 4.435722 3.487537 3.456215 2.393475

18 C 2.259998 3.783852 2.835056 5.052055 1.392480

19 O 2.401245 3.764117 2.981780 5.964399 2.242120

20 C 3.619345 5.174691 4.459662 4.423029 1.419299

21 O 4.625017 6.216884 5.673883 4.923463 2.243395

22 H 3.439816 4.230674 2.179437 4.859622 3.062255

23 H 4.265870 5.216303 4.001847 3.650601 3.303475

16 17 18 19 20

16 C 0.000000

17 C 1.471934 0.000000

18 C 1.507589 2.380899 0.000000

19 O 2.502842 3.585528 1.223506 0.000000

20 C 2.352191 1.501560 2.282819 3.424067 0.000000

21 O 3.564228 2.505161 3.406420 4.454456 1.222611

22 H 1.113704 2.139526 2.159390 2.931709 3.036777

23 H 2.191707 1.087362 3.308033 4.494834 2.223246

21 22 23

21 O 0.000000

22 H 4.195052 0.000000

23 H 2.939263 2.398418 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.939861 -0.871713 -0.526861

2 6 0 1.936627 -1.410757 0.379714

3 6 0 1.260035 0.923704 -0.578189

4 6 0 2.535213 0.354904 -1.043443

5 1 0 4.016354 -0.965671 -0.311962

6 1 0 3.345148 1.099214 -1.163216

7 6 0 1.693444 -0.445814 1.495533

8 1 0 0.851593 -0.847398 2.123738

9 1 0 2.595720 -0.353986 2.155125

10 6 0 1.280547 0.929169 0.947083

11 1 0 0.276504 1.207931 1.352913

12 1 0 2.004471 1.707705 1.303635

13 1 0 1.077350 1.934609 -1.023661

14 1 0 1.959584 -2.474629 0.657638

15 8 0 -2.470586 0.266932 0.330339

16 6 0 -0.458240 0.429600 -0.912839

17 6 0 -0.795894 -0.999953 -0.818197

18 6 0 -1.477075 1.155872 -0.071811

19 8 0 -1.569661 2.319762 0.293913

20 6 0 -2.140820 -1.026886 -0.151014

21 8 0 -2.907899 -1.926798 0.159671

22 1 0 -0.513436 0.782239 -1.967797

23 1 0 -0.670309 -1.597934 -1.717643

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3596746 0.6235302 0.5188930

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 453.0034083040 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.999015043583E-01 A.U. after 16 cycles

Convg = 0.4779D-08 -V/T = 1.0021

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.027084149 0.059271599 -0.010665836

2 6 -0.023313653 -0.026831784 -0.025301238

3 6 0.045903484 0.036448357 0.021470240

4 6 0.021964020 -0.028182493 -0.028567447

5 1 -0.000585057 -0.018976454 0.024377426

6 1 -0.009076846 0.008116167 0.025398269

7 6 0.021747844 0.019809492 0.024531533

8 1 0.000199945 -0.000483093 -0.003406091

9 1 -0.002361466 -0.002517848 0.002948163

10 6 -0.004034613 -0.012178743 -0.000870007

11 1 0.000004899 -0.000007544 -0.002705481

12 1 -0.000760369 -0.000158322 0.000516299

13 1 -0.005287579 -0.001196598 -0.008471753

14 1 0.005602704 0.004807434 0.011980218

15 8 -0.001531239 0.001309598 0.003236495

16 6 -0.053402587 -0.028880265 -0.008535425

17 6 0.006749818 0.030493839 -0.006748240

18 6 -0.003801918 -0.006085970 -0.003646054

19 8 0.003418474 -0.000240652 0.002846201

20 6 -0.023842450 -0.030122511 -0.018204434

21 8 -0.000134486 0.007074243 0.001930428

22 1 -0.004010721 0.003624807 0.001301960

23 1 -0.000532354 -0.015093259 -0.003415226

-------------------------------------------------------------------

Cartesian Forces: Max 0.059271599 RMS 0.018251242

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.052737091 RMS 0.008208081

Search for a saddle point.

Step number 9 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 8 9

ITU= 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.04405 -0.00660 0.00232 0.00340 0.00562

Eigenvalues --- 0.00818 0.00896 0.01131 0.01468 0.01852

Eigenvalues --- 0.01977 0.02129 0.02216 0.02398 0.02617

Eigenvalues --- 0.02974 0.03079 0.03203 0.03438 0.03664

Eigenvalues --- 0.03716 0.03775 0.03843 0.03980 0.04561

Eigenvalues --- 0.04757 0.05199 0.05819 0.06008 0.06145

Eigenvalues --- 0.06371 0.06770 0.07383 0.08662 0.09499

Eigenvalues --- 0.10952 0.12635 0.13667 0.14951 0.16525

Eigenvalues --- 0.19616 0.21111 0.24599 0.24895 0.25821

Eigenvalues --- 0.27682 0.28408 0.30817 0.31241 0.31515

Eigenvalues --- 0.31920 0.32240 0.32682 0.32850 0.34489

Eigenvalues --- 0.35724 0.37473 0.39579 0.40079 0.43266

Eigenvalues --- 0.45197 1.07993 1.10810

Eigenvectors required to have negative eigenvalues:

R6 R10 D41 A8 R22

1 -0.76818 -0.47389 -0.10080 0.10078 -0.08876

A15 D43 A12 D42 A14

1 0.08740 -0.08732 -0.08625 -0.08246 0.08162

RFO step: Lambda0=3.778471989D-02 Lambda=-7.17280658D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.341

Iteration 1 RMS(Cart)= 0.03557195 RMS(Int)= 0.00451176

Iteration 2 RMS(Cart)= 0.00711882 RMS(Int)= 0.00042968

Iteration 3 RMS(Cart)= 0.00001010 RMS(Int)= 0.00042962

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00042962

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.75079 -0.02168 0.00000 -0.01638 -0.01591 2.73487

R2 2.62882 -0.01726 0.00000 -0.00433 -0.00387 2.62494

R3 2.08200 -0.00216 0.00000 -0.00127 -0.00127 2.08073

R4 2.82532 -0.00312 0.00000 -0.01152 -0.01126 2.81406

R5 2.07835 -0.00060 0.00000 -0.00158 -0.00158 2.07677

R6 5.69132 -0.03368 0.00000 0.25961 0.25918 5.95049

R7 2.78122 -0.00725 0.00000 -0.01342 -0.01348 2.76774

R8 2.88263 0.00196 0.00000 0.00052 0.00031 2.88294

R9 2.11594 0.00001 0.00000 0.00361 0.00361 2.11955

R10 3.43733 -0.05274 0.00000 -0.05616 -0.05595 3.38138

R11 2.09098 -0.00124 0.00000 -0.00050 -0.00050 2.09048

R12 2.12510 0.00041 0.00000 0.00052 0.00052 2.12562

R13 2.11919 -0.00058 0.00000 0.00269 0.00269 2.12188

R14 2.90420 0.00092 0.00000 -0.00134 -0.00126 2.90293

R15 2.11321 0.00014 0.00000 0.00068 0.00068 2.11389

R16 2.11895 -0.00002 0.00000 0.00080 0.00080 2.11975

R17 2.63141 -0.00548 0.00000 -0.00570 -0.00571 2.62570

R18 2.68209 -0.00361 0.00000 0.00720 0.00730 2.68938

R19 2.78155 -0.00446 0.00000 -0.01967 -0.02002 2.76153

R20 2.84893 -0.00445 0.00000 0.00383 0.00373 2.85266

R21 2.10460 0.00479 0.00000 0.00817 0.00817 2.11277

R22 2.83754 -0.02632 0.00000 -0.02378 -0.02371 2.81383

R23 2.05482 0.00270 0.00000 -0.00067 -0.00067 2.05415

R24 2.31209 -0.00199 0.00000 0.00106 0.00106 2.31315

R25 2.31040 -0.00268 0.00000 0.00091 0.00091 2.31131

A1 1.93619 0.00929 0.00000 0.01406 0.01422 1.95041

A2 2.11805 -0.00333 0.00000 0.00618 0.00530 2.12335

A3 2.01733 0.00197 0.00000 0.01463 0.01387 2.03120

A4 1.91549 0.00510 0.00000 0.03051 0.02812 1.94361

A5 2.09578 0.00527 0.00000 0.02405 0.02205 2.11784

A6 1.90401 -0.01763 0.00000 -0.06690 -0.06622 1.83779

A7 2.02541 0.00326 0.00000 0.01787 0.01649 2.04190

A8 1.63207 0.00178 0.00000 -0.03660 -0.03612 1.59595

A9 1.82492 -0.00232 0.00000 0.00112 0.00149 1.82640

A10 1.88160 -0.00010 0.00000 0.00507 0.00436 1.88596

A11 1.94391 0.00243 0.00000 -0.00433 -0.00421 1.93970

A12 2.28542 -0.01821 0.00000 -0.02240 -0.02231 2.26311

A13 1.97879 0.00156 0.00000 0.00115 0.00134 1.98013

A14 1.76974 0.01052 0.00000 0.02306 0.02383 1.79357

A15 1.58872 0.00533 0.00000 -0.00193 -0.00248 1.58624

A16 2.06623 0.00362 0.00000 0.02045 0.01989 2.08613

A17 2.00469 0.00133 0.00000 0.00495 0.00415 2.00884

A18 1.99156 0.00331 0.00000 0.01228 0.01171 2.00327

A19 1.88410 0.00387 0.00000 0.01135 0.01111 1.89521

A20 1.94008 -0.00696 0.00000 -0.02409 -0.02394 1.91614

A21 1.93349 0.00294 0.00000 0.01652 0.01652 1.95001

A22 1.87862 0.00013 0.00000 -0.00080 -0.00074 1.87789

A23 1.89413 0.00005 0.00000 -0.00016 -0.00028 1.89385

A24 1.93136 0.00014 0.00000 -0.00244 -0.00250 1.92886

A25 1.93611 -0.00170 0.00000 0.01143 0.01102 1.94713

A26 1.93018 0.00070 0.00000 -0.00088 -0.00067 1.92951

A27 1.90617 0.00111 0.00000 -0.00418 -0.00415 1.90202

A28 1.91213 0.00005 0.00000 -0.00182 -0.00163 1.91050

A29 1.91162 0.00056 0.00000 -0.00536 -0.00531 1.90631

A30 1.86627 -0.00067 0.00000 0.00028 0.00020 1.86647

A31 1.89465 -0.00147 0.00000 -0.00314 -0.00322 1.89143

A32 2.05860 0.00734 0.00000 0.04091 0.04076 2.09936

A33 1.98767 -0.00684 0.00000 -0.02581 -0.02584 1.96183

A34 1.70629 0.00054 0.00000 -0.01437 -0.01454 1.69175

A35 1.85144 -0.00346 0.00000 -0.00566 -0.00538 1.84607

A36 1.93591 0.00084 0.00000 0.00332 0.00331 1.93922

A37 1.92027 0.00213 0.00000 0.00049 0.00020 1.92047

A38 1.52069 -0.00033 0.00000 -0.03663 -0.03719 1.48351

A39 2.25683 -0.00708 0.00000 -0.00317 -0.00268 2.25415

A40 1.72057 -0.00257 0.00000 -0.02314 -0.02256 1.69801

A41 1.82498 0.00502 0.00000 0.01544 0.01528 1.84026

A42 2.04252 0.00147 0.00000 0.02235 0.02136 2.06389

A43 2.05006 0.00286 0.00000 0.01718 0.01622 2.06628

A44 1.91320 -0.00150 0.00000 0.00083 0.00061 1.91381

A45 2.05665 -0.00320 0.00000 -0.00162 -0.00151 2.05514

A46 2.31334 0.00471 0.00000 0.00079 0.00090 2.31424

A47 1.92032 0.00241 0.00000 -0.00338 -0.00340 1.91692

A48 2.02531 -0.00645 0.00000 -0.00872 -0.00875 2.01656

A49 2.32963 0.00465 0.00000 0.01313 0.01313 2.34276

D1 -1.02008 0.01023 0.00000 0.05963 0.06026 -0.95982

D2 2.84860 -0.00796 0.00000 -0.03757 -0.03817 2.81042

D3 0.74505 0.00678 0.00000 0.00165 0.00132 0.74637

D4 1.43673 0.02257 0.00000 0.11425 0.11502 1.55175

D5 -0.97778 0.00438 0.00000 0.01705 0.01658 -0.96119

D6 -3.08132 0.01911 0.00000 0.05628 0.05607 -3.02525

D7 0.04678 -0.00251 0.00000 -0.01733 -0.01714 0.02964

D8 2.48411 0.01006 0.00000 0.03883 0.03894 2.52305

D9 -2.45274 -0.01158 0.00000 -0.06493 -0.06509 -2.51783

D10 -0.01542 0.00098 0.00000 -0.00877 -0.00901 -0.02443

D11 3.05418 -0.01064 0.00000 -0.04786 -0.04823 3.00595

D12 -1.17242 -0.01209 0.00000 -0.05567 -0.05612 -1.22854

D13 0.98255 -0.01476 0.00000 -0.06412 -0.06472 0.91782

D14 -0.78217 0.00761 0.00000 0.04751 0.04775 -0.73442

D15 1.27441 0.00616 0.00000 0.03971 0.03987 1.31428

D16 -2.85381 0.00349 0.00000 0.03126 0.03126 -2.82255

D17 1.10416 0.00666 0.00000 0.03324 0.03339 1.13755

D18 -3.12244 0.00520 0.00000 0.02543 0.02551 -3.09693

D19 -0.96748 0.00254 0.00000 0.01698 0.01690 -0.95057

D20 -0.95985 -0.00143 0.00000 0.00331 0.00262 -0.95723

D21 -2.81896 -0.00637 0.00000 0.01448 0.01405 -2.80490

D22 1.08060 -0.00005 0.00000 0.02018 0.01981 1.10041

D23 1.00018 0.00111 0.00000 0.00766 0.00818 1.00837

D24 -0.85892 -0.00383 0.00000 0.01883 0.01961 -0.83931

D25 3.04063 0.00250 0.00000 0.02454 0.02537 3.06600

D26 3.06081 0.00464 0.00000 0.01476 0.01427 3.07508

D27 1.20170 -0.00029 0.00000 0.02593 0.02570 1.22740

D28 -1.18193 0.00603 0.00000 0.03164 0.03146 -1.15047

D29 0.90488 -0.00410 0.00000 -0.02789 -0.02787 0.87701

D30 -1.53750 -0.01581 0.00000 -0.08078 -0.08086 -1.61835

D31 3.08616 -0.00059 0.00000 -0.02576 -0.02593 3.06023

D32 0.64378 -0.01231 0.00000 -0.07865 -0.07892 0.56487

D33 -1.25248 -0.00368 0.00000 -0.05045 -0.05054 -1.30302

D34 2.58833 -0.01539 0.00000 -0.10334 -0.10352 2.48481

D35 -0.86768 0.00601 0.00000 0.02438 0.02437 -0.84331

D36 -2.99301 0.00662 0.00000 0.01952 0.01936 -2.97365

D37 1.24098 0.00636 0.00000 0.02223 0.02200 1.26298

D38 -3.02797 0.00192 0.00000 0.02543 0.02565 -3.00231

D39 1.12989 0.00254 0.00000 0.02057 0.02065 1.15054

D40 -0.91931 0.00227 0.00000 0.02328 0.02329 -0.89602

D41 1.57715 -0.00922 0.00000 0.01677 0.01713 1.59428

D42 -0.54818 -0.00861 0.00000 0.01192 0.01213 -0.53606

D43 -2.59738 -0.00887 0.00000 0.01462 0.01476 -2.58262

D44 0.80304 0.00329 0.00000 0.03310 0.03278 0.83582

D45 2.98995 -0.00162 0.00000 0.03755 0.03690 3.02685

D46 -1.26872 -0.00137 0.00000 0.02059 0.02038 -1.24834

D47 -1.39628 0.00664 0.00000 0.01663 0.01689 -1.37939

D48 0.79063 0.00174 0.00000 0.02107 0.02101 0.81164

D49 2.81515 0.00199 0.00000 0.00412 0.00449 2.81963

D50 2.89538 0.00267 0.00000 0.01336 0.01338 2.90876

D51 -1.20090 -0.00223 0.00000 0.01780 0.01750 -1.18340

D52 0.82362 -0.00199 0.00000 0.00084 0.00098 0.82460

D53 -0.01703 0.00613 0.00000 0.02487 0.02462 0.00759

D54 2.11883 0.00592 0.00000 0.03011 0.03002 2.14885

D55 -2.12246 0.00546 0.00000 0.02629 0.02627 -2.09619

D56 -2.08259 -0.00034 0.00000 0.00146 0.00125 -2.08134

D57 0.05327 -0.00055 0.00000 0.00669 0.00665 0.05992

D58 2.09517 -0.00101 0.00000 0.00288 0.00290 2.09807

D59 2.14294 -0.00061 0.00000 0.00394 0.00375 2.14670

D60 -2.00438 -0.00082 0.00000 0.00918 0.00915 -1.99523

D61 0.03751 -0.00128 0.00000 0.00536 0.00540 0.04292

D62 0.04156 0.00128 0.00000 0.00337 0.00336 0.04492

D63 -3.09853 0.00181 0.00000 0.00465 0.00471 -3.09382

D64 0.08058 -0.00388 0.00000 -0.01584 -0.01594 0.06464

D65 3.10558 0.00096 0.00000 -0.00728 -0.00746 3.09811

D66 0.16869 -0.00418 0.00000 -0.01365 -0.01416 0.15453

D67 2.43698 -0.01091 0.00000 -0.02550 -0.02576 2.41123

D68 -1.54472 -0.00117 0.00000 0.03044 0.03075 -1.51397

D69 -2.08361 0.00261 0.00000 -0.00545 -0.00597 -2.08959

D70 0.18468 -0.00412 0.00000 -0.01729 -0.01757 0.16711

D71 2.48616 0.00562 0.00000 0.03864 0.03893 2.52509

D72 2.11476 0.00167 0.00000 -0.00445 -0.00478 2.10998

D73 -1.90014 -0.00506 0.00000 -0.01629 -0.01637 -1.91651

D74 0.40134 0.00468 0.00000 0.03964 0.04013 0.44147

D75 -2.44083 0.00119 0.00000 -0.01956 -0.01937 -2.46020

D76 0.69895 0.00055 0.00000 -0.02110 -0.02099 0.67796

D77 -0.14775 0.00280 0.00000 0.01050 0.01055 -0.13720

D78 2.99204 0.00216 0.00000 0.00895 0.00892 3.00096

D79 1.94728 0.00293 0.00000 0.01140 0.01145 1.95874

D80 -1.19612 0.00229 0.00000 0.00986 0.00983 -1.18629

D81 1.54785 0.00604 0.00000 -0.01712 -0.01746 1.53039

D82 -1.44920 0.00112 0.00000 -0.02533 -0.02570 -1.47490

D83 -0.16930 0.00485 0.00000 0.02010 0.02043 -0.14887

D84 3.11684 -0.00007 0.00000 0.01190 0.01219 3.12903

D85 -2.46643 -0.00415 0.00000 -0.03911 -0.03914 -2.50557

D86 0.81971 -0.00907 0.00000 -0.04731 -0.04737 0.77233

Item Value Threshold Converged?

Maximum Force 0.052737 0.000450 NO

RMS Force 0.008208 0.000300 NO

Maximum Displacement 0.163101 0.001800 NO

RMS Displacement 0.039001 0.001200 NO

Predicted change in Energy=-1.496996D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.520533 1.264144 0.133142

2 6 0 -0.125681 0.953372 -0.095530

3 6 0 -0.592563 3.548529 0.151424

4 6 0 -1.726564 2.630231 0.277527

5 1 0 -2.326908 0.696902 -0.357128

6 1 0 -2.678022 3.008151 -0.141586

7 6 0 0.413213 1.705003 -1.262650

8 1 0 1.525081 1.541958 -1.311736

9 1 0 -0.031109 1.302455 -2.212033

10 6 0 0.146362 3.212865 -1.140370

11 1 0 1.115742 3.768501 -1.194038

12 1 0 -0.472560 3.550351 -2.012895

13 1 0 -0.929052 4.616959 0.208515

14 1 0 0.269437 -0.058384 0.071748

15 8 0 3.055948 4.360235 1.105642

16 6 0 0.742471 3.878800 1.296140

17 6 0 1.471840 2.774599 1.916038

18 6 0 1.795051 4.785906 0.706212

19 8 0 1.728997 5.768421 -0.020864

20 6 0 2.904665 3.178521 1.884135

21 8 0 3.945370 2.662140 2.266542

22 1 0 0.136719 4.436261 2.052639

23 1 0 1.075696 2.347087 2.833583

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447232 0.000000

3 C 2.465740 2.648359 0.000000

4 C 1.389060 2.348160 1.464627 0.000000

5 H 1.101076 2.231504 3.376144 2.121546 0.000000

6 H 2.111117 3.276993 2.174167 1.106233 2.347682

7 C 2.425276 1.489136 2.531753 2.794072 3.056878

8 H 3.382398 2.133216 3.263676 3.779325 4.057489

9 H 2.778434 2.147182 3.308475 3.291727 3.012982

10 C 2.863194 2.504198 1.525586 2.420278 3.613945

11 H 3.870808 3.266926 2.185626 3.397038 4.689028

12 H 3.306125 3.246677 2.167643 2.768606 3.784487

13 H 3.405422 3.762940 1.121618 2.141933 4.200095

14 H 2.226397 1.098977 3.709341 3.354850 2.737773

15 O 5.610322 4.813761 3.857594 5.152777 6.673443

16 C 3.648311 3.353887 1.789349 2.948327 4.720048

17 C 3.796642 3.148865 2.823932 3.596575 4.890255

18 C 4.870761 4.361230 2.745833 4.151203 5.902643

19 O 5.556229 5.160437 3.216714 4.677412 6.502596

20 C 5.129638 4.248924 3.920433 4.932555 6.208949

21 O 6.031739 5.007267 5.084511 6.010660 7.077236

22 H 4.061191 4.100487 2.221383 3.143977 5.085198

23 H 3.899429 3.459111 3.379427 3.803453 4.947874

6 7 8 9 10

6 H 0.000000

7 C 3.537048 0.000000

8 H 4.602722 1.124831 0.000000

9 H 3.768594 1.122851 1.813732 0.000000

10 C 3.002769 1.536166 2.173054 2.197641 0.000000

11 H 4.009792 2.180889 2.266915 2.903957 1.118620

12 H 2.942761 2.180084 2.918190 2.299472 1.121722

13 H 2.402026 3.527816 4.217768 4.201344 2.224295

14 H 4.258717 2.216038 2.460034 2.675419 3.490766

15 O 6.021803 4.432055 4.016212 5.466892 3.850548

16 C 3.811149 3.373604 3.588081 4.420775 2.595264

17 C 4.637857 3.516929 3.455542 4.633254 3.360149

18 C 4.887490 3.908690 3.829909 4.897495 2.933002

19 O 5.201489 4.447998 4.423904 5.276747 3.207631

20 C 5.941293 4.275611 3.846451 5.377452 4.093537

21 O 7.056070 5.084038 4.462811 6.141560 5.132525

22 H 3.844071 4.304342 4.650114 5.294935 3.419371

23 H 4.835187 4.198842 4.246628 5.270153 4.171994

11 12 13 14 15

11 H 0.000000

12 H 1.800228 0.000000

13 H 2.620728 2.506132 0.000000

14 H 4.118677 4.233115 4.828449 0.000000

15 O 3.066443 4.778237 4.092794 5.325202 0.000000

16 C 2.520413 3.540323 2.126451 4.150218 2.370705

17 C 3.284390 4.451853 3.474795 3.587893 2.383355

18 C 2.259983 3.749960 2.774343 5.118319 1.389461

19 O 2.398353 3.706059 2.905805 6.007542 2.238929

20 C 3.608804 5.170178 4.424272 4.550464 1.423160

21 O 4.605045 6.214547 5.640636 5.072559 2.241046

22 H 3.456197 4.205309 2.137595 4.913591 3.069932

23 H 4.271270 5.228124 4.007781 3.750210 3.310580

16 17 18 19 20

16 C 0.000000

17 C 1.461339 0.000000

18 C 1.509564 2.369283 0.000000

19 O 2.505674 3.575009 1.224066 0.000000

20 C 2.347597 1.489013 2.280884 3.423273 0.000000

21 O 3.560969 2.500770 3.401306 4.448991 1.223091

22 H 1.118030 2.135960 2.164529 2.934181 3.044968

23 H 2.195658 1.087007 3.315271 4.503354 2.222130

21 22 23

21 O 0.000000

22 H 4.207028 0.000000

23 H 2.942078 2.419958 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.949933 -0.843449 -0.558312

2 6 0 2.034552 -1.406777 0.410822

3 6 0 1.220470 0.914008 -0.571538

4 6 0 2.483311 0.361918 -1.067077

5 1 0 4.041162 -0.936945 -0.444972

6 1 0 3.265135 1.114146 -1.283077

7 6 0 1.739293 -0.439712 1.504044

8 1 0 0.921122 -0.865358 2.147989

9 1 0 2.647391 -0.308935 2.151385

10 6 0 1.271075 0.915706 0.953207

11 1 0 0.267090 1.164441 1.379183

12 1 0 1.978288 1.717012 1.293824

13 1 0 1.020577 1.925673 -1.012678

14 1 0 2.073901 -2.470739 0.683196

15 8 0 -2.474905 0.275784 0.332844

16 6 0 -0.460576 0.403312 -0.910722

17 6 0 -0.833770 -1.006993 -0.825404

18 6 0 -1.468767 1.146247 -0.067881

19 8 0 -1.542531 2.311088 0.300957

20 6 0 -2.160086 -1.025838 -0.148876

21 8 0 -2.941619 -1.910222 0.172092

22 1 0 -0.501698 0.767518 -1.966966

23 1 0 -0.693149 -1.630546 -1.704603

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3628157 0.6166904 0.5171308

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 452.7330174872 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.853724883356E-01 A.U. after 16 cycles

Convg = 0.6447D-08 -V/T = 1.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.030677980 0.047736680 -0.013258890

2 6 -0.028813122 -0.022223693 -0.023060151

3 6 0.044713841 0.031003862 0.021320911

4 6 0.014773003 -0.021127495 -0.027894490

5 1 0.000148204 -0.017638571 0.024148697

6 1 -0.007223539 0.007218532 0.024965922

7 6 0.020625011 0.017633217 0.023472551

8 1 0.000046567 -0.000532358 -0.002839641

9 1 -0.001733567 -0.002066723 0.002051403

10 6 -0.003815553 -0.011813066 -0.000778600

11 1 0.000160424 -0.000199464 -0.002427296

12 1 -0.000678210 0.000100967 0.000622637

13 1 -0.005470235 -0.001102475 -0.010074007

14 1 0.004084457 0.003641187 0.009572317

15 8 -0.000520010 0.000893540 0.002643948

16 6 -0.052354840 -0.021925025 -0.008392636

17 6 0.007246105 0.027410083 -0.001722852

18 6 -0.002218136 -0.004185624 -0.003441145

19 8 0.002469765 0.000150936 0.002669529

20 6 -0.019420157 -0.027488402 -0.016776065

21 8 -0.000197696 0.006188982 0.002110610

22 1 -0.002466601 0.002529510 0.001232552

23 1 -0.000033692 -0.014204602 -0.004145303

-------------------------------------------------------------------

Cartesian Forces: Max 0.052354840 RMS 0.016723960

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.046173118 RMS 0.007279927

Search for a saddle point.

Step number 10 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 9 10

ITU= 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.04071 -0.00172 0.00246 0.00334 0.00556

Eigenvalues --- 0.00797 0.00863 0.00956 0.01464 0.01952

Eigenvalues --- 0.01991 0.02118 0.02189 0.02385 0.02594

Eigenvalues --- 0.02906 0.03067 0.03146 0.03408 0.03624

Eigenvalues --- 0.03664 0.03775 0.03809 0.03957 0.04496

Eigenvalues --- 0.04717 0.05214 0.05733 0.05978 0.06104

Eigenvalues --- 0.06335 0.06672 0.07379 0.08638 0.09443

Eigenvalues --- 0.10937 0.12549 0.13646 0.14807 0.16444

Eigenvalues --- 0.19472 0.21064 0.24614 0.24966 0.25809

Eigenvalues --- 0.27638 0.28326 0.30803 0.31230 0.31506

Eigenvalues --- 0.31919 0.32234 0.32677 0.32840 0.34472

Eigenvalues --- 0.35698 0.37456 0.39575 0.40078 0.43248

Eigenvalues --- 0.45075 1.07993 1.10809

Eigenvectors required to have negative eigenvalues:

R6 R10 D41 A8 A14

1 0.73098 0.53933 0.10069 -0.10017 -0.09754

A15 A12 D43 D42 D68

1 -0.09328 0.08629 0.08555 0.08070 0.08009

RFO step: Lambda0=3.327071584D-02 Lambda=-6.46766670D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.341

Iteration 1 RMS(Cart)= 0.03206436 RMS(Int)= 0.00478158

Iteration 2 RMS(Cart)= 0.00764827 RMS(Int)= 0.00041039

Iteration 3 RMS(Cart)= 0.00001097 RMS(Int)= 0.00041031

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00041031

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73487 -0.02317 0.00000 -0.05600 -0.05570 2.67917

R2 2.62494 -0.01139 0.00000 0.00970 0.01024 2.63519

R3 2.08073 -0.00177 0.00000 -0.00046 -0.00046 2.08027

R4 2.81406 -0.00207 0.00000 -0.00547 -0.00515 2.80891

R5 2.07677 -0.00043 0.00000 0.00097 0.00097 2.07774

R6 5.95049 -0.02756 0.00000 0.26331 0.26272 6.21321

R7 2.76774 -0.00537 0.00000 -0.01445 -0.01426 2.75348

R8 2.88294 0.00164 0.00000 -0.00231 -0.00257 2.88037

R9 2.11955 0.00008 0.00000 0.00249 0.00249 2.12204

R10 3.38138 -0.04617 0.00000 -0.00821 -0.00783 3.37355

R11 2.09048 -0.00078 0.00000 -0.00132 -0.00132 2.08916

R12 2.12562 0.00025 0.00000 0.00014 0.00014 2.12576

R13 2.12188 -0.00031 0.00000 0.00277 0.00277 2.12465

R14 2.90293 0.00033 0.00000 -0.00360 -0.00353 2.89941

R15 2.11389 0.00016 0.00000 0.00104 0.00104 2.11493

R16 2.11975 -0.00008 0.00000 0.00111 0.00111 2.12086

R17 2.62570 -0.00377 0.00000 -0.00290 -0.00288 2.62282

R18 2.68938 -0.00246 0.00000 0.00607 0.00613 2.69551

R19 2.76153 -0.00092 0.00000 -0.00606 -0.00635 2.75518

R20 2.85266 -0.00264 0.00000 0.00350 0.00345 2.85611

R21 2.11277 0.00343 0.00000 0.00500 0.00500 2.11777

R22 2.81383 -0.02194 0.00000 -0.04846 -0.04845 2.76537

R23 2.05415 0.00210 0.00000 -0.00050 -0.00050 2.05365

R24 2.31315 -0.00160 0.00000 0.00066 0.00066 2.31381

R25 2.31131 -0.00212 0.00000 0.00168 0.00168 2.31298

A1 1.95041 0.00897 0.00000 0.02203 0.02178 1.97219

A2 2.12335 -0.00388 0.00000 0.00331 0.00254 2.12589

A3 2.03120 0.00158 0.00000 0.00777 0.00709 2.03829

A4 1.94361 0.00460 0.00000 0.03536 0.03311 1.97672

A5 2.11784 0.00316 0.00000 0.01515 0.01368 2.13152

A6 1.83779 -0.01539 0.00000 -0.05746 -0.05672 1.78107

A7 2.04190 0.00242 0.00000 0.00717 0.00593 2.04783

A8 1.59595 0.00148 0.00000 -0.04047 -0.03962 1.55634

A9 1.82640 -0.00169 0.00000 0.00381 0.00382 1.83022

A10 1.88596 -0.00023 0.00000 0.01089 0.01000 1.89596

A11 1.93970 0.00204 0.00000 0.00062 0.00072 1.94042

A12 2.26311 -0.01621 0.00000 -0.02384 -0.02349 2.23962

A13 1.98013 0.00087 0.00000 -0.00177 -0.00147 1.97866

A14 1.79357 0.00998 0.00000 0.01548 0.01620 1.80977

A15 1.58624 0.00476 0.00000 -0.00326 -0.00379 1.58245

A16 2.08613 0.00181 0.00000 0.01049 0.01005 2.09618

A17 2.00884 0.00148 0.00000 0.00551 0.00471 2.01355

A18 2.00327 0.00334 0.00000 0.01704 0.01657 2.01983

A19 1.89521 0.00326 0.00000 0.00893 0.00870 1.90391

A20 1.91614 -0.00590 0.00000 -0.02082 -0.02061 1.89553

A21 1.95001 0.00262 0.00000 0.01406 0.01392 1.96393

A22 1.87789 0.00004 0.00000 -0.00143 -0.00140 1.87648

A23 1.89385 0.00018 0.00000 0.00293 0.00294 1.89679

A24 1.92886 -0.00013 0.00000 -0.00366 -0.00373 1.92513

A25 1.94713 -0.00125 0.00000 0.01139 0.01072 1.95784

A26 1.92951 0.00044 0.00000 -0.00100 -0.00070 1.92881

A27 1.90202 0.00100 0.00000 -0.00576 -0.00567 1.89634

A28 1.91050 0.00021 0.00000 -0.00053 -0.00028 1.91023

A29 1.90631 0.00017 0.00000 -0.00510 -0.00496 1.90135

A30 1.86647 -0.00054 0.00000 0.00042 0.00031 1.86678

A31 1.89143 -0.00097 0.00000 -0.00417 -0.00426 1.88717

A32 2.09936 0.00573 0.00000 0.02766 0.02743 2.12679

A33 1.96183 -0.00544 0.00000 -0.01719 -0.01697 1.94485

A34 1.69175 0.00120 0.00000 -0.00712 -0.00714 1.68462

A35 1.84607 -0.00314 0.00000 -0.01042 -0.01029 1.83578

A36 1.93922 0.00056 0.00000 0.00105 0.00104 1.94026

A37 1.92047 0.00155 0.00000 0.00667 0.00655 1.92703

A38 1.48351 -0.00046 0.00000 -0.03134 -0.03194 1.45157

A39 2.25415 -0.00579 0.00000 -0.00449 -0.00407 2.25007

A40 1.69801 -0.00267 0.00000 -0.02771 -0.02719 1.67082

A41 1.84026 0.00395 0.00000 0.01796 0.01791 1.85817

A42 2.06389 0.00164 0.00000 0.01573 0.01453 2.07842

A43 2.06628 0.00234 0.00000 0.01839 0.01745 2.08373

A44 1.91381 -0.00141 0.00000 -0.00105 -0.00122 1.91259

A45 2.05514 -0.00221 0.00000 -0.00084 -0.00076 2.05438

A46 2.31424 0.00362 0.00000 0.00187 0.00195 2.31619

A47 1.91692 0.00241 0.00000 0.00202 0.00190 1.91882

A48 2.01656 -0.00564 0.00000 -0.01221 -0.01222 2.00434

A49 2.34276 0.00373 0.00000 0.01176 0.01179 2.35455

D1 -0.95982 0.01000 0.00000 0.06569 0.06636 -0.89346

D2 2.81042 -0.00661 0.00000 -0.02638 -0.02680 2.78363

D3 0.74637 0.00653 0.00000 0.00706 0.00667 0.75304

D4 1.55175 0.02141 0.00000 0.12079 0.12152 1.67327

D5 -0.96119 0.00481 0.00000 0.02872 0.02836 -0.93283

D6 -3.02525 0.01794 0.00000 0.06216 0.06184 -2.96341

D7 0.02964 -0.00251 0.00000 -0.01780 -0.01764 0.01201

D8 2.52305 0.00893 0.00000 0.03928 0.03923 2.56227

D9 -2.51783 -0.01094 0.00000 -0.06762 -0.06769 -2.58552

D10 -0.02443 0.00049 0.00000 -0.01055 -0.01082 -0.03525

D11 3.00595 -0.00934 0.00000 -0.04763 -0.04812 2.95783

D12 -1.22854 -0.01073 0.00000 -0.05593 -0.05646 -1.28500

D13 0.91782 -0.01329 0.00000 -0.06569 -0.06639 0.85143

D14 -0.73442 0.00672 0.00000 0.04259 0.04265 -0.69177

D15 1.31428 0.00533 0.00000 0.03428 0.03431 1.34859

D16 -2.82255 0.00277 0.00000 0.02452 0.02438 -2.79817

D17 1.13755 0.00604 0.00000 0.02634 0.02664 1.16419

D18 -3.09693 0.00465 0.00000 0.01804 0.01830 -3.07863

D19 -0.95057 0.00210 0.00000 0.00828 0.00837 -0.94221

D20 -0.95723 -0.00221 0.00000 0.00112 0.00057 -0.95665

D21 -2.80490 -0.00614 0.00000 0.00420 0.00388 -2.80103

D22 1.10041 -0.00051 0.00000 0.01476 0.01440 1.11481

D23 1.00837 0.00088 0.00000 0.01758 0.01808 1.02645

D24 -0.83931 -0.00305 0.00000 0.02067 0.02139 -0.81793

D25 3.06600 0.00258 0.00000 0.03122 0.03191 3.09791

D26 3.07508 0.00359 0.00000 0.01317 0.01288 3.08796

D27 1.22740 -0.00034 0.00000 0.01625 0.01618 1.24358

D28 -1.15047 0.00529 0.00000 0.02681 0.02670 -1.12377

D29 0.87701 -0.00403 0.00000 -0.03406 -0.03418 0.84283

D30 -1.61835 -0.01479 0.00000 -0.08691 -0.08707 -1.70542

D31 3.06023 -0.00173 0.00000 -0.02823 -0.02847 3.03176

D32 0.56487 -0.01248 0.00000 -0.08109 -0.08136 0.48351

D33 -1.30302 -0.00414 0.00000 -0.04943 -0.04964 -1.35265

D34 2.48481 -0.01489 0.00000 -0.10228 -0.10252 2.38229

D35 -0.84331 0.00563 0.00000 0.03454 0.03447 -0.80884

D36 -2.97365 0.00592 0.00000 0.02806 0.02786 -2.94579

D37 1.26298 0.00572 0.00000 0.03158 0.03127 1.29425

D38 -3.00231 0.00259 0.00000 0.02689 0.02710 -2.97521

D39 1.15054 0.00287 0.00000 0.02042 0.02050 1.17103

D40 -0.89602 0.00267 0.00000 0.02393 0.02390 -0.87212

D41 1.59428 -0.00764 0.00000 0.02388 0.02429 1.61857

D42 -0.53606 -0.00735 0.00000 0.01740 0.01768 -0.51838

D43 -2.58262 -0.00755 0.00000 0.02092 0.02109 -2.56153

D44 0.83582 0.00332 0.00000 0.03760 0.03728 0.87311

D45 3.02685 -0.00155 0.00000 0.03031 0.02984 3.05669

D46 -1.24834 -0.00096 0.00000 0.02859 0.02825 -1.22009

D47 -1.37939 0.00632 0.00000 0.02327 0.02354 -1.35584

D48 0.81164 0.00146 0.00000 0.01598 0.01611 0.82775

D49 2.81963 0.00205 0.00000 0.01425 0.01452 2.83415

D50 2.90876 0.00302 0.00000 0.02408 0.02411 2.93287

D51 -1.18340 -0.00185 0.00000 0.01679 0.01667 -1.16673

D52 0.82460 -0.00126 0.00000 0.01506 0.01508 0.83968

D53 0.00759 0.00558 0.00000 0.02099 0.02072 0.02831

D54 2.14885 0.00545 0.00000 0.02702 0.02692 2.17576

D55 -2.09619 0.00501 0.00000 0.02431 0.02431 -2.07188

D56 -2.08134 -0.00017 0.00000 -0.00059 -0.00083 -2.08217

D57 0.05992 -0.00031 0.00000 0.00544 0.00536 0.06528

D58 2.09807 -0.00074 0.00000 0.00273 0.00276 2.10083

D59 2.14670 -0.00026 0.00000 0.00149 0.00126 2.14796

D60 -1.99523 -0.00039 0.00000 0.00752 0.00746 -1.98778

D61 0.04292 -0.00083 0.00000 0.00481 0.00485 0.04777

D62 0.04492 0.00103 0.00000 0.00250 0.00238 0.04729

D63 -3.09382 0.00159 0.00000 0.00742 0.00729 -3.08653

D64 0.06464 -0.00353 0.00000 -0.01656 -0.01666 0.04798

D65 3.09811 0.00075 0.00000 -0.00350 -0.00378 3.09433

D66 0.15453 -0.00439 0.00000 -0.02120 -0.02154 0.13300

D67 2.41123 -0.01011 0.00000 -0.03280 -0.03310 2.37813

D68 -1.51397 -0.00105 0.00000 0.02748 0.02771 -1.48626

D69 -2.08959 0.00167 0.00000 -0.00948 -0.00980 -2.09939

D70 0.16711 -0.00406 0.00000 -0.02108 -0.02136 0.14574

D71 2.52509 0.00501 0.00000 0.03921 0.03945 2.56454

D72 2.10998 0.00139 0.00000 -0.01179 -0.01204 2.09794

D73 -1.91651 -0.00433 0.00000 -0.02338 -0.02360 -1.94012

D74 0.44147 0.00473 0.00000 0.03690 0.03721 0.47868

D75 -2.46020 0.00189 0.00000 -0.00062 -0.00065 -2.46085

D76 0.67796 0.00120 0.00000 -0.00654 -0.00657 0.67138

D77 -0.13720 0.00270 0.00000 0.01422 0.01420 -0.12300

D78 3.00096 0.00201 0.00000 0.00830 0.00828 3.00923

D79 1.95874 0.00237 0.00000 0.01296 0.01291 1.97165

D80 -1.18629 0.00168 0.00000 0.00704 0.00699 -1.17930

D81 1.53039 0.00529 0.00000 -0.00526 -0.00564 1.52475

D82 -1.47490 0.00075 0.00000 -0.01941 -0.01979 -1.49469

D83 -0.14887 0.00468 0.00000 0.02315 0.02350 -0.12537

D84 3.12903 0.00014 0.00000 0.00901 0.00935 3.13838

D85 -2.50557 -0.00403 0.00000 -0.03579 -0.03597 -2.54154

D86 0.77233 -0.00857 0.00000 -0.04994 -0.05012 0.72221

Item Value Threshold Converged?

Maximum Force 0.046173 0.000450 NO

RMS Force 0.007280 0.000300 NO

Maximum Displacement 0.160802 0.001800 NO

RMS Displacement 0.035484 0.001200 NO

Predicted change in Energy=-1.396737D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.516835 1.262826 0.121360

2 6 0 -0.173115 0.911975 -0.163869

3 6 0 -0.569300 3.544866 0.138147

4 6 0 -1.698979 2.635958 0.282329

5 1 0 -2.364830 0.694899 -0.291192

6 1 0 -2.675922 3.027099 -0.056493

7 6 0 0.410027 1.688452 -1.289233

8 1 0 1.518144 1.499445 -1.331274

9 1 0 -0.033924 1.313553 -2.251756

10 6 0 0.174076 3.197760 -1.146442

11 1 0 1.155513 3.733985 -1.188719

12 1 0 -0.432526 3.555885 -2.020149

13 1 0 -0.902201 4.616319 0.184485

14 1 0 0.214066 -0.103484 0.002907

15 8 0 3.044819 4.394954 1.125712

16 6 0 0.738737 3.878952 1.306214

17 6 0 1.493163 2.806742 1.944114

18 6 0 1.781771 4.801368 0.718402

19 8 0 1.707356 5.778195 -0.016078

20 6 0 2.899629 3.208940 1.904762

21 8 0 3.951298 2.712477 2.286388

22 1 0 0.106834 4.427946 2.051344

23 1 0 1.095799 2.343898 2.843498

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.417757 0.000000

3 C 2.470994 2.679606 0.000000

4 C 1.394482 2.345095 1.457078 0.000000

5 H 1.100834 2.206116 3.395669 2.130726 0.000000

6 H 2.118437 3.278616 2.178032 1.105536 2.364534

7 C 2.425640 1.486410 2.538261 2.795619 3.111762

8 H 3.373015 2.137361 3.271141 3.774289 4.099579

9 H 2.798799 2.130706 3.313159 3.307983 3.108000

10 C 2.865392 2.512131 1.524224 2.421847 3.666307

11 H 3.868382 3.283186 2.184335 3.393784 4.736498

12 H 3.319624 3.240883 2.162653 2.784165 3.861130

13 H 3.409938 3.791448 1.122934 2.136881 4.212254

14 H 2.208360 1.099491 3.733953 3.352963 2.715625

15 O 5.623846 4.914190 3.841848 5.129229 6.705395

16 C 3.651794 3.434468 1.785205 2.921615 4.724619

17 C 3.842682 3.287890 2.839032 3.602842 4.933618

18 C 4.874273 4.441549 2.728191 4.122472 5.922555

19 O 5.550032 5.219014 3.192915 4.643902 6.519070

20 C 5.145195 4.358559 3.907332 4.909969 6.233549

21 O 6.057171 5.124095 5.073817 5.995644 7.113931

22 H 4.047113 4.165044 2.212987 3.098644 5.052943

23 H 3.924870 3.564379 3.396145 3.802061 4.951912

6 7 8 9 10

6 H 0.000000

7 C 3.582556 0.000000

8 H 4.642088 1.124906 0.000000

9 H 3.838694 1.124319 1.814044 0.000000

10 C 3.056076 1.534299 2.173696 2.194361 0.000000

11 H 4.057280 2.179463 2.268257 2.898845 1.119171

12 H 3.027933 2.175187 2.916951 2.289231 1.122312

13 H 2.393695 3.530750 4.227351 4.194930 2.223072

14 H 4.260999 2.217895 2.459682 2.674508 3.495828

15 O 5.999627 4.483218 4.092859 5.511895 3.851899

16 C 3.773926 3.412138 3.636738 4.453923 2.607371

17 C 4.629499 3.588634 3.526729 4.708178 3.382961

18 C 4.859991 3.950003 3.895300 4.927823 2.938347

19 O 5.175257 4.475487 4.480317 5.288038 3.207384

20 C 5.913236 4.325691 3.911879 5.429076 4.091284

21 O 7.036201 5.135591 4.525391 6.199495 5.127107

22 H 3.761526 4.330844 4.691483 5.313748 3.426910

23 H 4.806515 4.240207 4.280209 5.319727 4.183093

11 12 13 14 15

11 H 0.000000

12 H 1.801351 0.000000

13 H 2.626479 2.491089 0.000000

14 H 4.127040 4.231053 4.853407 0.000000

15 O 3.059894 4.763655 4.063727 5.432292 0.000000

16 C 2.533655 3.541316 2.120062 4.222994 2.369990

17 C 3.284574 4.470445 3.479745 3.724754 2.366397

18 C 2.273458 3.735505 2.742811 5.198769 1.387936

19 O 2.420416 3.678866 2.863559 6.068312 2.237375

20 C 3.589879 5.160286 4.403859 4.669202 1.426404

21 O 4.575615 6.202863 5.621304 5.206806 2.235978

22 H 3.475531 4.198625 2.130445 4.974077 3.080526

23 H 4.265522 5.240205 4.028181 3.851764 3.310030

16 17 18 19 20

16 C 0.000000

17 C 1.457981 0.000000

18 C 1.511388 2.358855 0.000000

19 O 2.508745 3.566197 1.224414 0.000000

20 C 2.340220 1.463372 2.278790 3.422311 0.000000

21 O 3.555553 2.483640 3.395423 4.442437 1.223978

22 H 1.120676 2.135815 2.172922 2.942631 3.050764

23 H 2.201619 1.086744 3.320504 4.510606 2.209824

21 22 23

21 O 0.000000

22 H 4.216395 0.000000

23 H 2.932593 2.439019 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.956608 -0.816047 -0.583115

2 6 0 2.140806 -1.389419 0.424728

3 6 0 1.195038 0.916612 -0.559160

4 6 0 2.442243 0.378429 -1.086338

5 1 0 4.052665 -0.917623 -0.569833

6 1 0 3.196001 1.126631 -1.393342

7 6 0 1.786308 -0.434118 1.506922

8 1 0 0.992257 -0.893767 2.157781

9 1 0 2.694146 -0.265879 2.148498

10 6 0 1.263473 0.902057 0.963457

11 1 0 0.256615 1.114871 1.403332

12 1 0 1.948285 1.725126 1.299869

13 1 0 0.979316 1.932766 -0.985631

14 1 0 2.202727 -2.454235 0.691583

15 8 0 -2.484180 0.269246 0.337539

16 6 0 -0.474149 0.391109 -0.912172

17 6 0 -0.873079 -1.008999 -0.833049

18 6 0 -1.478923 1.137453 -0.065005

19 8 0 -1.547749 2.301038 0.309856

20 6 0 -2.165441 -1.033918 -0.147019

21 8 0 -2.950898 -1.912122 0.184548

22 1 0 -0.503091 0.761021 -1.969642

23 1 0 -0.713616 -1.653170 -1.693647

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3632595 0.6090717 0.5139174

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 452.2460244838 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.720634289361E-01 A.U. after 16 cycles

Convg = 0.7265D-08 -V/T = 1.0015

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.017064713 0.042810250 -0.012367162

2 6 -0.017634291 -0.022789393 -0.023828870

3 6 0.037943308 0.025548129 0.019204630

4 6 0.011565623 -0.014414386 -0.027690170

5 1 0.000034739 -0.016239536 0.024525717

6 1 -0.005435873 0.006277853 0.024588171

7 6 0.020425946 0.015647182 0.022216530

8 1 -0.000052754 -0.000352047 -0.002323594

9 1 -0.001145296 -0.001846882 0.001664378

10 6 -0.002624938 -0.011230683 -0.000122952

11 1 0.000278093 -0.000242928 -0.001914105

12 1 -0.000579040 0.000432465 0.000711529

13 1 -0.004834449 -0.001391580 -0.010179701

14 1 0.003012813 0.002246549 0.006594243

15 8 -0.000484006 0.002225739 0.000964668

16 6 -0.044414750 -0.019706510 -0.002953699

17 6 -0.006666862 0.026596668 0.000819838

18 6 -0.001065913 -0.003222147 -0.004236638

19 8 0.001517224 0.000280976 0.002605668

20 6 -0.005426909 -0.023107824 -0.015630932

21 8 0.000855929 0.004998810 0.002656600

22 1 -0.002183718 0.001226008 -0.000432834

23 1 -0.000149592 -0.013746712 -0.004871314

-------------------------------------------------------------------

Cartesian Forces: Max 0.044414750 RMS 0.014497899

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.038819279 RMS 0.006104803

Search for a saddle point.

Step number 11 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 10 11

ITU= 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.04823 -0.00563 0.00276 0.00337 0.00530

Eigenvalues --- 0.00740 0.00820 0.00993 0.01531 0.01873

Eigenvalues --- 0.01979 0.02096 0.02181 0.02443 0.02608

Eigenvalues --- 0.02897 0.03079 0.03155 0.03464 0.03582

Eigenvalues --- 0.03713 0.03774 0.03847 0.03960 0.04551

Eigenvalues --- 0.04685 0.05343 0.05606 0.05999 0.06205

Eigenvalues --- 0.06453 0.07173 0.07375 0.08612 0.09500

Eigenvalues --- 0.11344 0.12567 0.13584 0.14681 0.16431

Eigenvalues --- 0.19315 0.20998 0.24594 0.25028 0.25735

Eigenvalues --- 0.27605 0.28257 0.30786 0.31220 0.31501

Eigenvalues --- 0.31919 0.32228 0.32670 0.32848 0.34461

Eigenvalues --- 0.35689 0.37439 0.39572 0.40085 0.43204

Eigenvalues --- 0.44992 1.07999 1.10808

Eigenvectors required to have negative eigenvalues:

R6 R10 R22 D4 A8

1 0.72033 0.47881 0.18510 0.10322 -0.10001

D41 D30 R19 R1 A15

1 0.09945 -0.09938 -0.09145 0.09136 -0.08700

RFO step: Lambda0=1.529101945D-02 Lambda=-6.31867643D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.435

Iteration 1 RMS(Cart)= 0.05870010 RMS(Int)= 0.00239036

Iteration 2 RMS(Cart)= 0.00283339 RMS(Int)= 0.00070522

Iteration 3 RMS(Cart)= 0.00000464 RMS(Int)= 0.00070521

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00070521

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.67917 -0.00917 0.00000 0.03101 0.03243 2.71160

R2 2.63519 -0.00782 0.00000 -0.01175 -0.01084 2.62435

R3 2.08027 -0.00084 0.00000 -0.00317 -0.00317 2.07711

R4 2.80891 -0.00112 0.00000 -0.01671 -0.01676 2.79215

R5 2.07774 -0.00001 0.00000 -0.00169 -0.00169 2.07605

R6 6.21321 -0.02272 0.00000 0.17241 0.17211 6.38533

R7 2.75348 -0.00490 0.00000 -0.02303 -0.02354 2.72994

R8 2.88037 0.00182 0.00000 0.00119 0.00113 2.88150

R9 2.12204 -0.00031 0.00000 0.00401 0.00401 2.12605

R10 3.37355 -0.03882 0.00000 -0.11099 -0.11113 3.26242

R11 2.08916 -0.00051 0.00000 -0.00087 -0.00087 2.08829

R12 2.12576 0.00009 0.00000 0.00079 0.00079 2.12656

R13 2.12465 -0.00036 0.00000 0.00279 0.00279 2.12745

R14 2.89941 0.00052 0.00000 -0.00397 -0.00412 2.89529

R15 2.11493 0.00020 0.00000 0.00142 0.00142 2.11635

R16 2.12086 -0.00010 0.00000 0.00088 0.00088 2.12174

R17 2.62282 -0.00265 0.00000 -0.00427 -0.00401 2.61881

R18 2.69551 -0.00063 0.00000 -0.00009 0.00027 2.69578

R19 2.75518 -0.00319 0.00000 -0.04282 -0.04390 2.71128

R20 2.85611 -0.00061 0.00000 0.00601 0.00585 2.86195

R21 2.11777 0.00154 0.00000 0.00482 0.00482 2.12259

R22 2.76537 -0.00747 0.00000 0.10899 0.10897 2.87434

R23 2.05365 0.00188 0.00000 -0.00320 -0.00320 2.05045

R24 2.31381 -0.00143 0.00000 0.00074 0.00074 2.31455

R25 2.31298 -0.00046 0.00000 -0.00288 -0.00288 2.31011

A1 1.97219 0.00570 0.00000 0.01846 0.01852 1.99070

A2 2.12589 -0.00224 0.00000 0.00440 0.00224 2.12813

A3 2.03829 0.00191 0.00000 0.02446 0.02260 2.06089

A4 1.97672 0.00402 0.00000 0.02838 0.02478 2.00150

A5 2.13152 0.00227 0.00000 0.01192 0.00997 2.14148

A6 1.78107 -0.01447 0.00000 -0.10567 -0.10429 1.67678

A7 2.04783 0.00158 0.00000 0.01540 0.01444 2.06227

A8 1.55634 0.00059 0.00000 -0.02853 -0.02791 1.52842

A9 1.83022 -0.00035 0.00000 0.02931 0.02892 1.85915

A10 1.89596 0.00112 0.00000 0.01725 0.01700 1.91296

A11 1.94042 0.00096 0.00000 -0.00641 -0.00616 1.93426

A12 2.23962 -0.01378 0.00000 -0.05666 -0.05751 2.18211

A13 1.97866 0.00063 0.00000 -0.00882 -0.00910 1.96956

A14 1.80977 0.00764 0.00000 0.04300 0.04458 1.85435

A15 1.58245 0.00421 0.00000 0.00935 0.00861 1.59106

A16 2.09618 0.00237 0.00000 0.02175 0.01961 2.11579

A17 2.01355 0.00062 0.00000 0.01565 0.01442 2.02798

A18 2.01983 0.00275 0.00000 0.01240 0.01127 2.03110

A19 1.90391 0.00253 0.00000 0.01008 0.00991 1.91381

A20 1.89553 -0.00461 0.00000 -0.02506 -0.02472 1.87081

A21 1.96393 0.00189 0.00000 0.01997 0.01937 1.98330

A22 1.87648 -0.00007 0.00000 -0.00350 -0.00353 1.87295

A23 1.89679 0.00055 0.00000 0.00221 0.00215 1.89894

A24 1.92513 -0.00032 0.00000 -0.00442 -0.00423 1.92090

A25 1.95784 -0.00009 0.00000 0.01645 0.01596 1.97381

A26 1.92881 0.00024 0.00000 -0.00012 0.00011 1.92892

A27 1.89634 0.00021 0.00000 -0.00995 -0.00991 1.88643

A28 1.91023 -0.00024 0.00000 -0.00409 -0.00391 1.90632

A29 1.90135 0.00016 0.00000 -0.00307 -0.00297 1.89838

A30 1.86678 -0.00029 0.00000 -0.00009 -0.00018 1.86660

A31 1.88717 -0.00086 0.00000 0.00395 0.00406 1.89123

A32 2.12679 0.00483 0.00000 0.02619 0.02545 2.15224

A33 1.94485 -0.00560 0.00000 -0.04351 -0.04345 1.90140

A34 1.68462 0.00073 0.00000 -0.00497 -0.00472 1.67989

A35 1.83578 -0.00176 0.00000 0.01380 0.01434 1.85012

A36 1.94026 0.00077 0.00000 0.00799 0.00765 1.94792

A37 1.92703 0.00132 0.00000 -0.00250 -0.00293 1.92410

A38 1.45157 0.00016 0.00000 -0.01345 -0.01464 1.43693

A39 2.25007 -0.00598 0.00000 -0.01262 -0.01143 2.23865

A40 1.67082 -0.00244 0.00000 -0.02658 -0.02626 1.64456

A41 1.85817 0.00266 0.00000 -0.00707 -0.00726 1.85091

A42 2.07842 0.00164 0.00000 0.04179 0.04130 2.11972

A43 2.08373 0.00252 0.00000 0.01443 0.01301 2.09674

A44 1.91259 0.00039 0.00000 0.01245 0.01207 1.92465

A45 2.05438 -0.00206 0.00000 -0.00683 -0.00664 2.04773

A46 2.31619 0.00166 0.00000 -0.00563 -0.00544 2.31075

A47 1.91882 0.00019 0.00000 -0.02037 -0.02062 1.89820

A48 2.00434 -0.00389 0.00000 0.01368 0.01375 2.01808

A49 2.35455 0.00409 0.00000 0.00816 0.00824 2.36280

D1 -0.89346 0.01054 0.00000 0.08940 0.09023 -0.80323

D2 2.78363 -0.00516 0.00000 -0.02320 -0.02287 2.76076

D3 0.75304 0.00572 0.00000 0.01730 0.01652 0.76957

D4 1.67327 0.02089 0.00000 0.18154 0.18222 1.85549

D5 -0.93283 0.00518 0.00000 0.06893 0.06911 -0.86372

D6 -2.96341 0.01606 0.00000 0.10944 0.10851 -2.85490

D7 0.01201 -0.00280 0.00000 -0.02391 -0.02366 -0.01165

D8 2.56227 0.00802 0.00000 0.06633 0.06679 2.62907

D9 -2.58552 -0.01103 0.00000 -0.10413 -0.10473 -2.69024

D10 -0.03525 -0.00022 0.00000 -0.01389 -0.01427 -0.04952

D11 2.95783 -0.00935 0.00000 -0.06960 -0.06987 2.88796

D12 -1.28500 -0.01061 0.00000 -0.08221 -0.08245 -1.36744

D13 0.85143 -0.01302 0.00000 -0.09227 -0.09268 0.75875

D14 -0.69177 0.00572 0.00000 0.03579 0.03611 -0.65567

D15 1.34859 0.00446 0.00000 0.02319 0.02352 1.37211

D16 -2.79817 0.00205 0.00000 0.01313 0.01329 -2.78488

D17 1.16419 0.00585 0.00000 0.05589 0.05578 1.21997

D18 -3.07863 0.00459 0.00000 0.04328 0.04320 -3.03543

D19 -0.94221 0.00219 0.00000 0.03322 0.03297 -0.90924

D20 -0.95665 -0.00243 0.00000 -0.00747 -0.00864 -0.96529

D21 -2.80103 -0.00538 0.00000 0.01375 0.01321 -2.78781

D22 1.11481 -0.00058 0.00000 0.03618 0.03516 1.14997

D23 1.02645 0.00070 0.00000 0.00697 0.00781 1.03426

D24 -0.81793 -0.00225 0.00000 0.02819 0.02966 -0.78826

D25 3.09791 0.00255 0.00000 0.05062 0.05161 -3.13367

D26 3.08796 0.00247 0.00000 0.01833 0.01788 3.10584

D27 1.24358 -0.00047 0.00000 0.03955 0.03973 1.28332

D28 -1.12377 0.00433 0.00000 0.06198 0.06168 -1.06209

D29 0.84283 -0.00442 0.00000 -0.04438 -0.04441 0.79841

D30 -1.70542 -0.01458 0.00000 -0.13598 -0.13604 -1.84146

D31 3.03176 -0.00216 0.00000 -0.04770 -0.04816 2.98360

D32 0.48351 -0.01232 0.00000 -0.13931 -0.13978 0.34373

D33 -1.35265 -0.00450 0.00000 -0.07882 -0.07870 -1.43136

D34 2.38229 -0.01467 0.00000 -0.17043 -0.17033 2.21195

D35 -0.80884 0.00466 0.00000 0.03836 0.03838 -0.77047

D36 -2.94579 0.00486 0.00000 0.03217 0.03201 -2.91378

D37 1.29425 0.00495 0.00000 0.03824 0.03799 1.33224

D38 -2.97521 0.00215 0.00000 0.03989 0.04005 -2.93516

D39 1.17103 0.00234 0.00000 0.03370 0.03368 1.20471

D40 -0.87212 0.00244 0.00000 0.03977 0.03967 -0.83245

D41 1.61857 -0.00634 0.00000 0.01199 0.01245 1.63102

D42 -0.51838 -0.00614 0.00000 0.00579 0.00608 -0.51229

D43 -2.56153 -0.00605 0.00000 0.01187 0.01207 -2.54946

D44 0.87311 0.00381 0.00000 0.06661 0.06552 0.93863

D45 3.05669 -0.00020 0.00000 0.06614 0.06457 3.12126

D46 -1.22009 -0.00011 0.00000 0.04749 0.04658 -1.17350

D47 -1.35584 0.00565 0.00000 0.04051 0.04081 -1.31503

D48 0.82775 0.00164 0.00000 0.04004 0.03986 0.86760

D49 2.83415 0.00173 0.00000 0.02139 0.02187 2.85602

D50 2.93287 0.00291 0.00000 0.04183 0.04157 2.97444

D51 -1.16673 -0.00110 0.00000 0.04136 0.04062 -1.12611

D52 0.83968 -0.00100 0.00000 0.02271 0.02263 0.86231

D53 0.02831 0.00442 0.00000 0.01901 0.01876 0.04707

D54 2.17576 0.00450 0.00000 0.02722 0.02712 2.20289

D55 -2.07188 0.00410 0.00000 0.02308 0.02306 -2.04882

D56 -2.08217 -0.00036 0.00000 -0.00802 -0.00820 -2.09037

D57 0.06528 -0.00028 0.00000 0.00019 0.00017 0.06545

D58 2.10083 -0.00068 0.00000 -0.00395 -0.00390 2.09693

D59 2.14796 -0.00042 0.00000 -0.00255 -0.00277 2.14518

D60 -1.98778 -0.00035 0.00000 0.00566 0.00559 -1.98218

D61 0.04777 -0.00074 0.00000 0.00152 0.00153 0.04930

D62 0.04729 0.00080 0.00000 0.00322 0.00361 0.05091

D63 -3.08653 0.00116 0.00000 0.00450 0.00516 -3.08136

D64 0.04798 -0.00322 0.00000 -0.01616 -0.01632 0.03167

D65 3.09433 0.00043 0.00000 -0.00301 -0.00318 3.09115

D66 0.13300 -0.00348 0.00000 -0.02654 -0.02805 0.10495

D67 2.37813 -0.00947 0.00000 -0.04412 -0.04443 2.33369

D68 -1.48626 -0.00061 0.00000 0.01527 0.01562 -1.47064

D69 -2.09939 0.00235 0.00000 0.00063 -0.00077 -2.10015

D70 0.14574 -0.00363 0.00000 -0.01696 -0.01715 0.12859

D71 2.56454 0.00522 0.00000 0.04244 0.04290 2.60744

D72 2.09794 0.00142 0.00000 -0.00888 -0.01018 2.08776

D73 -1.94012 -0.00456 0.00000 -0.02646 -0.02657 -1.96669

D74 0.47868 0.00429 0.00000 0.03293 0.03348 0.51217

D75 -2.46085 0.00135 0.00000 -0.00707 -0.00600 -2.46684

D76 0.67138 0.00089 0.00000 -0.00860 -0.00784 0.66354

D77 -0.12300 0.00203 0.00000 0.00559 0.00589 -0.11710

D78 3.00923 0.00157 0.00000 0.00405 0.00404 3.01328

D79 1.97165 0.00260 0.00000 0.02187 0.02198 1.99363

D80 -1.17930 0.00215 0.00000 0.02033 0.02013 -1.15917

D81 1.52475 0.00448 0.00000 -0.00782 -0.00840 1.51635

D82 -1.49469 0.00052 0.00000 -0.02450 -0.02508 -1.51977

D83 -0.12537 0.00421 0.00000 0.02057 0.02087 -0.10449

D84 3.13838 0.00024 0.00000 0.00389 0.00419 -3.14061

D85 -2.54154 -0.00424 0.00000 -0.05254 -0.05238 -2.59392

D86 0.72221 -0.00820 0.00000 -0.06922 -0.06906 0.65315

Item Value Threshold Converged?

Maximum Force 0.038819 0.000450 NO

RMS Force 0.006105 0.000300 NO

Maximum Displacement 0.289268 0.001800 NO

RMS Displacement 0.059213 0.001200 NO

Predicted change in Energy=-2.732134D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.517037 1.291357 0.129062

2 6 0 -0.200178 0.864948 -0.249149

3 6 0 -0.509264 3.545240 0.123774

4 6 0 -1.639544 2.663671 0.303299

5 1 0 -2.415131 0.723261 -0.151729

6 1 0 -2.635914 3.094614 0.096581

7 6 0 0.421751 1.664065 -1.325137

8 1 0 1.523789 1.441450 -1.373211

9 1 0 -0.031675 1.322904 -2.297469

10 6 0 0.230040 3.174858 -1.157372

11 1 0 1.229073 3.679650 -1.194020

12 1 0 -0.364581 3.562377 -2.027362

13 1 0 -0.834584 4.622032 0.144664

14 1 0 0.159711 -0.160925 -0.091087

15 8 0 3.004299 4.450341 1.141412

16 6 0 0.705858 3.852763 1.310940

17 6 0 1.454904 2.814801 1.959065

18 6 0 1.729448 4.806548 0.731104

19 8 0 1.627371 5.778920 -0.006613

20 6 0 2.909362 3.258070 1.918918

21 8 0 3.971735 2.792854 2.305362

22 1 0 0.036854 4.392963 2.033610

23 1 0 1.067312 2.296243 2.829817

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.434916 0.000000

3 C 2.468931 2.723705 0.000000

4 C 1.388745 2.369045 1.444620 0.000000

5 H 1.099158 2.221617 3.416401 2.138639 0.000000

6 H 2.122423 3.320203 2.174038 1.105078 2.394519

7 C 2.452041 1.477543 2.550481 2.810686 3.210903

8 H 3.394992 2.137272 3.286366 3.783013 4.186037

9 H 2.845232 2.105643 3.321036 3.338696 3.262611

10 C 2.873111 2.519055 1.524824 2.426977 3.744139

11 H 3.872417 3.295161 2.185513 3.391629 4.806957

12 H 3.337043 3.234995 2.156064 2.804494 3.972825

13 H 3.399910 3.830567 1.125056 2.123277 4.217392

14 H 2.229142 1.098599 3.772181 3.372121 2.723100

15 O 5.607719 5.005734 3.768278 5.045780 6.703249

16 C 3.591504 3.490246 1.726400 2.816060 4.655508

17 C 3.808179 3.378969 2.785640 3.512835 4.879258

18 C 4.822726 4.496728 2.640375 4.015601 5.884740

19 O 5.481235 5.248417 3.093790 4.524772 6.474764

20 C 5.163774 4.482944 3.871953 4.863752 6.250045

21 O 6.092404 5.258061 5.040314 5.959144 7.149305

22 H 3.957505 4.208808 2.159712 2.965593 4.924901

23 H 3.870754 3.624247 3.371684 3.720936 4.846782

6 7 8 9 10

6 H 0.000000

7 C 3.662932 0.000000

8 H 4.711303 1.125325 0.000000

9 H 3.956323 1.125796 1.813222 0.000000

10 C 3.129302 1.532120 2.173724 2.190445 0.000000

11 H 4.116558 2.175211 2.264621 2.891598 1.119922

12 H 3.144661 2.171411 2.914136 2.280137 1.122777

13 H 2.362225 3.533874 4.240516 4.182454 2.218792

14 H 4.295262 2.218588 2.464174 2.665802 3.502764

15 O 5.894206 4.529541 4.191499 5.551927 3.822011

16 C 3.635505 3.438025 3.699745 4.468194 2.603559

17 C 4.503547 3.630094 3.604844 4.749079 3.367805

18 C 4.731778 3.976606 3.974208 4.940606 2.911525

19 O 5.039022 4.485984 4.548843 5.277929 3.171422

20 C 5.839325 4.387819 4.007248 5.492949 4.080349

21 O 6.973578 5.201641 4.620675 6.274878 5.112409

22 H 3.547038 4.344676 4.746456 5.309256 3.421033

23 H 4.671387 4.252063 4.313292 5.333313 4.167813

11 12 13 14 15

11 H 0.000000

12 H 1.802206 0.000000

13 H 2.634168 2.462006 0.000000

14 H 4.136425 4.229305 4.890898 0.000000

15 O 3.033089 4.709454 3.969887 5.556483 0.000000

16 C 2.564868 3.517730 2.079648 4.286449 2.380897

17 C 3.277333 4.445335 3.435097 3.838696 2.396700

18 C 2.286127 3.679953 2.636706 5.274074 1.385814

19 O 2.444486 3.600606 2.724426 6.119062 2.231370

20 C 3.562511 5.136578 4.361824 4.825995 1.426548

21 O 4.533682 6.178050 5.578101 5.385100 2.244543

22 H 3.513944 4.164435 2.092843 5.026662 3.099200

23 H 4.258080 5.219732 4.029461 3.923403 3.353024

16 17 18 19 20

16 C 0.000000

17 C 1.434748 0.000000

18 C 1.514481 2.355911 0.000000

19 O 2.509026 3.560848 1.224808 0.000000

20 C 2.361933 1.521035 2.280544 3.421382 0.000000

21 O 3.574665 2.540637 3.400162 4.444981 1.222456

22 H 1.123225 2.122975 2.175419 2.934813 3.090702

23 H 2.204629 1.085053 3.338361 4.526372 2.268920

21 22 23

21 O 0.000000

22 H 4.256464 0.000000

23 H 2.992883 2.468203 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.941258 -0.762672 -0.644800

2 6 0 2.240667 -1.380431 0.444479

3 6 0 1.134211 0.914849 -0.517816

4 6 0 2.353195 0.408341 -1.104717

5 1 0 4.024322 -0.887316 -0.784744

6 1 0 3.037025 1.159056 -1.540608

7 6 0 1.830325 -0.453110 1.519109

8 1 0 1.073845 -0.955224 2.183921

9 1 0 2.742184 -0.246010 2.146037

10 6 0 1.237961 0.862061 1.002559

11 1 0 0.233227 1.022847 1.470407

12 1 0 1.894049 1.709693 1.336769

13 1 0 0.902442 1.945698 -0.904322

14 1 0 2.348769 -2.445344 0.691853

15 8 0 -2.480434 0.280021 0.337320

16 6 0 -0.456056 0.371102 -0.912588

17 6 0 -0.852855 -1.006770 -0.862400

18 6 0 -1.458337 1.125435 -0.064019

19 8 0 -1.509590 2.288995 0.314998

20 6 0 -2.190559 -1.033065 -0.138932

21 8 0 -2.985240 -1.902013 0.189415

22 1 0 -0.462538 0.765354 -1.964328

23 1 0 -0.670062 -1.679219 -1.694108

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3620848 0.6068851 0.5164332

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 452.3202531610 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.511591647727E-01 A.U. after 16 cycles

Convg = 0.4521D-08 -V/T = 1.0011

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.037849582 0.020969502 -0.020820488

2 6 -0.038950937 -0.006693659 -0.007548269

3 6 0.037987402 0.021862740 0.017365168

4 6 0.000277063 -0.011235319 -0.023375641

5 1 0.002612603 -0.013364373 0.021945599

6 1 -0.002747965 0.004300310 0.022101076

7 6 0.017184552 0.012083439 0.017804776

8 1 -0.000276677 -0.000236701 -0.001634992

9 1 -0.000329376 -0.001052569 0.000167803

10 6 -0.002144514 -0.009815426 -0.000049742

11 1 0.000193289 -0.000290849 -0.001275742

12 1 -0.000299033 0.000454466 0.000555615

13 1 -0.005477256 -0.000096663 -0.012226984

14 1 0.000357491 0.001609275 0.004078599

15 8 0.000473832 -0.004571874 0.004872017

16 6 -0.043703661 -0.007020963 -0.009860531

17 6 0.038274870 0.024801070 0.003813706

18 6 0.000018386 -0.000858391 -0.002808747

19 8 0.001084692 0.000143759 0.002854253

20 6 -0.038955790 -0.027350334 -0.013806056

21 8 -0.004894555 0.005711437 0.000854408

22 1 -0.001072722 0.001745887 0.002061203

23 1 0.002538723 -0.011094763 -0.005067029

-------------------------------------------------------------------

Cartesian Forces: Max 0.043703661 RMS 0.015207398

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.044376871 RMS 0.006715183

Search for a saddle point.

Step number 12 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 11 12

ITU= 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.04174 -0.01653 0.00271 0.00318 0.00458

Eigenvalues --- 0.00611 0.00816 0.00978 0.01525 0.01910

Eigenvalues --- 0.01974 0.02114 0.02187 0.02491 0.02628

Eigenvalues --- 0.02824 0.03063 0.03167 0.03417 0.03498

Eigenvalues --- 0.03672 0.03726 0.03889 0.03977 0.04394

Eigenvalues --- 0.04632 0.05425 0.05575 0.05991 0.06182

Eigenvalues --- 0.06297 0.07362 0.08177 0.08622 0.09791

Eigenvalues --- 0.11930 0.13481 0.14392 0.15036 0.17799

Eigenvalues --- 0.19418 0.20933 0.24559 0.25316 0.25646

Eigenvalues --- 0.27675 0.28125 0.30778 0.31206 0.31494

Eigenvalues --- 0.31920 0.32223 0.32664 0.32903 0.34436

Eigenvalues --- 0.35656 0.37416 0.39575 0.40136 0.43170

Eigenvalues --- 0.44881 1.08100 1.10812

Eigenvectors required to have negative eigenvalues:

R6 R10 A14 D41 A8

1 0.69858 0.57152 -0.11055 0.10054 -0.09948

A15 A12 A34 D68 D43

1 -0.09580 0.08972 -0.08531 0.08493 0.08313

RFO step: Lambda0=2.145556526D-02 Lambda=-7.30561500D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.382

Iteration 1 RMS(Cart)= 0.03371517 RMS(Int)= 0.00175193

Iteration 2 RMS(Cart)= 0.00237390 RMS(Int)= 0.00042495

Iteration 3 RMS(Cart)= 0.00000191 RMS(Int)= 0.00042494

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00042494

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.71160 -0.03059 0.00000 -0.09059 -0.09043 2.62117

R2 2.62435 -0.00193 0.00000 0.02387 0.02458 2.64892

R3 2.07711 -0.00083 0.00000 0.00051 0.00051 2.07762

R4 2.79215 0.00172 0.00000 0.00656 0.00678 2.79893

R5 2.07605 -0.00080 0.00000 0.00173 0.00173 2.07778

R6 6.38533 -0.01845 0.00000 0.21425 0.21342 6.59875

R7 2.72994 0.00052 0.00000 -0.01253 -0.01201 2.71792

R8 2.88150 0.00023 0.00000 -0.00935 -0.00956 2.87194

R9 2.12605 0.00126 0.00000 0.00169 0.00169 2.12774

R10 3.26242 -0.03035 0.00000 0.06166 0.06230 3.32472

R11 2.08829 0.00002 0.00000 -0.00253 -0.00253 2.08577

R12 2.12656 -0.00015 0.00000 -0.00098 -0.00098 2.12558

R13 2.12745 0.00031 0.00000 0.00298 0.00298 2.13043

R14 2.89529 -0.00093 0.00000 -0.00639 -0.00637 2.88892

R15 2.11635 0.00008 0.00000 0.00128 0.00128 2.11763

R16 2.12174 -0.00012 0.00000 0.00200 0.00200 2.12375

R17 2.61881 -0.00339 0.00000 -0.00003 0.00001 2.61882

R18 2.69578 -0.00475 0.00000 0.00276 0.00279 2.69858

R19 2.71128 0.00780 0.00000 0.00598 0.00581 2.71709

R20 2.86195 -0.00351 0.00000 0.00001 -0.00002 2.86194

R21 2.12259 0.00280 0.00000 0.00107 0.00107 2.12366

R22 2.87434 -0.04438 0.00000 -0.12973 -0.12975 2.74459

R23 2.05045 0.00033 0.00000 -0.00039 -0.00039 2.05007

R24 2.31455 -0.00170 0.00000 -0.00069 -0.00069 2.31386

R25 2.31011 -0.00616 0.00000 0.00240 0.00240 2.31251

A1 1.99070 0.00892 0.00000 0.03065 0.02978 2.02048

A2 2.12813 -0.00509 0.00000 -0.00382 -0.00482 2.12331

A3 2.06089 0.00006 0.00000 0.00448 0.00371 2.06460

A4 2.00150 0.00420 0.00000 0.03456 0.03255 2.03405

A5 2.14148 -0.00076 0.00000 -0.00022 -0.00098 2.14050

A6 1.67678 -0.00894 0.00000 -0.04528 -0.04463 1.63215

A7 2.06227 0.00087 0.00000 -0.00176 -0.00255 2.05972

A8 1.52842 0.00102 0.00000 -0.03645 -0.03539 1.49303

A9 1.85915 -0.00144 0.00000 0.00602 0.00565 1.86480

A10 1.91296 -0.00002 0.00000 0.02076 0.01964 1.93260

A11 1.93426 0.00198 0.00000 0.01073 0.01070 1.94496

A12 2.18211 -0.01245 0.00000 -0.03311 -0.03250 2.14960

A13 1.96956 -0.00085 0.00000 -0.00047 -0.00032 1.96924

A14 1.85435 0.00776 0.00000 0.00222 0.00289 1.85724

A15 1.59106 0.00426 0.00000 -0.00394 -0.00440 1.58666

A16 2.11579 -0.00243 0.00000 -0.00371 -0.00401 2.11178

A17 2.02798 0.00208 0.00000 0.00960 0.00860 2.03657

A18 2.03110 0.00380 0.00000 0.02214 0.02156 2.05266

A19 1.91381 0.00198 0.00000 0.00609 0.00594 1.91976

A20 1.87081 -0.00315 0.00000 -0.01411 -0.01384 1.85697

A21 1.98330 0.00156 0.00000 0.01019 0.00973 1.99303

A22 1.87295 -0.00019 0.00000 -0.00248 -0.00250 1.87046

A23 1.89894 0.00055 0.00000 0.00722 0.00735 1.90629

A24 1.92090 -0.00086 0.00000 -0.00783 -0.00783 1.91308

A25 1.97381 -0.00111 0.00000 0.00966 0.00882 1.98263

A26 1.92892 -0.00013 0.00000 -0.00197 -0.00166 1.92726

A27 1.88643 0.00105 0.00000 -0.00707 -0.00694 1.87949

A28 1.90632 0.00117 0.00000 0.00552 0.00578 1.91210

A29 1.89838 -0.00058 0.00000 -0.00676 -0.00652 1.89186

A30 1.86660 -0.00038 0.00000 -0.00018 -0.00030 1.86629

A31 1.89123 -0.00066 0.00000 -0.00960 -0.00967 1.88156

A32 2.15224 0.00231 0.00000 0.00601 0.00573 2.15797

A33 1.90140 -0.00156 0.00000 -0.00633 -0.00618 1.89522

A34 1.67989 0.00248 0.00000 -0.00838 -0.00843 1.67147

A35 1.85012 -0.00395 0.00000 -0.01510 -0.01510 1.83502

A36 1.94792 0.00031 0.00000 0.01259 0.01270 1.96062

A37 1.92410 0.00107 0.00000 0.01504 0.01502 1.93912

A38 1.43693 -0.00089 0.00000 -0.01728 -0.01765 1.41928

A39 2.23865 -0.00258 0.00000 -0.01808 -0.01788 2.22077

A40 1.64456 -0.00270 0.00000 -0.03083 -0.03045 1.61411

A41 1.85091 0.00355 0.00000 0.02368 0.02363 1.87455

A42 2.11972 0.00173 0.00000 0.01658 0.01530 2.13501

A43 2.09674 -0.00018 0.00000 0.01060 0.00888 2.10563

A44 1.92465 -0.00612 0.00000 -0.01403 -0.01416 1.91049

A45 2.04773 0.00167 0.00000 0.00632 0.00637 2.05410

A46 2.31075 0.00444 0.00000 0.00760 0.00763 2.31837

A47 1.89820 0.00771 0.00000 0.01877 0.01858 1.91678

A48 2.01808 -0.00589 0.00000 -0.02033 -0.02037 1.99771

A49 2.36280 -0.00150 0.00000 0.00348 0.00347 2.36627

D1 -0.80323 0.00856 0.00000 0.07561 0.07619 -0.72704

D2 2.76076 -0.00281 0.00000 -0.00833 -0.00827 2.75248

D3 0.76957 0.00602 0.00000 0.01820 0.01785 0.78742

D4 1.85549 0.01732 0.00000 0.14562 0.14601 2.00150

D5 -0.86372 0.00596 0.00000 0.06169 0.06155 -0.80216

D6 -2.85490 0.01479 0.00000 0.08822 0.08767 -2.76723

D7 -0.01165 -0.00192 0.00000 -0.01423 -0.01418 -0.02583

D8 2.62907 0.00663 0.00000 0.05243 0.05217 2.68124

D9 -2.69024 -0.00867 0.00000 -0.07851 -0.07868 -2.76892

D10 -0.04952 -0.00012 0.00000 -0.01185 -0.01233 -0.06185

D11 2.88796 -0.00602 0.00000 -0.05003 -0.05061 2.83735

D12 -1.36744 -0.00695 0.00000 -0.05755 -0.05810 -1.42554

D13 0.75875 -0.00927 0.00000 -0.07095 -0.07162 0.68713

D14 -0.65567 0.00433 0.00000 0.02972 0.02968 -0.62598

D15 1.37211 0.00340 0.00000 0.02220 0.02219 1.39431

D16 -2.78488 0.00107 0.00000 0.00880 0.00867 -2.77621

D17 1.21997 0.00335 0.00000 0.01640 0.01675 1.23672

D18 -3.03543 0.00242 0.00000 0.00887 0.00926 -3.02617

D19 -0.90924 0.00009 0.00000 -0.00452 -0.00426 -0.91350

D20 -0.96529 -0.00311 0.00000 -0.00984 -0.00988 -0.97517

D21 -2.78781 -0.00679 0.00000 -0.02540 -0.02532 -2.81313

D22 1.14997 -0.00106 0.00000 0.01029 0.00998 1.15995

D23 1.03426 0.00120 0.00000 0.02127 0.02173 1.05599

D24 -0.78826 -0.00248 0.00000 0.00570 0.00630 -0.78196

D25 -3.13367 0.00324 0.00000 0.04139 0.04159 -3.09208

D26 3.10584 0.00226 0.00000 0.00863 0.00868 3.11452

D27 1.28332 -0.00142 0.00000 -0.00693 -0.00675 1.27656

D28 -1.06209 0.00431 0.00000 0.02876 0.02854 -1.03355

D29 0.79841 -0.00391 0.00000 -0.04658 -0.04695 0.75147

D30 -1.84146 -0.01201 0.00000 -0.10994 -0.11030 -1.95176

D31 2.98360 -0.00361 0.00000 -0.02475 -0.02496 2.95864

D32 0.34373 -0.01171 0.00000 -0.08811 -0.08831 0.25541

D33 -1.43136 -0.00373 0.00000 -0.04131 -0.04177 -1.47313

D34 2.21195 -0.01183 0.00000 -0.10466 -0.10512 2.10683

D35 -0.77047 0.00562 0.00000 0.04906 0.04896 -0.72151

D36 -2.91378 0.00499 0.00000 0.03637 0.03622 -2.87756

D37 1.33224 0.00491 0.00000 0.04180 0.04151 1.37376

D38 -2.93516 0.00366 0.00000 0.01991 0.02003 -2.91513

D39 1.20471 0.00303 0.00000 0.00722 0.00730 1.21201

D40 -0.83245 0.00295 0.00000 0.01265 0.01259 -0.81986

D41 1.63102 -0.00454 0.00000 0.02354 0.02383 1.65484

D42 -0.51229 -0.00517 0.00000 0.01086 0.01109 -0.50121

D43 -2.54946 -0.00526 0.00000 0.01628 0.01638 -2.53308

D44 0.93863 0.00242 0.00000 0.02788 0.02760 0.96622

D45 3.12126 -0.00305 0.00000 0.00413 0.00384 3.12510

D46 -1.17350 -0.00125 0.00000 0.01527 0.01501 -1.15849

D47 -1.31503 0.00538 0.00000 0.02461 0.02468 -1.29035

D48 0.86760 -0.00009 0.00000 0.00086 0.00092 0.86853

D49 2.85602 0.00171 0.00000 0.01200 0.01210 2.86812

D50 2.97444 0.00368 0.00000 0.02606 0.02603 3.00047

D51 -1.12611 -0.00179 0.00000 0.00231 0.00227 -1.12383

D52 0.86231 0.00001 0.00000 0.01345 0.01345 0.87576

D53 0.04707 0.00392 0.00000 0.01300 0.01275 0.05983

D54 2.20289 0.00383 0.00000 0.02133 0.02124 2.22413

D55 -2.04882 0.00370 0.00000 0.02040 0.02040 -2.02841

D56 -2.09037 -0.00010 0.00000 -0.00708 -0.00730 -2.09767

D57 0.06545 -0.00018 0.00000 0.00124 0.00118 0.06663

D58 2.09693 -0.00031 0.00000 0.00031 0.00035 2.09727

D59 2.14518 0.00030 0.00000 -0.00385 -0.00409 2.14109

D60 -1.98218 0.00022 0.00000 0.00448 0.00439 -1.97779

D61 0.04930 0.00009 0.00000 0.00354 0.00356 0.05286

D62 0.05091 0.00078 0.00000 0.00428 0.00381 0.05472

D63 -3.08136 0.00167 0.00000 0.01470 0.01416 -3.06720

D64 0.03167 -0.00272 0.00000 -0.01987 -0.02004 0.01163

D65 3.09115 0.00052 0.00000 -0.00049 -0.00084 3.09031

D66 0.10495 -0.00522 0.00000 -0.02243 -0.02255 0.08241

D67 2.33369 -0.00796 0.00000 -0.04452 -0.04486 2.28883

D68 -1.47064 -0.00126 0.00000 0.02667 0.02706 -1.44358

D69 -2.10015 -0.00082 0.00000 -0.00272 -0.00292 -2.10307

D70 0.12859 -0.00355 0.00000 -0.02480 -0.02524 0.10335

D71 2.60744 0.00314 0.00000 0.04639 0.04668 2.65412

D72 2.08776 0.00017 0.00000 -0.01860 -0.01876 2.06900

D73 -1.96669 -0.00256 0.00000 -0.04069 -0.04108 -2.00776

D74 0.51217 0.00413 0.00000 0.03050 0.03085 0.54301

D75 -2.46684 0.00413 0.00000 0.02565 0.02541 -2.44143

D76 0.66354 0.00301 0.00000 0.01307 0.01288 0.67641

D77 -0.11710 0.00292 0.00000 0.01716 0.01698 -0.10012

D78 3.01328 0.00181 0.00000 0.00458 0.00445 3.01772

D79 1.99363 0.00151 0.00000 0.03156 0.03141 2.02504

D80 -1.15917 0.00040 0.00000 0.01898 0.01887 -1.14030

D81 1.51635 0.00490 0.00000 0.01846 0.01809 1.53444

D82 -1.51977 0.00088 0.00000 -0.00506 -0.00553 -1.52530

D83 -0.10449 0.00405 0.00000 0.02807 0.02855 -0.07595

D84 -3.14061 0.00003 0.00000 0.00455 0.00493 -3.13568

D85 -2.59392 -0.00339 0.00000 -0.04463 -0.04472 -2.63864

D86 0.65315 -0.00741 0.00000 -0.06815 -0.06834 0.58481

Item Value Threshold Converged?

Maximum Force 0.044377 0.000450 NO

RMS Force 0.006715 0.000300 NO

Maximum Displacement 0.189731 0.001800 NO

RMS Displacement 0.033980 0.001200 NO

Predicted change in Energy=-2.190373D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.489720 1.280439 0.121135

2 6 0 -0.242648 0.845253 -0.302385

3 6 0 -0.508655 3.549082 0.093651

4 6 0 -1.622114 2.663688 0.305517

5 1 0 -2.399032 0.689383 -0.059264

6 1 0 -2.637178 3.083340 0.196982

7 6 0 0.423909 1.659886 -1.344412

8 1 0 1.521370 1.415926 -1.379781

9 1 0 -0.019939 1.340562 -2.330314

10 6 0 0.249055 3.168264 -1.167514

11 1 0 1.252399 3.666948 -1.186518

12 1 0 -0.329632 3.563662 -2.046032

13 1 0 -0.833262 4.627211 0.099502

14 1 0 0.110069 -0.184626 -0.147874

15 8 0 2.998857 4.452945 1.160289

16 6 0 0.706067 3.878993 1.322869

17 6 0 1.472280 2.855409 1.980532

18 6 0 1.732113 4.830949 0.744394

19 8 0 1.642656 5.800810 0.002355

20 6 0 2.867703 3.254340 1.925405

21 8 0 3.928324 2.779201 2.308589

22 1 0 0.011703 4.411950 2.027654

23 1 0 1.089275 2.299391 2.829677

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.387064 0.000000

3 C 2.471839 2.745596 0.000000

4 C 1.401750 2.362029 1.438263 0.000000

5 H 1.099428 2.175638 3.431442 2.152801 0.000000

6 H 2.138426 3.315445 2.181331 1.103740 2.419382

7 C 2.440038 1.481129 2.550835 2.813555 3.249997

8 H 3.367160 2.144343 3.292773 3.778708 4.200141

9 H 2.858929 2.099387 3.315420 3.356372 3.352877

10 C 2.871906 2.527172 1.519764 2.434275 3.792814

11 H 3.863237 3.313430 2.180375 3.390505 4.844538

12 H 3.354926 3.230730 2.147208 2.830238 4.060929

13 H 3.410614 3.848837 1.125951 2.126065 4.240677

14 H 2.185888 1.099515 3.792325 3.364360 2.658445

15 O 5.593921 5.065788 3.775887 5.028463 6.692452

16 C 3.608064 3.570026 1.759365 2.816451 4.661067

17 C 3.835535 3.491907 2.822341 3.523877 4.882571

18 C 4.834747 4.569595 2.662272 4.017521 5.904642

19 O 5.500876 5.310817 3.115566 4.537859 6.516573

20 C 5.112613 4.521176 3.852530 4.809508 6.185178

21 O 6.032118 5.287188 5.018511 5.901950 7.071741

22 H 3.961748 4.267916 2.180753 2.948141 4.901467

23 H 3.876297 3.701128 3.406017 3.722328 4.806912

6 7 8 9 10

6 H 0.000000

7 C 3.711114 0.000000

8 H 4.749734 1.124806 0.000000

9 H 4.034159 1.127374 1.812409 0.000000

10 C 3.193651 1.528748 2.175898 2.182878 0.000000

11 H 4.169350 2.177068 2.275257 2.887764 1.120600

12 H 3.253704 2.164361 2.912537 2.262499 1.123838

13 H 2.376374 3.531343 4.247931 4.167441 2.214784

14 H 4.283211 2.220906 2.463967 2.665736 3.507258

15 O 5.879512 4.550281 4.225920 5.566360 3.824981

16 C 3.616348 3.481154 3.746429 4.507378 2.629829

17 C 4.485605 3.685595 3.655985 4.806753 3.391806

18 C 4.737563 4.016235 4.027271 4.970545 2.935877

19 O 5.073411 4.521767 4.599154 5.300884 3.200158

20 C 5.772383 4.382478 4.014552 5.487455 4.053501

21 O 6.903420 5.184420 4.610426 6.259224 5.076582

22 H 3.483265 4.372025 4.781827 5.331633 3.436887

23 H 4.629483 4.274892 4.322818 5.364254 4.175937

11 12 13 14 15

11 H 0.000000

12 H 1.803401 0.000000

13 H 2.631717 2.447059 0.000000

14 H 4.149496 4.224453 4.909668 0.000000

15 O 3.029094 4.706395 3.980046 5.618135 0.000000

16 C 2.576910 3.538587 2.103803 4.362487 2.369122

17 C 3.276759 4.467855 3.463102 3.953169 2.356980

18 C 2.305091 3.693682 2.653025 5.346322 1.385819

19 O 2.473679 3.618099 2.741704 6.180359 2.235360

20 C 3.530371 5.107929 4.349234 4.871295 1.428026

21 O 4.490484 6.140709 5.564882 5.421951 2.232470

22 H 3.524948 4.175047 2.116145 5.086365 3.110802

23 H 4.245780 5.232993 4.070473 3.999374 3.327334

16 17 18 19 20

16 C 0.000000

17 C 1.437820 0.000000

18 C 1.514472 2.344847 0.000000

19 O 2.512834 3.552126 1.224441 0.000000

20 C 2.329359 1.452374 2.273774 3.418095 0.000000

21 O 3.544592 2.479029 3.388173 4.435439 1.223726

22 H 1.123792 2.135023 2.186808 2.948012 3.083384

23 H 2.216407 1.084848 3.342219 4.534304 2.211886

21 22 23

21 O 0.000000

22 H 4.252613 0.000000

23 H 2.926081 2.503459 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.928613 -0.750776 -0.649853

2 6 0 2.324384 -1.341551 0.450073

3 6 0 1.127769 0.936445 -0.507605

4 6 0 2.321098 0.420608 -1.122812

5 1 0 3.989151 -0.919483 -0.885520

6 1 0 2.970895 1.135027 -1.657239

7 6 0 1.858984 -0.428535 1.519441

8 1 0 1.123490 -0.958981 2.184922

9 1 0 2.763230 -0.187792 2.148213

10 6 0 1.230483 0.867451 1.007114

11 1 0 0.221197 1.005072 1.474175

12 1 0 1.867991 1.728822 1.345693

13 1 0 0.885391 1.970154 -0.882389

14 1 0 2.456008 -2.404291 0.699456

15 8 0 -2.485140 0.245800 0.345167

16 6 0 -0.487865 0.376867 -0.922292

17 6 0 -0.892685 -1.001580 -0.864578

18 6 0 -1.491009 1.119918 -0.064853

19 8 0 -1.558185 2.279772 0.321775

20 6 0 -2.149209 -1.055270 -0.138179

21 8 0 -2.923248 -1.938770 0.205036

22 1 0 -0.479400 0.775858 -1.972836

23 1 0 -0.688763 -1.700265 -1.669036

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3538879 0.6058037 0.5162106

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 452.2354103725 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.351464329816E-01 A.U. after 16 cycles

Convg = 0.4950D-08 -V/T = 1.0008

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.005915794 0.024614009 -0.011652477

2 6 -0.008602798 -0.012568023 -0.015390413

3 6 0.023870360 0.015815670 0.013831820

4 6 0.003309621 -0.003876364 -0.023247796

5 1 0.001865773 -0.010772363 0.022107900

6 1 -0.000948952 0.003314583 0.020995046

7 6 0.016547569 0.008491836 0.016083923

8 1 -0.000281084 0.000132784 -0.000960742

9 1 0.000284221 -0.001194447 0.000551809

10 6 -0.000358113 -0.008595607 0.000915569

11 1 0.000263210 -0.000605830 -0.001080230

12 1 -0.000088653 0.000947980 0.000595534

13 1 -0.003570391 -0.001562131 -0.010157105

14 1 0.000319796 -0.000144441 0.000626426

15 8 0.000923529 0.002003435 -0.000175469

16 6 -0.035279731 -0.008322153 0.000985506

17 6 -0.007069289 0.020070252 0.003966972

18 6 0.000613734 -0.001154304 -0.004826437

19 8 0.000429828 0.000397517 0.002973586

20 6 0.002205447 -0.018594229 -0.012329053

21 8 0.001377705 0.003408833 0.002732989

22 1 -0.001168791 -0.000476744 -0.001170805

23 1 -0.000558785 -0.011330263 -0.005376553

-------------------------------------------------------------------

Cartesian Forces: Max 0.035279731 RMS 0.010211397

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.023265590 RMS 0.004334969

Search for a saddle point.

Step number 13 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 12 13

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.05886 0.00141 0.00251 0.00388 0.00570

Eigenvalues --- 0.00638 0.00839 0.01082 0.01533 0.01888

Eigenvalues --- 0.01947 0.02135 0.02224 0.02498 0.02605

Eigenvalues --- 0.02765 0.03042 0.03137 0.03336 0.03462

Eigenvalues --- 0.03670 0.03706 0.03865 0.03942 0.04446

Eigenvalues --- 0.04603 0.05379 0.05552 0.05971 0.06107

Eigenvalues --- 0.06190 0.07357 0.08264 0.08615 0.09867

Eigenvalues --- 0.11851 0.13433 0.14322 0.15462 0.18859

Eigenvalues --- 0.20682 0.22623 0.24535 0.25557 0.26559

Eigenvalues --- 0.27938 0.28768 0.30759 0.31207 0.31541

Eigenvalues --- 0.31934 0.32228 0.32666 0.33469 0.34443

Eigenvalues --- 0.35700 0.37412 0.39583 0.40357 0.43163

Eigenvalues --- 0.45216 1.08241 1.10814

Eigenvectors required to have negative eigenvalues:

R6 R10 D4 D30 R22

1 0.67844 0.54897 0.12001 -0.11515 0.11276

A14 A8 D41 D68 A15

1 -0.09930 -0.09749 0.09726 0.08950 -0.08889

RFO step: Lambda0=4.133236905D-03 Lambda=-4.59061931D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.948

Iteration 1 RMS(Cart)= 0.07917434 RMS(Int)= 0.01168879

Iteration 2 RMS(Cart)= 0.01197033 RMS(Int)= 0.00186406

Iteration 3 RMS(Cart)= 0.00023799 RMS(Int)= 0.00184601

Iteration 4 RMS(Cart)= 0.00000019 RMS(Int)= 0.00184601

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62117 0.00074 0.00000 0.00171 0.00439 2.62556

R2 2.64892 -0.00138 0.00000 0.00367 0.00708 2.65601

R3 2.07762 0.00062 0.00000 -0.00050 -0.00050 2.07712

R4 2.79893 0.00052 0.00000 -0.01396 -0.01469 2.78424

R5 2.07778 0.00033 0.00000 0.00064 0.00064 2.07843

R6 6.59875 -0.01562 0.00000 0.06817 0.06611 6.66485

R7 2.71792 -0.00331 0.00000 -0.04660 -0.04590 2.67202

R8 2.87194 0.00206 0.00000 -0.00502 -0.00517 2.86677

R9 2.12774 -0.00052 0.00000 -0.00006 -0.00006 2.12768

R10 3.32472 -0.02327 0.00000 -0.03114 -0.02983 3.29489

R11 2.08577 0.00007 0.00000 -0.00316 -0.00316 2.08260

R12 2.12558 -0.00027 0.00000 -0.00138 -0.00138 2.12420

R13 2.13043 -0.00026 0.00000 0.00287 0.00287 2.13329

R14 2.88892 0.00086 0.00000 -0.00832 -0.00948 2.87943

R15 2.11763 -0.00002 0.00000 0.00213 0.00213 2.11975

R16 2.12375 -0.00009 0.00000 0.00280 0.00280 2.12655

R17 2.61882 0.00009 0.00000 -0.00212 -0.00135 2.61747

R18 2.69858 0.00116 0.00000 0.00386 0.00436 2.70294

R19 2.71709 0.00096 0.00000 -0.02702 -0.02878 2.68830

R20 2.86194 0.00178 0.00000 0.00867 0.00866 2.87060

R21 2.12366 -0.00024 0.00000 -0.00512 -0.00512 2.11854

R22 2.74459 0.00057 0.00000 0.04794 0.04749 2.79208

R23 2.05007 0.00180 0.00000 -0.00050 -0.00050 2.04957

R24 2.31386 -0.00152 0.00000 -0.00118 -0.00118 2.31268

R25 2.31251 0.00073 0.00000 -0.00117 -0.00117 2.31133

A1 2.02048 0.00264 0.00000 0.03710 0.03384 2.05433

A2 2.12331 -0.00064 0.00000 0.00553 0.00014 2.12345

A3 2.06460 0.00075 0.00000 0.02017 0.01511 2.07970

A4 2.03405 0.00280 0.00000 0.05357 0.04657 2.08063

A5 2.14050 0.00037 0.00000 0.00024 -0.00261 2.13789

A6 1.63215 -0.00993 0.00000 -0.14481 -0.14239 1.48976

A7 2.05972 0.00004 0.00000 -0.00567 -0.00796 2.05176

A8 1.49303 0.00046 0.00000 -0.01874 -0.01539 1.47764

A9 1.86480 0.00046 0.00000 0.02820 0.02670 1.89150

A10 1.93260 0.00243 0.00000 0.05110 0.04926 1.98186

A11 1.94496 0.00021 0.00000 0.01682 0.01736 1.96232

A12 2.14960 -0.00993 0.00000 -0.12556 -0.12654 2.02307

A13 1.96924 -0.00030 0.00000 -0.00952 -0.01098 1.95825

A14 1.85724 0.00423 0.00000 0.04346 0.04751 1.90475

A15 1.58666 0.00346 0.00000 0.01564 0.01446 1.60112

A16 2.11178 0.00087 0.00000 0.00711 0.00230 2.11408

A17 2.03657 0.00015 0.00000 0.02415 0.02038 2.05695

A18 2.05266 0.00202 0.00000 0.03074 0.02738 2.08004

A19 1.91976 0.00119 0.00000 0.01020 0.01077 1.93053

A20 1.85697 -0.00184 0.00000 -0.01879 -0.01804 1.83893

A21 1.99303 0.00046 0.00000 0.01246 0.00970 2.00273

A22 1.87046 -0.00029 0.00000 -0.00710 -0.00736 1.86310

A23 1.90629 0.00111 0.00000 0.01286 0.01322 1.91951

A24 1.91308 -0.00077 0.00000 -0.01185 -0.01093 1.90215

A25 1.98263 0.00089 0.00000 0.02609 0.02419 2.00682

A26 1.92726 0.00012 0.00000 0.00058 0.00094 1.92820

A27 1.87949 -0.00047 0.00000 -0.02018 -0.01957 1.85991

A28 1.91210 -0.00046 0.00000 -0.00161 -0.00082 1.91127

A29 1.89186 -0.00003 0.00000 -0.00461 -0.00430 1.88756

A30 1.86629 -0.00010 0.00000 -0.00232 -0.00265 1.86365

A31 1.88156 -0.00004 0.00000 0.00042 0.00043 1.88199

A32 2.15797 0.00191 0.00000 -0.02210 -0.02425 2.13373

A33 1.89522 -0.00306 0.00000 -0.03648 -0.03651 1.85871

A34 1.67147 0.00102 0.00000 0.01143 0.01310 1.68457

A35 1.83502 -0.00168 0.00000 -0.00212 -0.00278 1.83224

A36 1.96062 0.00096 0.00000 0.02911 0.02833 1.98894

A37 1.93912 0.00112 0.00000 0.02570 0.02549 1.96461

A38 1.41928 0.00078 0.00000 0.02642 0.02499 1.44426

A39 2.22077 -0.00489 0.00000 -0.08675 -0.08522 2.13554

A40 1.61411 -0.00246 0.00000 -0.06584 -0.06711 1.54700

A41 1.87455 0.00167 0.00000 0.01050 0.01143 1.88597

A42 2.13501 0.00100 0.00000 0.04173 0.03845 2.17346

A43 2.10563 0.00171 0.00000 0.03812 0.02843 2.13405

A44 1.91049 0.00110 0.00000 0.01135 0.01092 1.92141

A45 2.05410 -0.00126 0.00000 -0.00791 -0.00777 2.04633

A46 2.31837 0.00015 0.00000 -0.00371 -0.00352 2.31486

A47 1.91678 -0.00074 0.00000 -0.01504 -0.01647 1.90031

A48 1.99771 -0.00222 0.00000 -0.00277 -0.00255 1.99516

A49 2.36627 0.00317 0.00000 0.02080 0.02107 2.38734

D1 -0.72704 0.00907 0.00000 0.15924 0.16202 -0.56502

D2 2.75248 -0.00170 0.00000 -0.00118 0.00031 2.75279

D3 0.78742 0.00474 0.00000 0.06813 0.06543 0.85285

D4 2.00150 0.01651 0.00000 0.32923 0.33129 2.33279

D5 -0.80216 0.00574 0.00000 0.16882 0.16959 -0.63258

D6 -2.76723 0.01219 0.00000 0.23812 0.23471 -2.53253

D7 -0.02583 -0.00223 0.00000 -0.03334 -0.03332 -0.05915

D8 2.68124 0.00587 0.00000 0.12946 0.12940 2.81064

D9 -2.76892 -0.00904 0.00000 -0.19352 -0.19435 -2.96327

D10 -0.06185 -0.00095 0.00000 -0.03072 -0.03162 -0.09347

D11 2.83735 -0.00729 0.00000 -0.12314 -0.12381 2.71354

D12 -1.42554 -0.00804 0.00000 -0.13662 -0.13699 -1.56254

D13 0.68713 -0.01001 0.00000 -0.15705 -0.15740 0.52972

D14 -0.62598 0.00299 0.00000 0.03008 0.03035 -0.59563

D15 1.39431 0.00225 0.00000 0.01660 0.01717 1.41148

D16 -2.77621 0.00028 0.00000 -0.00383 -0.00324 -2.77945

D17 1.23672 0.00377 0.00000 0.05169 0.05192 1.28865

D18 -3.02617 0.00302 0.00000 0.03820 0.03874 -2.98743

D19 -0.91350 0.00105 0.00000 0.01778 0.01833 -0.89517

D20 -0.97517 -0.00244 0.00000 -0.04864 -0.04763 -1.02280

D21 -2.81313 -0.00488 0.00000 -0.07724 -0.07399 -2.88712

D22 1.15995 -0.00108 0.00000 0.00250 0.00016 1.16011

D23 1.05599 0.00094 0.00000 0.01273 0.01486 1.07085

D24 -0.78196 -0.00150 0.00000 -0.01586 -0.01150 -0.79347

D25 -3.09208 0.00230 0.00000 0.06388 0.06265 -3.02942

D26 3.11452 0.00115 0.00000 0.00319 0.00352 3.11804

D27 1.27656 -0.00128 0.00000 -0.02540 -0.02284 1.25372

D28 -1.03355 0.00251 0.00000 0.05434 0.05131 -0.98223

D29 0.75147 -0.00453 0.00000 -0.09764 -0.09784 0.65362

D30 -1.95176 -0.01225 0.00000 -0.26024 -0.26090 -2.21266

D31 2.95864 -0.00291 0.00000 -0.05814 -0.05797 2.90067

D32 0.25541 -0.01062 0.00000 -0.22074 -0.22102 0.03439

D33 -1.47313 -0.00405 0.00000 -0.09887 -0.09926 -1.57238

D34 2.10683 -0.01177 0.00000 -0.26147 -0.26231 1.84452

D35 -0.72151 0.00385 0.00000 0.08902 0.08973 -0.63178

D36 -2.87756 0.00371 0.00000 0.07148 0.07181 -2.80574

D37 1.37376 0.00403 0.00000 0.08553 0.08554 1.45929

D38 -2.91513 0.00188 0.00000 0.03360 0.03422 -2.88090

D39 1.21201 0.00174 0.00000 0.01606 0.01631 1.22832

D40 -0.81986 0.00207 0.00000 0.03011 0.03003 -0.78983

D41 1.65484 -0.00393 0.00000 -0.00118 -0.00054 1.65431

D42 -0.50121 -0.00407 0.00000 -0.01872 -0.01845 -0.51966

D43 -2.53308 -0.00375 0.00000 -0.00467 -0.00473 -2.53781

D44 0.96622 0.00382 0.00000 0.07121 0.06783 1.03405

D45 3.12510 -0.00015 0.00000 0.01199 0.00986 3.13496

D46 -1.15849 0.00068 0.00000 0.03505 0.03291 -1.12558

D47 -1.29035 0.00467 0.00000 0.06207 0.06067 -1.22969

D48 0.86853 0.00070 0.00000 0.00285 0.00270 0.87122

D49 2.86812 0.00153 0.00000 0.02590 0.02575 2.89387

D50 3.00047 0.00322 0.00000 0.06043 0.05907 3.05954

D51 -1.12383 -0.00076 0.00000 0.00122 0.00111 -1.12273

D52 0.87576 0.00008 0.00000 0.02427 0.02416 0.89992

D53 0.05983 0.00220 0.00000 0.01684 0.01672 0.07655

D54 2.22413 0.00265 0.00000 0.03524 0.03524 2.25937

D55 -2.02841 0.00226 0.00000 0.02900 0.02924 -1.99917

D56 -2.09767 -0.00054 0.00000 -0.01538 -0.01536 -2.11303

D57 0.06663 -0.00009 0.00000 0.00302 0.00317 0.06979

D58 2.09727 -0.00048 0.00000 -0.00321 -0.00283 2.09444

D59 2.14109 -0.00040 0.00000 -0.00745 -0.00775 2.13335

D60 -1.97779 0.00005 0.00000 0.01095 0.01077 -1.96702

D61 0.05286 -0.00034 0.00000 0.00472 0.00478 0.05763

D62 0.05472 0.00054 0.00000 0.00652 0.00714 0.06186

D63 -3.06720 0.00093 0.00000 0.01862 0.01951 -3.04769

D64 0.01163 -0.00245 0.00000 -0.03821 -0.03862 -0.02699

D65 3.09031 0.00036 0.00000 0.00147 0.00001 3.09031

D66 0.08241 -0.00273 0.00000 -0.03738 -0.03922 0.04318

D67 2.28883 -0.00757 0.00000 -0.12062 -0.12098 2.16786

D68 -1.44358 -0.00010 0.00000 0.03209 0.03288 -1.41069

D69 -2.10307 0.00184 0.00000 0.03512 0.03280 -2.07027

D70 0.10335 -0.00300 0.00000 -0.04811 -0.04895 0.05440

D71 2.65412 0.00447 0.00000 0.10459 0.10491 2.75903

D72 2.06900 0.00100 0.00000 -0.01120 -0.01351 2.05549

D73 -2.00776 -0.00384 0.00000 -0.09443 -0.09526 -2.10303

D74 0.54301 0.00363 0.00000 0.05827 0.05860 0.60161

D75 -2.44143 0.00259 0.00000 0.08118 0.08228 -2.35915

D76 0.67641 0.00209 0.00000 0.06655 0.06731 0.74373

D77 -0.10012 0.00163 0.00000 0.02593 0.02647 -0.07365

D78 3.01772 0.00114 0.00000 0.01131 0.01150 3.02923

D79 2.02504 0.00238 0.00000 0.07411 0.07421 2.09925

D80 -1.14030 0.00189 0.00000 0.05948 0.05925 -1.08106

D81 1.53444 0.00403 0.00000 0.06724 0.06555 1.59999

D82 -1.52530 0.00072 0.00000 0.01740 0.01602 -1.50927

D83 -0.07595 0.00341 0.00000 0.05455 0.05567 -0.02027

D84 -3.13568 0.00010 0.00000 0.00471 0.00615 -3.12953

D85 -2.63864 -0.00363 0.00000 -0.09675 -0.09822 -2.73686

D86 0.58481 -0.00694 0.00000 -0.14659 -0.14775 0.43707

Item Value Threshold Converged?

Maximum Force 0.023266 0.000450 NO

RMS Force 0.004335 0.000300 NO

Maximum Displacement 0.585039 0.001800 NO

RMS Displacement 0.088007 0.001200 NO

Predicted change in Energy=-3.767417D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.426869 1.312795 0.164319

2 6 0 -0.246886 0.832540 -0.390114

3 6 0 -0.479065 3.574070 0.031071

4 6 0 -1.548410 2.701992 0.339777

5 1 0 -2.322707 0.681731 0.250325

6 1 0 -2.560662 3.118008 0.469489

7 6 0 0.468878 1.654997 -1.381084

8 1 0 1.560277 1.386872 -1.403634

9 1 0 0.040124 1.357705 -2.382175

10 6 0 0.305899 3.158996 -1.198936

11 1 0 1.315179 3.648481 -1.204016

12 1 0 -0.254627 3.561064 -2.088034

13 1 0 -0.802745 4.651503 -0.014397

14 1 0 0.095425 -0.202637 -0.245493

15 8 0 2.948621 4.433975 1.163715

16 6 0 0.632195 3.907585 1.332584

17 6 0 1.366505 2.879295 1.986166

18 6 0 1.686114 4.845894 0.770123

19 8 0 1.618696 5.826193 0.040606

20 6 0 2.802754 3.214150 1.896248

21 8 0 3.859130 2.712512 2.254596

22 1 0 -0.102679 4.434038 1.995634

23 1 0 0.968452 2.241247 2.767685

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.389388 0.000000

3 C 2.455494 2.783395 0.000000

4 C 1.405498 2.391977 1.413972 0.000000

5 H 1.099166 2.177599 3.436962 2.165408 0.000000

6 H 2.153465 3.363903 2.175603 1.102066 2.457662

7 C 2.469662 1.473356 2.564297 2.850791 3.376639

8 H 3.374463 2.144841 3.316795 3.799072 4.279061

9 H 2.939169 2.080019 3.317467 3.426305 3.601384

10 C 2.875657 2.524314 1.517027 2.452539 3.891884

11 H 3.853128 3.321447 2.179516 3.388108 4.914359

12 H 3.391453 3.213695 2.130997 2.882038 4.246814

13 H 3.401241 3.877451 1.125922 2.117085 4.259044

14 H 2.186746 1.099856 3.830149 3.388451 2.622081

15 O 5.466760 5.059248 3.710977 4.888959 6.534563

16 C 3.512481 3.632681 1.743579 2.682193 4.506535

17 C 3.684560 3.526889 2.776912 3.352426 4.631708

18 C 4.747678 4.603222 2.617582 3.904313 5.803541

19 O 5.446240 5.348129 3.077783 4.458777 6.484144

20 C 4.950196 4.494421 3.791934 4.649466 5.949165

21 O 5.854079 5.233369 4.950382 5.736561 6.808545

22 H 3.853486 4.322428 2.177319 2.798569 4.696215

23 H 3.657472 3.665133 3.370575 3.527267 4.427293

6 7 8 9 10

6 H 0.000000

7 C 3.839679 0.000000

8 H 4.846396 1.124078 0.000000

9 H 4.242021 1.128890 1.808109 0.000000

10 C 3.317000 1.523730 2.180777 2.171483 0.000000

11 H 4.254899 2.172914 2.283592 2.874278 1.121725

12 H 3.472034 2.157852 2.913656 2.242362 1.125319

13 H 2.382441 3.530426 4.262824 4.143176 2.204496

14 H 4.311923 2.209036 2.452269 2.646344 3.500562

15 O 5.706655 4.510859 4.219433 5.522330 3.767183

16 C 3.400397 3.530555 3.834347 4.544433 2.659971

17 C 4.216626 3.693645 3.708856 4.812164 3.368678

18 C 4.594679 4.036233 4.087283 4.981338 2.937314

19 O 4.998523 4.554356 4.668705 5.322512 3.220844

20 C 5.550776 4.314956 3.971386 5.420647 3.977121

21 O 6.675684 5.082354 4.519368 6.157917 4.975106

22 H 3.178480 4.410439 4.858566 5.352516 3.463805

23 H 4.301751 4.219662 4.298850 5.306929 4.124963

11 12 13 14 15

11 H 0.000000

12 H 1.803724 0.000000

13 H 2.628088 2.406130 0.000000

14 H 4.151828 4.205109 4.941943 0.000000

15 O 2.981826 4.647219 3.938021 5.623590 0.000000

16 C 2.639686 3.550656 2.104002 4.435355 2.381477

17 C 3.282003 4.437565 3.442182 4.011764 2.365702

18 C 2.338507 3.685963 2.616806 5.389753 1.385105

19 O 2.526586 3.629223 2.691894 6.224869 2.228978

20 C 3.466001 5.034127 4.326219 4.857069 1.430334

21 O 4.394283 6.041645 5.535440 5.377175 2.232148

22 H 3.586807 4.178698 2.139534 5.153703 3.162676

23 H 4.227876 5.178401 4.084905 3.976680 3.361821

16 17 18 19 20

16 C 0.000000

17 C 1.422589 0.000000

18 C 1.519056 2.334186 0.000000

19 O 2.514647 3.540199 1.223816 0.000000

20 C 2.347317 1.477506 2.275441 3.415870 0.000000

21 O 3.562501 2.512578 3.387769 4.429030 1.223104

22 H 1.121084 2.139116 2.207098 2.953533 3.152705

23 H 2.224694 1.084584 3.359981 4.551001 2.251801

21 22 23

21 O 0.000000

22 H 4.327430 0.000000

23 H 2.973444 2.559632 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.838539 -0.697696 -0.711026

2 6 0 2.387081 -1.294278 0.459732

3 6 0 1.083478 0.997046 -0.433433

4 6 0 2.196863 0.478946 -1.134334

5 1 0 3.796032 -0.980617 -1.170731

6 1 0 2.726917 1.124410 -1.853340

7 6 0 1.856107 -0.445609 1.540753

8 1 0 1.149532 -1.029514 2.191413

9 1 0 2.748067 -0.184620 2.181600

10 6 0 1.188941 0.841572 1.071917

11 1 0 0.177384 0.934027 1.547807

12 1 0 1.802540 1.709311 1.441875

13 1 0 0.839120 2.053694 -0.735896

14 1 0 2.555415 -2.357817 0.683857

15 8 0 -2.450374 0.183569 0.354916

16 6 0 -0.479100 0.429029 -0.958575

17 6 0 -0.830017 -0.949522 -0.943966

18 6 0 -1.505989 1.105067 -0.066385

19 8 0 -1.616046 2.250504 0.350254

20 6 0 -2.062489 -1.099940 -0.143083

21 8 0 -2.789988 -2.017791 0.209449

22 1 0 -0.439238 0.877783 -1.985152

23 1 0 -0.544986 -1.664602 -1.707995

---------------------------------------------------------------------

Rotational constants (GHZ): 1.3191936 0.6239262 0.5326236

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 453.3925129525 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = 0.282031660754E-02 A.U. after 16 cycles

Convg = 0.2603D-08 -V/T = 1.0001

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.015584068 0.003843627 -0.016226214

2 6 -0.018827888 0.000312323 0.004543882

3 6 0.020070403 0.014923399 0.006361348

4 6 -0.008652781 -0.007759248 -0.016062708

5 1 0.005118057 -0.005396631 0.015511212

6 1 0.001780112 0.001453765 0.015476577

7 6 0.009157071 0.005463952 0.008582623

8 1 -0.000052625 0.000587215 0.000299372

9 1 0.001253300 -0.000703940 -0.000859521

10 6 0.000777316 -0.003617647 0.001666238

11 1 -0.000027227 -0.000487647 -0.000126301

12 1 0.000462948 0.000875501 0.000170376

13 1 -0.002275992 -0.000619578 -0.009297850

14 1 -0.002975900 -0.001179186 -0.001934873

15 8 0.000100109 -0.003901263 0.001838124

16 6 -0.017785274 -0.001280838 0.002319113

17 6 0.015168149 0.014522767 0.003226472

18 6 -0.000253241 0.000386506 -0.004359434

19 8 -0.000597184 0.001322582 0.002705307

20 6 -0.014737564 -0.013413646 -0.008186606

21 8 -0.003768912 0.002285106 0.001123384

22 1 -0.000939212 -0.000162996 -0.001491397

23 1 0.001422267 -0.007454124 -0.005279125

-------------------------------------------------------------------

Cartesian Forces: Max 0.020070403 RMS 0.007807198

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.019266543 RMS 0.003556277

Search for a saddle point.

Step number 14 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 13 14

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.05440 0.00178 0.00249 0.00353 0.00585

Eigenvalues --- 0.00797 0.00932 0.01199 0.01529 0.01804

Eigenvalues --- 0.01954 0.02086 0.02234 0.02425 0.02542

Eigenvalues --- 0.02687 0.02920 0.03055 0.03122 0.03339

Eigenvalues --- 0.03636 0.03665 0.03813 0.03884 0.04292

Eigenvalues --- 0.04541 0.05197 0.05422 0.05675 0.05966

Eigenvalues --- 0.06095 0.07339 0.08078 0.08579 0.09789

Eigenvalues --- 0.11550 0.13252 0.14060 0.15249 0.18600

Eigenvalues --- 0.20496 0.22787 0.24446 0.25385 0.26722

Eigenvalues --- 0.27828 0.29074 0.30730 0.31181 0.31542

Eigenvalues --- 0.31934 0.32218 0.32634 0.33679 0.34398

Eigenvalues --- 0.35649 0.37375 0.39581 0.40386 0.43094

Eigenvalues --- 0.45197 1.08281 1.10816

Eigenvectors required to have negative eigenvalues:

R6 R10 A14 A8 D41

1 0.68716 0.56351 -0.11246 -0.10036 0.09953

R22 A15 D68 A34 A12

1 0.09425 -0.09359 0.09085 -0.09009 0.08653

RFO step: Lambda0=4.198034985D-03 Lambda=-2.97529431D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.915

Iteration 1 RMS(Cart)= 0.06886468 RMS(Int)= 0.00612437

Iteration 2 RMS(Cart)= 0.00629349 RMS(Int)= 0.00153664

Iteration 3 RMS(Cart)= 0.00005694 RMS(Int)= 0.00153535

Iteration 4 RMS(Cart)= 0.00000005 RMS(Int)= 0.00153535

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62556 -0.01521 0.00000 -0.07890 -0.07853 2.54703

R2 2.65601 0.00135 0.00000 0.01739 0.01986 2.67586

R3 2.07712 0.00014 0.00000 0.00262 0.00262 2.07974

R4 2.78424 0.00425 0.00000 0.02304 0.02299 2.80723

R5 2.07843 -0.00007 0.00000 0.00381 0.00381 2.08224

R6 6.66485 -0.01048 0.00000 0.08078 0.07841 6.74326

R7 2.67202 0.00706 0.00000 0.00729 0.00952 2.68154

R8 2.86677 -0.00099 0.00000 -0.02320 -0.02341 2.84336

R9 2.12768 0.00044 0.00000 -0.00533 -0.00533 2.12235

R10 3.29489 -0.01106 0.00000 0.14301 0.14476 3.43965

R11 2.08260 0.00074 0.00000 -0.00390 -0.00390 2.07870

R12 2.12420 -0.00020 0.00000 -0.00160 -0.00160 2.12260

R13 2.13329 0.00047 0.00000 0.00246 0.00246 2.13576

R14 2.87943 0.00069 0.00000 -0.00232 -0.00260 2.87683

R15 2.11975 -0.00024 0.00000 0.00049 0.00049 2.12024

R16 2.12655 -0.00005 0.00000 0.00357 0.00357 2.13012

R17 2.61747 -0.00021 0.00000 0.01025 0.01072 2.62819

R18 2.70294 -0.00176 0.00000 -0.00170 -0.00188 2.70106

R19 2.68830 0.00274 0.00000 -0.04214 -0.04309 2.64521

R20 2.87060 -0.00138 0.00000 -0.00087 -0.00042 2.87018

R21 2.11854 -0.00034 0.00000 -0.01127 -0.01127 2.10727

R22 2.79208 -0.01927 0.00000 -0.05290 -0.05346 2.73863

R23 2.04957 0.00006 0.00000 -0.00039 -0.00039 2.04917

R24 2.31268 -0.00052 0.00000 -0.00225 -0.00225 2.31043

R25 2.31133 -0.00386 0.00000 -0.00126 -0.00126 2.31008

A1 2.05433 0.00380 0.00000 0.03051 0.02775 2.08207

A2 2.12345 -0.00232 0.00000 -0.00493 -0.00763 2.11582

A3 2.07970 -0.00045 0.00000 0.00271 0.00024 2.07994

A4 2.08063 0.00250 0.00000 0.03590 0.03100 2.11163

A5 2.13789 -0.00179 0.00000 -0.00291 -0.00209 2.13580

A6 1.48976 -0.00362 0.00000 -0.07163 -0.07070 1.41906

A7 2.05176 0.00007 0.00000 -0.01794 -0.01827 2.03349

A8 1.47764 -0.00063 0.00000 -0.04178 -0.03950 1.43815

A9 1.89150 0.00045 0.00000 0.03540 0.03460 1.92609

A10 1.98186 0.00076 0.00000 0.03366 0.03015 2.01201

A11 1.96232 0.00181 0.00000 0.03660 0.03677 1.99910

A12 2.02307 -0.00669 0.00000 -0.08095 -0.07965 1.94342

A13 1.95825 -0.00142 0.00000 -0.00352 -0.00414 1.95411

A14 1.90475 0.00301 0.00000 -0.00741 -0.00635 1.89840

A15 1.60112 0.00271 0.00000 0.01478 0.01471 1.61584

A16 2.11408 -0.00193 0.00000 0.00323 0.00170 2.11578

A17 2.05695 0.00133 0.00000 0.01972 0.01526 2.07222

A18 2.08004 0.00190 0.00000 0.01314 0.00893 2.08896

A19 1.93053 0.00022 0.00000 -0.00715 -0.00735 1.92317

A20 1.83893 -0.00061 0.00000 -0.00124 -0.00044 1.83849

A21 2.00273 0.00119 0.00000 0.01614 0.01495 2.01768

A22 1.86310 -0.00013 0.00000 -0.00502 -0.00517 1.85792

A23 1.91951 0.00017 0.00000 0.01092 0.01162 1.93113

A24 1.90215 -0.00100 0.00000 -0.01611 -0.01612 1.88603

A25 2.00682 -0.00113 0.00000 0.01004 0.00871 2.01553

A26 1.92820 -0.00014 0.00000 0.00305 0.00373 1.93193

A27 1.85991 0.00082 0.00000 -0.01139 -0.01141 1.84850

A28 1.91127 0.00121 0.00000 0.00712 0.00731 1.91858

A29 1.88756 -0.00038 0.00000 -0.00499 -0.00448 1.88308

A30 1.86365 -0.00037 0.00000 -0.00581 -0.00597 1.85767

A31 1.88199 0.00015 0.00000 -0.00612 -0.00643 1.87556

A32 2.13373 -0.00051 0.00000 -0.04283 -0.04389 2.08983

A33 1.85871 -0.00193 0.00000 -0.02833 -0.02833 1.83038

A34 1.68457 0.00187 0.00000 -0.00791 -0.00687 1.67770

A35 1.83224 -0.00050 0.00000 0.00124 -0.00062 1.83162

A36 1.98894 0.00063 0.00000 0.05080 0.05038 2.03932

A37 1.96461 0.00048 0.00000 0.02717 0.02610 1.99071

A38 1.44426 0.00125 0.00000 0.04266 0.04261 1.48688

A39 2.13554 -0.00225 0.00000 -0.08651 -0.08764 2.04790

A40 1.54700 -0.00284 0.00000 -0.07574 -0.07729 1.46970

A41 1.88597 0.00125 0.00000 0.02085 0.02252 1.90850

A42 2.17346 0.00118 0.00000 0.03520 0.03283 2.20630

A43 2.13405 -0.00030 0.00000 0.00785 -0.00295 2.13110

A44 1.92141 -0.00402 0.00000 -0.01387 -0.01356 1.90785

A45 2.04633 0.00238 0.00000 0.00843 0.00822 2.05455

A46 2.31486 0.00162 0.00000 0.00492 0.00470 2.31956

A47 1.90031 0.00322 0.00000 0.00017 -0.00119 1.89912

A48 1.99516 -0.00091 0.00000 0.00495 0.00532 2.00048

A49 2.38734 -0.00226 0.00000 -0.00415 -0.00379 2.38355

D1 -0.56502 0.00638 0.00000 0.14802 0.14896 -0.41606

D2 2.75279 0.00110 0.00000 0.04780 0.04766 2.80045

D3 0.85285 0.00313 0.00000 0.05218 0.05137 0.90421

D4 2.33279 0.01116 0.00000 0.28044 0.28085 2.61364

D5 -0.63258 0.00588 0.00000 0.18022 0.17955 -0.45303

D6 -2.53253 0.00791 0.00000 0.18460 0.18326 -2.34927

D7 -0.05915 -0.00142 0.00000 -0.03419 -0.03506 -0.09421

D8 2.81064 0.00427 0.00000 0.11742 0.11670 2.92734

D9 -2.96327 -0.00579 0.00000 -0.16194 -0.16297 -3.12623

D10 -0.09347 -0.00009 0.00000 -0.01034 -0.01121 -0.10468

D11 2.71354 -0.00381 0.00000 -0.10028 -0.10127 2.61226

D12 -1.56254 -0.00418 0.00000 -0.11025 -0.11103 -1.67357

D13 0.52972 -0.00516 0.00000 -0.12178 -0.12278 0.40695

D14 -0.59563 0.00101 0.00000 -0.00380 -0.00441 -0.60004

D15 1.41148 0.00063 0.00000 -0.01377 -0.01417 1.39732

D16 -2.77945 -0.00034 0.00000 -0.02531 -0.02591 -2.80536

D17 1.28865 0.00120 0.00000 0.01328 0.01379 1.30244

D18 -2.98743 0.00082 0.00000 0.00331 0.00404 -2.98339

D19 -0.89517 -0.00015 0.00000 -0.00823 -0.00771 -0.90288

D20 -1.02280 -0.00238 0.00000 -0.02452 -0.02404 -1.04684

D21 -2.88712 -0.00451 0.00000 -0.07076 -0.06767 -2.95479

D22 1.16011 -0.00084 0.00000 0.01920 0.01646 1.17657

D23 1.07085 0.00080 0.00000 0.02917 0.03051 1.10136

D24 -0.79347 -0.00132 0.00000 -0.01707 -0.01312 -0.80659

D25 -3.02942 0.00235 0.00000 0.07288 0.07101 -2.95841

D26 3.11804 0.00070 0.00000 -0.00103 -0.00050 3.11754

D27 1.25372 -0.00143 0.00000 -0.04727 -0.04413 1.20960

D28 -0.98223 0.00224 0.00000 0.04268 0.04000 -0.94223

D29 0.65362 -0.00282 0.00000 -0.08353 -0.08471 0.56892

D30 -2.21266 -0.00849 0.00000 -0.23806 -0.23885 -2.45150

D31 2.90067 -0.00253 0.00000 -0.02628 -0.02635 2.87432

D32 0.03439 -0.00820 0.00000 -0.18082 -0.18049 -0.14610

D33 -1.57238 -0.00172 0.00000 -0.03000 -0.03196 -1.60434

D34 1.84452 -0.00739 0.00000 -0.18454 -0.18610 1.65842

D35 -0.63178 0.00420 0.00000 0.10183 0.10169 -0.53009

D36 -2.80574 0.00356 0.00000 0.08195 0.08173 -2.72401

D37 1.45929 0.00361 0.00000 0.09361 0.09323 1.55252

D38 -2.88090 0.00226 0.00000 0.02430 0.02446 -2.85645

D39 1.22832 0.00163 0.00000 0.00442 0.00450 1.23282

D40 -0.78983 0.00167 0.00000 0.01608 0.01600 -0.77384

D41 1.65431 -0.00172 0.00000 0.01217 0.01218 1.66649

D42 -0.51966 -0.00235 0.00000 -0.00771 -0.00777 -0.52743

D43 -2.53781 -0.00231 0.00000 0.00395 0.00372 -2.53409

D44 1.03405 0.00090 0.00000 0.02404 0.02357 1.05762

D45 3.13496 -0.00191 0.00000 -0.03042 -0.02967 3.10529

D46 -1.12558 -0.00120 0.00000 -0.01186 -0.01169 -1.13727

D47 -1.22969 0.00278 0.00000 0.05281 0.05146 -1.17823

D48 0.87122 -0.00003 0.00000 -0.00164 -0.00178 0.86944

D49 2.89387 0.00068 0.00000 0.01692 0.01620 2.91007

D50 3.05954 0.00266 0.00000 0.05217 0.05137 3.11092

D51 -1.12273 -0.00015 0.00000 -0.00228 -0.00187 -1.12460

D52 0.89992 0.00056 0.00000 0.01628 0.01611 0.91602

D53 0.07655 0.00132 0.00000 0.00092 0.00019 0.07674

D54 2.25937 0.00126 0.00000 0.01846 0.01812 2.27748

D55 -1.99917 0.00126 0.00000 0.01261 0.01243 -1.98674

D56 -2.11303 -0.00004 0.00000 -0.01097 -0.01151 -2.12454

D57 0.06979 -0.00011 0.00000 0.00657 0.00641 0.07620

D58 2.09444 -0.00010 0.00000 0.00072 0.00073 2.09517

D59 2.13335 0.00060 0.00000 -0.00177 -0.00242 2.13093

D60 -1.96702 0.00053 0.00000 0.01577 0.01551 -1.95151

D61 0.05763 0.00054 0.00000 0.00992 0.00982 0.06746

D62 0.06186 0.00002 0.00000 -0.00054 -0.00030 0.06157

D63 -3.04769 0.00051 0.00000 0.01385 0.01393 -3.03376

D64 -0.02699 -0.00147 0.00000 -0.03163 -0.03173 -0.05872

D65 3.09031 0.00019 0.00000 0.00017 -0.00002 3.09030

D66 0.04318 -0.00356 0.00000 -0.03942 -0.03906 0.00412

D67 2.16786 -0.00549 0.00000 -0.11644 -0.11620 2.05165

D68 -1.41069 -0.00070 0.00000 0.03103 0.03304 -1.37766

D69 -2.07027 -0.00011 0.00000 0.02796 0.02737 -2.04290

D70 0.05440 -0.00204 0.00000 -0.04906 -0.04977 0.00463

D71 2.75903 0.00276 0.00000 0.09841 0.09947 2.85850

D72 2.05549 -0.00074 0.00000 -0.03837 -0.03954 2.01595

D73 -2.10303 -0.00267 0.00000 -0.11539 -0.11668 -2.21971

D74 0.60161 0.00213 0.00000 0.03208 0.03256 0.63416

D75 -2.35915 0.00359 0.00000 0.10068 0.10063 -2.25852

D76 0.74373 0.00299 0.00000 0.08328 0.08343 0.82716

D77 -0.07365 0.00148 0.00000 0.03238 0.03204 -0.04160

D78 3.02923 0.00087 0.00000 0.01498 0.01485 3.04407

D79 2.09925 0.00221 0.00000 0.11295 0.11280 2.21205

D80 -1.08106 0.00160 0.00000 0.09555 0.09560 -0.98546

D81 1.59999 0.00383 0.00000 0.08754 0.08507 1.68506

D82 -1.50927 0.00154 0.00000 0.04498 0.04293 -1.46635

D83 -0.02027 0.00228 0.00000 0.05217 0.05293 0.03266

D84 -3.12953 0.00000 0.00000 0.00962 0.01079 -3.11875

D85 -2.73686 -0.00282 0.00000 -0.09944 -0.09911 -2.83596

D86 0.43707 -0.00510 0.00000 -0.14200 -0.14125 0.29581

Item Value Threshold Converged?

Maximum Force 0.019267 0.000450 NO

RMS Force 0.003556 0.000300 NO

Maximum Displacement 0.410689 0.001800 NO

RMS Displacement 0.072487 0.001200 NO

Predicted change in Energy=-2.135382D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.379090 1.305544 0.182164

2 6 0 -0.276153 0.824281 -0.424929

3 6 0 -0.496791 3.602341 -0.037445

4 6 0 -1.531469 2.705111 0.334046

5 1 0 -2.208978 0.641465 0.467652

6 1 0 -2.511524 3.100189 0.639669

7 6 0 0.500614 1.661194 -1.375180

8 1 0 1.585544 1.371513 -1.349478

9 1 0 0.118766 1.381071 -2.401368

10 6 0 0.342728 3.166014 -1.207388

11 1 0 1.351953 3.655191 -1.175485

12 1 0 -0.175904 3.564329 -2.125520

13 1 0 -0.819296 4.674285 -0.128444

14 1 0 0.057463 -0.218638 -0.301872

15 8 0 2.925818 4.394023 1.141832

16 6 0 0.601159 3.966115 1.367990

17 6 0 1.308074 2.926793 1.984012

18 6 0 1.669819 4.884095 0.800420

19 8 0 1.621083 5.883344 0.097608

20 6 0 2.730695 3.157930 1.832497

21 8 0 3.762064 2.581407 2.145961

22 1 0 -0.165836 4.488916 1.985961

23 1 0 0.912860 2.216495 2.701756

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.347830 0.000000

3 C 2.470214 2.813618 0.000000

4 C 1.416006 2.385242 1.419008 0.000000

5 H 1.100554 2.136805 3.457382 2.176121 0.000000

6 H 2.170822 3.363036 2.183984 1.100000 2.483233

7 C 2.466799 1.485520 2.559767 2.853170 3.431875

8 H 3.337565 2.149459 3.321769 3.785301 4.270051

9 H 2.987293 2.091002 3.301679 3.458156 3.767849

10 C 2.890824 2.545382 1.504640 2.470033 3.961100

11 H 3.850019 3.350838 2.171585 3.390495 4.945975

12 H 3.446037 3.226441 2.112930 2.936882 4.404664

13 H 3.429032 3.899415 1.123100 2.144466 4.306992

14 H 2.149676 1.101873 3.870013 3.387832 2.543364

15 O 5.384412 5.044841 3.705632 4.834495 6.395493

16 C 3.522245 3.722279 1.820185 2.684636 4.445309

17 C 3.618833 3.568379 2.792883 3.291585 4.460014

18 C 4.741742 4.665874 2.653133 3.900477 5.758100

19 O 5.473978 5.428321 3.115542 4.482817 6.502583

20 C 4.800549 4.425272 3.756442 4.540533 5.709271

21 O 5.649406 5.099428 4.893609 5.596411 6.498725

22 H 3.854806 4.387951 2.233768 2.788501 4.613304

23 H 3.525793 3.623282 3.378004 3.437956 4.149436

6 7 8 9 10

6 H 0.000000

7 C 3.899141 0.000000

8 H 4.871447 1.123231 0.000000

9 H 4.372836 1.130194 1.804994 0.000000

10 C 3.400398 1.522355 2.187468 2.159113 0.000000

11 H 4.304563 2.177310 2.302178 2.862719 1.121984

12 H 3.649221 2.154671 2.917770 2.220256 1.127208

13 H 2.435448 3.517845 4.264092 4.109915 2.188447

14 H 4.301256 2.209557 2.441535 2.640211 3.515282

15 O 5.611672 4.436814 4.139870 5.432466 3.701242

16 C 3.311959 3.584376 3.884020 4.596000 2.709155

17 C 4.052981 3.679389 3.688908 4.799507 3.342777

18 C 4.548823 4.060464 4.119150 4.992834 2.957071

19 O 5.011808 4.609892 4.738348 5.363981 3.274307

20 C 5.376526 4.183620 3.824608 5.282521 3.865664

21 O 6.472708 4.886950 4.291756 5.949170 4.824787

22 H 3.040283 4.442684 4.889856 5.384084 3.493736

23 H 4.093840 4.135180 4.192732 5.231673 4.063010

11 12 13 14 15

11 H 0.000000

12 H 1.801435 0.000000

13 H 2.617092 2.373662 0.000000

14 H 4.176776 4.206066 4.973880 0.000000

15 O 2.897047 4.580901 3.964597 5.620354 0.000000

16 C 2.670137 3.601371 2.181401 4.538304 2.374509

17 C 3.242670 4.415529 3.470145 4.084486 2.340754

18 C 2.348498 3.702648 2.665052 5.463756 1.390779

19 O 2.580283 3.680936 2.732832 6.311789 2.238485

20 C 3.346066 4.927411 4.329788 4.806550 1.429341

21 O 4.241892 5.892306 5.526473 5.249400 2.234537

22 H 3.604653 4.214172 2.220829 5.238808 3.206225

23 H 4.158803 5.128807 4.129301 3.960222 3.350670

16 17 18 19 20

16 C 0.000000

17 C 1.399787 0.000000

18 C 1.518835 2.315769 0.000000

19 O 2.515926 3.521036 1.222627 0.000000

20 C 2.324619 1.449218 2.273827 3.415986 0.000000

21 O 3.537510 2.483462 3.389740 4.436478 1.222440

22 H 1.115119 2.147706 2.220654 2.950150 3.191389

23 H 2.221995 1.084377 3.362166 4.552906 2.224058

21 22 23

21 O 0.000000

22 H 4.369506 0.000000

23 H 2.925753 2.615310 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.799488 -0.627978 -0.730523

2 6 0 2.447864 -1.234773 0.420479

3 6 0 1.066158 1.091007 -0.352878

4 6 0 2.152567 0.574489 -1.105546

5 1 0 3.648145 -0.990187 -1.330360

6 1 0 2.577035 1.168984 -1.927984

7 6 0 1.825247 -0.468039 1.530090

8 1 0 1.132397 -1.129110 2.117110

9 1 0 2.676782 -0.200913 2.223538

10 6 0 1.123299 0.821048 1.126243

11 1 0 0.095561 0.853640 1.575173

12 1 0 1.695132 1.682217 1.575679

13 1 0 0.812484 2.162334 -0.574830

14 1 0 2.665405 -2.296760 0.617919

15 8 0 -2.423265 0.076821 0.373113

16 6 0 -0.528631 0.494236 -0.995982

17 6 0 -0.799358 -0.878982 -1.015590

18 6 0 -1.571094 1.085687 -0.063075

19 8 0 -1.746729 2.210604 0.382496

20 6 0 -1.938059 -1.156104 -0.163066

21 8 0 -2.564179 -2.145576 0.188043

22 1 0 -0.458468 1.007802 -1.983310

23 1 0 -0.435978 -1.596352 -1.743057

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2870807 0.6412620 0.5435664

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 454.1162776495 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.159141880023E-01 A.U. after 15 cycles

Convg = 0.5972D-08 -V/T = 0.9997

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.012840590 0.007453224 0.001969082

2 6 0.017700055 -0.003646848 -0.011161650

3 6 -0.014763658 -0.007145225 -0.001500808

4 6 0.007968739 0.015239822 -0.012902567

5 1 0.003311885 -0.001010384 0.010632597

6 1 0.002562327 0.000679854 0.010000765

7 6 0.002674195 -0.001238302 0.005904191

8 1 -0.000110881 0.001424251 0.001194428

9 1 0.001705261 -0.001106466 0.000148080

10 6 0.002119640 -0.004220909 0.000816301

11 1 0.000397501 -0.001106432 -0.000044999

12 1 0.000926587 0.000705593 -0.000280321

13 1 0.000237708 -0.002292431 -0.002364822

14 1 -0.003287989 -0.001307791 -0.004187001

15 8 0.000003999 -0.000094745 -0.001616292

16 6 -0.008271109 0.010812147 0.012155138

17 6 -0.005183043 -0.001672354 0.008534858

18 6 0.000240748 -0.000578561 -0.006639621

19 8 0.000384459 0.000746473 0.003907602

20 6 0.009239295 -0.005609954 -0.006527518

21 8 -0.000567301 0.001680102 0.000484747

22 1 -0.003423214 -0.001684246 -0.004968589

23 1 -0.001024614 -0.006026818 -0.003553601

-------------------------------------------------------------------

Cartesian Forces: Max 0.017700055 RMS 0.006030947

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.017317149 RMS 0.002989158

Search for a saddle point.

Step number 15 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 14 15

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.05769 -0.00182 0.00184 0.00342 0.00584

Eigenvalues --- 0.00743 0.00879 0.01303 0.01531 0.01695

Eigenvalues --- 0.01941 0.02066 0.02282 0.02400 0.02520

Eigenvalues --- 0.02597 0.02693 0.02944 0.03078 0.03236

Eigenvalues --- 0.03613 0.03631 0.03810 0.03846 0.04296

Eigenvalues --- 0.04477 0.04903 0.05206 0.05474 0.05929

Eigenvalues --- 0.06051 0.07330 0.07965 0.08563 0.09707

Eigenvalues --- 0.11311 0.13116 0.13875 0.15090 0.18565

Eigenvalues --- 0.20420 0.22748 0.24403 0.25315 0.27046

Eigenvalues --- 0.27716 0.29332 0.30671 0.31169 0.31556

Eigenvalues --- 0.31934 0.32213 0.32619 0.34030 0.34395

Eigenvalues --- 0.35618 0.37349 0.39576 0.40426 0.43037

Eigenvalues --- 0.45317 1.08276 1.10816

Eigenvectors required to have negative eigenvalues:

R6 R10 A14 D30 R22

1 0.65672 0.57740 -0.10897 -0.10475 0.10109

D4 D41 A15 D68 D79

1 0.09891 0.09633 -0.09449 0.09324 0.08983

RFO step: Lambda0=1.949043267D-04 Lambda=-2.57142788D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.484

Iteration 1 RMS(Cart)= 0.06751497 RMS(Int)= 0.00221706

Iteration 2 RMS(Cart)= 0.00277530 RMS(Int)= 0.00068921

Iteration 3 RMS(Cart)= 0.00000594 RMS(Int)= 0.00068920

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00068920

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.54703 0.01732 0.00000 0.03473 0.03499 2.58202

R2 2.67586 0.00422 0.00000 0.00845 0.00942 2.68528

R3 2.07974 0.00087 0.00000 -0.00176 -0.00176 2.07798

R4 2.80723 -0.00440 0.00000 -0.02778 -0.02838 2.77884

R5 2.08224 -0.00023 0.00000 -0.00139 -0.00139 2.08085

R6 6.74326 -0.00664 0.00000 -0.20240 -0.20210 6.54116

R7 2.68154 -0.01592 0.00000 -0.06517 -0.06458 2.61696

R8 2.84336 0.00414 0.00000 0.00396 0.00370 2.84706

R9 2.12235 -0.00206 0.00000 -0.00383 -0.00383 2.11853

R10 3.43965 0.00157 0.00000 0.06286 0.06256 3.50221

R11 2.07870 0.00074 0.00000 0.00020 0.00020 2.07890

R12 2.12260 -0.00045 0.00000 0.00129 0.00129 2.12389

R13 2.13576 -0.00044 0.00000 -0.00067 -0.00067 2.13509

R14 2.87683 0.00003 0.00000 -0.00894 -0.01004 2.86679

R15 2.12024 -0.00013 0.00000 0.00101 0.00101 2.12125

R16 2.13012 0.00005 0.00000 0.00019 0.00019 2.13030

R17 2.62819 0.00123 0.00000 0.00757 0.00806 2.63625

R18 2.70106 0.00117 0.00000 -0.00286 -0.00288 2.69818

R19 2.64521 0.00785 0.00000 0.02811 0.02776 2.67297

R20 2.87018 0.00199 0.00000 -0.00721 -0.00687 2.86331

R21 2.10727 -0.00119 0.00000 -0.01024 -0.01024 2.09703

R22 2.73863 0.00763 0.00000 -0.00292 -0.00343 2.73520

R23 2.04917 0.00197 0.00000 0.00098 0.00098 2.05016

R24 2.31043 -0.00165 0.00000 -0.00180 -0.00180 2.30863

R25 2.31008 -0.00115 0.00000 -0.00138 -0.00138 2.30870

A1 2.08207 -0.00155 0.00000 0.01948 0.01809 2.10017

A2 2.11582 0.00224 0.00000 -0.00763 -0.00813 2.10769

A3 2.07994 -0.00045 0.00000 -0.00467 -0.00520 2.07474

A4 2.11163 -0.00087 0.00000 0.01475 0.01490 2.12653

A5 2.13580 0.00147 0.00000 -0.01952 -0.01912 2.11668

A6 1.41906 -0.00565 0.00000 -0.05566 -0.05659 1.36246

A7 2.03349 -0.00041 0.00000 0.00605 0.00530 2.03879

A8 1.43815 0.00272 0.00000 0.04260 0.04333 1.48148

A9 1.92609 0.00043 0.00000 0.00337 0.00275 1.92885

A10 2.01201 0.00384 0.00000 0.05150 0.05181 2.06382

A11 1.99910 -0.00097 0.00000 0.01514 0.01426 2.01336

A12 1.94342 -0.00481 0.00000 -0.09135 -0.09247 1.85094

A13 1.95411 -0.00002 0.00000 -0.01424 -0.01573 1.93838

A14 1.89840 0.00009 0.00000 0.02140 0.02293 1.92133

A15 1.61584 0.00092 0.00000 0.00191 0.00247 1.61831

A16 2.11578 0.00088 0.00000 -0.03308 -0.03403 2.08176

A17 2.07222 -0.00006 0.00000 0.02659 0.02622 2.09844

A18 2.08896 -0.00050 0.00000 0.01329 0.01281 2.10177

A19 1.92317 -0.00037 0.00000 0.00719 0.00780 1.93098

A20 1.83849 0.00115 0.00000 0.01280 0.01242 1.85091

A21 2.01768 -0.00088 0.00000 -0.01607 -0.01656 2.00112

A22 1.85792 -0.00024 0.00000 -0.00789 -0.00799 1.84993

A23 1.93113 0.00116 0.00000 -0.00367 -0.00396 1.92717

A24 1.88603 -0.00080 0.00000 0.00897 0.00962 1.89564

A25 2.01553 0.00196 0.00000 0.00758 0.00753 2.02305

A26 1.93193 0.00049 0.00000 -0.00321 -0.00372 1.92821

A27 1.84850 -0.00095 0.00000 -0.00084 -0.00033 1.84817

A28 1.91858 -0.00166 0.00000 -0.00654 -0.00600 1.91258

A29 1.88308 -0.00006 0.00000 0.00399 0.00347 1.88656

A30 1.85767 0.00012 0.00000 -0.00111 -0.00112 1.85655

A31 1.87556 0.00219 0.00000 0.00543 0.00549 1.88105

A32 2.08983 -0.00208 0.00000 -0.05961 -0.06064 2.02919

A33 1.83038 0.00029 0.00000 -0.01541 -0.01591 1.81446

A34 1.67770 -0.00105 0.00000 0.01574 0.01659 1.69429

A35 1.83162 -0.00100 0.00000 0.00067 -0.00069 1.83094

A36 2.03932 0.00279 0.00000 0.02876 0.02849 2.06782

A37 1.99071 0.00095 0.00000 0.02667 0.02634 2.01705

A38 1.48688 0.00166 0.00000 0.05444 0.05470 1.54157

A39 2.04790 -0.00352 0.00000 -0.07167 -0.07202 1.97588

A40 1.46970 -0.00118 0.00000 -0.03416 -0.03477 1.43493

A41 1.90850 -0.00096 0.00000 -0.00552 -0.00389 1.90461

A42 2.20630 0.00072 0.00000 0.01222 0.01164 2.21794

A43 2.13110 0.00117 0.00000 0.00941 0.00661 2.13771

A44 1.90785 0.00117 0.00000 -0.00211 -0.00173 1.90612

A45 2.05455 -0.00121 0.00000 -0.00464 -0.00484 2.04971

A46 2.31956 0.00005 0.00000 0.00660 0.00642 2.32598

A47 1.89912 -0.00144 0.00000 0.00188 0.00096 1.90008

A48 2.00048 -0.00011 0.00000 -0.00109 -0.00066 1.99982

A49 2.38355 0.00154 0.00000 -0.00089 -0.00046 2.38309

D1 -0.41606 0.00426 0.00000 0.04127 0.04145 -0.37462

D2 2.80045 0.00119 0.00000 0.02003 0.02055 2.82100

D3 0.90421 0.00409 0.00000 0.05143 0.05104 0.95526

D4 2.61364 0.00664 0.00000 0.11583 0.11615 2.72979

D5 -0.45303 0.00357 0.00000 0.09459 0.09525 -0.35778

D6 -2.34927 0.00648 0.00000 0.12599 0.12574 -2.22353

D7 -0.09421 -0.00057 0.00000 0.00922 0.00946 -0.08476

D8 2.92734 0.00250 0.00000 0.07563 0.07671 3.00405

D9 -3.12623 -0.00308 0.00000 -0.06356 -0.06362 3.09333

D10 -0.10468 -0.00001 0.00000 0.00285 0.00363 -0.10105

D11 2.61226 -0.00446 0.00000 -0.05618 -0.05607 2.55620

D12 -1.67357 -0.00431 0.00000 -0.05523 -0.05501 -1.72858

D13 0.40695 -0.00502 0.00000 -0.04436 -0.04404 0.36291

D14 -0.60004 -0.00148 0.00000 -0.03723 -0.03709 -0.63713

D15 1.39732 -0.00133 0.00000 -0.03628 -0.03603 1.36128

D16 -2.80536 -0.00204 0.00000 -0.02541 -0.02506 -2.83042

D17 1.30244 0.00030 0.00000 -0.01276 -0.01229 1.29015

D18 -2.98339 0.00045 0.00000 -0.01181 -0.01123 -2.99462

D19 -0.90288 -0.00026 0.00000 -0.00094 -0.00026 -0.90314

D20 -1.04684 -0.00011 0.00000 -0.01515 -0.01387 -1.06071

D21 -2.95479 0.00044 0.00000 -0.03053 -0.02801 -2.98280

D22 1.17657 0.00052 0.00000 -0.00685 -0.00692 1.16965

D23 1.10136 -0.00029 0.00000 0.00318 0.00349 1.10485

D24 -0.80659 0.00026 0.00000 -0.01220 -0.01065 -0.81724

D25 -2.95841 0.00035 0.00000 0.01148 0.01044 -2.94798

D26 3.11754 0.00023 0.00000 0.02453 0.02494 -3.14070

D27 1.20960 0.00078 0.00000 0.00915 0.01080 1.22039

D28 -0.94223 0.00087 0.00000 0.03284 0.03189 -0.91034

D29 0.56892 -0.00353 0.00000 -0.05525 -0.05514 0.51377

D30 -2.45150 -0.00667 0.00000 -0.12314 -0.12342 -2.57493

D31 2.87432 -0.00058 0.00000 -0.00736 -0.00583 2.86849

D32 -0.14610 -0.00371 0.00000 -0.07525 -0.07411 -0.22021

D33 -1.60434 -0.00267 0.00000 -0.04869 -0.04733 -1.65167

D34 1.65842 -0.00580 0.00000 -0.11659 -0.11561 1.54281

D35 -0.53009 0.00185 0.00000 0.04055 0.04145 -0.48864

D36 -2.72401 0.00212 0.00000 0.04614 0.04681 -2.67720

D37 1.55252 0.00226 0.00000 0.04948 0.05012 1.60264

D38 -2.85645 -0.00052 0.00000 -0.01880 -0.01817 -2.87462

D39 1.23282 -0.00024 0.00000 -0.01321 -0.01282 1.22000

D40 -0.77384 -0.00010 0.00000 -0.00987 -0.00951 -0.78334

D41 1.66649 -0.00161 0.00000 -0.02517 -0.02497 1.64152

D42 -0.52743 -0.00134 0.00000 -0.01958 -0.01961 -0.54704

D43 -2.53409 -0.00120 0.00000 -0.01624 -0.01630 -2.55039

D44 1.05762 0.00359 0.00000 0.04634 0.04496 1.10258

D45 3.10529 0.00129 0.00000 -0.00023 -0.00042 3.10488

D46 -1.13727 0.00200 0.00000 0.02981 0.02927 -1.10801

D47 -1.17823 0.00208 0.00000 0.03035 0.02900 -1.14922

D48 0.86944 -0.00023 0.00000 -0.01621 -0.01638 0.85307

D49 2.91007 0.00048 0.00000 0.01382 0.01331 2.92337

D50 3.11092 0.00172 0.00000 0.04058 0.04025 -3.13202

D51 -1.12460 -0.00059 0.00000 -0.00598 -0.00513 -1.12973

D52 0.91602 0.00012 0.00000 0.02405 0.02455 0.94057

D53 0.07674 -0.00103 0.00000 -0.01599 -0.01505 0.06169

D54 2.27748 -0.00022 0.00000 -0.01991 -0.01928 2.25820

D55 -1.98674 -0.00100 0.00000 -0.02249 -0.02188 -2.00862

D56 -2.12454 -0.00081 0.00000 -0.00959 -0.00905 -2.13359

D57 0.07620 0.00000 0.00000 -0.01351 -0.01328 0.06293

D58 2.09517 -0.00078 0.00000 -0.01609 -0.01588 2.07929

D59 2.13093 -0.00069 0.00000 -0.00331 -0.00283 2.12810

D60 -1.95151 0.00012 0.00000 -0.00722 -0.00706 -1.95857

D61 0.06746 -0.00066 0.00000 -0.00980 -0.00966 0.05780

D62 0.06157 0.00063 0.00000 -0.00914 -0.00903 0.05254

D63 -3.03376 0.00063 0.00000 -0.00659 -0.00642 -3.04019

D64 -0.05872 -0.00098 0.00000 -0.00246 -0.00255 -0.06127

D65 3.09030 -0.00045 0.00000 0.00776 0.00766 3.09796

D66 0.00412 0.00086 0.00000 -0.01592 -0.01512 -0.01099

D67 2.05165 -0.00238 0.00000 -0.07346 -0.07251 1.97915

D68 -1.37766 0.00125 0.00000 -0.01176 -0.01100 -1.38866

D69 -2.04290 0.00251 0.00000 0.03899 0.03894 -2.00396

D70 0.00463 -0.00073 0.00000 -0.01855 -0.01845 -0.01382

D71 2.85850 0.00289 0.00000 0.04315 0.04306 2.90156

D72 2.01595 0.00007 0.00000 -0.01797 -0.01836 1.99759

D73 -2.21971 -0.00317 0.00000 -0.07551 -0.07575 -2.29546

D74 0.63416 0.00045 0.00000 -0.01381 -0.01424 0.61992

D75 -2.25852 0.00296 0.00000 0.09498 0.09551 -2.16301

D76 0.82716 0.00292 0.00000 0.09141 0.09185 0.91901

D77 -0.04160 0.00015 0.00000 0.01768 0.01748 -0.02412

D78 3.04407 0.00012 0.00000 0.01412 0.01382 3.05790

D79 2.21205 0.00366 0.00000 0.07457 0.07467 2.28672

D80 -0.98546 0.00363 0.00000 0.07100 0.07101 -0.91445

D81 1.68506 0.00111 0.00000 0.04757 0.04756 1.73262

D82 -1.46635 0.00040 0.00000 0.03404 0.03405 -1.43229

D83 0.03266 0.00104 0.00000 0.01393 0.01385 0.04651

D84 -3.11875 0.00033 0.00000 0.00041 0.00035 -3.11840

D85 -2.83596 -0.00233 0.00000 -0.04531 -0.04537 -2.88133

D86 0.29581 -0.00304 0.00000 -0.05883 -0.05887 0.23694

Item Value Threshold Converged?

Maximum Force 0.017317 0.000450 NO

RMS Force 0.002989 0.000300 NO

Maximum Displacement 0.316576 0.001800 NO

RMS Displacement 0.068359 0.001200 NO

Predicted change in Energy=-1.341514D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.313750 1.349552 0.233158

2 6 0 -0.218762 0.855708 -0.418012

3 6 0 -0.511613 3.610960 -0.089618

4 6 0 -1.499979 2.752400 0.361793

5 1 0 -2.081658 0.672893 0.635177

6 1 0 -2.440658 3.151191 0.769622

7 6 0 0.539685 1.664553 -1.383878

8 1 0 1.631935 1.401927 -1.349191

9 1 0 0.176540 1.351345 -2.406895

10 6 0 0.350830 3.162983 -1.240857

11 1 0 1.353333 3.666310 -1.199639

12 1 0 -0.157128 3.542352 -2.172995

13 1 0 -0.824239 4.680496 -0.212775

14 1 0 0.106636 -0.187096 -0.279523

15 8 0 2.878855 4.331991 1.120029

16 6 0 0.544062 3.996946 1.383898

17 6 0 1.229845 2.905231 1.965790

18 6 0 1.634268 4.890701 0.828495

19 8 0 1.619158 5.916993 0.165933

20 6 0 2.653543 3.083681 1.775481

21 8 0 3.669312 2.461140 2.046094

22 1 0 -0.237683 4.509952 1.981505

23 1 0 0.821069 2.160799 2.640865

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.366346 0.000000

3 C 2.421069 2.790164 0.000000

4 C 1.420989 2.418068 1.384834 0.000000

5 H 1.099622 2.147791 3.409194 2.176565 0.000000

6 H 2.191716 3.408304 2.161225 1.100107 2.507772

7 C 2.479769 1.470500 2.562974 2.896724 3.454188

8 H 3.344194 2.142552 3.325830 3.815774 4.273169

9 H 3.031641 2.087480 3.308955 3.526939 3.848890

10 C 2.869160 2.514960 1.506599 2.482450 3.954370

11 H 3.812297 3.313896 2.170999 3.378564 4.911848

12 H 3.454811 3.209645 2.114433 2.975302 4.452352

13 H 3.396125 3.877851 1.121076 2.122335 4.284974

14 H 2.154443 1.101137 3.852729 3.410738 2.522873

15 O 5.221055 4.903606 3.671295 4.716378 6.183103

16 C 3.432836 3.700832 1.853290 2.602249 4.301664

17 C 3.448482 3.461433 2.784858 3.169875 4.209503

18 C 4.645964 4.611797 2.661856 3.822781 5.624534

19 O 5.428442 5.416230 3.150124 4.447699 6.435589

20 C 4.596235 4.245634 3.711446 4.400001 5.434548

21 O 5.417866 4.875075 4.833579 5.444564 6.185642

22 H 3.768655 4.371674 2.274374 2.702933 4.464959

23 H 3.318528 3.484428 3.366682 3.306271 3.829161

6 7 8 9 10

6 H 0.000000

7 C 3.966119 0.000000

8 H 4.912770 1.123914 0.000000

9 H 4.492152 1.129840 1.799852 0.000000

10 C 3.440141 1.517041 2.180432 2.161493 0.000000

11 H 4.305543 2.168639 2.286354 2.863804 1.122519

12 H 3.745198 2.152762 2.908748 2.228577 1.127308

13 H 2.432424 3.511080 4.251264 4.110835 2.177289

14 H 4.328230 2.199031 2.448616 2.626289 3.493826

15 O 5.460247 4.342406 4.029533 5.350322 3.651202

16 C 3.162465 3.619483 3.922674 4.637282 2.760828

17 C 3.868321 3.638115 3.662062 4.758612 3.334919

18 C 4.431070 4.062110 4.112647 5.011962 2.985706

19 O 4.949364 4.653001 4.762519 5.435599 3.342497

20 C 5.192994 4.057569 3.692635 5.160310 3.795664

21 O 6.279911 4.711032 4.098878 5.767167 4.723235

22 H 2.857969 4.475086 4.924310 5.422769 3.541792

23 H 3.888611 4.064971 4.141731 5.152719 4.036491

11 12 13 14 15

11 H 0.000000

12 H 1.801189 0.000000

13 H 2.596978 2.362810 0.000000

14 H 4.153264 4.190894 4.956252 0.000000

15 O 2.855032 4.548047 3.951042 5.483256 0.000000

16 C 2.727435 3.653739 2.211075 4.523773 2.373424

17 C 3.257980 4.411254 3.480945 3.983154 2.338844

18 C 2.385662 3.746477 2.678188 5.417139 1.395044

19 O 2.645945 3.776863 2.764514 6.304447 2.238162

20 C 3.298687 4.868338 4.312534 4.626852 1.427817

21 O 4.165450 5.797532 5.497275 5.011419 2.232151

22 H 3.655508 4.266451 2.277718 5.224276 3.238305

23 H 4.159247 5.102823 4.147189 3.814668 3.355816

16 17 18 19 20

16 C 0.000000

17 C 1.414475 0.000000

18 C 1.515197 2.323595 0.000000

19 O 2.515124 3.530122 1.221675 0.000000

20 C 2.331802 1.447404 2.280576 3.418809 0.000000

21 O 3.544629 2.480860 3.395102 4.436333 1.221710

22 H 1.109700 2.174630 2.231279 2.953629 3.230462

23 H 2.242351 1.084898 3.376144 4.568504 2.226782

21 22 23

21 O 0.000000

22 H 4.412076 0.000000

23 H 2.925140 2.659743 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.696597 -0.561395 -0.776743

2 6 0 2.389215 -1.213033 0.384199

3 6 0 1.059329 1.149822 -0.274086

4 6 0 2.063201 0.669334 -1.098184

5 1 0 3.460610 -0.959714 -1.459967

6 1 0 2.402064 1.257076 -1.964191

7 6 0 1.793878 -0.513297 1.532378

8 1 0 1.090433 -1.191192 2.088082

9 1 0 2.645530 -0.298370 2.243034

10 6 0 1.107442 0.795369 1.189434

11 1 0 0.075087 0.805491 1.630104

12 1 0 1.675154 1.630344 1.690776

13 1 0 0.795282 2.229733 -0.418591

14 1 0 2.623630 -2.280322 0.520019

15 8 0 -2.363053 -0.004192 0.384672

16 6 0 -0.535858 0.568934 -1.017478

17 6 0 -0.728797 -0.831347 -1.069705

18 6 0 -1.592368 1.072294 -0.055066

19 8 0 -1.839152 2.171543 0.417414

20 6 0 -1.817705 -1.193255 -0.187503

21 8 0 -2.374332 -2.224700 0.157261

22 1 0 -0.452959 1.127617 -1.972693

23 1 0 -0.312146 -1.522433 -1.794828

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2551909 0.6708937 0.5644973

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 455.8872278331 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.256188957174E-01 A.U. after 15 cycles

Convg = 0.3651D-08 -V/T = 0.9995

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.003959164 -0.005458592 -0.003988536

2 6 -0.010124527 0.001123691 0.008938859

3 6 -0.000728627 0.014107255 -0.017142450

4 6 -0.006366423 -0.009240177 -0.008288850

5 1 0.002979159 -0.000593311 0.007047905

6 1 0.002090834 -0.001511349 0.007173688

7 6 0.005013480 0.001848831 0.000303670

8 1 0.000127998 0.000709155 0.001376644

9 1 0.001153017 -0.000633323 -0.000372543

10 6 0.001768802 0.001259261 0.002333011

11 1 0.000143863 -0.000001279 0.000679208

12 1 0.000584258 0.000736457 0.000005241

13 1 0.001843000 0.000095196 -0.000586169

14 1 -0.003302688 -0.001791618 -0.003570490

15 8 -0.001534873 0.001440203 -0.002550653

16 6 0.011397133 -0.005258598 0.025050751

17 6 -0.015743503 0.012973956 0.000159294

18 6 0.002368752 -0.003668296 -0.005303170

19 8 -0.000045372 0.000997410 0.003422743

20 6 0.008612955 -0.002013267 -0.005672539

21 8 0.000776345 0.000300902 0.000395655

22 1 -0.003519584 -0.001715761 -0.005699381

23 1 -0.001453165 -0.003706746 -0.003711888

-------------------------------------------------------------------

Cartesian Forces: Max 0.025050751 RMS 0.006121954

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011242145 RMS 0.002471129

Search for a saddle point.

Step number 16 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 15 16

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.05764 -0.01505 0.00189 0.00344 0.00587

Eigenvalues --- 0.00838 0.00977 0.01353 0.01624 0.01667

Eigenvalues --- 0.01976 0.02082 0.02182 0.02391 0.02491

Eigenvalues --- 0.02551 0.02889 0.03015 0.03086 0.03209

Eigenvalues --- 0.03608 0.03685 0.03827 0.03886 0.04242

Eigenvalues --- 0.04478 0.04790 0.05208 0.05441 0.05933

Eigenvalues --- 0.06198 0.07325 0.07940 0.08627 0.09679

Eigenvalues --- 0.11244 0.13044 0.13900 0.15268 0.18741

Eigenvalues --- 0.21223 0.22908 0.24653 0.25423 0.27561

Eigenvalues --- 0.28327 0.29659 0.30760 0.31159 0.31569

Eigenvalues --- 0.31932 0.32218 0.32617 0.34318 0.34748

Eigenvalues --- 0.35638 0.37344 0.39576 0.40449 0.43173

Eigenvalues --- 0.45464 1.08276 1.10816

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 0.60109 0.58805 -0.14179 0.13261 0.11463

D73 A14 R22 D80 A15

1 -0.11125 -0.10327 0.10083 0.09477 -0.09327

RFO step: Lambda0=1.624938007D-03 Lambda=-2.86002844D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.404

Iteration 1 RMS(Cart)= 0.04791985 RMS(Int)= 0.00378613

Iteration 2 RMS(Cart)= 0.00642235 RMS(Int)= 0.00042420

Iteration 3 RMS(Cart)= 0.00000747 RMS(Int)= 0.00042417

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00042417

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58202 -0.00800 0.00000 -0.05947 -0.05968 2.52234

R2 2.68528 0.00051 0.00000 -0.01567 -0.01539 2.66989

R3 2.07798 0.00086 0.00000 0.00153 0.00153 2.07951

R4 2.77884 0.00687 0.00000 0.02874 0.02861 2.80745

R5 2.08085 0.00027 0.00000 0.00275 0.00275 2.08359

R6 6.54116 -0.00184 0.00000 -0.24937 -0.24996 6.29120

R7 2.61696 0.01124 0.00000 0.03751 0.03808 2.65503

R8 2.84706 -0.00234 0.00000 -0.01190 -0.01197 2.83509

R9 2.11853 -0.00036 0.00000 -0.00535 -0.00535 2.11318

R10 3.50221 0.00763 0.00000 0.03250 0.03316 3.53537

R11 2.07890 0.00032 0.00000 -0.00392 -0.00392 2.07498

R12 2.12389 0.00000 0.00000 -0.00067 -0.00067 2.12323

R13 2.13509 0.00014 0.00000 -0.00163 -0.00163 2.13346

R14 2.86679 0.00298 0.00000 0.00588 0.00566 2.87245

R15 2.12125 0.00015 0.00000 0.00135 0.00135 2.12260

R16 2.13030 -0.00002 0.00000 -0.00063 -0.00063 2.12967

R17 2.63625 -0.00305 0.00000 -0.00335 -0.00304 2.63321

R18 2.69818 -0.00026 0.00000 -0.00018 -0.00028 2.69790

R19 2.67297 -0.01090 0.00000 -0.04536 -0.04520 2.62777

R20 2.86331 0.00138 0.00000 -0.00176 -0.00147 2.86183

R21 2.09703 -0.00138 0.00000 -0.00560 -0.00560 2.09143

R22 2.73520 0.01010 0.00000 0.02108 0.02072 2.75591

R23 2.05016 0.00078 0.00000 0.00178 0.00178 2.05194

R24 2.30863 -0.00102 0.00000 -0.00061 -0.00061 2.30802

R25 2.30870 0.00058 0.00000 -0.00150 -0.00150 2.30720

A1 2.10017 -0.00110 0.00000 -0.00851 -0.00884 2.09133

A2 2.10769 0.00093 0.00000 -0.01535 -0.01538 2.09232

A3 2.07474 0.00024 0.00000 0.02478 0.02478 2.09952

A4 2.12653 0.00197 0.00000 0.01967 0.01947 2.14600

A5 2.11668 -0.00158 0.00000 -0.00592 -0.00558 2.11109

A6 1.36246 0.00065 0.00000 -0.00429 -0.00467 1.35780

A7 2.03879 -0.00033 0.00000 -0.01443 -0.01466 2.02414

A8 1.48148 -0.00245 0.00000 0.01488 0.01468 1.49616

A9 1.92885 0.00139 0.00000 0.00858 0.00915 1.93800

A10 2.06382 0.00006 0.00000 -0.00172 -0.00226 2.06156

A11 2.01336 0.00231 0.00000 0.02272 0.02299 2.03635

A12 1.85094 -0.00324 0.00000 -0.05549 -0.05582 1.79512

A13 1.93838 0.00011 0.00000 0.00567 0.00530 1.94368

A14 1.92133 -0.00047 0.00000 0.00116 0.00045 1.92178

A15 1.61831 0.00092 0.00000 0.02758 0.02792 1.64623

A16 2.08176 0.00154 0.00000 0.01422 0.01416 2.09592

A17 2.09844 -0.00249 0.00000 -0.02652 -0.02746 2.07098

A18 2.10177 0.00115 0.00000 0.01541 0.01443 2.11620

A19 1.93098 -0.00101 0.00000 -0.01378 -0.01392 1.91706

A20 1.85091 -0.00016 0.00000 0.00838 0.00842 1.85933

A21 2.00112 0.00193 0.00000 0.00220 0.00238 2.00350

A22 1.84993 0.00031 0.00000 0.00138 0.00144 1.85137

A23 1.92717 -0.00052 0.00000 0.00273 0.00259 1.92975

A24 1.89564 -0.00064 0.00000 -0.00043 -0.00045 1.89520

A25 2.02305 -0.00252 0.00000 -0.01115 -0.01094 2.01212

A26 1.92821 0.00021 0.00000 0.00223 0.00223 1.93045

A27 1.84817 0.00096 0.00000 0.00318 0.00305 1.85122

A28 1.91258 0.00131 0.00000 -0.00041 -0.00076 1.91183

A29 1.88656 0.00062 0.00000 0.00954 0.00977 1.89632

A30 1.85655 -0.00046 0.00000 -0.00241 -0.00239 1.85416

A31 1.88105 -0.00181 0.00000 -0.00379 -0.00372 1.87733

A32 2.02919 -0.00052 0.00000 -0.02764 -0.02740 2.00179

A33 1.81446 -0.00365 0.00000 -0.03520 -0.03523 1.77923

A34 1.69429 -0.00006 0.00000 0.00792 0.00803 1.70232

A35 1.83094 0.00198 0.00000 0.01016 0.00912 1.84006

A36 2.06782 0.00080 0.00000 0.02320 0.02288 2.09070

A37 2.01705 0.00056 0.00000 0.01106 0.01073 2.02778

A38 1.54157 0.00316 0.00000 0.05444 0.05467 1.59625

A39 1.97588 -0.00148 0.00000 -0.04646 -0.04713 1.92875

A40 1.43493 -0.00352 0.00000 -0.03005 -0.03066 1.40427

A41 1.90461 -0.00128 0.00000 0.00115 0.00225 1.90685

A42 2.21794 0.00054 0.00000 0.01353 0.01352 2.23145

A43 2.13771 0.00126 0.00000 -0.00869 -0.01017 2.12753

A44 1.90612 0.00177 0.00000 -0.00117 -0.00077 1.90535

A45 2.04971 -0.00087 0.00000 0.00230 0.00210 2.05181

A46 2.32598 -0.00088 0.00000 -0.00092 -0.00112 2.32486

A47 1.90008 -0.00068 0.00000 -0.00611 -0.00669 1.89339

A48 1.99982 -0.00022 0.00000 0.00335 0.00363 2.00345

A49 2.38309 0.00089 0.00000 0.00267 0.00296 2.38605

D1 -0.37462 0.00355 0.00000 0.03343 0.03336 -0.34126

D2 2.82100 0.00230 0.00000 0.04935 0.04929 2.87029

D3 0.95526 0.00024 0.00000 0.04154 0.04103 0.99629

D4 2.72979 0.00550 0.00000 0.06338 0.06288 2.79267

D5 -0.35778 0.00425 0.00000 0.07930 0.07881 -0.27897

D6 -2.22353 0.00219 0.00000 0.07149 0.07055 -2.15298

D7 -0.08476 -0.00098 0.00000 -0.02417 -0.02442 -0.10918

D8 3.00405 0.00314 0.00000 0.04355 0.04238 3.04643

D9 3.09333 -0.00290 0.00000 -0.05272 -0.05321 3.04012

D10 -0.10105 0.00121 0.00000 0.01500 0.01359 -0.08746

D11 2.55620 -0.00158 0.00000 -0.01469 -0.01478 2.54142

D12 -1.72858 -0.00180 0.00000 -0.01521 -0.01537 -1.74395

D13 0.36291 -0.00157 0.00000 -0.00863 -0.00860 0.35431

D14 -0.63713 -0.00043 0.00000 -0.02974 -0.02977 -0.66690

D15 1.36128 -0.00064 0.00000 -0.03027 -0.03036 1.33092

D16 -2.83042 -0.00041 0.00000 -0.02368 -0.02359 -2.85401

D17 1.29015 -0.00014 0.00000 -0.01390 -0.01367 1.27648

D18 -2.99462 -0.00035 0.00000 -0.01443 -0.01426 -3.00888

D19 -0.90314 -0.00012 0.00000 -0.00785 -0.00748 -0.91062

D20 -1.06071 -0.00181 0.00000 -0.00829 -0.00803 -1.06874

D21 -2.98280 -0.00163 0.00000 -0.02798 -0.02684 -3.00965

D22 1.16965 -0.00138 0.00000 -0.00085 -0.00118 1.16846

D23 1.10485 0.00087 0.00000 0.00879 0.00897 1.11382

D24 -0.81724 0.00106 0.00000 -0.01090 -0.00985 -0.82709

D25 -2.94798 0.00131 0.00000 0.01623 0.01581 -2.93217

D26 -3.14070 -0.00028 0.00000 -0.00035 -0.00027 -3.14097

D27 1.22039 -0.00010 0.00000 -0.02004 -0.01908 1.20131

D28 -0.91034 0.00016 0.00000 0.00709 0.00658 -0.90377

D29 0.51377 -0.00113 0.00000 -0.00322 -0.00313 0.51064

D30 -2.57493 -0.00514 0.00000 -0.06977 -0.07041 -2.64534

D31 2.86849 0.00197 0.00000 0.03206 0.03230 2.90079

D32 -0.22021 -0.00204 0.00000 -0.03449 -0.03498 -0.25519

D33 -1.65167 0.00218 0.00000 0.04324 0.04259 -1.60908

D34 1.54281 -0.00183 0.00000 -0.02331 -0.02469 1.51812

D35 -0.48864 0.00342 0.00000 0.03141 0.03113 -0.45750

D36 -2.67720 0.00346 0.00000 0.03901 0.03898 -2.63822

D37 1.60264 0.00337 0.00000 0.03903 0.03903 1.64167

D38 -2.87462 -0.00048 0.00000 -0.00982 -0.01023 -2.88485

D39 1.22000 -0.00044 0.00000 -0.00222 -0.00238 1.21762

D40 -0.78334 -0.00053 0.00000 -0.00220 -0.00233 -0.78567

D41 1.64152 -0.00137 0.00000 -0.04496 -0.04545 1.59607

D42 -0.54704 -0.00134 0.00000 -0.03736 -0.03761 -0.58465

D43 -2.55039 -0.00143 0.00000 -0.03734 -0.03755 -2.58794

D44 1.10258 -0.00144 0.00000 -0.00567 -0.00571 1.09687

D45 3.10488 -0.00167 0.00000 -0.03025 -0.02947 3.07540

D46 -1.10801 -0.00211 0.00000 -0.02542 -0.02500 -1.13300

D47 -1.14922 0.00108 0.00000 0.03477 0.03388 -1.11535

D48 0.85307 0.00084 0.00000 0.01019 0.01011 0.86318

D49 2.92337 0.00041 0.00000 0.01502 0.01459 2.93796

D50 -3.13202 0.00067 0.00000 0.01679 0.01604 -3.11599

D51 -1.12973 0.00044 0.00000 -0.00778 -0.00772 -1.13746

D52 0.94057 0.00000 0.00000 -0.00296 -0.00325 0.93732

D53 0.06169 0.00002 0.00000 -0.01200 -0.01217 0.04952

D54 2.25820 -0.00056 0.00000 -0.01812 -0.01833 2.23987

D55 -2.00862 -0.00006 0.00000 -0.01595 -0.01618 -2.02480

D56 -2.13359 0.00029 0.00000 0.00264 0.00264 -2.13094

D57 0.06293 -0.00028 0.00000 -0.00348 -0.00351 0.05941

D58 2.07929 0.00022 0.00000 -0.00131 -0.00136 2.07793

D59 2.12810 0.00058 0.00000 -0.00029 -0.00027 2.12784

D60 -1.95857 0.00000 0.00000 -0.00641 -0.00642 -1.96499

D61 0.05780 0.00050 0.00000 -0.00424 -0.00427 0.05352

D62 0.05254 0.00018 0.00000 -0.00826 -0.00822 0.04432

D63 -3.04019 -0.00014 0.00000 -0.01191 -0.01198 -3.05217

D64 -0.06127 -0.00010 0.00000 0.00332 0.00342 -0.05786

D65 3.09796 0.00017 0.00000 0.00728 0.00730 3.10526

D66 -0.01099 -0.00290 0.00000 -0.02969 -0.02945 -0.04044

D67 1.97915 -0.00347 0.00000 -0.05909 -0.05886 1.92029

D68 -1.38866 -0.00079 0.00000 -0.03148 -0.03121 -1.41986

D69 -2.00396 0.00054 0.00000 0.02101 0.02106 -1.98291

D70 -0.01382 -0.00004 0.00000 -0.00839 -0.00835 -0.02217

D71 2.90156 0.00265 0.00000 0.01922 0.01930 2.92086

D72 1.99759 -0.00278 0.00000 -0.02308 -0.02325 1.97433

D73 -2.29546 -0.00335 0.00000 -0.05248 -0.05266 -2.34812

D74 0.61992 -0.00067 0.00000 -0.02487 -0.02501 0.59491

D75 -2.16301 0.00130 0.00000 0.05370 0.05333 -2.10968

D76 0.91901 0.00172 0.00000 0.05827 0.05804 0.97704

D77 -0.02412 -0.00009 0.00000 0.01037 0.01040 -0.01372

D78 3.05790 0.00032 0.00000 0.01494 0.01510 3.07300

D79 2.28672 0.00322 0.00000 0.05993 0.05982 2.34655

D80 -0.91445 0.00363 0.00000 0.06450 0.06453 -0.84992

D81 1.73262 0.00260 0.00000 0.04888 0.04852 1.78114

D82 -1.43229 0.00222 0.00000 0.04361 0.04335 -1.38895

D83 0.04651 0.00014 0.00000 0.00378 0.00370 0.05022

D84 -3.11840 -0.00025 0.00000 -0.00150 -0.00147 -3.11987

D85 -2.88133 -0.00230 0.00000 -0.02568 -0.02554 -2.90687

D86 0.23694 -0.00269 0.00000 -0.03095 -0.03071 0.20623

Item Value Threshold Converged?

Maximum Force 0.011242 0.000450 NO

RMS Force 0.002471 0.000300 NO

Maximum Displacement 0.219123 0.001800 NO

RMS Displacement 0.053193 0.001200 NO

Predicted change in Energy=-9.322834D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.271989 1.364667 0.277488

2 6 0 -0.199000 0.892072 -0.360435

3 6 0 -0.512632 3.649222 -0.128170

4 6 0 -1.487977 2.758943 0.351499

5 1 0 -1.988088 0.666860 0.737067

6 1 0 -2.420997 3.124179 0.800670

7 6 0 0.567146 1.688830 -1.353067

8 1 0 1.658398 1.428806 -1.290220

9 1 0 0.222862 1.348314 -2.372923

10 6 0 0.369870 3.192634 -1.252232

11 1 0 1.370559 3.700159 -1.200369

12 1 0 -0.119147 3.556354 -2.200198

13 1 0 -0.827830 4.713466 -0.264207

14 1 0 0.129991 -0.151018 -0.221024

15 8 0 2.847452 4.277818 1.069753

16 6 0 0.515473 4.000258 1.394922

17 6 0 1.165152 2.891216 1.925571

18 6 0 1.613296 4.880974 0.835828

19 8 0 1.606689 5.931109 0.212228

20 6 0 2.600118 3.020887 1.699982

21 8 0 3.599379 2.358209 1.930139

22 1 0 -0.268737 4.512359 1.984526

23 1 0 0.753612 2.126688 2.577631

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.334765 0.000000

3 C 2.441388 2.784635 0.000000

4 C 1.412846 2.377714 1.404983 0.000000

5 H 1.100430 2.110940 3.438036 2.185311 0.000000

6 H 2.165600 3.356745 2.186383 1.098034 2.495971

7 C 2.479155 1.485639 2.551359 2.876494 3.455764

8 H 3.324002 2.145346 3.315718 3.790011 4.241145

9 H 3.042947 2.106237 3.297582 3.512737 3.876173

10 C 2.894340 2.532094 1.500266 2.492315 3.987080

11 H 3.823826 3.324810 2.167628 3.386061 4.922913

12 H 3.503065 3.238751 2.111103 3.003451 4.524339

13 H 3.421281 3.873983 1.118244 2.152916 4.327097

14 H 2.123997 1.102590 3.855310 3.378384 2.464370

15 O 5.107243 4.773844 3.622198 4.649603 6.044183

16 C 3.374911 3.640409 1.870839 2.577481 4.220443

17 C 3.314542 3.329161 2.758149 3.087764 4.037725

18 C 4.582688 4.541674 2.639332 3.788862 5.544229

19 O 5.398466 5.383340 3.132794 4.433845 6.396108

20 C 4.445196 4.075811 3.664173 4.312719 5.245978

21 O 5.239142 4.671613 4.776190 5.341711 5.958513

22 H 3.718663 4.313952 2.295207 2.688454 4.393197

23 H 3.158226 3.326255 3.353035 3.221820 3.610498

6 7 8 9 10

6 H 0.000000

7 C 3.953202 0.000000

8 H 4.887491 1.123562 0.000000

9 H 4.496152 1.128977 1.799858 0.000000

10 C 3.465260 1.520037 2.184682 2.163117 0.000000

11 H 4.325714 2.171229 2.291282 2.867624 1.123232

12 H 3.806639 2.162470 2.917908 2.241037 1.126974

13 H 2.489573 3.504283 4.245353 4.107906 2.173386

14 H 4.275314 2.204011 2.444391 2.624365 3.507269

15 O 5.399985 4.215770 3.885897 5.227092 3.564779

16 C 3.121459 3.591214 3.889555 4.616827 2.771440

17 C 3.765652 3.542995 3.566966 4.663208 3.289644

18 C 4.400350 4.009423 4.054575 4.970823 2.959154

19 O 4.944428 4.639798 4.746658 5.440588 3.342695

20 C 5.102061 3.902366 3.516088 5.003740 3.703927

21 O 6.173114 4.519065 3.873231 5.562113 4.610149

22 H 2.821485 4.450904 4.893476 5.407422 3.553321

23 H 3.772363 3.959403 4.033107 5.039400 3.993913

11 12 13 14 15

11 H 0.000000

12 H 1.799878 0.000000

13 H 2.595400 2.364149 0.000000

14 H 4.162894 4.209965 4.958073 0.000000

15 O 2.769179 4.473678 3.934074 5.353998 0.000000

16 C 2.748957 3.677592 2.250742 4.471351 2.370844

17 C 3.235442 4.371934 3.476737 3.864533 2.342056

18 C 2.366293 3.738105 2.682765 5.351455 1.393434

19 O 2.651099 3.799706 2.763427 6.273803 2.237903

20 C 3.222617 4.784614 4.298104 4.455646 1.427669

21 O 4.070448 5.685303 5.473808 4.791699 2.233956

22 H 3.672943 4.295141 2.325904 5.174023 3.256141

23 H 4.138806 5.062934 4.155529 3.661873 3.359349

16 17 18 19 20

16 C 0.000000

17 C 1.390556 0.000000

18 C 1.514418 2.312469 0.000000

19 O 2.513504 3.517307 1.221353 0.000000

20 C 2.323354 1.458367 2.276073 3.416095 0.000000

21 O 3.534580 2.491903 3.392107 4.437076 1.220916

22 H 1.106736 2.165091 2.235494 2.944676 3.245887

23 H 2.228402 1.085840 3.370315 4.560317 2.231467

21 22 23

21 O 0.000000

22 H 4.427826 0.000000

23 H 2.927667 2.662404 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.643144 -0.518371 -0.775009

2 6 0 2.331207 -1.180338 0.341276

3 6 0 1.022989 1.216532 -0.204410

4 6 0 2.041837 0.731993 -1.041755

5 1 0 3.372609 -0.945138 -1.479775

6 1 0 2.378338 1.301939 -1.917887

7 6 0 1.719573 -0.524439 1.525684

8 1 0 1.008531 -1.233630 2.029529

9 1 0 2.556652 -0.345450 2.261790

10 6 0 1.035909 0.802226 1.237458

11 1 0 -0.007379 0.785366 1.653291

12 1 0 1.582722 1.617289 1.791298

13 1 0 0.752548 2.295855 -0.315728

14 1 0 2.578763 -2.248737 0.455053

15 8 0 -2.311879 -0.071321 0.379039

16 6 0 -0.531988 0.594814 -1.038407

17 6 0 -0.644226 -0.789831 -1.100118

18 6 0 -1.607278 1.043441 -0.070964

19 8 0 -1.913139 2.130723 0.393761

20 6 0 -1.707836 -1.226573 -0.202998

21 8 0 -2.202263 -2.289532 0.138024

22 1 0 -0.440031 1.181158 -1.972543

23 1 0 -0.184491 -1.464337 -1.816173

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2439527 0.7018210 0.5836811

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 458.2417694537 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.300239113275E-01 A.U. after 15 cycles

Convg = 0.2729D-08 -V/T = 0.9994

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.019443649 0.000434753 0.010971109

2 6 0.028387456 -0.011938297 -0.018996525

3 6 -0.024315158 -0.005995692 -0.010162536

4 6 0.003533251 0.018486179 -0.009913358

5 1 -0.000229072 0.001905895 0.006912718

6 1 0.001422836 0.002577928 0.004926326

7 6 0.000455032 -0.001659993 0.004788532

8 1 -0.000016610 0.001227976 0.001173980

9 1 0.000673642 -0.000789069 0.000642648

10 6 0.002705480 -0.002802402 0.001790200

11 1 0.000003685 -0.000268846 0.000307184

12 1 0.000583538 -0.000140249 -0.000344754

13 1 0.001062998 -0.000842200 0.001695932

14 1 -0.001134236 -0.001676729 -0.003713150

15 8 0.000203194 -0.000304161 -0.001618494

16 6 0.004515049 0.010537026 0.018215497

17 6 0.001943320 -0.004822273 0.008716981

18 6 0.001276166 0.000126346 -0.005309577

19 8 0.000324021 0.001278842 0.002989825

20 6 0.004246904 -0.001756562 -0.004046190

21 8 -0.000123445 0.000227502 0.000108650

22 1 -0.004734780 -0.000710277 -0.005874954

23 1 -0.001339623 -0.003095698 -0.003260044

-------------------------------------------------------------------

Cartesian Forces: Max 0.028387456 RMS 0.007492625

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.030477213 RMS 0.003543031

Search for a saddle point.

Step number 17 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 16 17

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.05699 -0.01504 0.00191 0.00344 0.00588

Eigenvalues --- 0.00859 0.00970 0.01355 0.01594 0.01670

Eigenvalues --- 0.01959 0.02079 0.02279 0.02378 0.02510

Eigenvalues --- 0.02648 0.02857 0.03031 0.03171 0.03256

Eigenvalues --- 0.03608 0.03728 0.03822 0.03876 0.04221

Eigenvalues --- 0.04450 0.04601 0.05172 0.05445 0.05945

Eigenvalues --- 0.06253 0.07329 0.07988 0.08622 0.09671

Eigenvalues --- 0.11262 0.12994 0.13890 0.15204 0.18814

Eigenvalues --- 0.21959 0.23169 0.24717 0.25684 0.27658

Eigenvalues --- 0.28686 0.30483 0.31131 0.31188 0.31758

Eigenvalues --- 0.31932 0.32237 0.32630 0.34318 0.35631

Eigenvalues --- 0.37337 0.39017 0.39614 0.40653 0.43239

Eigenvalues --- 0.46805 1.08276 1.10817

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 -0.63706 -0.37547 0.19589 -0.17605 -0.16566

D73 D80 D5 D6 A14

1 0.15562 -0.14833 -0.12200 -0.11189 0.10865

RFO step: Lambda0=5.733253241D-03 Lambda=-2.29162639D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.408

Iteration 1 RMS(Cart)= 0.03801697 RMS(Int)= 0.00507779

Iteration 2 RMS(Cart)= 0.00821490 RMS(Int)= 0.00017333

Iteration 3 RMS(Cart)= 0.00001246 RMS(Int)= 0.00017309

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00017309

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.52234 0.03048 0.00000 0.04707 0.04690 2.56925

R2 2.66989 0.01125 0.00000 0.00778 0.00766 2.67755

R3 2.07951 0.00183 0.00000 -0.00065 -0.00065 2.07886

R4 2.80745 -0.00536 0.00000 -0.01656 -0.01658 2.79087

R5 2.08359 0.00078 0.00000 -0.00023 -0.00023 2.08337

R6 6.29120 0.00044 0.00000 -0.26881 -0.26910 6.02210

R7 2.65503 -0.01285 0.00000 -0.01529 -0.01521 2.63982

R8 2.83509 0.00407 0.00000 0.01167 0.01161 2.84671

R9 2.11318 -0.00131 0.00000 -0.00012 -0.00012 2.11305

R10 3.53537 0.01128 0.00000 -0.06129 -0.06084 3.47454

R11 2.07498 0.00166 0.00000 0.00110 0.00110 2.07608

R12 2.12323 -0.00023 0.00000 0.00105 0.00105 2.12428

R13 2.13346 -0.00055 0.00000 -0.00084 -0.00084 2.13262

R14 2.87245 0.00211 0.00000 -0.00118 -0.00128 2.87118

R15 2.12260 -0.00010 0.00000 0.00058 0.00058 2.12318

R16 2.12967 -0.00001 0.00000 -0.00098 -0.00098 2.12869

R17 2.63321 0.00076 0.00000 0.00007 0.00022 2.63343

R18 2.69790 0.00079 0.00000 0.00166 0.00169 2.69960

R19 2.62777 0.00924 0.00000 0.02629 0.02660 2.65437

R20 2.86183 0.00309 0.00000 0.00326 0.00332 2.86515

R21 2.09143 -0.00010 0.00000 -0.00074 -0.00074 2.09069

R22 2.75591 0.00427 0.00000 -0.02829 -0.02841 2.72751

R23 2.05194 0.00073 0.00000 0.00068 0.00068 2.05262

R24 2.30802 -0.00043 0.00000 -0.00044 -0.00044 2.30758

R25 2.30720 -0.00020 0.00000 0.00068 0.00068 2.30787

A1 2.09133 -0.00380 0.00000 0.00219 0.00208 2.09340

A2 2.09232 0.00580 0.00000 0.02236 0.02240 2.11472

A3 2.09952 -0.00199 0.00000 -0.02450 -0.02446 2.07506

A4 2.14600 -0.00301 0.00000 -0.01263 -0.01264 2.13336

A5 2.11109 0.00252 0.00000 0.01019 0.01014 2.12123

A6 1.35780 -0.00236 0.00000 -0.00410 -0.00433 1.35347

A7 2.02414 0.00058 0.00000 0.00086 0.00061 2.02475

A8 1.49616 0.00023 0.00000 0.02287 0.02287 1.51903

A9 1.93800 0.00002 0.00000 0.00029 0.00067 1.93866

A10 2.06156 0.00372 0.00000 -0.00409 -0.00427 2.05729

A11 2.03635 -0.00220 0.00000 0.00414 0.00430 2.04065

A12 1.79512 -0.00118 0.00000 -0.02661 -0.02648 1.76864

A13 1.94368 0.00123 0.00000 -0.00617 -0.00631 1.93736

A14 1.92178 -0.00424 0.00000 -0.00096 -0.00137 1.92041

A15 1.64623 0.00124 0.00000 0.04118 0.04129 1.68752

A16 2.09592 0.00071 0.00000 -0.00294 -0.00288 2.09304

A17 2.07098 0.00180 0.00000 0.02569 0.02557 2.09655

A18 2.11620 -0.00253 0.00000 -0.02298 -0.02308 2.09312

A19 1.91706 -0.00120 0.00000 -0.00545 -0.00541 1.91164

A20 1.85933 0.00074 0.00000 0.00367 0.00359 1.86292

A21 2.00350 0.00050 0.00000 0.00130 0.00135 2.00485

A22 1.85137 0.00027 0.00000 0.00146 0.00148 1.85285

A23 1.92975 0.00076 0.00000 -0.00300 -0.00324 1.92652

A24 1.89520 -0.00109 0.00000 0.00248 0.00266 1.89786

A25 2.01212 0.00375 0.00000 0.00842 0.00842 2.02053

A26 1.93045 -0.00031 0.00000 -0.00430 -0.00433 1.92612

A27 1.85122 -0.00160 0.00000 0.00131 0.00134 1.85256

A28 1.91183 -0.00217 0.00000 -0.00685 -0.00689 1.90493

A29 1.89632 -0.00039 0.00000 0.00073 0.00076 1.89709

A30 1.85416 0.00054 0.00000 0.00056 0.00056 1.85473

A31 1.87733 0.00166 0.00000 0.00221 0.00232 1.87965

A32 2.00179 -0.00229 0.00000 -0.01947 -0.01917 1.98263

A33 1.77923 0.00186 0.00000 0.00096 0.00087 1.78011

A34 1.70232 -0.00259 0.00000 0.01121 0.01109 1.71341

A35 1.84006 -0.00157 0.00000 -0.00452 -0.00482 1.83524

A36 2.09070 0.00369 0.00000 0.01074 0.01085 2.10154

A37 2.02778 0.00049 0.00000 -0.00116 -0.00111 2.02668

A38 1.59625 0.00304 0.00000 0.04360 0.04379 1.64004

A39 1.92875 -0.00339 0.00000 -0.02630 -0.02655 1.90220

A40 1.40427 -0.00118 0.00000 -0.01355 -0.01350 1.39077

A41 1.90685 -0.00124 0.00000 -0.00069 -0.00042 1.90644

A42 2.23145 0.00060 0.00000 -0.00159 -0.00159 2.22987

A43 2.12753 0.00096 0.00000 0.00122 0.00093 2.12846

A44 1.90535 0.00098 0.00000 -0.00383 -0.00375 1.90160

A45 2.05181 -0.00077 0.00000 0.00314 0.00310 2.05491

A46 2.32486 -0.00021 0.00000 0.00097 0.00092 2.32578

A47 1.89339 0.00015 0.00000 0.00702 0.00684 1.90023

A48 2.00345 -0.00013 0.00000 -0.00525 -0.00517 1.99829

A49 2.38605 -0.00003 0.00000 -0.00186 -0.00177 2.38427

D1 -0.34126 0.00289 0.00000 -0.00617 -0.00621 -0.34746

D2 2.87029 0.00123 0.00000 0.02186 0.02170 2.89199

D3 0.99629 0.00262 0.00000 0.02422 0.02378 1.02006

D4 2.79267 0.00404 0.00000 0.00064 0.00085 2.79352

D5 -0.27897 0.00237 0.00000 0.02867 0.02875 -0.25022

D6 -2.15298 0.00376 0.00000 0.03103 0.03083 -2.12214

D7 -0.10918 -0.00003 0.00000 -0.00709 -0.00715 -0.11633

D8 3.04643 0.00203 0.00000 0.01186 0.01213 3.05856

D9 3.04012 -0.00121 0.00000 -0.01414 -0.01425 3.02586

D10 -0.08746 0.00085 0.00000 0.00481 0.00502 -0.08243

D11 2.54142 -0.00281 0.00000 0.00258 0.00230 2.54372

D12 -1.74395 -0.00268 0.00000 0.00357 0.00328 -1.74067

D13 0.35431 -0.00323 0.00000 0.01009 0.01003 0.36434

D14 -0.66690 -0.00114 0.00000 -0.02378 -0.02376 -0.69066

D15 1.33092 -0.00101 0.00000 -0.02279 -0.02278 1.30814

D16 -2.85401 -0.00156 0.00000 -0.01627 -0.01603 -2.87003

D17 1.27648 -0.00094 0.00000 -0.01207 -0.01151 1.26498

D18 -3.00888 -0.00081 0.00000 -0.01108 -0.01053 -3.01941

D19 -0.91062 -0.00136 0.00000 -0.00455 -0.00378 -0.91440

D20 -1.06874 0.00139 0.00000 0.01039 0.01015 -1.05859

D21 -3.00965 0.00207 0.00000 -0.00225 -0.00201 -3.01166

D22 1.16846 0.00153 0.00000 0.00167 0.00146 1.16993

D23 1.11382 -0.00127 0.00000 -0.00914 -0.00918 1.10464

D24 -0.82709 -0.00059 0.00000 -0.02178 -0.02134 -0.84843

D25 -2.93217 -0.00113 0.00000 -0.01786 -0.01787 -2.95003

D26 -3.14097 -0.00055 0.00000 0.00078 0.00068 -3.14028

D27 1.20131 0.00013 0.00000 -0.01186 -0.01148 1.18983

D28 -0.90377 -0.00041 0.00000 -0.00793 -0.00800 -0.91177

D29 0.51064 -0.00272 0.00000 0.01148 0.01155 0.52219

D30 -2.64534 -0.00480 0.00000 -0.00757 -0.00729 -2.65263

D31 2.90079 0.00135 0.00000 0.00090 0.00075 2.90154

D32 -0.25519 -0.00073 0.00000 -0.01815 -0.01809 -0.27328

D33 -1.60908 0.00139 0.00000 0.03551 0.03546 -1.57362

D34 1.51812 -0.00069 0.00000 0.01647 0.01662 1.53474

D35 -0.45750 0.00063 0.00000 -0.00921 -0.00940 -0.46691

D36 -2.63822 0.00089 0.00000 -0.00295 -0.00301 -2.64124

D37 1.64167 0.00128 0.00000 -0.00222 -0.00228 1.63939

D38 -2.88485 -0.00177 0.00000 -0.00329 -0.00346 -2.88830

D39 1.21762 -0.00151 0.00000 0.00297 0.00293 1.22055

D40 -0.78567 -0.00112 0.00000 0.00370 0.00367 -0.78201

D41 1.59607 -0.00172 0.00000 -0.04818 -0.04824 1.54783

D42 -0.58465 -0.00147 0.00000 -0.04191 -0.04185 -0.62650

D43 -2.58794 -0.00108 0.00000 -0.04119 -0.04112 -2.62906

D44 1.09687 0.00360 0.00000 0.00407 0.00434 1.10121

D45 3.07540 0.00187 0.00000 -0.00906 -0.00887 3.06653

D46 -1.13300 0.00207 0.00000 -0.00650 -0.00627 -1.13928

D47 -1.11535 0.00223 0.00000 0.02621 0.02627 -1.08908

D48 0.86318 0.00050 0.00000 0.01309 0.01306 0.87624

D49 2.93796 0.00070 0.00000 0.01565 0.01566 2.95362

D50 -3.11599 0.00142 0.00000 0.01520 0.01510 -3.10088

D51 -1.13746 -0.00032 0.00000 0.00207 0.00189 -1.13556

D52 0.93732 -0.00012 0.00000 0.00463 0.00449 0.94181

D53 0.04952 -0.00145 0.00000 -0.00685 -0.00678 0.04274

D54 2.23987 -0.00078 0.00000 -0.01184 -0.01190 2.22798

D55 -2.02480 -0.00154 0.00000 -0.01449 -0.01455 -2.03934

D56 -2.13094 -0.00084 0.00000 0.00198 0.00213 -2.12882

D57 0.05941 -0.00018 0.00000 -0.00302 -0.00299 0.05642

D58 2.07793 -0.00093 0.00000 -0.00567 -0.00564 2.07228

D59 2.12784 -0.00096 0.00000 0.00044 0.00060 2.12844

D60 -1.96499 -0.00030 0.00000 -0.00455 -0.00452 -1.96951

D61 0.05352 -0.00105 0.00000 -0.00720 -0.00717 0.04635

D62 0.04432 0.00040 0.00000 -0.00581 -0.00586 0.03846

D63 -3.05217 0.00041 0.00000 -0.01131 -0.01141 -3.06357

D64 -0.05786 -0.00039 0.00000 0.00315 0.00320 -0.05466

D65 3.10526 -0.00019 0.00000 0.00670 0.00673 3.11199

D66 -0.04044 0.00291 0.00000 -0.00288 -0.00287 -0.04332

D67 1.92029 0.00024 0.00000 -0.01430 -0.01421 1.90608

D68 -1.41986 0.00209 0.00000 -0.02014 -0.02006 -1.43992

D69 -1.98291 0.00271 0.00000 0.00794 0.00782 -1.97509

D70 -0.02217 0.00004 0.00000 -0.00348 -0.00352 -0.02569

D71 2.92086 0.00189 0.00000 -0.00932 -0.00937 2.91149

D72 1.97433 0.00024 0.00000 0.00452 0.00452 1.97886

D73 -2.34812 -0.00243 0.00000 -0.00689 -0.00681 -2.35493

D74 0.59491 -0.00058 0.00000 -0.01273 -0.01266 0.58225

D75 -2.10968 0.00214 0.00000 0.02879 0.02856 -2.08112

D76 0.97704 0.00212 0.00000 0.03552 0.03535 1.01240

D77 -0.01372 -0.00022 0.00000 0.00571 0.00574 -0.00798

D78 3.07300 -0.00024 0.00000 0.01244 0.01253 3.08553

D79 2.34655 0.00395 0.00000 0.01556 0.01550 2.36205

D80 -0.84992 0.00393 0.00000 0.02229 0.02230 -0.82762

D81 1.78114 0.00170 0.00000 0.03897 0.03895 1.82010

D82 -1.38895 0.00144 0.00000 0.03426 0.03425 -1.35469

D83 0.05022 0.00017 0.00000 0.00024 0.00025 0.05046

D84 -3.11987 -0.00009 0.00000 -0.00447 -0.00446 -3.12433

D85 -2.90687 -0.00153 0.00000 0.00602 0.00602 -2.90085

D86 0.20623 -0.00179 0.00000 0.00131 0.00132 0.20755

Item Value Threshold Converged?

Maximum Force 0.030477 0.000450 NO

RMS Force 0.003543 0.000300 NO

Maximum Displacement 0.154741 0.001800 NO

RMS Displacement 0.045261 0.001200 NO

Predicted change in Energy=-3.907505D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.235655 1.389523 0.319531

2 6 0 -0.133588 0.911074 -0.316872

3 6 0 -0.520095 3.673972 -0.130970

4 6 0 -1.479257 2.784749 0.359655

5 1 0 -1.950178 0.710930 0.808566

6 1 0 -2.407129 3.169882 0.804271

7 6 0 0.598925 1.702347 -1.326053

8 1 0 1.696917 1.470375 -1.260878

9 1 0 0.259462 1.333617 -2.337187

10 6 0 0.369686 3.202456 -1.251345

11 1 0 1.363200 3.725311 -1.207910

12 1 0 -0.123258 3.540377 -2.206181

13 1 0 -0.846803 4.730512 -0.296229

14 1 0 0.210155 -0.126574 -0.173449

15 8 0 2.815183 4.232311 1.042970

16 6 0 0.481881 3.993099 1.377281

17 6 0 1.126690 2.849354 1.876344

18 6 0 1.593792 4.870856 0.836931

19 8 0 1.604500 5.943258 0.253004

20 6 0 2.546286 2.963595 1.642014

21 8 0 3.537598 2.280751 1.848254

22 1 0 -0.294737 4.504552 1.976680

23 1 0 0.710027 2.076679 2.516032

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.359586 0.000000

3 C 2.435915 2.795988 0.000000

4 C 1.416900 2.403991 1.396933 0.000000

5 H 1.100085 2.146315 3.421620 2.173480 0.000000

6 H 2.185636 3.395315 2.165567 1.098617 2.501054

7 C 2.484249 1.476867 2.562759 2.886529 3.469501

8 H 3.332298 2.134178 3.323804 3.800235 4.261532

9 H 3.049040 2.101119 3.309435 3.521630 3.894356

10 C 2.886433 2.525263 1.506412 2.487647 3.979033

11 H 3.813532 3.309721 2.170077 3.379568 4.912346

12 H 3.498974 3.237720 2.117033 2.998870 4.520189

13 H 3.419441 3.885513 1.118180 2.148529 4.312198

14 H 2.152196 1.102471 3.870299 3.407948 2.516507

15 O 5.001409 4.644894 3.579658 4.583074 5.929902

16 C 3.293535 3.570411 1.838646 2.518280 4.124437

17 C 3.183622 3.186759 2.724189 3.015871 3.896168

18 C 4.515878 4.471575 2.614935 3.744766 5.464935

19 O 5.367253 5.354306 3.132252 4.415553 6.349933

20 C 4.304619 3.902795 3.612589 4.228644 5.097776

21 O 5.090700 4.476761 4.724749 5.257259 5.801807

22 H 3.651694 4.266080 2.276584 2.641132 4.300761

23 H 3.013715 3.177368 3.327335 3.153457 3.443457

6 7 8 9 10

6 H 0.000000

7 C 3.965893 0.000000

8 H 4.898608 1.124119 0.000000

9 H 4.511245 1.128534 1.800950 0.000000

10 C 3.455042 1.519361 2.182140 2.164200 0.000000

11 H 4.309612 2.165747 2.280112 2.865956 1.123537

12 H 3.796861 2.162066 2.914025 2.243530 1.126453

13 H 2.466025 3.510051 4.246123 4.114393 2.174178

14 H 4.321196 2.196495 2.437869 2.610814 3.502820

15 O 5.334630 4.113975 3.766501 5.134160 3.507840

16 C 3.058171 3.545315 3.847119 4.573793 2.747249

17 C 3.706745 3.442312 3.474033 4.561073 3.237310

18 C 4.347615 3.963296 3.996838 4.936347 2.939880

19 O 4.908022 4.635724 4.723036 5.455915 3.361522

20 C 5.027991 3.767278 3.373117 4.870363 3.628522

21 O 6.100839 4.364238 3.702906 5.400106 4.526888

22 H 2.760088 4.422559 4.863609 5.382510 3.543594

23 H 3.720468 3.861876 3.950520 4.930404 3.946686

11 12 13 14 15

11 H 0.000000

12 H 1.800085 0.000000

13 H 2.593397 2.363865 0.000000

14 H 4.151703 4.205912 4.972275 0.000000

15 O 2.726126 4.435109 3.930878 5.221659 0.000000

16 C 2.744384 3.662288 2.260490 4.410249 2.369236

17 C 3.214944 4.325148 3.486188 3.727980 2.336256

18 C 2.355169 3.738846 2.694486 5.282956 1.393552

19 O 2.666793 3.847932 2.789498 6.242509 2.239897

20 C 3.178360 4.718872 4.288571 4.278148 1.428566

21 O 4.019316 5.605976 5.461054 4.577594 2.231357

22 H 3.673906 4.295971 2.349882 5.130818 3.258455

23 H 4.124605 5.013589 4.168376 3.512478 3.353855

16 17 18 19 20

16 C 0.000000

17 C 1.404633 0.000000

18 C 1.516174 2.320568 0.000000

19 O 2.515431 3.526440 1.221119 0.000000

20 C 2.322009 1.443335 2.278826 3.419752 0.000000

21 O 3.534311 2.477212 3.392610 4.437978 1.221274

22 H 1.106345 2.184079 2.236012 2.940754 3.249302

23 H 2.240863 1.086202 3.377551 4.568568 2.218642

21 22 23

21 O 0.000000

22 H 4.432671 0.000000

23 H 2.912513 2.682353 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.589363 -0.464652 -0.783461

2 6 0 2.255428 -1.183172 0.321388

3 6 0 0.989220 1.262812 -0.159687

4 6 0 2.006679 0.808259 -1.002054

5 1 0 3.309543 -0.852913 -1.518840

6 1 0 2.331665 1.424928 -1.851207

7 6 0 1.656688 -0.556580 1.517226

8 1 0 0.929175 -1.270553 1.991157

9 1 0 2.491582 -0.417291 2.263643

10 6 0 0.993689 0.787937 1.269911

11 1 0 -0.053311 0.762859 1.676725

12 1 0 1.542628 1.575136 1.859725

13 1 0 0.728831 2.348548 -0.220522

14 1 0 2.501013 -2.254400 0.408572

15 8 0 -2.267905 -0.128183 0.360145

16 6 0 -0.505523 0.635200 -1.027133

17 6 0 -0.563608 -0.766072 -1.104970

18 6 0 -1.613276 1.025080 -0.068145

19 8 0 -1.979120 2.092693 0.398215

20 6 0 -1.607363 -1.247824 -0.232213

21 8 0 -2.064731 -2.333679 0.089104

22 1 0 -0.420831 1.244131 -1.946932

23 1 0 -0.074035 -1.413013 -1.827203

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2346566 0.7323973 0.6011013

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 460.4410333176 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.315672633251E-01 A.U. after 15 cycles

Convg = 0.2887D-08 -V/T = 0.9993

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001452188 -0.000695117 -0.000050784

2 6 -0.000594315 -0.001347662 -0.000575772

3 6 -0.006248212 0.001136488 -0.011991762

4 6 -0.003991058 -0.000484100 -0.007714697

5 1 0.002162476 -0.000010527 0.004887196

6 1 0.000239713 -0.000586033 0.004676572

7 6 0.002608075 0.001321166 0.002873570

8 1 0.000466078 0.001243885 0.000478171

9 1 0.000596811 -0.000749668 0.000050520

10 6 0.001777600 -0.000082617 0.001598118

11 1 -0.000186337 0.000124426 0.000235785

12 1 0.000382915 -0.000191585 -0.000256874

13 1 0.001143331 -0.000321212 0.001748178

14 1 -0.002152577 -0.000751216 -0.001387758

15 8 0.000086671 0.002024160 -0.003052193

16 6 0.004199052 0.003619596 0.011659677

17 6 -0.010838872 0.000262059 0.006830637

18 6 0.002413305 -0.002012254 -0.002013264

19 8 0.000303059 0.001306651 0.002432564

20 6 0.011660706 -0.000214723 -0.003635094

21 8 0.002348622 -0.001193341 -0.000090246

22 1 -0.002877202 -0.000394564 -0.003263687

23 1 -0.002047652 -0.002003815 -0.003438857

-------------------------------------------------------------------

Cartesian Forces: Max 0.011991762 RMS 0.003640311

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.013934675 RMS 0.001725581

Search for a saddle point.

Step number 18 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 17 18

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06065 -0.00598 0.00194 0.00348 0.00589

Eigenvalues --- 0.00894 0.01028 0.01344 0.01639 0.01731

Eigenvalues --- 0.02010 0.02171 0.02318 0.02417 0.02513

Eigenvalues --- 0.02667 0.02879 0.03032 0.03183 0.03260

Eigenvalues --- 0.03612 0.03732 0.03848 0.03873 0.04234

Eigenvalues --- 0.04456 0.04619 0.05169 0.05561 0.05946

Eigenvalues --- 0.06258 0.07325 0.08038 0.08641 0.09680

Eigenvalues --- 0.11321 0.13017 0.13910 0.15213 0.18803

Eigenvalues --- 0.22010 0.23557 0.24948 0.25805 0.27682

Eigenvalues --- 0.28776 0.30522 0.31162 0.31308 0.31837

Eigenvalues --- 0.31932 0.32296 0.32648 0.34318 0.35637

Eigenvalues --- 0.37339 0.39574 0.40309 0.42533 0.43254

Eigenvalues --- 0.48254 1.08341 1.10819

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 0.62562 0.41238 -0.18769 0.16816 0.16581

D73 D80 D5 D35 D6

1 -0.15697 0.14708 0.11390 0.10506 0.10278

RFO step: Lambda0=2.341520040D-03 Lambda=-1.27659241D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.359

Iteration 1 RMS(Cart)= 0.03973658 RMS(Int)= 0.00565840

Iteration 2 RMS(Cart)= 0.00929710 RMS(Int)= 0.00021595

Iteration 3 RMS(Cart)= 0.00001575 RMS(Int)= 0.00021566

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00021566

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.56925 0.00144 0.00000 -0.00543 -0.00520 2.56404

R2 2.67755 0.00153 0.00000 -0.02109 -0.02073 2.65682

R3 2.07886 0.00077 0.00000 -0.00029 -0.00029 2.07857

R4 2.79087 0.00124 0.00000 -0.00308 -0.00315 2.78773

R5 2.08337 -0.00014 0.00000 -0.00112 -0.00112 2.08225

R6 6.02210 -0.00094 0.00000 -0.27682 -0.27739 5.74471

R7 2.63982 0.00331 0.00000 0.01745 0.01763 2.65745

R8 2.84671 -0.00054 0.00000 -0.00214 -0.00211 2.84459

R9 2.11305 -0.00090 0.00000 -0.00360 -0.00360 2.10946

R10 3.47454 0.00829 0.00000 0.01537 0.01586 3.49040

R11 2.07608 0.00148 0.00000 -0.00036 -0.00036 2.07572

R12 2.12428 0.00023 0.00000 0.00073 0.00073 2.12500

R13 2.13262 0.00002 0.00000 -0.00026 -0.00026 2.13236

R14 2.87118 0.00026 0.00000 0.00046 0.00043 2.87160

R15 2.12318 -0.00010 0.00000 0.00056 0.00056 2.12373

R16 2.12869 -0.00001 0.00000 -0.00042 -0.00042 2.12827

R17 2.63343 0.00007 0.00000 -0.00239 -0.00227 2.63116

R18 2.69960 0.00165 0.00000 -0.00086 -0.00076 2.69884

R19 2.65437 0.00073 0.00000 0.02401 0.02378 2.67815

R20 2.86515 0.00299 0.00000 0.00290 0.00287 2.86802

R21 2.09069 0.00007 0.00000 -0.00010 -0.00010 2.09059

R22 2.72751 0.01393 0.00000 0.03169 0.03164 2.75915

R23 2.05262 0.00019 0.00000 -0.00163 -0.00163 2.05099

R24 2.30758 -0.00001 0.00000 0.00069 0.00069 2.30827

R25 2.30787 0.00256 0.00000 0.00053 0.00053 2.30841

A1 2.09340 -0.00057 0.00000 0.00225 0.00245 2.09585

A2 2.11472 0.00044 0.00000 -0.03768 -0.03788 2.07684

A3 2.07506 0.00013 0.00000 0.03544 0.03521 2.11027

A4 2.13336 0.00043 0.00000 0.00469 0.00429 2.13765

A5 2.12123 -0.00059 0.00000 -0.01237 -0.01221 2.10902

A6 1.35347 0.00103 0.00000 0.02119 0.02119 1.37465

A7 2.02475 0.00024 0.00000 0.00604 0.00611 2.03086

A8 1.51903 -0.00143 0.00000 0.01506 0.01490 1.53393

A9 1.93866 -0.00040 0.00000 -0.02027 -0.02013 1.91854

A10 2.05729 0.00091 0.00000 -0.00278 -0.00321 2.05408

A11 2.04065 0.00005 0.00000 0.00213 0.00230 2.04295

A12 1.76864 -0.00033 0.00000 -0.01326 -0.01357 1.75507

A13 1.93736 0.00078 0.00000 0.00678 0.00696 1.94432

A14 1.92041 -0.00224 0.00000 -0.02255 -0.02245 1.89796

A15 1.68752 0.00013 0.00000 0.03032 0.03023 1.71775

A16 2.09304 -0.00029 0.00000 -0.00589 -0.00602 2.08702

A17 2.09655 -0.00127 0.00000 -0.01262 -0.01306 2.08350

A18 2.09312 0.00149 0.00000 0.01703 0.01645 2.10957

A19 1.91164 -0.00013 0.00000 0.00555 0.00551 1.91715

A20 1.86292 -0.00015 0.00000 -0.00032 -0.00039 1.86254

A21 2.00485 0.00094 0.00000 -0.00261 -0.00246 2.00239

A22 1.85285 0.00018 0.00000 0.00111 0.00114 1.85399

A23 1.92652 -0.00031 0.00000 -0.00720 -0.00724 1.91928

A24 1.89786 -0.00058 0.00000 0.00401 0.00397 1.90183

A25 2.02053 -0.00033 0.00000 -0.00482 -0.00457 2.01596

A26 1.92612 0.00005 0.00000 -0.00249 -0.00261 1.92351

A27 1.85256 0.00025 0.00000 0.00731 0.00726 1.85983

A28 1.90493 0.00026 0.00000 -0.00115 -0.00125 1.90368

A29 1.89709 -0.00014 0.00000 0.00225 0.00218 1.89926

A30 1.85473 -0.00008 0.00000 -0.00044 -0.00040 1.85432

A31 1.87965 0.00034 0.00000 0.00520 0.00517 1.88482

A32 1.98263 -0.00141 0.00000 -0.01912 -0.01886 1.96377

A33 1.78011 0.00067 0.00000 0.01284 0.01270 1.79280

A34 1.71341 -0.00064 0.00000 0.01264 0.01254 1.72594

A35 1.83524 -0.00031 0.00000 -0.00584 -0.00586 1.82938

A36 2.10154 0.00112 0.00000 0.00038 0.00032 2.10186

A37 2.02668 0.00038 0.00000 0.00089 0.00087 2.02754

A38 1.64004 0.00166 0.00000 0.03922 0.03893 1.67897

A39 1.90220 -0.00071 0.00000 -0.01644 -0.01612 1.88608

A40 1.39077 -0.00229 0.00000 -0.02088 -0.02036 1.37041

A41 1.90644 -0.00111 0.00000 -0.00495 -0.00480 1.90164

A42 2.22987 -0.00017 0.00000 -0.01714 -0.01702 2.21285

A43 2.12846 0.00160 0.00000 0.02120 0.02094 2.14940

A44 1.90160 0.00293 0.00000 0.01009 0.00994 1.91153

A45 2.05491 -0.00165 0.00000 -0.00463 -0.00457 2.05034

A46 2.32578 -0.00128 0.00000 -0.00511 -0.00505 2.32073

A47 1.90023 -0.00186 0.00000 -0.00393 -0.00412 1.89611

A48 1.99829 0.00031 0.00000 0.00214 0.00223 2.00051

A49 2.38427 0.00155 0.00000 0.00196 0.00204 2.38632

D1 -0.34746 0.00240 0.00000 0.00734 0.00741 -0.34005

D2 2.89199 0.00135 0.00000 0.02773 0.02776 2.91975

D3 1.02006 0.00120 0.00000 0.03887 0.03882 1.05888

D4 2.79352 0.00352 0.00000 0.03056 0.03012 2.82364

D5 -0.25022 0.00247 0.00000 0.05095 0.05047 -0.19975

D6 -2.12214 0.00232 0.00000 0.06209 0.06153 -2.06062

D7 -0.11633 -0.00076 0.00000 -0.02268 -0.02270 -0.13903

D8 3.05856 0.00184 0.00000 0.02836 0.02785 3.08641

D9 3.02586 -0.00185 0.00000 -0.04535 -0.04583 2.98004

D10 -0.08243 0.00074 0.00000 0.00569 0.00473 -0.07771

D11 2.54372 -0.00126 0.00000 -0.00387 -0.00381 2.53991

D12 -1.74067 -0.00120 0.00000 0.00000 0.00004 -1.74063

D13 0.36434 -0.00145 0.00000 0.00322 0.00325 0.36759

D14 -0.69066 -0.00031 0.00000 -0.02417 -0.02427 -0.71493

D15 1.30814 -0.00024 0.00000 -0.02031 -0.02042 1.28772

D16 -2.87003 -0.00049 0.00000 -0.01708 -0.01721 -2.88724

D17 1.26498 -0.00145 0.00000 -0.03844 -0.03838 1.22660

D18 -3.01941 -0.00138 0.00000 -0.03458 -0.03453 -3.05394

D19 -0.91440 -0.00163 0.00000 -0.03136 -0.03131 -0.94571

D20 -1.05859 -0.00013 0.00000 0.01062 0.01058 -1.04801

D21 -3.01166 0.00056 0.00000 0.00383 0.00402 -3.00764

D22 1.16993 -0.00047 0.00000 -0.01264 -0.01285 1.15708

D23 1.10464 0.00053 0.00000 0.00652 0.00673 1.11137

D24 -0.84843 0.00122 0.00000 -0.00027 0.00017 -0.84826

D25 -2.95003 0.00019 0.00000 -0.01673 -0.01670 -2.96673

D26 -3.14028 0.00016 0.00000 0.01639 0.01639 -3.12389

D27 1.18983 0.00085 0.00000 0.00960 0.00983 1.19966

D28 -0.91177 -0.00018 0.00000 -0.00687 -0.00704 -0.91881

D29 0.52219 -0.00077 0.00000 0.02657 0.02658 0.54877

D30 -2.65263 -0.00341 0.00000 -0.02494 -0.02532 -2.67795

D31 2.90154 0.00181 0.00000 0.03739 0.03740 2.93894

D32 -0.27328 -0.00084 0.00000 -0.01412 -0.01450 -0.28778

D33 -1.57362 0.00179 0.00000 0.06597 0.06571 -1.50791

D34 1.53474 -0.00086 0.00000 0.01446 0.01381 1.54855

D35 -0.46691 0.00128 0.00000 -0.01459 -0.01462 -0.48152

D36 -2.64124 0.00115 0.00000 -0.00714 -0.00720 -2.64844

D37 1.63939 0.00109 0.00000 -0.00936 -0.00938 1.63000

D38 -2.88830 -0.00084 0.00000 -0.02319 -0.02325 -2.91156

D39 1.22055 -0.00098 0.00000 -0.01575 -0.01584 1.20471

D40 -0.78201 -0.00104 0.00000 -0.01797 -0.01802 -0.80003

D41 1.54783 -0.00025 0.00000 -0.05086 -0.05073 1.49710

D42 -0.62650 -0.00038 0.00000 -0.04342 -0.04332 -0.66981

D43 -2.62906 -0.00045 0.00000 -0.04564 -0.04550 -2.67456

D44 1.10121 0.00006 0.00000 -0.00652 -0.00651 1.09470

D45 3.06653 -0.00051 0.00000 -0.01400 -0.01410 3.05243

D46 -1.13928 -0.00013 0.00000 -0.00535 -0.00523 -1.14451

D47 -1.08908 0.00031 0.00000 0.01601 0.01567 -1.07341

D48 0.87624 -0.00025 0.00000 0.00853 0.00808 0.88432

D49 2.95362 0.00013 0.00000 0.01718 0.01695 2.97057

D50 -3.10088 0.00006 0.00000 0.00141 0.00134 -3.09954

D51 -1.13556 -0.00050 0.00000 -0.00607 -0.00625 -1.14182

D52 0.94181 -0.00012 0.00000 0.00258 0.00262 0.94443

D53 0.04274 -0.00017 0.00000 0.00197 0.00202 0.04476

D54 2.22798 -0.00014 0.00000 -0.00604 -0.00599 2.22199

D55 -2.03934 -0.00017 0.00000 -0.00597 -0.00595 -2.04530

D56 -2.12882 -0.00046 0.00000 0.00240 0.00239 -2.12642

D57 0.05642 -0.00043 0.00000 -0.00562 -0.00561 0.05080

D58 2.07228 -0.00046 0.00000 -0.00554 -0.00558 2.06670

D59 2.12844 -0.00017 0.00000 0.00276 0.00279 2.13123

D60 -1.96951 -0.00014 0.00000 -0.00525 -0.00522 -1.97473

D61 0.04635 -0.00017 0.00000 -0.00518 -0.00518 0.04117

D62 0.03846 -0.00023 0.00000 -0.01922 -0.01936 0.01911

D63 -3.06357 -0.00016 0.00000 -0.02670 -0.02683 -3.09041

D64 -0.05466 0.00002 0.00000 0.01281 0.01271 -0.04195

D65 3.11199 0.00002 0.00000 0.00724 0.00718 3.11917

D66 -0.04332 -0.00025 0.00000 -0.00466 -0.00494 -0.04826

D67 1.90608 -0.00058 0.00000 -0.00767 -0.00767 1.89842

D68 -1.43992 0.00135 0.00000 -0.00970 -0.00952 -1.44944

D69 -1.97509 -0.00022 0.00000 -0.00783 -0.00817 -1.98326

D70 -0.02569 -0.00055 0.00000 -0.01084 -0.01089 -0.03658

D71 2.91149 0.00138 0.00000 -0.01287 -0.01274 2.89875

D72 1.97886 -0.00150 0.00000 -0.00328 -0.00354 1.97532

D73 -2.35493 -0.00183 0.00000 -0.00630 -0.00626 -2.36119

D74 0.58225 0.00010 0.00000 -0.00832 -0.00811 0.57414

D75 -2.08112 0.00198 0.00000 0.03714 0.03706 -2.04406

D76 1.01240 0.00192 0.00000 0.04635 0.04624 1.05863

D77 -0.00798 0.00058 0.00000 0.01915 0.01923 0.01125

D78 3.08553 0.00052 0.00000 0.02836 0.02841 3.11395

D79 2.36205 0.00222 0.00000 0.01475 0.01473 2.37678

D80 -0.82762 0.00215 0.00000 0.02397 0.02391 -0.80371

D81 1.82010 0.00150 0.00000 0.03502 0.03493 1.85502

D82 -1.35469 0.00145 0.00000 0.04237 0.04223 -1.31246

D83 0.05046 0.00038 0.00000 -0.00060 -0.00047 0.04999

D84 -3.12433 0.00033 0.00000 0.00675 0.00683 -3.11749

D85 -2.90085 -0.00121 0.00000 0.00639 0.00644 -2.89441

D86 0.20755 -0.00125 0.00000 0.01373 0.01374 0.22129

Item Value Threshold Converged?

Maximum Force 0.013935 0.000450 NO

RMS Force 0.001726 0.000300 NO

Maximum Displacement 0.192254 0.001800 NO

RMS Displacement 0.047489 0.001200 NO

Predicted change in Energy=-3.246875D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.219542 1.420575 0.348388

2 6 0 -0.101094 0.951249 -0.259725

3 6 0 -0.544331 3.699486 -0.158234

4 6 0 -1.503157 2.797549 0.336480

5 1 0 -1.883240 0.711439 0.864603

6 1 0 -2.437588 3.159119 0.786637

7 6 0 0.626639 1.723367 -1.284644

8 1 0 1.730220 1.524660 -1.200196

9 1 0 0.308238 1.313525 -2.286606

10 6 0 0.365326 3.220073 -1.257596

11 1 0 1.347933 3.763678 -1.213171

12 1 0 -0.118175 3.522077 -2.228893

13 1 0 -0.878910 4.749618 -0.335294

14 1 0 0.245267 -0.080384 -0.086786

15 8 0 2.806806 4.189313 1.009743

16 6 0 0.463667 3.989491 1.362091

17 6 0 1.094970 2.809281 1.827990

18 6 0 1.596955 4.859834 0.850673

19 8 0 1.628131 5.961271 0.323521

20 6 0 2.529918 2.908251 1.577077

21 8 0 3.513130 2.203423 1.746517

22 1 0 -0.300873 4.497190 1.979835

23 1 0 0.653309 2.038925 2.452045

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.356832 0.000000

3 C 2.430229 2.785599 0.000000

4 C 1.405929 2.393755 1.406264 0.000000

5 H 1.099930 2.120770 3.430349 2.185230 0.000000

6 H 2.167542 3.380646 2.183850 1.098425 2.510880

7 C 2.483316 1.475201 2.558322 2.884083 3.455828

8 H 3.333173 2.137053 3.314986 3.799519 4.240497

9 H 3.047747 2.099295 3.309026 3.516256 3.885254

10 C 2.886032 2.522073 1.505293 2.492153 3.981585

11 H 3.810581 3.304314 2.167412 3.385784 4.906504

12 H 3.503098 3.238374 2.121488 3.004039 4.537054

13 H 3.415550 3.877927 1.116276 2.156743 4.330741

14 H 2.141943 1.101881 3.862122 3.393912 2.462248

15 O 4.931001 4.533485 3.582487 4.578872 5.840650

16 C 3.234211 3.490008 1.847038 2.518134 4.062154

17 C 3.078098 3.039968 2.724859 2.995831 3.768128

18 C 4.473639 4.403793 2.636173 3.758737 5.414899

19 O 5.359830 5.332046 3.172908 4.451322 6.339024

20 C 4.216788 3.758446 3.617783 4.221022 4.980919

21 O 4.996579 4.319209 4.725385 5.244457 5.667856

22 H 3.601546 4.198719 2.294982 2.652335 4.252004

23 H 2.883626 3.017592 3.317432 3.114718 3.273571

6 7 8 9 10

6 H 0.000000

7 C 3.967502 0.000000

8 H 4.897917 1.124504 0.000000

9 H 4.515596 1.128396 1.801915 0.000000

10 C 3.469716 1.519587 2.177305 2.167267 0.000000

11 H 4.323760 2.165235 2.271456 2.869927 1.123832

12 H 3.821627 2.163727 2.909374 2.250081 1.126232

13 H 2.493571 3.510860 4.237449 4.125976 2.176758

14 H 4.295924 2.198596 2.453759 2.605024 3.504029

15 O 5.349275 4.012260 3.625361 5.037748 3.470025

16 C 3.072124 3.488135 3.774237 4.527465 2.732112

17 C 3.699428 3.329720 3.350180 4.448160 3.197182

18 C 4.378821 3.916442 3.917551 4.907099 2.941177

19 O 4.959496 4.642091 4.692084 5.491486 3.407165

20 C 5.036253 3.635363 3.204229 4.733609 3.580232

21 O 6.102932 4.213101 3.510357 5.227746 4.468439

22 H 2.789213 4.383057 4.803527 5.358102 3.543417

23 H 3.685385 3.750084 3.842274 4.806255 3.903777

11 12 13 14 15

11 H 0.000000

12 H 1.799872 0.000000

13 H 2.588741 2.381448 0.000000

14 H 4.154687 4.206951 4.965325 0.000000

15 O 2.692734 4.414689 3.963277 5.098447 0.000000

16 C 2.732195 3.667722 2.293779 4.325602 2.377893

17 C 3.197425 4.293961 3.512963 3.569107 2.346146

18 C 2.350111 3.770278 2.747467 5.206884 1.392350

19 O 2.696173 3.938790 2.861362 6.211462 2.236070

20 C 3.148702 4.677027 4.320636 4.113393 1.428165

21 O 3.985251 5.543385 5.486990 4.388132 2.232821

22 H 3.667681 4.324074 2.399514 5.052066 3.270097

23 H 4.109876 4.970524 4.179092 3.332211 3.367781

16 17 18 19 20

16 C 0.000000

17 C 1.417216 0.000000

18 C 1.517691 2.326350 0.000000

19 O 2.514462 3.533091 1.221485 0.000000

20 C 2.341942 1.460078 2.281832 3.421338 0.000000

21 O 3.554863 2.494234 3.395701 4.438419 1.221556

22 H 1.106294 2.195557 2.237916 2.933933 3.271134

23 H 2.242470 1.085337 3.378222 4.567897 2.245653

21 22 23

21 O 0.000000

22 H 4.456728 0.000000

23 H 2.950154 2.678901 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.557532 -0.423704 -0.773582

2 6 0 2.175770 -1.186787 0.281386

3 6 0 0.997279 1.309723 -0.090313

4 6 0 2.036495 0.872606 -0.930871

5 1 0 3.260200 -0.843242 -1.508490

6 1 0 2.392668 1.499603 -1.759456

7 6 0 1.572891 -0.611069 1.498473

8 1 0 0.808233 -1.320793 1.918114

9 1 0 2.395859 -0.543452 2.267518

10 6 0 0.956395 0.765336 1.312498

11 1 0 -0.101427 0.748198 1.691598

12 1 0 1.510884 1.502160 1.959050

13 1 0 0.750368 2.398129 -0.112217

14 1 0 2.405216 -2.264089 0.311636

15 8 0 -2.240476 -0.163798 0.333823

16 6 0 -0.472892 0.680231 -1.014374

17 6 0 -0.485787 -0.733299 -1.115706

18 6 0 -1.622108 1.012875 -0.080546

19 8 0 -2.049884 2.063812 0.371741

20 6 0 -1.543055 -1.260682 -0.257872

21 8 0 -1.973880 -2.362117 0.047795

22 1 0 -0.385068 1.306258 -1.922264

23 1 0 0.041875 -1.337330 -1.846921

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2310312 0.7534305 0.6104657

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 461.7106309882 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.333467016910E-01 A.U. after 15 cycles

Convg = 0.2518D-08 -V/T = 0.9993

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.003458666 -0.007404412 0.001922520

2 6 0.007038053 -0.003525848 -0.002820463

3 6 -0.008861434 -0.002523108 -0.005882166

4 6 -0.001374888 0.009162851 -0.005181249

5 1 -0.001511225 0.002413510 0.004959566

6 1 0.000223773 0.001721298 0.002712935

7 6 0.003167734 0.001824397 0.001047398

8 1 0.000148607 0.000464314 0.000575936

9 1 0.000700699 -0.000393929 -0.000151467

10 6 0.001214728 0.000126494 0.000725664

11 1 -0.000277115 0.000243231 -0.000048458

12 1 0.000158645 -0.000236964 -0.000036650

13 1 0.001421410 -0.000402394 0.002591336

14 1 -0.000197619 -0.001029696 -0.001121142

15 8 -0.000210659 -0.000784767 -0.001022403

16 6 0.011831647 -0.005528511 0.011491348

17 6 -0.003313802 0.009603669 -0.000693094

18 6 -0.001465143 -0.001665276 -0.002105678

19 8 0.000235196 0.000664025 0.002129782

20 6 -0.002933124 0.000147784 -0.001607696

21 8 -0.000325236 -0.000096794 -0.000287156

22 1 -0.002237785 -0.000688119 -0.003957642

23 1 0.000026204 -0.002091754 -0.003241222

-------------------------------------------------------------------

Cartesian Forces: Max 0.011831647 RMS 0.003640910

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.009231985 RMS 0.001665802

Search for a saddle point.

Step number 19 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 18 19

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06040 -0.00987 0.00196 0.00358 0.00589

Eigenvalues --- 0.00958 0.01026 0.01388 0.01634 0.01731

Eigenvalues --- 0.02036 0.02189 0.02331 0.02495 0.02674

Eigenvalues --- 0.02824 0.03026 0.03135 0.03228 0.03273

Eigenvalues --- 0.03621 0.03740 0.03849 0.03966 0.04257

Eigenvalues --- 0.04410 0.04654 0.05187 0.05595 0.05950

Eigenvalues --- 0.06265 0.07327 0.08086 0.08649 0.09716

Eigenvalues --- 0.11393 0.13120 0.13958 0.15241 0.19197

Eigenvalues --- 0.22112 0.24045 0.25318 0.25886 0.27691

Eigenvalues --- 0.28773 0.30515 0.31172 0.31296 0.31847

Eigenvalues --- 0.31934 0.32293 0.32653 0.34323 0.35646

Eigenvalues --- 0.37352 0.39577 0.40356 0.43072 0.43958

Eigenvalues --- 0.48410 1.08390 1.10826

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 -0.63605 -0.40933 0.19062 -0.16685 -0.16085

D73 D80 D5 D35 D6

1 0.15363 -0.14277 -0.11515 -0.10625 -0.10615

RFO step: Lambda0=1.229149119D-03 Lambda=-1.58742102D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.421

Iteration 1 RMS(Cart)= 0.04454218 RMS(Int)= 0.00473226

Iteration 2 RMS(Cart)= 0.00774245 RMS(Int)= 0.00028818

Iteration 3 RMS(Cart)= 0.00001131 RMS(Int)= 0.00028807

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00028807

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.56404 0.00923 0.00000 0.00340 0.00325 2.56729

R2 2.65682 0.00697 0.00000 0.02097 0.02083 2.67766

R3 2.07857 0.00168 0.00000 0.00269 0.00269 2.08126

R4 2.78773 0.00204 0.00000 0.00924 0.00900 2.79673

R5 2.08225 0.00073 0.00000 0.00063 0.00063 2.08288

R6 5.74471 -0.00202 0.00000 -0.26312 -0.26290 5.48180

R7 2.65745 -0.00412 0.00000 -0.00589 -0.00591 2.65154

R8 2.84459 0.00094 0.00000 0.00057 0.00054 2.84513

R9 2.10946 -0.00122 0.00000 -0.00394 -0.00394 2.10552

R10 3.49040 0.00407 0.00000 -0.02498 -0.02494 3.46546

R11 2.07572 0.00149 0.00000 0.00131 0.00131 2.07703

R12 2.12500 0.00011 0.00000 0.00012 0.00012 2.12512

R13 2.13236 0.00008 0.00000 -0.00035 -0.00035 2.13201

R14 2.87160 0.00112 0.00000 0.00268 0.00232 2.87393

R15 2.12373 -0.00013 0.00000 0.00033 0.00033 2.12407

R16 2.12827 -0.00010 0.00000 -0.00112 -0.00112 2.12715

R17 2.63116 -0.00173 0.00000 0.00178 0.00198 2.63314

R18 2.69884 -0.00167 0.00000 0.00148 0.00162 2.70046

R19 2.67815 -0.00735 0.00000 -0.04022 -0.03995 2.63820

R20 2.86802 -0.00126 0.00000 -0.00431 -0.00432 2.86370

R21 2.09059 -0.00098 0.00000 0.00006 0.00006 2.09065

R22 2.75915 -0.00213 0.00000 -0.01630 -0.01642 2.74273

R23 2.05099 -0.00039 0.00000 -0.00019 -0.00019 2.05080

R24 2.30827 -0.00031 0.00000 -0.00031 -0.00031 2.30796

R25 2.30841 -0.00025 0.00000 0.00102 0.00102 2.30943

A1 2.09585 -0.00234 0.00000 -0.00177 -0.00190 2.09395

A2 2.07684 0.00531 0.00000 0.06780 0.06768 2.14452

A3 2.11027 -0.00301 0.00000 -0.06652 -0.06653 2.04374

A4 2.13765 -0.00034 0.00000 -0.00043 -0.00023 2.13742

A5 2.10902 0.00023 0.00000 -0.00169 -0.00172 2.10730

A6 1.37465 -0.00036 0.00000 0.00759 0.00730 1.38195

A7 2.03086 0.00025 0.00000 0.00101 0.00082 2.03169

A8 1.53393 -0.00172 0.00000 0.00428 0.00421 1.53813

A9 1.91854 0.00078 0.00000 -0.00296 -0.00270 1.91584

A10 2.05408 0.00258 0.00000 0.00565 0.00554 2.05962

A11 2.04295 -0.00149 0.00000 -0.00454 -0.00462 2.03833

A12 1.75507 -0.00025 0.00000 -0.01951 -0.01957 1.73550

A13 1.94432 0.00074 0.00000 0.01356 0.01339 1.95771

A14 1.89796 -0.00291 0.00000 -0.01230 -0.01238 1.88558

A15 1.71775 0.00037 0.00000 0.01181 0.01206 1.72981

A16 2.08702 0.00013 0.00000 -0.00726 -0.00734 2.07968

A17 2.08350 0.00104 0.00000 0.01622 0.01597 2.09946

A18 2.10957 -0.00131 0.00000 -0.01122 -0.01131 2.09826

A19 1.91715 -0.00036 0.00000 -0.00192 -0.00188 1.91526

A20 1.86254 0.00039 0.00000 0.00039 0.00042 1.86296

A21 2.00239 0.00005 0.00000 0.00010 -0.00004 2.00236

A22 1.85399 -0.00003 0.00000 0.00120 0.00118 1.85517

A23 1.91928 0.00013 0.00000 -0.00302 -0.00321 1.91607

A24 1.90183 -0.00017 0.00000 0.00356 0.00384 1.90567

A25 2.01596 0.00076 0.00000 -0.00297 -0.00294 2.01303

A26 1.92351 -0.00024 0.00000 -0.00468 -0.00469 1.91882

A27 1.85983 -0.00021 0.00000 0.00761 0.00759 1.86742

A28 1.90368 -0.00054 0.00000 -0.00020 -0.00035 1.90334

A29 1.89926 0.00014 0.00000 0.00114 0.00125 1.90051

A30 1.85432 0.00006 0.00000 -0.00048 -0.00046 1.85386

A31 1.88482 -0.00207 0.00000 -0.00649 -0.00642 1.87840

A32 1.96377 -0.00009 0.00000 -0.02133 -0.02109 1.94268

A33 1.79280 -0.00083 0.00000 0.00859 0.00878 1.80158

A34 1.72594 -0.00128 0.00000 0.00070 0.00063 1.72657

A35 1.82938 0.00092 0.00000 0.00711 0.00687 1.83625

A36 2.10186 0.00095 0.00000 0.01167 0.01168 2.11354

A37 2.02754 -0.00014 0.00000 -0.00956 -0.00954 2.01801

A38 1.67897 0.00272 0.00000 0.05375 0.05437 1.73334

A39 1.88608 -0.00231 0.00000 -0.03181 -0.03239 1.85369

A40 1.37041 -0.00169 0.00000 -0.04028 -0.04086 1.32954

A41 1.90164 -0.00008 0.00000 0.00674 0.00696 1.90860

A42 2.21285 0.00068 0.00000 0.00666 0.00726 2.22011

A43 2.14940 -0.00030 0.00000 -0.00913 -0.01022 2.13918

A44 1.91153 0.00008 0.00000 -0.00693 -0.00703 1.90450

A45 2.05034 -0.00011 0.00000 0.00425 0.00430 2.05463

A46 2.32073 0.00004 0.00000 0.00285 0.00289 2.32362

A47 1.89611 0.00114 0.00000 -0.00094 -0.00119 1.89492

A48 2.00051 -0.00041 0.00000 -0.00033 -0.00020 2.00031

A49 2.38632 -0.00073 0.00000 0.00131 0.00144 2.38776

D1 -0.34005 0.00150 0.00000 0.00086 0.00080 -0.33925

D2 2.91975 -0.00005 0.00000 0.01229 0.01198 2.93173

D3 1.05888 -0.00075 0.00000 0.01141 0.01096 1.06984

D4 2.82364 0.00313 0.00000 0.02660 0.02744 2.85108

D5 -0.19975 0.00159 0.00000 0.03802 0.03863 -0.16112

D6 -2.06062 0.00089 0.00000 0.03714 0.03761 -2.02301

D7 -0.13903 0.00004 0.00000 -0.00549 -0.00562 -0.14465

D8 3.08641 0.00197 0.00000 0.02555 0.02564 3.11205

D9 2.98004 -0.00152 0.00000 -0.02999 -0.02908 2.95096

D10 -0.07771 0.00041 0.00000 0.00106 0.00218 -0.07552

D11 2.53991 -0.00156 0.00000 -0.00757 -0.00772 2.53219

D12 -1.74063 -0.00157 0.00000 -0.00692 -0.00704 -1.74767

D13 0.36759 -0.00148 0.00000 -0.00207 -0.00190 0.36569

D14 -0.71493 -0.00008 0.00000 -0.01869 -0.01861 -0.73354

D15 1.28772 -0.00009 0.00000 -0.01803 -0.01793 1.26978

D16 -2.88724 0.00000 0.00000 -0.01318 -0.01279 -2.90003

D17 1.22660 -0.00006 0.00000 -0.01965 -0.01934 1.20727

D18 -3.05394 -0.00006 0.00000 -0.01899 -0.01866 -3.07260

D19 -0.94571 0.00003 0.00000 -0.01414 -0.01352 -0.95923

D20 -1.04801 -0.00009 0.00000 0.00629 0.00614 -1.04186

D21 -3.00764 -0.00050 0.00000 -0.01436 -0.01372 -3.02136

D22 1.15708 0.00017 0.00000 0.00441 0.00371 1.16078

D23 1.11137 0.00008 0.00000 0.00338 0.00357 1.11494

D24 -0.84826 -0.00033 0.00000 -0.01727 -0.01630 -0.86456

D25 -2.96673 0.00034 0.00000 0.00150 0.00114 -2.96560

D26 -3.12389 -0.00020 0.00000 0.00569 0.00569 -3.11820

D27 1.19966 -0.00061 0.00000 -0.01495 -0.01418 1.18548

D28 -0.91881 0.00005 0.00000 0.00381 0.00326 -0.91556

D29 0.54877 -0.00066 0.00000 0.01512 0.01534 0.56410

D30 -2.67795 -0.00251 0.00000 -0.01504 -0.01456 -2.69252

D31 2.93894 0.00204 0.00000 0.04000 0.03993 2.97887

D32 -0.28778 0.00019 0.00000 0.00983 0.01004 -0.27775

D33 -1.50791 0.00183 0.00000 0.04100 0.04128 -1.46663

D34 1.54855 -0.00001 0.00000 0.01083 0.01139 1.55994

D35 -0.48152 0.00001 0.00000 -0.01752 -0.01769 -0.49921

D36 -2.64844 0.00036 0.00000 -0.01110 -0.01115 -2.65959

D37 1.63000 0.00052 0.00000 -0.01235 -0.01237 1.61763

D38 -2.91156 -0.00157 0.00000 -0.03390 -0.03405 -2.94561

D39 1.20471 -0.00122 0.00000 -0.02748 -0.02751 1.17720

D40 -0.80003 -0.00106 0.00000 -0.02873 -0.02874 -0.82877

D41 1.49710 -0.00086 0.00000 -0.04791 -0.04814 1.44896

D42 -0.66981 -0.00051 0.00000 -0.04149 -0.04159 -0.71141

D43 -2.67456 -0.00035 0.00000 -0.04273 -0.04282 -2.71738

D44 1.09470 0.00153 0.00000 0.00402 0.00424 1.09894

D45 3.05243 0.00212 0.00000 0.00809 0.00809 3.06052

D46 -1.14451 0.00127 0.00000 0.00074 0.00080 -1.14371

D47 -1.07341 0.00003 0.00000 0.01361 0.01349 -1.05991

D48 0.88432 0.00061 0.00000 0.01768 0.01735 0.90167

D49 2.97057 -0.00024 0.00000 0.01034 0.01006 2.98063

D50 -3.09954 0.00000 0.00000 -0.00264 -0.00255 -3.10209

D51 -1.14182 0.00059 0.00000 0.00144 0.00130 -1.14051

D52 0.94443 -0.00026 0.00000 -0.00591 -0.00598 0.93845

D53 0.04476 -0.00023 0.00000 0.00820 0.00813 0.05289

D54 2.22199 -0.00042 0.00000 -0.00046 -0.00061 2.22139

D55 -2.04530 -0.00057 0.00000 -0.00051 -0.00066 -2.04596

D56 -2.12642 0.00012 0.00000 0.01313 0.01324 -2.11318

D57 0.05080 -0.00008 0.00000 0.00447 0.00451 0.05532

D58 2.06670 -0.00022 0.00000 0.00442 0.00446 2.07116

D59 2.13123 0.00018 0.00000 0.01134 0.01143 2.14267

D60 -1.97473 -0.00002 0.00000 0.00268 0.00270 -1.97202

D61 0.04117 -0.00016 0.00000 0.00263 0.00265 0.04382

D62 0.01911 -0.00021 0.00000 -0.01714 -0.01707 0.00204

D63 -3.09041 -0.00035 0.00000 -0.02187 -0.02194 -3.11234

D64 -0.04195 0.00010 0.00000 0.00394 0.00416 -0.03779

D65 3.11917 0.00015 0.00000 0.00222 0.00235 3.12152

D66 -0.04826 0.00073 0.00000 -0.00613 -0.00637 -0.05464

D67 1.89842 -0.00069 0.00000 -0.01686 -0.01676 1.88166

D68 -1.44944 0.00084 0.00000 0.00450 0.00447 -1.44497

D69 -1.98326 0.00123 0.00000 -0.01063 -0.01095 -1.99421

D70 -0.03658 -0.00018 0.00000 -0.02136 -0.02133 -0.05791

D71 2.89875 0.00135 0.00000 0.00000 -0.00011 2.89864

D72 1.97532 -0.00040 0.00000 -0.01469 -0.01496 1.96036

D73 -2.36119 -0.00182 0.00000 -0.02542 -0.02535 -2.38653

D74 0.57414 -0.00029 0.00000 -0.00405 -0.00412 0.57002

D75 -2.04406 0.00033 0.00000 0.04124 0.04094 -2.00312

D76 1.05863 0.00050 0.00000 0.04696 0.04684 1.10547

D77 0.01125 0.00025 0.00000 0.02401 0.02398 0.03523

D78 3.11395 0.00042 0.00000 0.02973 0.02987 -3.13937

D79 2.37678 0.00237 0.00000 0.03909 0.03884 2.41562

D80 -0.80371 0.00254 0.00000 0.04481 0.04473 -0.75898

D81 1.85502 0.00217 0.00000 0.06230 0.06225 1.91727

D82 -1.31246 0.00213 0.00000 0.06455 0.06461 -1.24785

D83 0.04999 0.00011 0.00000 0.01209 0.01192 0.06192

D84 -3.11749 0.00007 0.00000 0.01434 0.01428 -3.10321

D85 -2.89441 -0.00149 0.00000 -0.01049 -0.01049 -2.90490

D86 0.22129 -0.00153 0.00000 -0.00824 -0.00813 0.21315

Item Value Threshold Converged?

Maximum Force 0.009232 0.000450 NO

RMS Force 0.001666 0.000300 NO

Maximum Displacement 0.229476 0.001800 NO

RMS Displacement 0.051247 0.001200 NO

Predicted change in Energy=-3.972285D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.188092 1.429983 0.381240

2 6 0 -0.052978 0.971652 -0.207921

3 6 0 -0.552393 3.711413 -0.170842

4 6 0 -1.503056 2.810638 0.332782

5 1 0 -1.873126 0.778683 0.946500

6 1 0 -2.433727 3.183100 0.783540

7 6 0 0.667847 1.739065 -1.248008

8 1 0 1.775130 1.572563 -1.143836

9 1 0 0.373137 1.294901 -2.242354

10 6 0 0.370379 3.230466 -1.258934

11 1 0 1.339592 3.798243 -1.218351

12 1 0 -0.110438 3.499009 -2.240649

13 1 0 -0.893455 4.758365 -0.341118

14 1 0 0.307889 -0.051884 -0.015500

15 8 0 2.780305 4.151938 0.972410

16 6 0 0.445615 3.974042 1.345066

17 6 0 1.052721 2.788876 1.764395

18 6 0 1.581643 4.854093 0.864019

19 8 0 1.624515 5.983129 0.400277

20 6 0 2.477745 2.857898 1.497785

21 8 0 3.444711 2.121493 1.625084

22 1 0 -0.317929 4.476526 1.968334

23 1 0 0.607566 1.998817 2.360535

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.358551 0.000000

3 C 2.431837 2.785153 0.000000

4 C 1.416954 2.403529 1.403136 0.000000

5 H 1.101355 2.163993 3.404952 2.154633 0.000000

6 H 2.187892 3.397272 2.174713 1.099117 2.474278

7 C 2.488873 1.479964 2.557230 2.891364 3.492097

8 H 3.335696 2.139862 3.307380 3.802596 4.278963

9 H 3.055966 2.103564 3.314709 3.528298 3.934587

10 C 2.891495 2.527073 1.505577 2.493907 3.988546

11 H 3.815303 3.309054 2.164353 3.385561 4.911811

12 H 3.509489 3.243890 2.127097 3.005959 4.545896

13 H 3.418588 3.881152 1.114193 2.149278 4.295997

14 H 2.142730 1.102215 3.863498 3.405122 2.524304

15 O 4.848370 4.419829 3.550769 4.533805 5.747516

16 C 3.173357 3.416827 1.833840 2.485064 3.968090

17 C 2.963267 2.900846 2.678172 2.929502 3.642858

18 C 4.430467 4.346767 2.632635 3.738086 5.343333

19 O 5.351847 5.319661 3.197781 4.455441 6.294293

20 C 4.089496 3.587746 3.562940 4.148040 4.853569

21 O 4.846462 4.112891 4.661549 5.159977 5.526573

22 H 3.543653 4.134057 2.283954 2.618155 4.139666

23 H 2.732319 2.844003 3.268999 3.037360 3.105166

6 7 8 9 10

6 H 0.000000

7 C 3.978968 0.000000

8 H 4.901335 1.124567 0.000000

9 H 4.538702 1.128211 1.802615 0.000000

10 C 3.469431 1.520817 2.176055 2.171067 0.000000

11 H 4.315542 2.166180 2.269118 2.872166 1.124007

12 H 3.826643 2.165287 2.910251 2.256533 1.125640

13 H 2.473611 3.517995 4.232616 4.149041 2.184980

14 H 4.315095 2.203666 2.462675 2.603260 3.510535

15 O 5.306642 3.900601 3.484544 4.928673 3.411121

16 C 3.038340 3.430530 3.705313 4.478016 2.709129

17 C 3.643187 3.213223 3.234053 4.329877 3.130673

18 C 4.349930 3.872864 3.851929 4.876257 2.934324

19 O 4.945339 4.652326 4.675475 5.525299 3.450072

20 C 4.973777 3.473744 3.020582 4.567382 3.489885

21 O 6.032515 4.013961 3.279594 5.007484 4.358773

22 H 2.748325 4.337085 4.743364 5.322613 3.527279

23 H 3.624762 3.618382 3.718268 4.662300 3.830636

11 12 13 14 15

11 H 0.000000

12 H 1.799228 0.000000

13 H 2.584158 2.409837 0.000000

14 H 4.163501 4.211310 4.968677 0.000000

15 O 2.645786 4.371093 3.948370 4.976036 0.000000

16 C 2.720516 3.659536 2.291612 4.251845 2.370928

17 C 3.161944 4.230557 3.478459 3.434054 2.338744

18 C 2.347269 3.786602 2.754566 5.144377 1.393398

19 O 2.734020 4.019379 2.896530 6.190942 2.239743

20 C 3.091445 4.591907 4.284662 3.932575 1.429021

21 O 3.915116 5.429597 5.444147 4.153882 2.233859

22 H 3.655463 4.325984 2.396713 4.983347 3.270517

23 H 4.072127 4.892546 4.143320 3.152892 3.359110

16 17 18 19 20

16 C 0.000000

17 C 1.396078 0.000000

18 C 1.515406 2.314207 0.000000

19 O 2.513735 3.520088 1.221318 0.000000

20 C 2.323500 1.451391 2.278036 3.420467 0.000000

21 O 3.536231 2.487252 3.393721 4.441340 1.222097

22 H 1.106324 2.183675 2.229449 2.915775 3.264532

23 H 2.226863 1.085237 3.367638 4.555386 2.231575

21 22 23

21 O 0.000000

22 H 4.452131 0.000000

23 H 2.933485 2.673837 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.526467 -0.337481 -0.769792

2 6 0 2.123819 -1.159595 0.234032

3 6 0 0.953399 1.355596 -0.012972

4 6 0 2.007184 0.977874 -0.858935

5 1 0 3.218741 -0.658430 -1.563979

6 1 0 2.350074 1.656658 -1.652495

7 6 0 1.499691 -0.650618 1.475684

8 1 0 0.720471 -1.377660 1.834680

9 1 0 2.307177 -0.637458 2.263499

10 6 0 0.892436 0.738820 1.359118

11 1 0 -0.172452 0.705079 1.717262

12 1 0 1.436943 1.434249 2.056941

13 1 0 0.682010 2.436162 -0.000621

14 1 0 2.359631 -2.236010 0.209516

15 8 0 -2.199772 -0.245244 0.307636

16 6 0 -0.460273 0.712269 -0.987976

17 6 0 -0.396687 -0.676273 -1.118135

18 6 0 -1.650246 0.973009 -0.086625

19 8 0 -2.158921 1.993718 0.350435

20 6 0 -1.423035 -1.284391 -0.291491

21 8 0 -1.784528 -2.417172 -0.009266

22 1 0 -0.374882 1.373445 -1.870874

23 1 0 0.181528 -1.241697 -1.841809

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2322502 0.7842398 0.6268830

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 464.2332509785 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.350687900800E-01 A.U. after 15 cycles

Convg = 0.4185D-08 -V/T = 0.9993

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.009562042 0.007568558 0.002923820

2 6 0.004186247 -0.000918289 -0.000696868

3 6 -0.006082153 -0.000834615 -0.007208759

4 6 -0.000264491 -0.002897056 -0.005684445

5 1 0.003261464 -0.002172513 0.001501918

6 1 0.000120722 -0.000584825 0.001874970

7 6 0.000756017 0.000668769 0.002717767

8 1 0.000051010 0.000206142 0.000766009

9 1 0.000601068 0.000035489 0.000069424

10 6 0.000672670 -0.000462625 0.000331754

11 1 -0.000176320 0.000128683 -0.000403830

12 1 -0.000282717 -0.000197901 0.000175904

13 1 0.001584966 0.000773712 0.000884495

14 1 0.000200988 -0.000354426 -0.000791356

15 8 0.000435909 0.000179709 -0.001030657

16 6 -0.001741900 0.014608768 0.005649783

17 6 -0.000169917 -0.014394044 0.007688657

18 6 0.001145128 0.000957131 -0.003890790

19 8 0.000484354 -0.000175400 0.002047323

20 6 0.008428595 -0.000024234 -0.002149457

21 8 -0.000478637 0.000217782 -0.000528028

22 1 -0.002466419 0.000065072 -0.002574752

23 1 -0.000704542 -0.002393884 -0.001672882

-------------------------------------------------------------------

Cartesian Forces: Max 0.014608768 RMS 0.003766810

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.012805174 RMS 0.001726243

Search for a saddle point.

Step number 20 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 19 20

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06011 -0.01269 0.00197 0.00365 0.00589

Eigenvalues --- 0.00962 0.01025 0.01412 0.01681 0.01786

Eigenvalues --- 0.02057 0.02174 0.02300 0.02470 0.02668

Eigenvalues --- 0.02837 0.03034 0.03216 0.03271 0.03397

Eigenvalues --- 0.03619 0.03785 0.03866 0.04083 0.04364

Eigenvalues --- 0.04425 0.05176 0.05381 0.05739 0.05953

Eigenvalues --- 0.06328 0.07329 0.08186 0.08682 0.09766

Eigenvalues --- 0.11454 0.13310 0.13972 0.15308 0.19881

Eigenvalues --- 0.22279 0.24502 0.25859 0.26159 0.27773

Eigenvalues --- 0.29068 0.30491 0.31174 0.31347 0.31850

Eigenvalues --- 0.31944 0.32326 0.32671 0.34327 0.35653

Eigenvalues --- 0.37379 0.39575 0.40371 0.43078 0.45089

Eigenvalues --- 0.48609 1.08393 1.10825

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 -0.62726 -0.40405 0.19077 -0.17292 -0.16299

D73 D80 D5 D6 D35

1 0.15582 -0.14410 -0.11964 -0.10898 -0.10753

RFO step: Lambda0=6.498892525D-04 Lambda=-1.76206493D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.480

Iteration 1 RMS(Cart)= 0.04187931 RMS(Int)= 0.00511772

Iteration 2 RMS(Cart)= 0.00839923 RMS(Int)= 0.00023767

Iteration 3 RMS(Cart)= 0.00001328 RMS(Int)= 0.00023748

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00023748

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.56729 0.00629 0.00000 0.02278 0.02320 2.59049

R2 2.67766 -0.00082 0.00000 -0.01810 -0.01774 2.65992

R3 2.08126 0.00003 0.00000 -0.00167 -0.00167 2.07959

R4 2.79673 -0.00118 0.00000 0.00131 0.00116 2.79788

R5 2.08288 0.00026 0.00000 0.00014 0.00014 2.08303

R6 5.48180 -0.00249 0.00000 -0.26907 -0.26966 5.21214

R7 2.65154 0.00247 0.00000 0.01271 0.01272 2.66427

R8 2.84513 -0.00042 0.00000 -0.00416 -0.00409 2.84104

R9 2.10552 0.00011 0.00000 -0.00241 -0.00241 2.10311

R10 3.46546 0.00626 0.00000 0.02339 0.02393 3.48938

R11 2.07703 0.00047 0.00000 0.00066 0.00066 2.07769

R12 2.12512 0.00009 0.00000 0.00078 0.00078 2.12590

R13 2.13201 -0.00023 0.00000 -0.00064 -0.00064 2.13136

R14 2.87393 -0.00047 0.00000 -0.00329 -0.00339 2.87054

R15 2.12407 -0.00010 0.00000 0.00002 0.00002 2.12408

R16 2.12715 -0.00008 0.00000 -0.00060 -0.00060 2.12655

R17 2.63314 0.00218 0.00000 0.00185 0.00195 2.63510

R18 2.70046 0.00168 0.00000 -0.00591 -0.00584 2.69462

R19 2.63820 0.01281 0.00000 0.04847 0.04824 2.68645

R20 2.86370 0.00260 0.00000 -0.00028 -0.00029 2.86341

R21 2.09065 0.00028 0.00000 -0.00325 -0.00325 2.08740

R22 2.74273 0.00738 0.00000 0.00867 0.00862 2.75135

R23 2.05080 0.00111 0.00000 -0.00126 -0.00126 2.04954

R24 2.30796 -0.00092 0.00000 -0.00085 -0.00085 2.30711

R25 2.30943 -0.00056 0.00000 -0.00027 -0.00027 2.30916

A1 2.09395 -0.00097 0.00000 -0.00621 -0.00590 2.08805

A2 2.14452 -0.00301 0.00000 -0.05141 -0.05161 2.09291

A3 2.04374 0.00398 0.00000 0.05668 0.05634 2.10007

A4 2.13742 -0.00062 0.00000 -0.00402 -0.00444 2.13298

A5 2.10730 0.00088 0.00000 0.01405 0.01439 2.12169

A6 1.38195 0.00166 0.00000 0.03571 0.03583 1.41778

A7 2.03169 -0.00025 0.00000 -0.01223 -0.01234 2.01934

A8 1.53813 -0.00015 0.00000 0.00661 0.00654 1.54468

A9 1.91584 -0.00174 0.00000 -0.02704 -0.02712 1.88873

A10 2.05962 0.00004 0.00000 -0.00257 -0.00293 2.05669

A11 2.03833 0.00064 0.00000 0.00504 0.00523 2.04356

A12 1.73550 0.00051 0.00000 -0.00211 -0.00235 1.73315

A13 1.95771 0.00013 0.00000 0.00609 0.00611 1.96382

A14 1.88558 -0.00151 0.00000 -0.02568 -0.02532 1.86026

A15 1.72981 -0.00015 0.00000 0.01663 0.01642 1.74623

A16 2.07968 0.00053 0.00000 0.00015 -0.00010 2.07957

A17 2.09946 -0.00128 0.00000 -0.00700 -0.00712 2.09234

A18 2.09826 0.00064 0.00000 0.00294 0.00265 2.10091

A19 1.91526 -0.00084 0.00000 -0.00821 -0.00821 1.90705

A20 1.86296 0.00008 0.00000 0.00449 0.00448 1.86744

A21 2.00236 0.00114 0.00000 0.00298 0.00300 2.00536

A22 1.85517 0.00022 0.00000 0.00173 0.00174 1.85691

A23 1.91607 0.00045 0.00000 0.00247 0.00249 1.91856

A24 1.90567 -0.00114 0.00000 -0.00346 -0.00350 1.90217

A25 2.01303 0.00033 0.00000 -0.00625 -0.00598 2.00705

A26 1.91882 0.00010 0.00000 0.00148 0.00136 1.92018

A27 1.86742 -0.00033 0.00000 0.00270 0.00263 1.87005

A28 1.90334 -0.00013 0.00000 -0.00250 -0.00256 1.90077

A29 1.90051 -0.00002 0.00000 0.00654 0.00644 1.90695

A30 1.85386 0.00003 0.00000 -0.00144 -0.00139 1.85247

A31 1.87840 0.00290 0.00000 0.00524 0.00525 1.88366

A32 1.94268 -0.00194 0.00000 -0.02119 -0.02090 1.92178

A33 1.80158 0.00154 0.00000 0.00371 0.00329 1.80487

A34 1.72657 -0.00069 0.00000 0.00006 0.00018 1.72676

A35 1.83625 -0.00128 0.00000 -0.00802 -0.00803 1.82822

A36 2.11354 0.00156 0.00000 0.01273 0.01245 2.12599

A37 2.01801 0.00075 0.00000 0.00986 0.00990 2.02791

A38 1.73334 -0.00013 0.00000 0.03663 0.03608 1.76942

A39 1.85369 0.00050 0.00000 -0.02093 -0.02032 1.83337

A40 1.32954 -0.00081 0.00000 -0.02424 -0.02436 1.30518

A41 1.90860 -0.00175 0.00000 -0.00943 -0.00925 1.89936

A42 2.22011 0.00069 0.00000 0.00882 0.00897 2.22908

A43 2.13918 0.00123 0.00000 0.00278 0.00240 2.14157

A44 1.90450 0.00098 0.00000 0.00670 0.00661 1.91112

A45 2.05463 -0.00087 0.00000 -0.00607 -0.00604 2.04859

A46 2.32362 -0.00010 0.00000 -0.00036 -0.00033 2.32329

A47 1.89492 -0.00086 0.00000 0.00520 0.00504 1.89995

A48 2.00031 0.00036 0.00000 0.00009 0.00016 2.00047

A49 2.38776 0.00051 0.00000 -0.00512 -0.00506 2.38270

D1 -0.33925 0.00116 0.00000 -0.00668 -0.00655 -0.34580

D2 2.93173 0.00116 0.00000 0.01508 0.01544 2.94717

D3 1.06984 0.00228 0.00000 0.02672 0.02641 1.09625

D4 2.85108 0.00113 0.00000 0.01533 0.01483 2.86591

D5 -0.16112 0.00113 0.00000 0.03709 0.03682 -0.12430

D6 -2.02301 0.00224 0.00000 0.04873 0.04779 -1.97522

D7 -0.14465 -0.00040 0.00000 -0.01113 -0.01114 -0.15579

D8 3.11205 0.00064 0.00000 0.02737 0.02730 3.13935

D9 2.95096 -0.00055 0.00000 -0.03476 -0.03557 2.91539

D10 -0.07552 0.00049 0.00000 0.00374 0.00287 -0.07266

D11 2.53219 0.00011 0.00000 0.00792 0.00783 2.54002

D12 -1.74767 0.00000 0.00000 0.00826 0.00816 -1.73951

D13 0.36569 -0.00067 0.00000 0.00897 0.00885 0.37455

D14 -0.73354 0.00020 0.00000 -0.01115 -0.01112 -0.74466

D15 1.26978 0.00008 0.00000 -0.01081 -0.01079 1.25900

D16 -2.90003 -0.00059 0.00000 -0.01009 -0.01010 -2.91013

D17 1.20727 -0.00189 0.00000 -0.04013 -0.04009 1.16718

D18 -3.07260 -0.00200 0.00000 -0.03979 -0.03976 -3.11236

D19 -0.95923 -0.00268 0.00000 -0.03908 -0.03907 -0.99830

D20 -1.04186 0.00058 0.00000 0.01992 0.01962 -1.02224

D21 -3.02136 0.00238 0.00000 0.02232 0.02232 -2.99904

D22 1.16078 0.00130 0.00000 0.02167 0.02124 1.18203

D23 1.11494 -0.00029 0.00000 0.00818 0.00827 1.12321

D24 -0.86456 0.00150 0.00000 0.01058 0.01098 -0.85358

D25 -2.96560 0.00043 0.00000 0.00994 0.00990 -2.95570

D26 -3.11820 -0.00089 0.00000 -0.00643 -0.00634 -3.12454

D27 1.18548 0.00091 0.00000 -0.00403 -0.00363 1.18185

D28 -0.91556 -0.00017 0.00000 -0.00468 -0.00472 -0.92027

D29 0.56410 -0.00033 0.00000 0.02980 0.02977 0.59388

D30 -2.69252 -0.00149 0.00000 -0.00935 -0.00952 -2.70203

D31 2.97887 0.00084 0.00000 0.04397 0.04386 3.02274

D32 -0.27775 -0.00032 0.00000 0.00482 0.00458 -0.27317

D33 -1.46663 0.00115 0.00000 0.06366 0.06330 -1.40333

D34 1.55994 -0.00002 0.00000 0.02451 0.02401 1.58395

D35 -0.49921 0.00046 0.00000 -0.02556 -0.02557 -0.52478

D36 -2.65959 0.00032 0.00000 -0.01870 -0.01877 -2.67836

D37 1.61763 0.00041 0.00000 -0.01922 -0.01925 1.59838

D38 -2.94561 -0.00085 0.00000 -0.03891 -0.03892 -2.98452

D39 1.17720 -0.00100 0.00000 -0.03205 -0.03212 1.14508

D40 -0.82877 -0.00091 0.00000 -0.03257 -0.03260 -0.86136

D41 1.44896 0.00007 0.00000 -0.04768 -0.04749 1.40148

D42 -0.71141 -0.00008 0.00000 -0.04082 -0.04069 -0.75210

D43 -2.71738 0.00002 0.00000 -0.04133 -0.04117 -2.75855

D44 1.09894 -0.00001 0.00000 -0.00234 -0.00262 1.09632

D45 3.06052 -0.00148 0.00000 -0.01844 -0.01866 3.04185

D46 -1.14371 -0.00045 0.00000 -0.00669 -0.00692 -1.15063

D47 -1.05991 0.00032 0.00000 0.01233 0.01197 -1.04794

D48 0.90167 -0.00116 0.00000 -0.00377 -0.00407 0.89760

D49 2.98063 -0.00012 0.00000 0.00799 0.00767 2.98830

D50 -3.10209 0.00076 0.00000 0.00704 0.00690 -3.09519

D51 -1.14051 -0.00071 0.00000 -0.00906 -0.00914 -1.14965

D52 0.93845 0.00032 0.00000 0.00269 0.00260 0.94105

D53 0.05289 -0.00014 0.00000 0.00725 0.00725 0.06014

D54 2.22139 0.00012 0.00000 0.00257 0.00262 2.22401

D55 -2.04596 0.00008 0.00000 0.00307 0.00308 -2.04288

D56 -2.11318 -0.00025 0.00000 0.01397 0.01395 -2.09923

D57 0.05532 0.00002 0.00000 0.00929 0.00932 0.06463

D58 2.07116 -0.00002 0.00000 0.00979 0.00977 2.08093

D59 2.14267 -0.00012 0.00000 0.01247 0.01245 2.15512

D60 -1.97202 0.00014 0.00000 0.00779 0.00782 -1.96420

D61 0.04382 0.00010 0.00000 0.00829 0.00828 0.05210

D62 0.00204 0.00033 0.00000 -0.00902 -0.00914 -0.00710

D63 -3.11234 0.00026 0.00000 -0.01794 -0.01804 -3.13038

D64 -0.03779 -0.00044 0.00000 0.00405 0.00399 -0.03380

D65 3.12152 -0.00076 0.00000 -0.00322 -0.00331 3.11821

D66 -0.05464 0.00030 0.00000 -0.00613 -0.00655 -0.06118

D67 1.88166 0.00025 0.00000 -0.01609 -0.01623 1.86543

D68 -1.44497 0.00139 0.00000 -0.00310 -0.00313 -1.44811

D69 -1.99421 0.00004 0.00000 0.00314 0.00273 -1.99148

D70 -0.05791 -0.00001 0.00000 -0.00683 -0.00695 -0.06487

D71 2.89864 0.00113 0.00000 0.00616 0.00614 2.90478

D72 1.96036 -0.00118 0.00000 -0.01497 -0.01536 1.94500

D73 -2.38653 -0.00123 0.00000 -0.02494 -0.02504 -2.41157

D74 0.57002 -0.00008 0.00000 -0.01195 -0.01194 0.55807

D75 -2.00312 0.00184 0.00000 0.03523 0.03512 -1.96800

D76 1.10547 0.00192 0.00000 0.04595 0.04585 1.15132

D77 0.03523 -0.00017 0.00000 0.01004 0.01016 0.04538

D78 -3.13937 -0.00009 0.00000 0.02077 0.02089 -3.11848

D79 2.41562 0.00148 0.00000 0.02919 0.02907 2.44469

D80 -0.75898 0.00156 0.00000 0.03991 0.03980 -0.71917

D81 1.91727 -0.00043 0.00000 0.03028 0.03011 1.94738

D82 -1.24785 -0.00001 0.00000 0.04007 0.03988 -1.20797

D83 0.06192 0.00020 0.00000 0.00197 0.00210 0.06402

D84 -3.10321 0.00061 0.00000 0.01176 0.01187 -3.09134

D85 -2.90490 -0.00083 0.00000 -0.01115 -0.01113 -2.91603

D86 0.21315 -0.00042 0.00000 -0.00136 -0.00135 0.21180

Item Value Threshold Converged?

Maximum Force 0.012805 0.000450 NO

RMS Force 0.001726 0.000300 NO

Maximum Displacement 0.224607 0.001800 NO

RMS Displacement 0.048950 0.001200 NO

Predicted change in Energy=-4.327276D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.192969 1.460252 0.407908

2 6 0 -0.020982 1.011193 -0.143419

3 6 0 -0.578511 3.733161 -0.190947

4 6 0 -1.532813 2.822417 0.306632

5 1 0 -1.828949 0.770156 0.982653

6 1 0 -2.472822 3.186563 0.745507

7 6 0 0.697966 1.767728 -1.193595

8 1 0 1.806108 1.628602 -1.058511

9 1 0 0.435399 1.291103 -2.181510

10 6 0 0.365931 3.248719 -1.255650

11 1 0 1.322249 3.838223 -1.218895

12 1 0 -0.107148 3.481727 -2.249761

13 1 0 -0.918619 4.778231 -0.366290

14 1 0 0.366245 0.001018 0.067879

15 8 0 2.767209 4.104576 0.927963

16 6 0 0.429190 3.974328 1.337434

17 6 0 1.030982 2.746071 1.724986

18 6 0 1.582196 4.836909 0.865715

19 8 0 1.651043 5.981641 0.446937

20 6 0 2.454679 2.805539 1.426074

21 8 0 3.409895 2.047709 1.506227

22 1 0 -0.329023 4.474958 1.965635

23 1 0 0.586344 1.942181 2.301487

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.370828 0.000000

3 C 2.429465 2.778886 0.000000

4 C 1.407567 2.401814 1.409869 0.000000

5 H 1.100470 2.143567 3.423497 2.180935 0.000000

6 H 2.175350 3.396166 2.182688 1.099468 2.511938

7 C 2.496996 1.480575 2.549044 2.887806 3.480877

8 H 3.342632 2.134676 3.296702 3.799632 4.256397

9 H 3.063540 2.107237 3.309683 3.522731 3.925632

10 C 2.897621 2.528494 1.503412 2.495533 3.996345

11 H 3.824598 3.309534 2.163471 3.392709 4.918322

12 H 3.511207 3.247713 2.126997 3.000392 4.556942

13 H 3.418133 3.878917 1.112919 2.157607 4.325854

14 H 2.162437 1.102291 3.858555 3.409358 2.499452

15 O 4.790189 4.300102 3.547359 4.529920 5.678557

16 C 3.133049 3.343015 1.846503 2.497781 3.935960

17 C 2.886864 2.758145 2.689910 2.930973 3.554504

18 C 4.394649 4.269031 2.646403 3.751537 5.309243

19 O 5.341618 5.277266 3.230088 4.487462 6.289428

20 C 4.018930 3.436842 3.560265 4.141682 4.763284

21 O 4.768414 3.945454 4.650648 5.144858 5.417726

22 H 3.501624 4.067021 2.294200 2.632925 4.116016

23 H 2.642698 2.685730 3.282792 3.040574 2.991088

6 7 8 9 10

6 H 0.000000

7 C 3.978330 0.000000

8 H 4.898057 1.124980 0.000000

9 H 4.540699 1.127869 1.803850 0.000000

10 C 3.473760 1.519023 2.176638 2.166634 0.000000

11 H 4.322743 2.162710 2.267657 2.863730 1.124015

12 H 3.828207 2.168292 2.917825 2.257842 1.125324

13 H 2.486976 3.515808 4.221785 4.157938 2.186421

14 H 4.320553 2.196047 2.447650 2.594003 3.507035

15 O 5.322966 3.774073 3.316661 4.798102 3.356605

16 C 3.064739 3.368594 3.624760 4.425234 2.693435

17 C 3.664704 3.096154 3.097970 4.210981 3.095019

18 C 4.379642 3.800327 3.747801 4.813882 2.915791

19 O 4.990778 4.621337 4.608619 5.512501 3.466869

20 C 4.988850 3.320505 2.824711 4.402916 3.427962

21 O 6.040037 3.836923 3.053795 4.797862 4.282068

22 H 2.782904 4.285386 4.669688 5.283946 3.516149

23 H 3.650762 3.501212 3.588278 4.532543 3.795898

11 12 13 14 15

11 H 0.000000

12 H 1.798041 0.000000

13 H 2.575275 2.426287 0.000000

14 H 4.158591 4.208432 4.965999 0.000000

15 O 2.601510 4.329873 3.964118 4.831518 0.000000

16 C 2.711254 3.660366 2.316360 4.171682 2.377175

17 C 3.153422 4.199422 3.507713 3.274630 2.344198

18 C 2.326058 3.794284 2.788432 5.049844 1.394433

19 O 2.734473 4.075903 2.951727 6.128804 2.236199

20 C 3.056909 4.531220 4.299212 3.751212 1.425933

21 O 3.871756 5.341671 5.449596 3.939746 2.231173

22 H 3.643263 4.336508 2.424351 4.909279 3.286426

23 H 4.065663 4.854378 4.174341 2.967417 3.364325

16 17 18 19 20

16 C 0.000000

17 C 1.421606 0.000000

18 C 1.515251 2.326754 0.000000

19 O 2.513009 3.533666 1.220871 0.000000

20 C 2.340199 1.455953 2.280722 3.419380 0.000000

21 O 3.553161 2.488934 3.395640 4.437508 1.221952

22 H 1.104606 2.212820 2.234634 2.914995 3.290453

23 H 2.254710 1.084571 3.381214 4.570576 2.236607

21 22 23

21 O 0.000000

22 H 4.481305 0.000000

23 H 2.935304 2.713973 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.512104 -0.298775 -0.748377

2 6 0 2.037298 -1.166998 0.200262

3 6 0 0.959465 1.390015 0.051372

4 6 0 2.043803 1.028359 -0.773944

5 1 0 3.204629 -0.658666 -1.524214

6 1 0 2.423456 1.728706 -1.531709

7 6 0 1.393705 -0.697516 1.448251

8 1 0 0.578602 -1.416417 1.738716

9 1 0 2.172525 -0.753598 2.262121

10 6 0 0.840681 0.716062 1.390000

11 1 0 -0.234005 0.700549 1.718967

12 1 0 1.386551 1.359194 2.134823

13 1 0 0.691830 2.469495 0.092407

14 1 0 2.237962 -2.249401 0.143832

15 8 0 -2.167564 -0.270035 0.274263

16 6 0 -0.429757 0.752699 -0.984708

17 6 0 -0.327403 -0.658246 -1.125153

18 6 0 -1.647800 0.965855 -0.108967

19 8 0 -2.208248 1.965477 0.311961

20 6 0 -1.358916 -1.287304 -0.312709

21 8 0 -1.693749 -2.428615 -0.032594

22 1 0 -0.325461 1.432919 -1.848754

23 1 0 0.281319 -1.212297 -1.831396

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2331452 0.8085740 0.6374042

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 465.8764713724 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.376580871098E-01 A.U. after 15 cycles

Convg = 0.2919D-08 -V/T = 0.9992

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001556114 -0.001023523 -0.002564471

2 6 0.002201574 0.006581483 0.002466946

3 6 -0.003389458 -0.001732048 -0.000431138

4 6 -0.000106660 -0.001119414 -0.001212201

5 1 -0.000941127 0.001505771 0.001474393

6 1 -0.000049115 0.000337345 0.000519038

7 6 0.000128424 -0.000999093 0.001337134

8 1 0.000365714 0.000520035 0.000482200

9 1 0.000633114 -0.000363875 -0.000034750

10 6 0.000219427 0.000167906 -0.000831579

11 1 -0.000172257 0.000428586 -0.000850897

12 1 -0.000320699 -0.000612469 -0.000069906

13 1 0.001134844 0.000285378 0.001102310

14 1 -0.000875336 0.000252217 0.000993144

15 8 -0.000226154 0.000230795 -0.000734233

16 6 0.006769106 -0.005998528 0.004842492

17 6 -0.006989301 0.002287955 -0.003762213

18 6 -0.000894412 -0.001037471 -0.000861805

19 8 0.000225134 0.000679833 0.001107305

20 6 0.001964044 0.001292815 -0.000897581

21 8 0.000305072 -0.000761789 -0.000374763

22 1 -0.000873587 -0.000696076 -0.001475351

23 1 -0.000664462 -0.000225833 -0.000224073

-------------------------------------------------------------------

Cartesian Forces: Max 0.006989301 RMS 0.002041548

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.006596196 RMS 0.000921886

Search for a saddle point.

Step number 21 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 20 21

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0

Eigenvalues --- -0.06231 -0.00486 0.00202 0.00374 0.00590

Eigenvalues --- 0.00966 0.01024 0.01408 0.01785 0.01829

Eigenvalues --- 0.02056 0.02178 0.02302 0.02457 0.02772

Eigenvalues --- 0.02850 0.03035 0.03223 0.03281 0.03396

Eigenvalues --- 0.03617 0.03779 0.03890 0.04104 0.04353

Eigenvalues --- 0.04428 0.05173 0.05534 0.05864 0.05957

Eigenvalues --- 0.06411 0.07336 0.08289 0.08687 0.09797

Eigenvalues --- 0.11490 0.13412 0.13987 0.15346 0.20275

Eigenvalues --- 0.22348 0.24511 0.25937 0.26457 0.27965

Eigenvalues --- 0.29592 0.30499 0.31187 0.31459 0.31855

Eigenvalues --- 0.31958 0.32382 0.32697 0.34378 0.35740

Eigenvalues --- 0.37387 0.39575 0.40370 0.43098 0.45241

Eigenvalues --- 0.49441 1.08394 1.10825

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 0.60479 0.48538 -0.18447 0.16341 0.14856

D73 D80 D35 D29 D5

1 -0.14452 0.12737 0.11451 -0.10832 0.10515

RFO step: Lambda0=3.489339095D-10 Lambda=-1.06057203D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.386

Iteration 1 RMS(Cart)= 0.04731486 RMS(Int)= 0.00396100

Iteration 2 RMS(Cart)= 0.00657786 RMS(Int)= 0.00023273

Iteration 3 RMS(Cart)= 0.00000771 RMS(Int)= 0.00023267

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00023267

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.59049 -0.00119 0.00000 0.00136 0.00155 2.59204

R2 2.65992 -0.00237 0.00000 -0.01412 -0.01388 2.64604

R3 2.07959 0.00037 0.00000 0.00091 0.00091 2.08050

R4 2.79788 -0.00118 0.00000 -0.01703 -0.01718 2.78070

R5 2.08303 -0.00035 0.00000 -0.00065 -0.00065 2.08238

R6 5.21214 -0.00516 0.00000 -0.25286 -0.25290 4.95924

R7 2.66427 -0.00163 0.00000 -0.00419 -0.00418 2.66009

R8 2.84104 0.00070 0.00000 0.00160 0.00179 2.84282

R9 2.10311 -0.00025 0.00000 -0.00451 -0.00451 2.09860

R10 3.48938 0.00160 0.00000 0.09731 0.09720 3.58658

R11 2.07769 0.00036 0.00000 -0.00047 -0.00047 2.07722

R12 2.12590 0.00035 0.00000 0.00164 0.00164 2.12755

R13 2.13136 0.00004 0.00000 -0.00041 -0.00041 2.13095

R14 2.87054 -0.00040 0.00000 0.00412 0.00416 2.87469

R15 2.12408 0.00005 0.00000 0.00052 0.00052 2.12460

R16 2.12655 0.00007 0.00000 -0.00047 -0.00047 2.12609

R17 2.63510 -0.00068 0.00000 0.00551 0.00565 2.64074

R18 2.69462 -0.00045 0.00000 -0.00463 -0.00456 2.69006

R19 2.68645 -0.00660 0.00000 -0.02156 -0.02198 2.66447

R20 2.86341 -0.00037 0.00000 -0.00719 -0.00718 2.85623

R21 2.08740 -0.00055 0.00000 -0.00264 -0.00264 2.08476

R22 2.75135 0.00255 0.00000 0.01780 0.01771 2.76907

R23 2.04954 0.00032 0.00000 0.00060 0.00060 2.05014

R24 2.30711 0.00027 0.00000 -0.00001 -0.00001 2.30710

R25 2.30916 0.00069 0.00000 0.00036 0.00036 2.30951

A1 2.08805 0.00009 0.00000 -0.00078 -0.00046 2.08759

A2 2.09291 0.00199 0.00000 0.03600 0.03549 2.12840

A3 2.10007 -0.00214 0.00000 -0.03737 -0.03769 2.06238

A4 2.13298 0.00085 0.00000 0.01338 0.01296 2.14595

A5 2.12169 -0.00082 0.00000 -0.02762 -0.02743 2.09426

A6 1.41778 0.00049 0.00000 0.03432 0.03433 1.45211

A7 2.01934 -0.00002 0.00000 0.01325 0.01346 2.03280

A8 1.54468 0.00030 0.00000 0.01423 0.01386 1.55854

A9 1.88873 -0.00070 0.00000 -0.04209 -0.04212 1.84660

A10 2.05669 0.00078 0.00000 0.00444 0.00376 2.06045

A11 2.04356 -0.00029 0.00000 0.01198 0.01198 2.05554

A12 1.73315 -0.00005 0.00000 -0.00884 -0.00898 1.72417

A13 1.96382 -0.00006 0.00000 0.00806 0.00786 1.97168

A14 1.86026 -0.00095 0.00000 -0.03670 -0.03644 1.82382

A15 1.74623 0.00034 0.00000 0.01032 0.01037 1.75660

A16 2.07957 -0.00040 0.00000 -0.01005 -0.00995 2.06963

A17 2.09234 0.00027 0.00000 0.01700 0.01648 2.10882

A18 2.10091 0.00004 0.00000 -0.01232 -0.01262 2.08830

A19 1.90705 0.00033 0.00000 0.00786 0.00772 1.91478

A20 1.86744 0.00006 0.00000 0.00450 0.00458 1.87202

A21 2.00536 -0.00051 0.00000 -0.01366 -0.01364 1.99172

A22 1.85691 -0.00009 0.00000 -0.00033 -0.00035 1.85656

A23 1.91856 -0.00008 0.00000 -0.00410 -0.00407 1.91449

A24 1.90217 0.00033 0.00000 0.00688 0.00688 1.90905

A25 2.00705 -0.00104 0.00000 -0.00218 -0.00180 2.00525

A26 1.92018 0.00040 0.00000 -0.00410 -0.00417 1.91602

A27 1.87005 0.00044 0.00000 0.00504 0.00485 1.87490

A28 1.90077 0.00004 0.00000 -0.00210 -0.00223 1.89854

A29 1.90695 0.00046 0.00000 0.00382 0.00369 1.91064

A30 1.85247 -0.00025 0.00000 -0.00014 -0.00007 1.85240

A31 1.88366 -0.00123 0.00000 -0.00248 -0.00250 1.88116

A32 1.92178 0.00002 0.00000 -0.02327 -0.02343 1.89835

A33 1.80487 -0.00046 0.00000 0.00746 0.00764 1.81251

A34 1.72676 -0.00033 0.00000 -0.01402 -0.01381 1.71295

A35 1.82822 0.00106 0.00000 0.00684 0.00674 1.83496

A36 2.12599 -0.00033 0.00000 0.01468 0.01437 2.14036

A37 2.02791 -0.00014 0.00000 0.00304 0.00288 2.03079

A38 1.76942 0.00099 0.00000 0.04420 0.04404 1.81347

A39 1.83337 -0.00088 0.00000 -0.03562 -0.03532 1.79806

A40 1.30518 -0.00048 0.00000 -0.02145 -0.02151 1.28367

A41 1.89936 0.00008 0.00000 -0.00187 -0.00160 1.89776

A42 2.22908 -0.00041 0.00000 0.00266 0.00293 2.23200

A43 2.14157 0.00039 0.00000 0.00146 0.00084 2.14241

A44 1.91112 0.00037 0.00000 -0.00043 -0.00050 1.91061

A45 2.04859 -0.00022 0.00000 -0.00272 -0.00268 2.04591

A46 2.32329 -0.00014 0.00000 0.00322 0.00325 2.32654

A47 1.89995 -0.00029 0.00000 -0.00292 -0.00314 1.89682

A48 2.00047 0.00040 0.00000 0.00761 0.00772 2.00819

A49 2.38270 -0.00011 0.00000 -0.00465 -0.00454 2.37815

D1 -0.34580 -0.00058 0.00000 -0.01523 -0.01530 -0.36110

D2 2.94717 -0.00065 0.00000 -0.00820 -0.00838 2.93879

D3 1.09625 -0.00010 0.00000 0.02124 0.02130 1.11755

D4 2.86591 0.00039 0.00000 0.02128 0.02177 2.88769

D5 -0.12430 0.00033 0.00000 0.02831 0.02869 -0.09561

D6 -1.97522 0.00088 0.00000 0.05775 0.05838 -1.91684

D7 -0.15579 0.00028 0.00000 0.00734 0.00710 -0.14868

D8 3.13935 0.00101 0.00000 0.04805 0.04806 -3.09578

D9 2.91539 -0.00054 0.00000 -0.02632 -0.02564 2.88975

D10 -0.07266 0.00020 0.00000 0.01439 0.01531 -0.05734

D11 2.54002 -0.00016 0.00000 -0.00759 -0.00754 2.53248

D12 -1.73951 -0.00007 0.00000 -0.00169 -0.00161 -1.74112

D13 0.37455 0.00006 0.00000 0.00164 0.00174 0.37629

D14 -0.74466 -0.00017 0.00000 -0.01759 -0.01757 -0.76223

D15 1.25900 -0.00008 0.00000 -0.01170 -0.01164 1.24735

D16 -2.91013 0.00005 0.00000 -0.00837 -0.00829 -2.91842

D17 1.16718 -0.00080 0.00000 -0.05566 -0.05586 1.11131

D18 -3.11236 -0.00072 0.00000 -0.04976 -0.04994 3.12089

D19 -0.99830 -0.00059 0.00000 -0.04643 -0.04659 -1.04488

D20 -1.02224 0.00008 0.00000 0.00634 0.00578 -1.01647

D21 -2.99904 -0.00008 0.00000 0.00354 0.00370 -2.99534

D22 1.18203 -0.00056 0.00000 -0.00035 -0.00095 1.18107

D23 1.12321 0.00082 0.00000 0.01264 0.01266 1.13587

D24 -0.85358 0.00066 0.00000 0.00983 0.01059 -0.84299

D25 -2.95570 0.00018 0.00000 0.00594 0.00593 -2.94977

D26 -3.12454 0.00082 0.00000 0.02605 0.02582 -3.09873

D27 1.18185 0.00065 0.00000 0.02324 0.02374 1.20559

D28 -0.92027 0.00018 0.00000 0.01935 0.01909 -0.90119

D29 0.59388 0.00036 0.00000 0.00862 0.00861 0.60249

D30 -2.70203 -0.00036 0.00000 -0.02965 -0.02923 -2.73126

D31 3.02274 0.00093 0.00000 0.04604 0.04593 3.06866

D32 -0.27317 0.00021 0.00000 0.00777 0.00809 -0.26509

D33 -1.40333 0.00121 0.00000 0.05681 0.05664 -1.34669

D34 1.58395 0.00049 0.00000 0.01854 0.01880 1.60275

D35 -0.52478 -0.00060 0.00000 -0.02188 -0.02189 -0.54667

D36 -2.67836 -0.00020 0.00000 -0.01419 -0.01431 -2.69267

D37 1.59838 -0.00036 0.00000 -0.01468 -0.01473 1.58365

D38 -2.98452 -0.00104 0.00000 -0.05929 -0.05920 -3.04372

D39 1.14508 -0.00064 0.00000 -0.05160 -0.05162 1.09347

D40 -0.86136 -0.00080 0.00000 -0.05209 -0.05204 -0.91340

D41 1.40148 -0.00090 0.00000 -0.05531 -0.05520 1.34628

D42 -0.75210 -0.00050 0.00000 -0.04762 -0.04762 -0.79972

D43 -2.75855 -0.00066 0.00000 -0.04811 -0.04804 -2.80659

D44 1.09632 -0.00022 0.00000 -0.01285 -0.01263 1.08369

D45 3.04185 0.00077 0.00000 -0.01075 -0.01074 3.03111

D46 -1.15063 0.00036 0.00000 -0.01022 -0.01031 -1.16094

D47 -1.04794 -0.00070 0.00000 0.00049 0.00042 -1.04751

D48 0.89760 0.00030 0.00000 0.00259 0.00232 0.89991

D49 2.98830 -0.00012 0.00000 0.00312 0.00275 2.99105

D50 -3.09519 -0.00044 0.00000 0.00017 0.00032 -3.09487

D51 -1.14965 0.00056 0.00000 0.00227 0.00221 -1.14745

D52 0.94105 0.00014 0.00000 0.00280 0.00264 0.94369

D53 0.06014 0.00031 0.00000 0.01472 0.01458 0.07473

D54 2.22401 0.00012 0.00000 0.00606 0.00604 2.23006

D55 -2.04288 0.00010 0.00000 0.00682 0.00674 -2.03614

D56 -2.09923 0.00031 0.00000 0.01773 0.01761 -2.08162

D57 0.06463 0.00012 0.00000 0.00906 0.00907 0.07371

D58 2.08093 0.00010 0.00000 0.00982 0.00977 2.09070

D59 2.15512 0.00028 0.00000 0.01649 0.01639 2.17151

D60 -1.96420 0.00009 0.00000 0.00782 0.00785 -1.95635

D61 0.05210 0.00007 0.00000 0.00858 0.00855 0.06065

D62 -0.00710 -0.00021 0.00000 -0.01330 -0.01321 -0.02031

D63 -3.13038 -0.00040 0.00000 -0.01657 -0.01650 3.13630

D64 -0.03380 0.00019 0.00000 0.00502 0.00502 -0.02877

D65 3.11821 0.00011 0.00000 0.00179 0.00170 3.11991

D66 -0.06118 0.00035 0.00000 0.00925 0.00901 -0.05217

D67 1.86543 -0.00016 0.00000 -0.01156 -0.01152 1.85392

D68 -1.44811 0.00024 0.00000 0.00311 0.00312 -1.44499

D69 -1.99148 0.00034 0.00000 0.00711 0.00688 -1.98460

D70 -0.06487 -0.00017 0.00000 -0.01370 -0.01364 -0.07851

D71 2.90478 0.00023 0.00000 0.00098 0.00099 2.90577

D72 1.94500 -0.00032 0.00000 -0.01961 -0.02001 1.92499

D73 -2.41157 -0.00083 0.00000 -0.04041 -0.04054 -2.45211

D74 0.55807 -0.00043 0.00000 -0.02574 -0.02591 0.53217

D75 -1.96800 0.00006 0.00000 0.03728 0.03740 -1.93060

D76 1.15132 0.00029 0.00000 0.04115 0.04132 1.19264

D77 0.04538 0.00031 0.00000 0.01724 0.01721 0.06260

D78 -3.11848 0.00054 0.00000 0.02112 0.02113 -3.09735

D79 2.44469 0.00078 0.00000 0.04827 0.04811 2.49280

D80 -0.71917 0.00101 0.00000 0.05214 0.05202 -0.66715

D81 1.94738 0.00080 0.00000 0.03939 0.03922 1.98660

D82 -1.20797 0.00091 0.00000 0.04377 0.04370 -1.16427

D83 0.06402 0.00005 0.00000 0.00616 0.00609 0.07010

D84 -3.09134 0.00016 0.00000 0.01054 0.01056 -3.08078

D85 -2.91603 -0.00024 0.00000 -0.00779 -0.00790 -2.92393

D86 0.21180 -0.00013 0.00000 -0.00341 -0.00343 0.20837

Item Value Threshold Converged?

Maximum Force 0.006596 0.000450 NO

RMS Force 0.000922 0.000300 NO

Maximum Displacement 0.235968 0.001800 NO

RMS Displacement 0.052706 0.001200 NO

Predicted change in Energy=-3.446181D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.180232 1.479872 0.419037

2 6 0 0.020512 1.060258 -0.094341

3 6 0 -0.620316 3.739423 -0.220432

4 6 0 -1.560988 2.820282 0.281378

5 1 0 -1.817159 0.818463 1.026460

6 1 0 -2.498561 3.187646 0.722151

7 6 0 0.739729 1.792176 -1.148989

8 1 0 1.849744 1.705033 -0.982229

9 1 0 0.523064 1.271000 -2.125222

10 6 0 0.352055 3.258761 -1.262809

11 1 0 1.286043 3.883694 -1.228804

12 1 0 -0.113325 3.446601 -2.269753

13 1 0 -0.957318 4.783762 -0.390936

14 1 0 0.415899 0.066486 0.170938

15 8 0 2.760507 4.058173 0.885037

16 6 0 0.431266 3.961319 1.343889

17 6 0 1.005799 2.719490 1.684198

18 6 0 1.587997 4.818439 0.883665

19 8 0 1.675710 5.979551 0.516729

20 6 0 2.432028 2.753325 1.349671

21 8 0 3.365319 1.964914 1.381358

22 1 0 -0.326827 4.458361 1.972627

23 1 0 0.552655 1.905979 2.240834

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.371648 0.000000

3 C 2.414125 2.757623 0.000000

4 C 1.400223 2.395827 1.407657 0.000000

5 H 1.100954 2.166032 3.393992 2.151290 0.000000

6 H 2.178615 3.396788 2.172723 1.099218 2.483937

7 C 2.498498 1.471482 2.550238 2.897628 3.495479

8 H 3.345893 2.133113 3.289419 3.804415 4.273993

9 H 3.068892 2.102724 3.320942 3.540518 3.951523

10 C 2.888072 2.511703 1.504358 2.497300 3.987643

11 H 3.817887 3.295507 2.161443 3.393683 4.910369

12 H 3.497987 3.231867 2.131315 2.999379 4.546997

13 H 3.409023 3.861165 1.110533 2.161406 4.297899

14 H 2.146357 1.101947 3.836324 3.391706 2.506778

15 O 4.732253 4.177828 3.571222 4.535647 5.609880

16 C 3.099977 3.263951 1.897936 2.529816 3.877335

17 C 2.813541 2.624317 2.704094 2.926851 3.466355

18 C 4.361766 4.187772 2.694430 3.777762 5.255026

19 O 5.330390 5.226139 3.291399 4.529082 6.252743

20 C 3.941597 3.281320 3.571332 4.133994 4.680144

21 O 4.671548 3.766142 4.647569 5.119581 5.319623

22 H 3.466026 3.992506 2.326481 2.658341 4.045390

23 H 2.550178 2.539973 3.285606 3.023723 2.876355

6 7 8 9 10

6 H 0.000000

7 C 3.991869 0.000000

8 H 4.900083 1.125849 0.000000

9 H 4.572885 1.127652 1.804133 0.000000

10 C 3.474354 1.521222 2.176206 2.173521 0.000000

11 H 4.314387 2.163164 2.263874 2.865637 1.124292

12 H 3.835088 2.172771 2.923084 2.271370 1.125077

13 H 2.482333 3.521959 4.208063 4.187932 2.190947

14 H 4.305758 2.196607 2.463847 2.595128 3.500047

15 O 5.333118 3.654524 3.139019 4.672916 3.324597

16 C 3.093383 3.318850 3.537475 4.391010 2.700877

17 C 3.664048 2.992933 2.975097 4.104002 3.066438

18 C 4.402901 3.742928 3.639144 4.771981 2.927030

19 O 5.026079 4.602693 4.533064 5.520774 3.510202

20 C 4.989301 3.167173 2.622162 4.232766 3.377397

21 O 6.026170 3.650509 2.819761 4.566840 4.212532

22 H 2.809775 4.241529 4.587969 5.260604 3.516812

23 H 3.641289 3.396888 3.480080 4.412088 3.761087

11 12 13 14 15

11 H 0.000000

12 H 1.798015 0.000000

13 H 2.558284 2.455662 0.000000

14 H 4.157825 4.202646 4.945110 0.000000

15 O 2.583178 4.311106 3.997100 4.684089 0.000000

16 C 2.712088 3.690518 2.369429 4.067650 2.375982

17 C 3.149522 4.173111 3.524376 3.110686 2.347282

18 C 2.329689 3.836728 2.846830 4.945994 1.397421

19 O 2.755239 4.169048 3.030941 6.055661 2.236991

20 C 3.039663 4.478804 4.317412 3.559957 1.423520

21 O 3.849422 5.256137 5.456383 3.710556 2.234696

22 H 3.630531 4.366582 2.467759 4.804820 3.297671

23 H 4.060493 4.812737 4.181849 2.772527 3.368195

16 17 18 19 20

16 C 0.000000

17 C 1.409977 0.000000

18 C 1.511452 2.320645 0.000000

19 O 2.511194 3.527005 1.220867 0.000000

20 C 2.337162 1.465326 2.279088 3.416773 0.000000

21 O 3.549042 2.495683 3.398408 4.440684 1.222141

22 H 1.103208 2.209696 2.232050 2.905824 3.302499

23 H 2.245811 1.084888 3.375835 4.563746 2.245932

21 22 23

21 O 0.000000

22 H 4.494310 0.000000

23 H 2.941641 2.712946 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.488637 -0.272655 -0.726639

2 6 0 1.943063 -1.167983 0.157758

3 6 0 0.990904 1.419799 0.122125

4 6 0 2.081242 1.066621 -0.695144

5 1 0 3.168566 -0.590208 -1.532217

6 1 0 2.473260 1.791888 -1.422186

7 6 0 1.293829 -0.758528 1.413187

8 1 0 0.430774 -1.446240 1.636178

9 1 0 2.043182 -0.909753 2.242162

10 6 0 0.814636 0.685215 1.423051

11 1 0 -0.267389 0.705342 1.727767

12 1 0 1.372630 1.260183 2.212893

13 1 0 0.723724 2.495435 0.192163

14 1 0 2.108521 -2.248703 0.020084

15 8 0 -2.140678 -0.291693 0.254839

16 6 0 -0.416182 0.780004 -0.979207

17 6 0 -0.274505 -0.614508 -1.131855

18 6 0 -1.652225 0.960292 -0.128218

19 8 0 -2.255157 1.942275 0.275143

20 6 0 -1.300286 -1.282705 -0.326580

21 8 0 -1.596501 -2.436869 -0.054934

22 1 0 -0.291657 1.485966 -1.817765

23 1 0 0.362394 -1.146929 -1.830333

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2360403 0.8307812 0.6475182

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 467.5803064138 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.402062175453E-01 A.U. after 15 cycles

Convg = 0.5621D-08 -V/T = 0.9991

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.002464157 -0.003628895 -0.000526656

2 6 -0.000570122 -0.000378713 0.010849722

3 6 -0.004668769 -0.003293215 -0.007509695

4 6 0.002867808 0.010991693 -0.000974670

5 1 0.001364339 -0.002208666 -0.000388186

6 1 -0.001067362 -0.001008384 -0.000128648

7 6 0.001313496 0.003725745 -0.003692974

8 1 0.000186817 -0.000063653 0.000456844

9 1 0.000586898 0.000338593 -0.000379253

10 6 0.000090863 0.001408157 -0.000522389

11 1 -0.000359552 0.000519758 -0.001270386

12 1 -0.000580696 -0.000825070 0.000276967

13 1 0.001808511 0.000182671 0.002239481

14 1 0.000936230 -0.000379182 0.000064151

15 8 -0.000414881 -0.000889947 0.000290926

16 6 0.005193143 0.000606335 0.008482656

17 6 -0.001654468 -0.006210562 -0.004362930

18 6 -0.001305404 0.000710462 -0.003185421

19 8 0.000427651 -0.000445589 0.001248450

20 6 0.000739184 0.000935476 0.000045330

21 8 -0.001311724 0.000803199 -0.000463790

22 1 -0.001736782 -0.000925439 -0.002652402

23 1 0.000618980 0.000035227 0.002102876

-------------------------------------------------------------------

Cartesian Forces: Max 0.010991693 RMS 0.002961849

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.006152980 RMS 0.001126432

Search for a saddle point.

Step number 22 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 21 22

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0

Eigenvalues --- -0.06230 -0.00922 0.00206 0.00374 0.00591

Eigenvalues --- 0.00966 0.01023 0.01408 0.01814 0.01984

Eigenvalues --- 0.02063 0.02224 0.02435 0.02550 0.02752

Eigenvalues --- 0.02917 0.03045 0.03233 0.03316 0.03539

Eigenvalues --- 0.03630 0.03775 0.03902 0.04100 0.04276

Eigenvalues --- 0.04543 0.05166 0.05665 0.05961 0.06019

Eigenvalues --- 0.06661 0.07338 0.08331 0.08693 0.09806

Eigenvalues --- 0.11519 0.13427 0.14047 0.15369 0.20384

Eigenvalues --- 0.22436 0.24839 0.26031 0.26449 0.27987

Eigenvalues --- 0.29771 0.30488 0.31193 0.31466 0.31866

Eigenvalues --- 0.31969 0.32378 0.32706 0.34412 0.35801

Eigenvalues --- 0.37404 0.39578 0.40370 0.43131 0.45232

Eigenvalues --- 0.49634 1.08416 1.10830

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D79

1 0.60837 0.47529 -0.18435 0.16614 0.14952

D73 D80 D35 D5 D29

1 -0.14750 0.12871 0.11379 0.10882 -0.10798

RFO step: Lambda0=3.982777660D-06 Lambda=-1.49785425D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.402

Iteration 1 RMS(Cart)= 0.04141430 RMS(Int)= 0.00279887

Iteration 2 RMS(Cart)= 0.00451475 RMS(Int)= 0.00028478

Iteration 3 RMS(Cart)= 0.00000437 RMS(Int)= 0.00028476

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00028476

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.59204 -0.00037 0.00000 0.00179 0.00178 2.59382

R2 2.64604 0.00615 0.00000 0.02539 0.02561 2.67165

R3 2.08050 0.00032 0.00000 -0.00183 -0.00183 2.07867

R4 2.78070 0.00611 0.00000 0.03360 0.03363 2.81433

R5 2.08238 0.00069 0.00000 0.00025 0.00025 2.08263

R6 4.95924 -0.00397 0.00000 -0.23634 -0.23674 4.72250

R7 2.66009 -0.00299 0.00000 -0.02517 -0.02490 2.63519

R8 2.84282 -0.00053 0.00000 -0.01754 -0.01738 2.82544

R9 2.09860 -0.00072 0.00000 -0.00476 -0.00476 2.09384

R10 3.58658 0.00370 0.00000 0.10492 0.10505 3.69163

R11 2.07722 0.00052 0.00000 0.00083 0.00083 2.07805

R12 2.12755 0.00026 0.00000 0.00036 0.00036 2.12791

R13 2.13095 0.00006 0.00000 -0.00140 -0.00140 2.12955

R14 2.87469 -0.00006 0.00000 -0.00479 -0.00453 2.87016

R15 2.12460 -0.00005 0.00000 0.00070 0.00070 2.12530

R16 2.12609 -0.00015 0.00000 -0.00019 -0.00019 2.12590

R17 2.64074 -0.00022 0.00000 0.00643 0.00644 2.64718

R18 2.69006 -0.00077 0.00000 -0.00548 -0.00558 2.68448

R19 2.66447 0.00130 0.00000 -0.01161 -0.01201 2.65246

R20 2.85623 -0.00030 0.00000 -0.01106 -0.01096 2.84528

R21 2.08476 -0.00074 0.00000 -0.00500 -0.00500 2.07976

R22 2.76907 -0.00054 0.00000 -0.00215 -0.00222 2.76685

R23 2.05014 0.00079 0.00000 0.00213 0.00213 2.05227

R24 2.30710 -0.00077 0.00000 -0.00081 -0.00081 2.30630

R25 2.30951 -0.00153 0.00000 -0.00024 -0.00024 2.30927

A1 2.08759 -0.00129 0.00000 -0.00205 -0.00201 2.08558

A2 2.12840 -0.00212 0.00000 -0.04759 -0.04771 2.08069

A3 2.06238 0.00336 0.00000 0.04648 0.04605 2.10843

A4 2.14595 -0.00121 0.00000 -0.01111 -0.01196 2.13398

A5 2.09426 0.00075 0.00000 0.01536 0.01584 2.11010

A6 1.45211 0.00094 0.00000 0.03469 0.03500 1.48711

A7 2.03280 0.00038 0.00000 -0.00722 -0.00708 2.02571

A8 1.55854 0.00010 0.00000 0.01758 0.01799 1.57653

A9 1.84660 -0.00083 0.00000 -0.03692 -0.03718 1.80942

A10 2.06045 0.00180 0.00000 0.03460 0.03386 2.09431

A11 2.05554 -0.00045 0.00000 -0.00403 -0.00500 2.05055

A12 1.72417 -0.00159 0.00000 -0.03524 -0.03478 1.68939

A13 1.97168 -0.00051 0.00000 0.00787 0.00739 1.97907

A14 1.82382 -0.00016 0.00000 -0.01858 -0.01786 1.80596

A15 1.75660 0.00047 0.00000 -0.00600 -0.00632 1.75028

A16 2.06963 0.00043 0.00000 -0.01610 -0.01558 2.05404

A17 2.10882 -0.00161 0.00000 -0.03975 -0.03988 2.06894

A18 2.08830 0.00122 0.00000 0.05457 0.05418 2.14247

A19 1.91478 -0.00061 0.00000 -0.00940 -0.00957 1.90521

A20 1.87202 0.00038 0.00000 0.00189 0.00189 1.87391

A21 1.99172 0.00072 0.00000 0.00419 0.00447 1.99619

A22 1.85656 0.00005 0.00000 0.00239 0.00243 1.85899

A23 1.91449 0.00002 0.00000 0.00110 0.00120 1.91568

A24 1.90905 -0.00061 0.00000 -0.00021 -0.00047 1.90857

A25 2.00525 -0.00063 0.00000 -0.01792 -0.01747 1.98778

A26 1.91602 0.00059 0.00000 0.00293 0.00286 1.91887

A27 1.87490 -0.00009 0.00000 0.00543 0.00525 1.88015

A28 1.89854 -0.00029 0.00000 0.00418 0.00400 1.90254

A29 1.91064 0.00066 0.00000 0.00841 0.00831 1.91895

A30 1.85240 -0.00019 0.00000 -0.00188 -0.00184 1.85056

A31 1.88116 0.00042 0.00000 -0.00266 -0.00276 1.87840

A32 1.89835 0.00056 0.00000 -0.00809 -0.00821 1.89014

A33 1.81251 -0.00136 0.00000 -0.01470 -0.01451 1.79800

A34 1.71295 -0.00065 0.00000 -0.02695 -0.02668 1.68627

A35 1.83496 0.00045 0.00000 0.01028 0.01007 1.84503

A36 2.14036 0.00021 0.00000 0.02048 0.02010 2.16045

A37 2.03079 0.00037 0.00000 0.00718 0.00638 2.03716

A38 1.81347 0.00018 0.00000 0.02720 0.02655 1.84002

A39 1.79806 0.00007 0.00000 -0.02376 -0.02350 1.77456

A40 1.28367 0.00029 0.00000 -0.00207 -0.00208 1.28160

A41 1.89776 -0.00091 0.00000 -0.00648 -0.00618 1.89157

A42 2.23200 0.00067 0.00000 0.01320 0.01304 2.24504

A43 2.14241 0.00018 0.00000 -0.00688 -0.00700 2.13541

A44 1.91061 -0.00051 0.00000 -0.00585 -0.00574 1.90487

A45 2.04591 -0.00009 0.00000 -0.00232 -0.00238 2.04353

A46 2.32654 0.00061 0.00000 0.00823 0.00818 2.33471

A47 1.89682 0.00058 0.00000 0.00400 0.00387 1.90069

A48 2.00819 -0.00021 0.00000 0.00183 0.00190 2.01008

A49 2.37815 -0.00036 0.00000 -0.00582 -0.00575 2.37240

D1 -0.36110 -0.00068 0.00000 -0.03267 -0.03248 -0.39358

D2 2.93879 -0.00012 0.00000 -0.00917 -0.00874 2.93005

D3 1.11755 0.00028 0.00000 0.01348 0.01349 1.13105

D4 2.88769 -0.00037 0.00000 -0.00056 -0.00122 2.88647

D5 -0.09561 0.00019 0.00000 0.02294 0.02252 -0.07309

D6 -1.91684 0.00060 0.00000 0.04559 0.04475 -1.87209

D7 -0.14868 0.00123 0.00000 0.03799 0.03823 -0.11045

D8 -3.09578 0.00085 0.00000 0.03932 0.03925 -3.05653

D9 2.88975 0.00061 0.00000 0.00145 0.00068 2.89044

D10 -0.05734 0.00023 0.00000 0.00278 0.00170 -0.05564

D11 2.53248 0.00052 0.00000 0.00949 0.00936 2.54184

D12 -1.74112 0.00048 0.00000 0.00852 0.00835 -1.73277

D13 0.37629 0.00044 0.00000 0.01228 0.01197 0.38826

D14 -0.76223 0.00002 0.00000 -0.01131 -0.01132 -0.77355

D15 1.24735 -0.00002 0.00000 -0.01228 -0.01233 1.23503

D16 -2.91842 -0.00006 0.00000 -0.00852 -0.00871 -2.92713

D17 1.11131 -0.00080 0.00000 -0.04481 -0.04489 1.06643

D18 3.12089 -0.00085 0.00000 -0.04578 -0.04589 3.07500

D19 -1.04488 -0.00088 0.00000 -0.04202 -0.04228 -1.08716

D20 -1.01647 0.00017 0.00000 0.01413 0.01367 -1.00279

D21 -2.99534 0.00107 0.00000 0.02023 0.02002 -2.97532

D22 1.18107 0.00086 0.00000 0.02272 0.02245 1.20353

D23 1.13587 -0.00116 0.00000 -0.00298 -0.00303 1.13285

D24 -0.84299 -0.00026 0.00000 0.00311 0.00331 -0.83968

D25 -2.94977 -0.00046 0.00000 0.00561 0.00575 -2.94402

D26 -3.09873 -0.00084 0.00000 -0.00996 -0.01001 -3.10873

D27 1.20559 0.00006 0.00000 -0.00386 -0.00367 1.20192

D28 -0.90119 -0.00015 0.00000 -0.00137 -0.00123 -0.90241

D29 0.60249 0.00024 0.00000 -0.00068 -0.00091 0.60158

D30 -2.73126 0.00029 0.00000 -0.01265 -0.01310 -2.74436

D31 3.06866 0.00131 0.00000 0.06024 0.06005 3.12871

D32 -0.26509 0.00136 0.00000 0.04827 0.04786 -0.21723

D33 -1.34669 0.00076 0.00000 0.03081 0.03086 -1.31583

D34 1.60275 0.00082 0.00000 0.01884 0.01867 1.62141

D35 -0.54667 -0.00047 0.00000 -0.02038 -0.02014 -0.56681

D36 -2.69267 -0.00009 0.00000 -0.01513 -0.01498 -2.70765

D37 1.58365 -0.00011 0.00000 -0.01737 -0.01715 1.56649

D38 -3.04372 -0.00147 0.00000 -0.07343 -0.07363 -3.11735

D39 1.09347 -0.00108 0.00000 -0.06818 -0.06847 1.02500

D40 -0.91340 -0.00111 0.00000 -0.07042 -0.07064 -0.98405

D41 1.34628 -0.00171 0.00000 -0.05981 -0.05977 1.28651

D42 -0.79972 -0.00132 0.00000 -0.05456 -0.05461 -0.85433

D43 -2.80659 -0.00135 0.00000 -0.05680 -0.05678 -2.86337

D44 1.08369 0.00079 0.00000 0.01511 0.01535 1.09903

D45 3.03111 0.00089 0.00000 0.01668 0.01686 3.04797

D46 -1.16094 0.00064 0.00000 0.01003 0.01023 -1.15070

D47 -1.04751 -0.00047 0.00000 -0.00198 -0.00214 -1.04965

D48 0.89991 -0.00036 0.00000 -0.00041 -0.00063 0.89929

D49 2.99105 -0.00062 0.00000 -0.00706 -0.00725 2.98380

D50 -3.09487 -0.00004 0.00000 -0.00182 -0.00177 -3.09664

D51 -1.14745 0.00007 0.00000 -0.00024 -0.00025 -1.14770

D52 0.94369 -0.00019 0.00000 -0.00689 -0.00688 0.93681

D53 0.07473 -0.00024 0.00000 0.00464 0.00451 0.07924

D54 2.23006 -0.00015 0.00000 -0.00106 -0.00105 2.22900

D55 -2.03614 -0.00019 0.00000 0.00362 0.00358 -2.03256

D56 -2.08162 0.00001 0.00000 0.01310 0.01293 -2.06869

D57 0.07371 0.00010 0.00000 0.00740 0.00736 0.08107

D58 2.09070 0.00007 0.00000 0.01208 0.01199 2.10269

D59 2.17151 0.00029 0.00000 0.00971 0.00959 2.18110

D60 -1.95635 0.00038 0.00000 0.00402 0.00402 -1.95233

D61 0.06065 0.00034 0.00000 0.00869 0.00865 0.06930

D62 -0.02031 0.00019 0.00000 -0.00524 -0.00512 -0.02544

D63 3.13630 -0.00029 0.00000 -0.00911 -0.00897 3.12733

D64 -0.02877 -0.00001 0.00000 0.00021 0.00015 -0.02862

D65 3.11991 -0.00029 0.00000 -0.00117 -0.00134 3.11857

D66 -0.05217 -0.00057 0.00000 -0.00655 -0.00648 -0.05865

D67 1.85392 -0.00075 0.00000 -0.02357 -0.02355 1.83037

D68 -1.44499 -0.00115 0.00000 -0.02569 -0.02559 -1.47058

D69 -1.98460 0.00053 0.00000 0.00873 0.00879 -1.97581

D70 -0.07851 0.00035 0.00000 -0.00829 -0.00828 -0.08679

D71 2.90577 -0.00005 0.00000 -0.01040 -0.01032 2.89545

D72 1.92499 -0.00083 0.00000 -0.03658 -0.03680 1.88819

D73 -2.45211 -0.00101 0.00000 -0.05360 -0.05387 -2.50598

D74 0.53217 -0.00141 0.00000 -0.05571 -0.05591 0.47626

D75 -1.93060 -0.00058 0.00000 0.01965 0.01982 -1.91079

D76 1.19264 -0.00001 0.00000 0.02422 0.02439 1.21703

D77 0.06260 -0.00033 0.00000 0.00874 0.00868 0.07128

D78 -3.09735 0.00024 0.00000 0.01331 0.01326 -3.08409

D79 2.49280 0.00084 0.00000 0.05741 0.05739 2.55018

D80 -0.66715 0.00141 0.00000 0.06198 0.06197 -0.60518

D81 1.98660 -0.00035 0.00000 0.02263 0.02221 2.00882

D82 -1.16427 0.00001 0.00000 0.02451 0.02421 -1.14006

D83 0.07010 -0.00026 0.00000 0.00515 0.00516 0.07527

D84 -3.08078 0.00011 0.00000 0.00703 0.00716 -3.07362

D85 -2.92393 0.00006 0.00000 0.00495 0.00487 -2.91906

D86 0.20837 0.00042 0.00000 0.00683 0.00687 0.21524

Item Value Threshold Converged?

Maximum Force 0.006153 0.000450 NO

RMS Force 0.001126 0.000300 NO

Maximum Displacement 0.172177 0.001800 NO

RMS Displacement 0.045080 0.001200 NO

Predicted change in Energy=-4.538555D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.175635 1.510230 0.438055

2 6 0 0.049448 1.104803 -0.029717

3 6 0 -0.644843 3.746018 -0.265494

4 6 0 -1.577866 2.854140 0.262329

5 1 0 -1.769171 0.820857 1.056480

6 1 0 -2.525437 3.182276 0.713642

7 6 0 0.766001 1.830420 -1.115067

8 1 0 1.874628 1.779080 -0.924595

9 1 0 0.579566 1.269660 -2.074608

10 6 0 0.341127 3.278367 -1.287585

11 1 0 1.255179 3.933297 -1.266656

12 1 0 -0.122258 3.424088 -2.302286

13 1 0 -0.967541 4.795614 -0.413510

14 1 0 0.472289 0.129788 0.262050

15 8 0 2.748269 4.007164 0.855496

16 6 0 0.432972 3.937412 1.352513

17 6 0 0.985439 2.685409 1.664629

18 6 0 1.586489 4.788951 0.892863

19 8 0 1.691606 5.957005 0.555116

20 6 0 2.403746 2.703184 1.301537

21 8 0 3.319732 1.894305 1.299529

22 1 0 -0.337974 4.434852 1.960323

23 1 0 0.537833 1.866085 2.219412

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.372593 0.000000

3 C 2.403220 2.741103 0.000000

4 C 1.413776 2.406994 1.394481 0.000000

5 H 1.099986 2.137247 3.401219 2.191235 0.000000

6 H 2.166484 3.390946 2.193889 1.099658 2.503153

7 C 2.506922 1.489279 2.526216 2.904984 3.487396

8 H 3.351597 2.141667 3.263586 3.805819 4.256774

9 H 3.074424 2.118911 3.302184 3.553360 3.939759

10 C 2.899088 2.528179 1.495160 2.502946 3.998419

11 H 3.832251 3.314239 2.155802 3.395368 4.922493

12 H 3.504557 3.251636 2.127264 3.003479 4.557460

13 H 3.400326 3.847551 1.108015 2.144430 4.313024

14 H 2.156908 1.102078 3.821440 3.409579 2.476456

15 O 4.669684 4.060902 3.583019 4.516277 5.531745

16 C 3.052058 3.175110 1.953526 2.530899 3.827529

17 C 2.748776 2.499040 2.740088 2.926679 3.381460

18 C 4.311169 4.097144 2.721827 3.762208 5.199325

19 O 5.292313 5.155829 3.319768 4.516962 6.213562

20 C 3.870492 3.141620 3.582874 4.117764 4.584369

21 O 4.593253 3.617314 4.647149 5.097405 5.206563

22 H 3.401821 3.898664 2.350090 2.630431 3.990766

23 H 2.497166 2.424180 3.332811 3.046737 2.786966

6 7 8 9 10

6 H 0.000000

7 C 4.000657 0.000000

8 H 4.900343 1.126042 0.000000

9 H 4.590587 1.126911 1.805332 0.000000

10 C 3.497333 1.518825 2.175143 2.170521 0.000000

11 H 4.333437 2.164339 2.267459 2.864297 1.124661

12 H 3.863880 2.176757 2.931150 2.277270 1.124979

13 H 2.510055 3.505670 4.175957 4.193464 2.186015

14 H 4.302090 2.207910 2.468775 2.602074 3.511712

15 O 5.339713 3.542699 2.982671 4.558806 3.304281

16 C 3.119386 3.261790 3.452824 4.345521 2.722663

17 C 3.671172 2.916482 2.883777 4.018827 3.079335

18 C 4.418309 3.668499 3.527818 4.712238 2.930383

19 O 5.050515 4.546972 4.436000 5.488469 3.520574

20 C 4.987183 3.046949 2.467711 4.096459 3.359879

21 O 6.013995 3.515096 2.654869 4.391297 4.181014

22 H 2.812144 4.178498 4.502386 5.209701 3.513907

23 H 3.658323 3.342466 3.417510 4.335444 3.785798

11 12 13 14 15

11 H 0.000000

12 H 1.796985 0.000000

13 H 2.532180 2.482551 0.000000

14 H 4.173313 4.216837 4.929445 0.000000

15 O 2.595824 4.307144 4.004906 4.535009 0.000000

16 C 2.745194 3.732202 2.411801 3.960891 2.369070

17 C 3.197251 4.184382 3.547641 2.960025 2.347190

18 C 2.346366 3.871904 2.868750 4.831890 1.400828

19 O 2.757666 4.227353 3.059106 5.960628 2.238000

20 C 3.070505 4.459590 4.322642 3.381335 1.420568

21 O 3.873651 5.211584 5.452780 3.506824 2.233363

22 H 3.633605 4.386115 2.482255 4.698322 3.305820

23 H 4.115899 4.827923 4.216702 2.617306 3.366082

16 17 18 19 20

16 C 0.000000

17 C 1.403620 0.000000

18 C 1.505655 2.319864 0.000000

19 O 2.509732 3.526050 1.220440 0.000000

20 C 2.325913 1.464154 2.277136 3.413450 0.000000

21 O 3.537016 2.491600 3.398306 4.439649 1.222015

22 H 1.100561 2.213460 2.228993 2.900129 3.309033

23 H 2.247867 1.086015 3.376767 4.564723 2.241620

21 22 23

21 O 0.000000

22 H 4.502204 0.000000

23 H 2.930178 2.726303 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.455949 -0.294545 -0.714771

2 6 0 1.841057 -1.190770 0.123501

3 6 0 1.034832 1.428635 0.172100

4 6 0 2.100599 1.072478 -0.653653

5 1 0 3.117812 -0.669548 -1.509302

6 1 0 2.542432 1.763465 -1.386161

7 6 0 1.197627 -0.773068 1.400010

8 1 0 0.293295 -1.417630 1.586274

9 1 0 1.925310 -0.994167 2.231589

10 6 0 0.803178 0.692691 1.452813

11 1 0 -0.278836 0.770376 1.749584

12 1 0 1.385081 1.217917 2.259724

13 1 0 0.767189 2.502428 0.227164

14 1 0 1.947652 -2.276540 -0.032436

15 8 0 -2.114326 -0.278916 0.243507

16 6 0 -0.389514 0.773526 -0.993377

17 6 0 -0.242038 -0.615476 -1.131471

18 6 0 -1.627679 0.971221 -0.159793

19 8 0 -2.242572 1.955266 0.218409

20 6 0 -1.268190 -1.271716 -0.319001

21 8 0 -1.556075 -2.423889 -0.031008

22 1 0 -0.223969 1.490873 -1.811450

23 1 0 0.392890 -1.164712 -1.820408

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2334569 0.8538282 0.6597267

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 469.2271076374 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.427414240949E-01 A.U. after 15 cycles

Convg = 0.2911D-08 -V/T = 0.9991

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000053120 0.001069931 -0.002310865

2 6 0.003993752 0.008610073 -0.002239332

3 6 -0.011430197 0.005863040 -0.010895184

4 6 0.001898128 -0.012919072 0.003132306

5 1 -0.002919617 0.001727926 -0.000050553

6 1 0.000697234 0.002565933 -0.001772772

7 6 -0.001888012 -0.004880311 0.002267244

8 1 -0.000205162 -0.000428114 -0.000544506

9 1 0.000271235 0.000115096 0.000344622

10 6 0.001386520 -0.001338690 0.000224532

11 1 -0.000326341 0.000567049 -0.001189831

12 1 -0.000708044 -0.001144248 0.000197326

13 1 0.002183753 0.001936694 0.001959399

14 1 0.000105132 0.000578616 -0.000148456

15 8 -0.000417991 0.000071430 0.000163951

16 6 0.006441619 0.003763483 0.015510955

17 6 -0.005245031 -0.007142686 -0.003429756

18 6 0.000506484 0.000704688 -0.004077352

19 8 0.000315377 -0.000563596 0.001077101

20 6 0.007365245 0.000066115 -0.000150170

21 8 -0.000653264 0.000586358 -0.000102653

22 1 -0.002341147 -0.001091403 -0.002401264

23 1 0.000917207 0.001281686 0.004435260

-------------------------------------------------------------------

Cartesian Forces: Max 0.015510955 RMS 0.004057811

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.009660406 RMS 0.001464532

Search for a saddle point.

Step number 23 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 22 23

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0

Eigenvalues --- -0.06326 -0.00963 0.00218 0.00373 0.00592

Eigenvalues --- 0.00970 0.01023 0.01411 0.01920 0.02055

Eigenvalues --- 0.02069 0.02228 0.02459 0.02680 0.02755

Eigenvalues --- 0.02991 0.03074 0.03307 0.03356 0.03621

Eigenvalues --- 0.03729 0.03864 0.04081 0.04145 0.04541

Eigenvalues --- 0.04842 0.05569 0.05688 0.05970 0.06363

Eigenvalues --- 0.07008 0.07345 0.08338 0.08746 0.09807

Eigenvalues --- 0.11526 0.13475 0.14133 0.15452 0.20383

Eigenvalues --- 0.22563 0.25424 0.26282 0.26748 0.28045

Eigenvalues --- 0.29775 0.30492 0.31208 0.31459 0.31876

Eigenvalues --- 0.31972 0.32396 0.32752 0.34439 0.35847

Eigenvalues --- 0.37494 0.39578 0.40372 0.43159 0.45427

Eigenvalues --- 0.49624 1.08418 1.10829

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D79 D73

1 0.65527 0.34221 -0.18983 0.17481 -0.17359

D80 D4 D5 D6 D29

1 0.15729 0.15694 0.11606 0.11450 -0.10759

RFO step: Lambda0=8.072692368D-04 Lambda=-1.53614365D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.487

Iteration 1 RMS(Cart)= 0.03876216 RMS(Int)= 0.00279222

Iteration 2 RMS(Cart)= 0.00453030 RMS(Int)= 0.00044457

Iteration 3 RMS(Cart)= 0.00000357 RMS(Int)= 0.00044456

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00044456

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.59382 0.00122 0.00000 -0.01173 -0.01104 2.58279

R2 2.67165 -0.00533 0.00000 -0.03152 -0.03097 2.64068

R3 2.07867 0.00046 0.00000 0.00108 0.00108 2.07975

R4 2.81433 -0.00465 0.00000 -0.01408 -0.01351 2.80082

R5 2.08263 -0.00051 0.00000 0.00127 0.00127 2.08389

R6 4.72250 0.00151 0.00000 -0.23512 -0.23506 4.48744

R7 2.63519 0.00157 0.00000 0.01483 0.01464 2.64983

R8 2.82544 0.00155 0.00000 0.00492 0.00478 2.83022

R9 2.09384 0.00094 0.00000 -0.00247 -0.00247 2.09137

R10 3.69163 0.00966 0.00000 0.07481 0.07408 3.76571

R11 2.07805 -0.00056 0.00000 -0.00159 -0.00159 2.07646

R12 2.12791 -0.00027 0.00000 -0.00062 -0.00062 2.12729

R13 2.12955 -0.00040 0.00000 -0.00064 -0.00064 2.12891

R14 2.87016 0.00065 0.00000 0.00156 0.00211 2.87227

R15 2.12530 0.00004 0.00000 0.00033 0.00033 2.12563

R16 2.12590 -0.00003 0.00000 -0.00064 -0.00064 2.12526

R17 2.64718 0.00069 0.00000 0.00240 0.00225 2.64943

R18 2.68448 0.00026 0.00000 -0.00923 -0.00932 2.67517

R19 2.65246 0.00224 0.00000 0.01937 0.01838 2.67083

R20 2.84528 0.00173 0.00000 -0.00625 -0.00626 2.83901

R21 2.07976 -0.00018 0.00000 -0.00262 -0.00262 2.07714

R22 2.76685 0.00567 0.00000 0.01512 0.01521 2.78206

R23 2.05227 0.00092 0.00000 0.00234 0.00234 2.05462

R24 2.30630 -0.00081 0.00000 -0.00044 -0.00044 2.30586

R25 2.30927 -0.00088 0.00000 -0.00074 -0.00074 2.30853

A1 2.08558 -0.00020 0.00000 -0.01552 -0.01470 2.07088

A2 2.08069 0.00340 0.00000 0.04883 0.04843 2.12911

A3 2.10843 -0.00317 0.00000 -0.03391 -0.03428 2.07415

A4 2.13398 0.00055 0.00000 0.01784 0.01538 2.14936

A5 2.11010 0.00003 0.00000 -0.01026 -0.00931 2.10079

A6 1.48711 0.00112 0.00000 0.05643 0.05642 1.54353

A7 2.02571 -0.00086 0.00000 -0.01347 -0.01269 2.01302

A8 1.57653 0.00238 0.00000 0.04304 0.04265 1.61918

A9 1.80942 -0.00189 0.00000 -0.06594 -0.06645 1.74297

A10 2.09431 -0.00209 0.00000 -0.01402 -0.01489 2.07942

A11 2.05055 0.00177 0.00000 0.01837 0.01871 2.06925

A12 1.68939 -0.00060 0.00000 -0.01191 -0.01229 1.67710

A13 1.97907 0.00073 0.00000 0.00908 0.00938 1.98845

A14 1.80596 0.00009 0.00000 -0.01813 -0.01803 1.78793

A15 1.75028 -0.00013 0.00000 0.00830 0.00812 1.75840

A16 2.05404 0.00139 0.00000 0.00314 0.00318 2.05722

A17 2.06894 0.00223 0.00000 0.05342 0.05350 2.12244

A18 2.14247 -0.00358 0.00000 -0.05623 -0.05629 2.08618

A19 1.90521 0.00008 0.00000 0.00780 0.00758 1.91278

A20 1.87391 -0.00005 0.00000 0.00475 0.00453 1.87843

A21 1.99619 -0.00004 0.00000 -0.01920 -0.01843 1.97775

A22 1.85899 -0.00025 0.00000 -0.00415 -0.00408 1.85491

A23 1.91568 0.00028 0.00000 0.00759 0.00764 1.92332

A24 1.90857 -0.00004 0.00000 0.00400 0.00352 1.91209

A25 1.98778 -0.00020 0.00000 -0.00369 -0.00362 1.98416

A26 1.91887 0.00047 0.00000 -0.00162 -0.00164 1.91723

A27 1.88015 -0.00022 0.00000 -0.00105 -0.00108 1.87908

A28 1.90254 -0.00008 0.00000 0.00380 0.00397 1.90651

A29 1.91895 0.00007 0.00000 -0.00066 -0.00088 1.91807

A30 1.85056 -0.00003 0.00000 0.00367 0.00367 1.85423

A31 1.87840 0.00126 0.00000 0.00160 0.00136 1.87976

A32 1.89014 -0.00055 0.00000 0.00788 0.00702 1.89716

A33 1.79800 -0.00023 0.00000 -0.01500 -0.01466 1.78334

A34 1.68627 -0.00074 0.00000 -0.01799 -0.01759 1.66868

A35 1.84503 -0.00015 0.00000 0.00211 0.00235 1.84737

A36 2.16045 0.00047 0.00000 0.00173 0.00171 2.16216

A37 2.03716 0.00082 0.00000 0.01450 0.01410 2.05126

A38 1.84002 -0.00076 0.00000 -0.00181 -0.00218 1.83784

A39 1.77456 0.00065 0.00000 0.00285 0.00304 1.77760

A40 1.28160 0.00165 0.00000 0.05679 0.05694 1.33854

A41 1.89157 -0.00041 0.00000 -0.01048 -0.01066 1.88092

A42 2.24504 -0.00032 0.00000 -0.00041 -0.00138 2.24366

A43 2.13541 0.00048 0.00000 0.00103 -0.00004 2.13537

A44 1.90487 0.00045 0.00000 0.00362 0.00349 1.90836

A45 2.04353 -0.00047 0.00000 -0.00641 -0.00638 2.03714

A46 2.33471 0.00003 0.00000 0.00294 0.00297 2.33768

A47 1.90069 -0.00104 0.00000 0.00512 0.00519 1.90587

A48 2.01008 0.00047 0.00000 0.00283 0.00279 2.01287

A49 2.37240 0.00057 0.00000 -0.00791 -0.00796 2.36444

D1 -0.39358 -0.00174 0.00000 -0.05825 -0.05846 -0.45204

D2 2.93005 0.00021 0.00000 -0.01715 -0.01682 2.91323

D3 1.13105 0.00174 0.00000 0.02674 0.02770 1.15875

D4 2.88647 -0.00174 0.00000 -0.05062 -0.05112 2.83535

D5 -0.07309 0.00020 0.00000 -0.00953 -0.00948 -0.08256

D6 -1.87209 0.00174 0.00000 0.03437 0.03504 -1.83705

D7 -0.11045 0.00024 0.00000 0.01812 0.01781 -0.09264

D8 -3.05653 0.00048 0.00000 0.02291 0.02232 -3.03421

D9 2.89044 0.00078 0.00000 0.01710 0.01738 2.90782

D10 -0.05564 0.00103 0.00000 0.02188 0.02189 -0.03375

D11 2.54184 0.00173 0.00000 0.04429 0.04482 2.58666

D12 -1.73277 0.00145 0.00000 0.04590 0.04633 -1.68644

D13 0.38826 0.00133 0.00000 0.04205 0.04222 0.43048

D14 -0.77355 -0.00005 0.00000 0.00517 0.00524 -0.76830

D15 1.23503 -0.00033 0.00000 0.00678 0.00676 1.24179

D16 -2.92713 -0.00044 0.00000 0.00293 0.00265 -2.92448

D17 1.06643 -0.00108 0.00000 -0.04882 -0.04959 1.01684

D18 3.07500 -0.00135 0.00000 -0.04721 -0.04807 3.02693

D19 -1.08716 -0.00147 0.00000 -0.05106 -0.05218 -1.13934

D20 -1.00279 0.00013 0.00000 -0.00614 -0.00734 -1.01013

D21 -2.97532 0.00059 0.00000 0.00482 0.00387 -2.97145

D22 1.20353 0.00013 0.00000 0.00074 -0.00030 1.20323

D23 1.13285 0.00041 0.00000 0.00505 0.00581 1.13866

D24 -0.83968 0.00086 0.00000 0.01601 0.01702 -0.82266

D25 -2.94402 0.00040 0.00000 0.01193 0.01285 -2.93116

D26 -3.10873 -0.00007 0.00000 -0.00564 -0.00571 -3.11445

D27 1.20192 0.00038 0.00000 0.00533 0.00550 1.20742

D28 -0.90241 -0.00008 0.00000 0.00124 0.00133 -0.90108

D29 0.60158 -0.00014 0.00000 0.02288 0.02264 0.62422

D30 -2.74436 0.00033 0.00000 0.03139 0.03126 -2.71311

D31 3.12871 0.00087 0.00000 0.04951 0.04940 -3.10508

D32 -0.21723 0.00134 0.00000 0.05802 0.05802 -0.15921

D33 -1.31583 0.00084 0.00000 0.05720 0.05663 -1.25920

D34 1.62141 0.00131 0.00000 0.06571 0.06525 1.68666

D35 -0.56681 0.00030 0.00000 -0.03305 -0.03275 -0.59956

D36 -2.70765 0.00019 0.00000 -0.03415 -0.03410 -2.74175

D37 1.56649 0.00010 0.00000 -0.03707 -0.03700 1.52949

D38 -3.11735 -0.00106 0.00000 -0.06215 -0.06191 3.10392

D39 1.02500 -0.00117 0.00000 -0.06325 -0.06327 0.96173

D40 -0.98405 -0.00126 0.00000 -0.06617 -0.06617 -1.05022

D41 1.28651 -0.00124 0.00000 -0.06568 -0.06527 1.22124

D42 -0.85433 -0.00136 0.00000 -0.06678 -0.06662 -0.92095

D43 -2.86337 -0.00144 0.00000 -0.06970 -0.06953 -2.93290

D44 1.09903 -0.00139 0.00000 -0.02272 -0.02294 1.07609

D45 3.04797 -0.00188 0.00000 -0.02409 -0.02427 3.02370

D46 -1.15070 -0.00132 0.00000 -0.01863 -0.01866 -1.16936

D47 -1.04965 0.00103 0.00000 0.00204 0.00216 -1.04749

D48 0.89929 0.00055 0.00000 0.00068 0.00083 0.90012

D49 2.98380 0.00111 0.00000 0.00613 0.00645 2.99024

D50 -3.09664 0.00026 0.00000 -0.00484 -0.00491 -3.10155

D51 -1.14770 -0.00023 0.00000 -0.00620 -0.00624 -1.15394

D52 0.93681 0.00033 0.00000 -0.00074 -0.00063 0.93618

D53 0.07924 -0.00013 0.00000 0.00900 0.00901 0.08825

D54 2.22900 0.00029 0.00000 0.00718 0.00732 2.23633

D55 -2.03256 0.00024 0.00000 0.01338 0.01352 -2.01904

D56 -2.06869 -0.00041 0.00000 0.00676 0.00656 -2.06213

D57 0.08107 0.00000 0.00000 0.00493 0.00487 0.08594

D58 2.10269 -0.00004 0.00000 0.01114 0.01107 2.11376

D59 2.18110 -0.00025 0.00000 0.00512 0.00503 2.18613

D60 -1.95233 0.00016 0.00000 0.00330 0.00335 -1.94898

D61 0.06930 0.00012 0.00000 0.00951 0.00954 0.07884

D62 -0.02544 0.00056 0.00000 0.00137 0.00157 -0.02387

D63 3.12733 -0.00007 0.00000 -0.01039 -0.01006 3.11727

D64 -0.02862 0.00013 0.00000 0.01069 0.01065 -0.01798

D65 3.11857 -0.00025 0.00000 0.00527 0.00513 3.12370

D66 -0.05865 0.00033 0.00000 0.00935 0.00947 -0.04918

D67 1.83037 0.00056 0.00000 0.00758 0.00771 1.83808

D68 -1.47058 -0.00117 0.00000 -0.06240 -0.06217 -1.53275

D69 -1.97581 0.00089 0.00000 0.02210 0.02209 -1.95371

D70 -0.08679 0.00112 0.00000 0.02033 0.02034 -0.06645

D71 2.89545 -0.00060 0.00000 -0.04966 -0.04954 2.84591

D72 1.88819 -0.00085 0.00000 -0.00723 -0.00732 1.88086

D73 -2.50598 -0.00062 0.00000 -0.00900 -0.00908 -2.51506

D74 0.47626 -0.00234 0.00000 -0.07898 -0.07896 0.39730

D75 -1.91079 -0.00025 0.00000 -0.01684 -0.01633 -1.92712

D76 1.21703 0.00052 0.00000 -0.00243 -0.00199 1.21504

D77 0.07128 -0.00102 0.00000 -0.01346 -0.01368 0.05759

D78 -3.08409 -0.00024 0.00000 0.00095 0.00066 -3.08344

D79 2.55018 0.00045 0.00000 0.00771 0.00792 2.55810

D80 -0.60518 0.00122 0.00000 0.02213 0.02226 -0.58292

D81 2.00882 -0.00153 0.00000 -0.02465 -0.02499 1.98383

D82 -1.14006 -0.00104 0.00000 -0.01753 -0.01781 -1.15787

D83 0.07527 -0.00083 0.00000 -0.02025 -0.02018 0.05508

D84 -3.07362 -0.00034 0.00000 -0.01312 -0.01301 -3.08662

D85 -2.91906 0.00085 0.00000 0.04449 0.04448 -2.87458

D86 0.21524 0.00134 0.00000 0.05161 0.05166 0.26690

Item Value Threshold Converged?

Maximum Force 0.009660 0.000450 NO

RMS Force 0.001465 0.000300 NO

Maximum Displacement 0.174200 0.001800 NO

RMS Displacement 0.040966 0.001200 NO

Predicted change in Energy=-4.819168D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.166764 1.525784 0.440227

2 6 0 0.083210 1.173145 0.014523

3 6 0 -0.675984 3.758264 -0.285093

4 6 0 -1.596463 2.840419 0.240763

5 1 0 -1.786901 0.851305 1.049923

6 1 0 -2.549190 3.203331 0.650647

7 6 0 0.787361 1.863587 -1.091901

8 1 0 1.897017 1.844320 -0.903428

9 1 0 0.616135 1.265456 -2.031096

10 6 0 0.316135 3.292703 -1.305891

11 1 0 1.206994 3.979406 -1.313613

12 1 0 -0.164553 3.389743 -2.317987

13 1 0 -0.993362 4.810517 -0.414847

14 1 0 0.535636 0.221971 0.341071

15 8 0 2.749801 3.961547 0.838598

16 6 0 0.438377 3.906381 1.360274

17 6 0 0.983530 2.635967 1.654204

18 6 0 1.590052 4.747783 0.888346

19 8 0 1.705356 5.917037 0.559008

20 6 0 2.408658 2.662461 1.285843

21 8 0 3.321904 1.851100 1.279968

22 1 0 -0.333760 4.397634 1.969097

23 1 0 0.550411 1.833145 2.245820

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.366753 0.000000

3 C 2.398108 2.710901 0.000000

4 C 1.397387 2.377454 1.402229 0.000000

5 H 1.100555 2.161701 3.386269 2.155825 0.000000

6 H 2.183928 3.384648 2.166209 1.098817 2.504503

7 C 2.506018 1.482131 2.526285 2.900484 3.498420

8 H 3.360599 2.140795 3.265861 3.808646 4.286363

9 H 3.058420 2.115913 3.306386 3.540825 3.929221

10 C 2.893081 2.508042 1.497689 2.500946 3.991622

11 H 3.838091 3.301808 2.156933 3.401874 4.933024

12 H 3.476566 3.227274 2.128386 2.983174 4.518683

13 H 3.398630 3.817570 1.106707 2.162138 4.295418

14 H 2.146608 1.102749 3.790181 3.378192 2.508528

15 O 4.629376 3.945249 3.611095 4.528173 5.504538

16 C 3.014997 3.067209 1.992729 2.555417 3.792318

17 C 2.707400 2.374653 2.788263 2.948895 3.350443

18 C 4.264050 3.976453 2.736974 3.769785 5.158727

19 O 5.248455 5.043047 3.323188 4.524253 6.172398

20 C 3.845873 3.040069 3.630928 4.143049 4.575878

21 O 4.578114 3.542613 4.697850 5.123381 5.210796

22 H 3.358402 3.793620 2.367971 2.646975 3.941187

23 H 2.510643 2.373302 3.408174 3.105467 2.803072

6 7 8 9 10

6 H 0.000000

7 C 3.995492 0.000000

8 H 4.902123 1.125713 0.000000

9 H 4.578907 1.126572 1.802047 0.000000

10 C 3.470751 1.519940 2.181508 2.173856 0.000000

11 H 4.309237 2.168396 2.281004 2.868696 1.124834

12 H 3.812353 2.176828 2.939282 2.281310 1.124640

13 H 2.477685 3.509098 4.170291 4.215471 2.193741

14 H 4.301221 2.193553 2.456451 2.592781 3.491426

15 O 5.356260 3.461132 2.871332 4.478457 3.311935

16 C 3.150144 3.210601 3.391765 4.302031 2.738609

17 C 3.716065 2.859396 2.828895 3.949014 3.104655

18 C 4.424382 3.589468 3.425606 4.647392 2.924859

19 O 5.047153 4.471987 4.331567 5.434357 3.506410

20 C 5.027551 2.986715 2.392496 4.020801 3.390124

21 O 6.057583 3.471286 2.607214 4.315936 4.218949

22 H 2.841267 4.128924 4.443780 5.168596 3.516928

23 H 3.745599 3.346259 3.425089 4.314927 3.847057

11 12 13 14 15

11 H 0.000000

12 H 1.799336 0.000000

13 H 2.517953 2.515445 0.000000

14 H 4.160171 4.194715 4.895304 0.000000

15 O 2.648128 4.334103 4.037715 4.374299 0.000000

16 C 2.783123 3.762983 2.453240 3.824018 2.370205

17 C 3.265379 4.202925 3.594126 2.784297 2.354164

18 C 2.363421 3.899164 2.894180 4.679132 1.402020

19 O 2.740344 4.261557 3.075038 5.818034 2.234497

20 C 3.152065 4.487532 4.368092 3.218197 1.415638

21 O 3.966005 5.241000 5.500187 3.361380 2.230716

22 H 3.650345 4.407218 2.507735 4.565357 3.313088

23 H 4.207980 4.874680 4.281019 2.494829 3.368632

16 17 18 19 20

16 C 0.000000

17 C 1.413343 0.000000

18 C 1.502341 2.326838 0.000000

19 O 2.507987 3.533540 1.220210 0.000000

20 C 2.331284 1.472202 2.275234 3.408106 0.000000

21 O 3.541943 2.494806 3.397565 4.434507 1.221621

22 H 1.099177 2.222135 2.234207 2.907736 3.316402

23 H 2.257222 1.087256 3.379157 4.566990 2.249978

21 22 23

21 O 0.000000

22 H 4.508172 0.000000

23 H 2.935023 2.726708 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.420393 -0.420128 -0.692625

2 6 0 1.691980 -1.241820 0.121163

3 6 0 1.130668 1.409942 0.166662

4 6 0 2.184443 0.956170 -0.639499

5 1 0 3.083606 -0.815156 -1.477050

6 1 0 2.668482 1.650889 -1.339835

7 6 0 1.096522 -0.793339 1.402180

8 1 0 0.140560 -1.356717 1.591841

9 1 0 1.804530 -1.085605 2.228297

10 6 0 0.842568 0.704273 1.455888

11 1 0 -0.223989 0.888522 1.762089

12 1 0 1.483815 1.172923 2.252120

13 1 0 0.911315 2.494447 0.189772

14 1 0 1.693530 -2.332381 -0.042329

15 8 0 -2.107540 -0.186391 0.242423

16 6 0 -0.335440 0.759342 -1.015800

17 6 0 -0.243473 -0.647184 -1.119565

18 6 0 -1.557030 1.030351 -0.184355

19 8 0 -2.130914 2.046844 0.171048

20 6 0 -1.318782 -1.229430 -0.299760

21 8 0 -1.667419 -2.360202 0.003824

22 1 0 -0.120611 1.450193 -1.843305

23 1 0 0.334659 -1.238182 -1.825688

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2337487 0.8669665 0.6664561

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.2351986359 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.453246452461E-01 A.U. after 16 cycles

Convg = 0.2572D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.017461083 0.002155103 0.002989405

2 6 0.019862772 -0.005709677 0.001361621

3 6 -0.004321418 0.000639631 -0.007398351

4 6 0.000573947 0.008026533 -0.000766395

5 1 0.000725478 -0.001910547 -0.000468915

6 1 -0.001125345 -0.001867781 0.000214695

7 6 -0.001952529 0.000050317 -0.002395513

8 1 -0.000251005 -0.000190065 -0.001164797

9 1 0.000031884 0.000356514 -0.000139447

10 6 0.001115624 0.001293515 0.000471777

11 1 -0.000521225 0.000289425 -0.001119470

12 1 -0.000499191 -0.000929437 0.000123231

13 1 0.001742146 0.000567248 0.002191102

14 1 0.000105316 -0.000856932 -0.000134874

15 8 -0.000529740 0.000093804 -0.000077577

16 6 0.005116103 -0.001181778 0.009865622

17 6 -0.005468402 -0.002295400 -0.007868623

18 6 -0.000694544 0.000933126 -0.001270122

19 8 0.000059896 0.000252288 0.000160569

20 6 0.002931429 -0.001260844 0.001429152

21 8 0.000093171 -0.000225376 0.000266524

22 1 -0.001381670 -0.000926183 -0.001925696

23 1 0.001848387 0.002696513 0.005656081

-------------------------------------------------------------------

Cartesian Forces: Max 0.019862772 RMS 0.004185245

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.015234134 RMS 0.001632169

Search for a saddle point.

Step number 24 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 23 24

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0

Eigenvalues --- -0.06345 -0.00389 0.00220 0.00380 0.00592

Eigenvalues --- 0.00977 0.01024 0.01412 0.01948 0.02067

Eigenvalues --- 0.02199 0.02266 0.02461 0.02728 0.02821

Eigenvalues --- 0.03016 0.03085 0.03370 0.03534 0.03645

Eigenvalues --- 0.03813 0.03859 0.04110 0.04151 0.04583

Eigenvalues --- 0.04968 0.05582 0.05709 0.05995 0.06465

Eigenvalues --- 0.07344 0.07968 0.08476 0.08761 0.09833

Eigenvalues --- 0.11686 0.13561 0.14167 0.15614 0.20450

Eigenvalues --- 0.22602 0.25485 0.26331 0.26829 0.28245

Eigenvalues --- 0.29840 0.30511 0.31221 0.31480 0.31894

Eigenvalues --- 0.31976 0.32416 0.32807 0.34438 0.35956

Eigenvalues --- 0.37494 0.39580 0.40374 0.43221 0.46055

Eigenvalues --- 0.50280 1.08421 1.10832

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D79 D73

1 0.65302 0.34104 -0.18780 0.17450 -0.17411

D4 D80 D5 D6 D72

1 0.16161 0.15714 0.11762 0.11733 -0.10865

RFO step: Lambda0=2.309197171D-04 Lambda=-1.09022077D-02.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.483

Iteration 1 RMS(Cart)= 0.04568688 RMS(Int)= 0.00180643

Iteration 2 RMS(Cart)= 0.00180928 RMS(Int)= 0.00062244

Iteration 3 RMS(Cart)= 0.00000325 RMS(Int)= 0.00062243

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00062243

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58279 0.01523 0.00000 0.05669 0.05697 2.63976

R2 2.64068 0.00331 0.00000 -0.01650 -0.01591 2.62477

R3 2.07975 0.00050 0.00000 -0.00400 -0.00400 2.07575

R4 2.80082 0.00223 0.00000 0.00647 0.00686 2.80768

R5 2.08389 0.00074 0.00000 -0.00258 -0.00258 2.08132

R6 4.48744 0.00137 0.00000 -0.21328 -0.21456 4.27289

R7 2.64983 0.00021 0.00000 0.00549 0.00582 2.65565

R8 2.83022 0.00138 0.00000 -0.00963 -0.00973 2.82050

R9 2.09137 -0.00022 0.00000 -0.00426 -0.00426 2.08711

R10 3.76571 0.00505 0.00000 0.10397 0.10468 3.87039

R11 2.07646 0.00044 0.00000 -0.00213 -0.00213 2.07433

R12 2.12729 -0.00044 0.00000 -0.00173 -0.00173 2.12556

R13 2.12891 -0.00008 0.00000 0.00011 0.00011 2.12903

R14 2.87227 0.00206 0.00000 0.00901 0.00939 2.88166

R15 2.12563 -0.00023 0.00000 -0.00069 -0.00069 2.12494

R16 2.12526 0.00002 0.00000 0.00125 0.00125 2.12651

R17 2.64943 0.00042 0.00000 0.00653 0.00630 2.65574

R18 2.67517 0.00033 0.00000 -0.00185 -0.00202 2.67315

R19 2.67083 0.00049 0.00000 -0.01933 -0.01999 2.65084

R20 2.83901 0.00045 0.00000 -0.01070 -0.01066 2.82835

R21 2.07714 -0.00051 0.00000 -0.00119 -0.00119 2.07596

R22 2.78206 0.00179 0.00000 0.00314 0.00326 2.78532

R23 2.05462 0.00035 0.00000 0.00497 0.00497 2.05958

R24 2.30586 0.00020 0.00000 0.00061 0.00061 2.30648

R25 2.30853 0.00022 0.00000 0.00036 0.00036 2.30889

A1 2.07088 -0.00160 0.00000 0.00386 0.00364 2.07452

A2 2.12911 -0.00122 0.00000 -0.04684 -0.04676 2.08235

A3 2.07415 0.00272 0.00000 0.03946 0.03922 2.11337

A4 2.14936 -0.00281 0.00000 -0.04111 -0.04335 2.10601

A5 2.10079 0.00096 0.00000 -0.00420 -0.00378 2.09701

A6 1.54353 -0.00031 0.00000 0.05627 0.05766 1.60119

A7 2.01302 0.00158 0.00000 0.03330 0.03331 2.04634

A8 1.61918 0.00110 0.00000 0.03997 0.04134 1.66052

A9 1.74297 0.00021 0.00000 -0.04775 -0.04814 1.69483

A10 2.07942 0.00101 0.00000 -0.00286 -0.00436 2.07507

A11 2.06925 -0.00094 0.00000 0.00868 0.00891 2.07816

A12 1.67710 -0.00026 0.00000 -0.00522 -0.00486 1.67224

A13 1.98845 0.00028 0.00000 0.01653 0.01665 2.00510

A14 1.78793 -0.00069 0.00000 -0.02855 -0.02778 1.76016

A15 1.75840 0.00030 0.00000 -0.00643 -0.00700 1.75140

A16 2.05722 0.00060 0.00000 -0.00496 -0.00501 2.05221

A17 2.12244 -0.00258 0.00000 -0.03406 -0.03399 2.08845

A18 2.08618 0.00202 0.00000 0.04064 0.04061 2.12679

A19 1.91278 0.00000 0.00000 0.01058 0.01012 1.92291

A20 1.87843 0.00035 0.00000 -0.00111 -0.00088 1.87755

A21 1.97775 0.00049 0.00000 0.00426 0.00467 1.98242

A22 1.85491 -0.00020 0.00000 -0.00553 -0.00549 1.84942

A23 1.92332 -0.00059 0.00000 -0.00701 -0.00677 1.91655

A24 1.91209 -0.00006 0.00000 -0.00172 -0.00226 1.90984

A25 1.98416 0.00136 0.00000 -0.00462 -0.00466 1.97950

A26 1.91723 0.00043 0.00000 0.00179 0.00213 1.91936

A27 1.87908 -0.00109 0.00000 -0.00381 -0.00418 1.87490

A28 1.90651 -0.00129 0.00000 0.00791 0.00801 1.91451

A29 1.91807 0.00038 0.00000 -0.00582 -0.00596 1.91212

A30 1.85423 0.00015 0.00000 0.00500 0.00502 1.85925

A31 1.87976 0.00067 0.00000 -0.00065 -0.00094 1.87881

A32 1.89716 0.00127 0.00000 0.01676 0.01636 1.91352

A33 1.78334 -0.00089 0.00000 -0.00188 -0.00172 1.78162

A34 1.66868 -0.00122 0.00000 -0.03934 -0.03912 1.62956

A35 1.84737 -0.00023 0.00000 0.00739 0.00756 1.85494

A36 2.16216 0.00057 0.00000 0.00580 0.00570 2.16786

A37 2.05126 0.00025 0.00000 0.00556 0.00501 2.05627

A38 1.83784 0.00040 0.00000 0.00840 0.00697 1.84481

A39 1.77760 -0.00090 0.00000 -0.00735 -0.00660 1.77100

A40 1.33854 0.00218 0.00000 0.08377 0.08455 1.42310

A41 1.88092 0.00047 0.00000 0.00216 0.00188 1.88279

A42 2.24366 -0.00022 0.00000 -0.00034 -0.00340 2.24026

A43 2.13537 -0.00073 0.00000 -0.02404 -0.02589 2.10948

A44 1.90836 0.00007 0.00000 -0.00392 -0.00393 1.90443

A45 2.03714 -0.00003 0.00000 -0.00181 -0.00181 2.03533

A46 2.33768 -0.00004 0.00000 0.00572 0.00572 2.34340

A47 1.90587 -0.00092 0.00000 -0.00400 -0.00388 1.90199

A48 2.01287 0.00068 0.00000 0.00584 0.00578 2.01865

A49 2.36444 0.00024 0.00000 -0.00184 -0.00190 2.36254

D1 -0.45204 -0.00159 0.00000 -0.08385 -0.08285 -0.53489

D2 2.91323 -0.00033 0.00000 -0.02191 -0.02249 2.89075

D3 1.15875 -0.00047 0.00000 0.00066 -0.00029 1.15846

D4 2.83535 -0.00106 0.00000 -0.05905 -0.05842 2.77694

D5 -0.08256 0.00020 0.00000 0.00289 0.00195 -0.08061

D6 -1.83705 0.00006 0.00000 0.02546 0.02415 -1.81290

D7 -0.09264 0.00125 0.00000 0.04553 0.04567 -0.04697

D8 -3.03421 0.00081 0.00000 0.03149 0.03173 -3.00247

D9 2.90782 0.00041 0.00000 0.01429 0.01344 2.92126

D10 -0.03375 -0.00002 0.00000 0.00024 -0.00049 -0.03424

D11 2.58666 0.00075 0.00000 0.06322 0.06245 2.64911

D12 -1.68644 0.00070 0.00000 0.06158 0.06073 -1.62571

D13 0.43048 0.00118 0.00000 0.06134 0.06022 0.49070

D14 -0.76830 -0.00049 0.00000 0.00028 -0.00024 -0.76855

D15 1.24179 -0.00054 0.00000 -0.00137 -0.00197 1.23982

D16 -2.92448 -0.00006 0.00000 -0.00161 -0.00247 -2.92695

D17 1.01684 0.00054 0.00000 -0.02818 -0.02746 0.98938

D18 3.02693 0.00048 0.00000 -0.02983 -0.02918 2.99775

D19 -1.13934 0.00096 0.00000 -0.03007 -0.02969 -1.16902

D20 -1.01013 0.00074 0.00000 0.00711 0.00574 -1.00440

D21 -2.97145 0.00044 0.00000 0.00471 0.00387 -2.96758

D22 1.20323 0.00083 0.00000 0.01979 0.01910 1.22233

D23 1.13866 -0.00209 0.00000 -0.03183 -0.03118 1.10748

D24 -0.82266 -0.00239 0.00000 -0.03423 -0.03304 -0.85570

D25 -2.93116 -0.00200 0.00000 -0.01915 -0.01782 -2.94899

D26 -3.11445 -0.00020 0.00000 0.00432 0.00386 -3.11058

D27 1.20742 -0.00050 0.00000 0.00192 0.00200 1.20942

D28 -0.90108 -0.00011 0.00000 0.01700 0.01722 -0.88386

D29 0.62422 0.00033 0.00000 0.02005 0.02009 0.64431

D30 -2.71311 0.00022 0.00000 0.02506 0.02538 -2.68772

D31 -3.10508 0.00107 0.00000 0.06619 0.06573 -3.03934

D32 -0.15921 0.00095 0.00000 0.07120 0.07103 -0.08818

D33 -1.25920 0.00102 0.00000 0.05786 0.05695 -1.20225

D34 1.68666 0.00090 0.00000 0.06288 0.06224 1.74891

D35 -0.59956 -0.00136 0.00000 -0.03772 -0.03777 -0.63732

D36 -2.74175 -0.00097 0.00000 -0.04608 -0.04648 -2.78823

D37 1.52949 -0.00078 0.00000 -0.05084 -0.05123 1.47826

D38 3.10392 -0.00165 0.00000 -0.07967 -0.07945 3.02447

D39 0.96173 -0.00126 0.00000 -0.08803 -0.08817 0.87356

D40 -1.05022 -0.00107 0.00000 -0.09280 -0.09292 -1.14314

D41 1.22124 -0.00174 0.00000 -0.06309 -0.06232 1.15892

D42 -0.92095 -0.00135 0.00000 -0.07146 -0.07104 -0.99199

D43 -2.93290 -0.00116 0.00000 -0.07622 -0.07579 -3.00869

D44 1.07609 0.00150 0.00000 -0.02576 -0.02628 1.04982

D45 3.02370 0.00131 0.00000 -0.01221 -0.01249 3.01121

D46 -1.16936 0.00098 0.00000 -0.01880 -0.01903 -1.18839

D47 -1.04749 0.00070 0.00000 -0.01357 -0.01335 -1.06084

D48 0.90012 0.00051 0.00000 -0.00002 0.00044 0.90056

D49 2.99024 0.00018 0.00000 -0.00661 -0.00610 2.98414

D50 -3.10155 0.00052 0.00000 -0.01969 -0.01996 -3.12151

D51 -1.15394 0.00033 0.00000 -0.00614 -0.00618 -1.16011

D52 0.93618 0.00000 0.00000 -0.01273 -0.01271 0.92347

D53 0.08825 -0.00089 0.00000 -0.00900 -0.00968 0.07858

D54 2.23633 -0.00034 0.00000 -0.00399 -0.00419 2.23214

D55 -2.01904 -0.00068 0.00000 0.00328 0.00307 -2.01597

D56 -2.06213 -0.00079 0.00000 -0.02060 -0.02115 -2.08329

D57 0.08594 -0.00024 0.00000 -0.01559 -0.01566 0.07028

D58 2.11376 -0.00058 0.00000 -0.00832 -0.00841 2.10535

D59 2.18613 -0.00016 0.00000 -0.00880 -0.00931 2.17682

D60 -1.94898 0.00038 0.00000 -0.00379 -0.00382 -1.95280

D61 0.07884 0.00004 0.00000 0.00348 0.00343 0.08228

D62 -0.02387 -0.00004 0.00000 -0.01291 -0.01271 -0.03658

D63 3.11727 -0.00046 0.00000 -0.01878 -0.01851 3.09876

D64 -0.01798 0.00056 0.00000 0.02192 0.02148 0.00350

D65 3.12370 0.00049 0.00000 0.02514 0.02447 -3.13501

D66 -0.04918 0.00087 0.00000 0.02565 0.02563 -0.02356

D67 1.83808 0.00022 0.00000 0.02184 0.02195 1.86003

D68 -1.53275 -0.00221 0.00000 -0.08928 -0.08911 -1.62186

D69 -1.95371 0.00146 0.00000 0.01740 0.01704 -1.93667

D70 -0.06645 0.00080 0.00000 0.01359 0.01336 -0.05309

D71 2.84591 -0.00163 0.00000 -0.09752 -0.09769 2.74821

D72 1.88086 0.00064 0.00000 -0.00983 -0.01004 1.87083

D73 -2.51506 -0.00002 0.00000 -0.01364 -0.01372 -2.52878

D74 0.39730 -0.00245 0.00000 -0.12476 -0.12477 0.27253

D75 -1.92712 -0.00146 0.00000 -0.02106 -0.02079 -1.94791

D76 1.21504 -0.00094 0.00000 -0.01377 -0.01355 1.20149

D77 0.05759 -0.00050 0.00000 -0.00072 -0.00069 0.05690

D78 -3.08344 0.00001 0.00000 0.00657 0.00655 -3.07688

D79 2.55810 0.00042 0.00000 0.02450 0.02456 2.58267

D80 -0.58292 0.00094 0.00000 0.03179 0.03181 -0.55112

D81 1.98383 -0.00065 0.00000 -0.01568 -0.01663 1.96720

D82 -1.15787 -0.00056 0.00000 -0.01983 -0.02047 -1.17834

D83 0.05508 -0.00087 0.00000 -0.02261 -0.02219 0.03289

D84 -3.08662 -0.00079 0.00000 -0.02676 -0.02603 -3.11266

D85 -2.87458 0.00131 0.00000 0.07663 0.07571 -2.79887

D86 0.26690 0.00139 0.00000 0.07248 0.07187 0.33877

Item Value Threshold Converged?

Maximum Force 0.015234 0.000450 NO

RMS Force 0.001632 0.000300 NO

Maximum Displacement 0.185015 0.001800 NO

RMS Displacement 0.046087 0.001200 NO

Predicted change in Energy=-4.844441D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.177154 1.553867 0.426547

2 6 0 0.132702 1.226433 0.068227

3 6 0 -0.712357 3.777419 -0.316100

4 6 0 -1.628586 2.848888 0.206629

5 1 0 -1.767721 0.839864 1.016463

6 1 0 -2.605605 3.157750 0.600280

7 6 0 0.797952 1.904825 -1.074012

8 1 0 1.911380 1.928268 -0.916203

9 1 0 0.628193 1.272552 -1.990917

10 6 0 0.282304 3.317035 -1.329205

11 1 0 1.147233 4.034331 -1.371789

12 1 0 -0.218269 3.359032 -2.336164

13 1 0 -1.014757 4.835577 -0.409197

14 1 0 0.591574 0.296363 0.438977

15 8 0 2.765860 3.902013 0.828515

16 6 0 0.461452 3.876303 1.359370

17 6 0 0.982295 2.605684 1.645722

18 6 0 1.614114 4.705273 0.885780

19 8 0 1.746902 5.875254 0.564507

20 6 0 2.412584 2.612273 1.289791

21 8 0 3.316779 1.790729 1.307744

22 1 0 -0.317028 4.373125 1.954303

23 1 0 0.573752 1.840148 2.305187

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.396899 0.000000

3 C 2.389925 2.714657 0.000000

4 C 1.388969 2.398677 1.405308 0.000000

5 H 1.098440 2.158748 3.393928 2.170568 0.000000

6 H 2.154784 3.392844 2.192745 1.097690 2.499570

7 C 2.505174 1.485761 2.522315 2.901618 3.476623

8 H 3.388539 2.150668 3.265498 3.826180 4.295998

9 H 3.030272 2.118422 3.297945 3.522371 3.869361

10 C 2.884691 2.519090 1.492543 2.495887 3.980092

11 H 3.845710 3.314696 2.153731 3.406149 4.940173

12 H 3.436664 3.232995 2.121281 2.952125 4.470695

13 H 3.390348 3.817134 1.104450 2.168631 4.308733

14 H 2.170224 1.101385 3.793168 3.390941 2.489008

15 O 4.606813 3.830181 3.663831 4.561466 5.474069

16 C 2.991470 2.965963 2.048122 2.598586 3.782427

17 C 2.693683 2.261114 2.844917 2.991126 3.328164

18 C 4.234788 3.868501 2.778110 3.797699 5.137632

19 O 5.219532 4.946056 3.350274 4.547624 6.157271

20 C 3.840785 2.934388 3.701581 4.190499 4.548746

21 O 4.585635 3.463118 4.776792 5.175789 5.180843

22 H 3.319950 3.696107 2.380311 2.664178 3.932936

23 H 2.583972 2.361178 3.504031 3.204964 2.853747

6 7 8 9 10

6 H 0.000000

7 C 3.994656 0.000000

8 H 4.920823 1.124800 0.000000

9 H 4.552551 1.126633 1.797649 0.000000

10 C 3.476824 1.524911 2.180168 2.176560 0.000000

11 H 4.329116 2.178408 2.286259 2.877524 1.124468

12 H 3.789801 2.177258 2.932368 2.277958 1.125303

13 H 2.522884 3.509587 4.155933 4.230398 2.198807

14 H 4.293659 2.217854 2.498301 2.618906 3.513769

15 O 5.427583 3.388366 2.769448 4.408274 3.341557

16 C 3.240273 3.149810 3.327967 4.246380 2.751964

17 C 3.777665 2.814630 2.808122 3.889444 3.137865

18 C 4.503595 3.514173 3.323743 4.585956 2.933782

19 O 5.131318 4.398813 4.218798 5.382060 3.503666

20 C 5.094623 2.948743 2.363361 3.967612 3.448756

21 O 6.119141 3.468468 2.634389 4.286977 4.300133

22 H 2.923713 4.062804 4.379833 5.106051 3.500850

23 H 3.840715 3.387246 3.489178 4.333778 3.933819

11 12 13 14 15

11 H 0.000000

12 H 1.802955 0.000000

13 H 2.498555 2.554952 0.000000

14 H 4.190469 4.211555 4.889188 0.000000

15 O 2.734739 4.383498 4.086139 4.228471 0.000000

16 C 2.820372 3.792963 2.495441 3.698651 2.364903

17 C 3.342694 4.226619 3.630885 2.634741 2.351467

18 C 2.400991 3.943465 2.933412 4.547934 1.405356

19 O 2.738219 4.313602 3.107376 5.698646 2.236439

20 C 3.272211 4.541650 4.424511 3.066496 1.414570

21 O 4.113463 5.313588 5.566075 3.227170 2.233985

22 H 3.649894 4.409790 2.507353 4.443170 3.315652

23 H 4.320123 4.947367 4.343251 2.422051 3.352191

16 17 18 19 20

16 C 0.000000

17 C 1.402764 0.000000

18 C 1.496700 2.320556 0.000000

19 O 2.505992 3.527568 1.220535 0.000000

20 C 2.325839 1.473925 2.276274 3.408256 0.000000

21 O 3.536266 2.495636 3.401718 4.438497 1.221813

22 H 1.098548 2.215244 2.231899 2.906498 3.315562

23 H 2.247911 1.089884 3.362441 4.548442 2.237970

21 22 23

21 O 0.000000

22 H 4.504593 0.000000

23 H 2.919167 2.707873 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.383639 -0.571069 -0.666105

2 6 0 1.515752 -1.324623 0.127781

3 6 0 1.259435 1.377879 0.139817

4 6 0 2.280109 0.813866 -0.644406

5 1 0 3.014756 -1.081111 -1.406455

6 1 0 2.861719 1.413274 -1.356701

7 6 0 1.002658 -0.784234 1.413161

8 1 0 -0.003589 -1.229190 1.646947

9 1 0 1.694237 -1.135628 2.230193

10 6 0 0.914298 0.737817 1.443231

11 1 0 -0.116896 1.051264 1.763884

12 1 0 1.626204 1.141268 2.215709

13 1 0 1.092121 2.468822 0.099076

14 1 0 1.411258 -2.407918 -0.041341

15 8 0 -2.102282 -0.074273 0.257164

16 6 0 -0.287810 0.724376 -1.032262

17 6 0 -0.273883 -0.677000 -1.093049

18 6 0 -1.482112 1.096857 -0.210671

19 8 0 -1.999342 2.154926 0.109747

20 6 0 -1.388102 -1.176760 -0.267694

21 8 0 -1.812189 -2.279150 0.044901

22 1 0 -0.016474 1.381628 -1.869641

23 1 0 0.203254 -1.317093 -1.834985

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2323373 0.8722977 0.6673518

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4210566112 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.480734831595E-01 A.U. after 16 cycles

Convg = 0.3190D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.006712064 -0.007050112 -0.000764320

2 6 0.000521637 0.008750695 0.005802997

3 6 -0.001954709 0.000967175 0.000398114

4 6 0.002276649 0.001028320 0.000720570

5 1 -0.002380155 -0.000356125 -0.000285967

6 1 -0.000795941 0.002458297 -0.000860600

7 6 -0.001308816 -0.000620651 -0.002977415

8 1 -0.000152022 -0.000559514 -0.000640036

9 1 -0.000407231 0.000596910 -0.000134256

10 6 0.000995327 -0.002308909 -0.000212854

11 1 -0.000318370 -0.000298926 -0.000627493

12 1 0.000317377 -0.000680088 -0.000087990

13 1 0.001254648 0.000487637 0.001605397

14 1 0.000127363 -0.000478945 -0.002168933

15 8 0.000035856 -0.000012266 0.000188171

16 6 -0.007003861 0.014247576 0.003183946

17 6 -0.005107189 -0.020301551 -0.005092520

18 6 0.000816549 0.001863936 -0.002054241

19 8 0.000208020 -0.000766539 -0.000117325

20 6 0.007180146 -0.000207067 -0.000075146

21 8 -0.000904564 0.000860975 0.000020654

22 1 -0.000831285 -0.000693454 -0.001188589

23 1 0.000718506 0.003072626 0.005367837

-------------------------------------------------------------------

Cartesian Forces: Max 0.020301551 RMS 0.003974291

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011746089 RMS 0.001505391

Search for a saddle point.

Step number 25 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 24 25

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0

Eigenvalues --- -0.06558 -0.00175 0.00223 0.00412 0.00605

Eigenvalues --- 0.00987 0.01024 0.01425 0.01990 0.02088

Eigenvalues --- 0.02274 0.02300 0.02558 0.02875 0.02968

Eigenvalues --- 0.03046 0.03112 0.03420 0.03602 0.03674

Eigenvalues --- 0.03845 0.03877 0.04167 0.04276 0.04613

Eigenvalues --- 0.05165 0.05578 0.05842 0.06012 0.06466

Eigenvalues --- 0.07347 0.08275 0.08703 0.08811 0.09832

Eigenvalues --- 0.11891 0.13656 0.14242 0.15821 0.20534

Eigenvalues --- 0.22625 0.25573 0.26450 0.26852 0.28469

Eigenvalues --- 0.30195 0.30565 0.31239 0.31522 0.31942

Eigenvalues --- 0.31982 0.32425 0.32915 0.34453 0.35971

Eigenvalues --- 0.37499 0.39582 0.40378 0.43261 0.46572

Eigenvalues --- 0.50233 1.08426 1.10833

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D73

1 0.60665 0.41340 -0.19265 0.17336 -0.16252

D79 D80 D71 D86 D29

1 0.15816 0.13963 0.11928 -0.11510 -0.11168

RFO step: Lambda0=3.069164984D-04 Lambda=-8.08411494D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.508

Iteration 1 RMS(Cart)= 0.03651515 RMS(Int)= 0.00116993

Iteration 2 RMS(Cart)= 0.00111623 RMS(Int)= 0.00068688

Iteration 3 RMS(Cart)= 0.00000113 RMS(Int)= 0.00068688

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00068688

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63976 -0.00323 0.00000 -0.00295 -0.00306 2.63669

R2 2.62477 0.00437 0.00000 0.01702 0.01724 2.64201

R3 2.07575 0.00136 0.00000 0.00322 0.00322 2.07897

R4 2.80768 0.00086 0.00000 0.01785 0.01834 2.82602

R5 2.08132 -0.00027 0.00000 0.00198 0.00198 2.08329

R6 4.27289 -0.00195 0.00000 -0.18018 -0.18008 4.09280

R7 2.65565 -0.00203 0.00000 -0.00612 -0.00581 2.64983

R8 2.82050 0.00211 0.00000 -0.00974 -0.00996 2.81054

R9 2.08711 -0.00001 0.00000 -0.00746 -0.00746 2.07965

R10 3.87039 -0.00220 0.00000 0.12815 0.12772 3.99811

R11 2.07433 0.00109 0.00000 0.00164 0.00164 2.07597

R12 2.12556 -0.00025 0.00000 -0.00225 -0.00225 2.12332

R13 2.12903 -0.00016 0.00000 -0.00087 -0.00087 2.12816

R14 2.88166 -0.00144 0.00000 -0.01045 -0.01013 2.87153

R15 2.12494 -0.00041 0.00000 -0.00080 -0.00080 2.12413

R16 2.12651 -0.00009 0.00000 0.00116 0.00116 2.12767

R17 2.65574 0.00169 0.00000 0.00649 0.00613 2.66186

R18 2.67315 0.00116 0.00000 -0.01212 -0.01271 2.66044

R19 2.65084 0.01175 0.00000 0.04354 0.04359 2.69443

R20 2.82835 0.00194 0.00000 -0.01115 -0.01082 2.81753

R21 2.07596 -0.00037 0.00000 -0.01156 -0.01156 2.06440

R22 2.78532 0.00518 0.00000 0.03519 0.03519 2.82051

R23 2.05958 0.00082 0.00000 0.00300 0.00300 2.06259

R24 2.30648 -0.00068 0.00000 -0.00022 -0.00022 2.30625

R25 2.30889 -0.00125 0.00000 -0.00175 -0.00175 2.30714

A1 2.07452 -0.00065 0.00000 -0.02231 -0.02214 2.05238

A2 2.08235 0.00189 0.00000 0.04896 0.04840 2.13075

A3 2.11337 -0.00112 0.00000 -0.03107 -0.03102 2.08235

A4 2.10601 -0.00012 0.00000 0.00222 0.00024 2.10625

A5 2.09701 0.00028 0.00000 0.00923 0.00923 2.10624

A6 1.60119 -0.00068 0.00000 0.02412 0.02337 1.62456

A7 2.04634 -0.00068 0.00000 -0.02610 -0.02575 2.02059

A8 1.66052 0.00276 0.00000 0.06731 0.06792 1.72844

A9 1.69483 -0.00018 0.00000 -0.03821 -0.03792 1.65691

A10 2.07507 -0.00157 0.00000 0.01632 0.01535 2.09042

A11 2.07816 0.00110 0.00000 0.00667 0.00371 2.08187

A12 1.67224 -0.00116 0.00000 -0.03755 -0.03693 1.63531

A13 2.00510 0.00047 0.00000 0.02248 0.02200 2.02710

A14 1.76016 0.00255 0.00000 0.00871 0.00870 1.76886

A15 1.75140 -0.00138 0.00000 -0.05833 -0.05835 1.69304

A16 2.05221 0.00073 0.00000 -0.00286 -0.00217 2.05004

A17 2.08845 0.00215 0.00000 0.02863 0.02806 2.11651

A18 2.12679 -0.00273 0.00000 -0.02884 -0.02903 2.09776

A19 1.92291 -0.00001 0.00000 -0.00079 -0.00078 1.92213

A20 1.87755 0.00019 0.00000 0.00388 0.00343 1.88098

A21 1.98242 0.00020 0.00000 -0.00700 -0.00629 1.97613

A22 1.84942 -0.00006 0.00000 -0.00211 -0.00200 1.84742

A23 1.91655 -0.00006 0.00000 0.00870 0.00824 1.92479

A24 1.90984 -0.00028 0.00000 -0.00254 -0.00249 1.90734

A25 1.97950 0.00071 0.00000 -0.00739 -0.00745 1.97204

A26 1.91936 0.00017 0.00000 0.00572 0.00553 1.92489

A27 1.87490 0.00003 0.00000 -0.00382 -0.00363 1.87127

A28 1.91451 -0.00040 0.00000 0.00712 0.00732 1.92184

A29 1.91212 -0.00056 0.00000 -0.00305 -0.00327 1.90885

A30 1.85925 0.00001 0.00000 0.00166 0.00166 1.86091

A31 1.87881 0.00287 0.00000 0.00633 0.00586 1.88467

A32 1.91352 -0.00129 0.00000 -0.02477 -0.02556 1.88797

A33 1.78162 0.00010 0.00000 -0.02643 -0.02621 1.75541

A34 1.62956 0.00027 0.00000 -0.03952 -0.03856 1.59100

A35 1.85494 -0.00091 0.00000 -0.00098 -0.00181 1.85313

A36 2.16786 0.00089 0.00000 0.02966 0.02799 2.19585

A37 2.05627 0.00067 0.00000 0.03307 0.03108 2.08735

A38 1.84481 -0.00089 0.00000 0.00894 0.00879 1.85360

A39 1.77100 0.00116 0.00000 -0.02275 -0.02319 1.74781

A40 1.42310 0.00212 0.00000 0.09634 0.09738 1.52048

A41 1.88279 -0.00168 0.00000 -0.01511 -0.01502 1.86778

A42 2.24026 -0.00003 0.00000 -0.02157 -0.02498 2.21529

A43 2.10948 0.00096 0.00000 0.00567 0.00400 2.11349

A44 1.90443 0.00034 0.00000 0.00877 0.00933 1.91376

A45 2.03533 -0.00057 0.00000 -0.01318 -0.01345 2.02188

A46 2.34340 0.00023 0.00000 0.00441 0.00413 2.34753

A47 1.90199 -0.00055 0.00000 0.00202 0.00208 1.90406

A48 2.01865 0.00026 0.00000 0.00768 0.00765 2.02630

A49 2.36254 0.00029 0.00000 -0.00970 -0.00973 2.35282

D1 -0.53489 -0.00118 0.00000 -0.05181 -0.05175 -0.58664

D2 2.89075 0.00105 0.00000 0.01250 0.01308 2.90382

D3 1.15846 0.00162 0.00000 0.04148 0.04211 1.20057

D4 2.77694 -0.00186 0.00000 -0.01985 -0.01938 2.75756

D5 -0.08061 0.00037 0.00000 0.04446 0.04545 -0.03516

D6 -1.81290 0.00094 0.00000 0.07344 0.07449 -1.73842

D7 -0.04697 0.00015 0.00000 0.02824 0.02856 -0.01841

D8 -3.00247 -0.00039 0.00000 0.04945 0.04968 -2.95279

D9 2.92126 0.00115 0.00000 0.00378 0.00513 2.92639

D10 -0.03424 0.00061 0.00000 0.02498 0.02625 -0.00799

D11 2.64911 0.00136 0.00000 0.06046 0.06051 2.70962

D12 -1.62571 0.00139 0.00000 0.05969 0.05963 -1.56608

D13 0.49070 0.00130 0.00000 0.05476 0.05490 0.54560

D14 -0.76855 -0.00066 0.00000 0.00338 0.00401 -0.76454

D15 1.23982 -0.00063 0.00000 0.00261 0.00313 1.24295

D16 -2.92695 -0.00072 0.00000 -0.00232 -0.00160 -2.92855

D17 0.98938 0.00050 0.00000 -0.00872 -0.00879 0.98059

D18 2.99775 0.00053 0.00000 -0.00949 -0.00967 2.98807

D19 -1.16902 0.00044 0.00000 -0.01442 -0.01441 -1.18343

D20 -1.00440 -0.00118 0.00000 -0.03181 -0.03280 -1.03719

D21 -2.96758 0.00051 0.00000 -0.00949 -0.01035 -2.97793

D22 1.22233 -0.00073 0.00000 -0.03083 -0.03038 1.19194

D23 1.10748 -0.00113 0.00000 -0.02057 -0.02005 1.08742

D24 -0.85570 0.00055 0.00000 0.00175 0.00239 -0.85331

D25 -2.94899 -0.00068 0.00000 -0.01960 -0.01764 -2.96663

D26 -3.11058 -0.00134 0.00000 -0.04093 -0.04134 3.13126

D27 1.20942 0.00035 0.00000 -0.01860 -0.01890 1.19052

D28 -0.88386 -0.00088 0.00000 -0.03995 -0.03893 -0.92279

D29 0.64431 -0.00010 0.00000 -0.00036 -0.00061 0.64369

D30 -2.68772 0.00101 0.00000 -0.01547 -0.01506 -2.70278

D31 -3.03934 0.00004 0.00000 0.09714 0.09689 -2.94245

D32 -0.08818 0.00116 0.00000 0.08203 0.08245 -0.00573

D33 -1.20225 -0.00199 0.00000 0.00777 0.00785 -1.19440

D34 1.74891 -0.00087 0.00000 -0.00734 -0.00659 1.74232

D35 -0.63732 0.00009 0.00000 0.00248 0.00265 -0.63468

D36 -2.78823 -0.00003 0.00000 -0.00582 -0.00571 -2.79394

D37 1.47826 -0.00015 0.00000 -0.00867 -0.00856 1.46970

D38 3.02447 -0.00028 0.00000 -0.08640 -0.08647 2.93799

D39 0.87356 -0.00040 0.00000 -0.09471 -0.09483 0.77873

D40 -1.14314 -0.00051 0.00000 -0.09755 -0.09768 -1.24081

D41 1.15892 -0.00024 0.00000 -0.03150 -0.03107 1.12785

D42 -0.99199 -0.00035 0.00000 -0.03980 -0.03943 -1.03141

D43 -3.00869 -0.00047 0.00000 -0.04265 -0.04227 -3.05095

D44 1.04982 0.00008 0.00000 0.00132 0.00081 1.05063

D45 3.01121 -0.00138 0.00000 -0.02168 -0.02196 2.98925

D46 -1.18839 -0.00059 0.00000 -0.00329 -0.00386 -1.19225

D47 -1.06084 0.00145 0.00000 -0.00709 -0.00674 -1.06757

D48 0.90056 -0.00001 0.00000 -0.03009 -0.02951 0.87105

D49 2.98414 0.00078 0.00000 -0.01170 -0.01141 2.97273

D50 -3.12151 0.00060 0.00000 -0.01536 -0.01462 -3.13613

D51 -1.16011 -0.00086 0.00000 -0.03836 -0.03739 -1.19751

D52 0.92347 -0.00008 0.00000 -0.01997 -0.01929 0.90418

D53 0.07858 -0.00022 0.00000 -0.02788 -0.02752 0.05105

D54 2.23214 0.00021 0.00000 -0.02033 -0.02014 2.21200

D55 -2.01597 -0.00033 0.00000 -0.01598 -0.01580 -2.03177

D56 -2.08329 -0.00031 0.00000 -0.02843 -0.02823 -2.11151

D57 0.07028 0.00012 0.00000 -0.02088 -0.02085 0.04943

D58 2.10535 -0.00042 0.00000 -0.01654 -0.01651 2.08885

D59 2.17682 -0.00004 0.00000 -0.02937 -0.02906 2.14777

D60 -1.95280 0.00038 0.00000 -0.02182 -0.02168 -1.97448

D61 0.08228 -0.00015 0.00000 -0.01747 -0.01734 0.06494

D62 -0.03658 0.00052 0.00000 -0.01301 -0.01302 -0.04960

D63 3.09876 0.00042 0.00000 -0.01246 -0.01237 3.08639

D64 0.00350 0.00008 0.00000 0.02841 0.02864 0.03214

D65 -3.13501 -0.00019 0.00000 0.02811 0.02855 -3.10647

D66 -0.02356 0.00001 0.00000 0.01210 0.01290 -0.01066

D67 1.86003 0.00026 0.00000 -0.01567 -0.01537 1.84466

D68 -1.62186 -0.00205 0.00000 -0.11479 -0.11308 -1.73493

D69 -1.93667 0.00090 0.00000 0.05375 0.05431 -1.88236

D70 -0.05309 0.00114 0.00000 0.02598 0.02604 -0.02704

D71 2.74821 -0.00117 0.00000 -0.07314 -0.07166 2.67655

D72 1.87083 -0.00017 0.00000 -0.04413 -0.04448 1.82634

D73 -2.52878 0.00008 0.00000 -0.07190 -0.07275 -2.60153

D74 0.27253 -0.00223 0.00000 -0.17102 -0.17046 0.10207

D75 -1.94791 0.00061 0.00000 0.03032 0.03044 -1.91747

D76 1.20149 0.00074 0.00000 0.02972 0.02971 1.23120

D77 0.05690 -0.00111 0.00000 -0.00856 -0.00889 0.04802

D78 -3.07688 -0.00098 0.00000 -0.00917 -0.00962 -3.08651

D79 2.58267 0.00003 0.00000 0.08152 0.08219 2.66486

D80 -0.55112 0.00016 0.00000 0.08092 0.08145 -0.46967

D81 1.96720 -0.00189 0.00000 -0.03969 -0.03954 1.92766

D82 -1.17834 -0.00154 0.00000 -0.03925 -0.03936 -1.21771

D83 0.03289 -0.00083 0.00000 -0.03482 -0.03488 -0.00199

D84 -3.11266 -0.00048 0.00000 -0.03438 -0.03470 3.13583

D85 -2.79887 0.00146 0.00000 0.06135 0.06238 -2.73649

D86 0.33877 0.00180 0.00000 0.06179 0.06256 0.40133

Item Value Threshold Converged?

Maximum Force 0.011746 0.000450 NO

RMS Force 0.001505 0.000300 NO

Maximum Displacement 0.150596 0.001800 NO

RMS Displacement 0.036115 0.001200 NO

Predicted change in Energy=-4.002549D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.151743 1.554856 0.436853

2 6 0 0.174099 1.280865 0.099400

3 6 0 -0.732085 3.773061 -0.358333

4 6 0 -1.629488 2.845312 0.189576

5 1 0 -1.753804 0.865449 1.047223

6 1 0 -2.597202 3.180898 0.586734

7 6 0 0.810872 1.935228 -1.084977

8 1 0 1.926266 1.970572 -0.954026

9 1 0 0.627042 1.278112 -1.980897

10 6 0 0.268888 3.327158 -1.363922

11 1 0 1.113993 4.065630 -1.426593

12 1 0 -0.240910 3.335127 -2.367780

13 1 0 -1.010713 4.837224 -0.390358

14 1 0 0.671267 0.368481 0.467819

15 8 0 2.749475 3.851189 0.811848

16 6 0 0.451272 3.868788 1.392876

17 6 0 0.958444 2.563006 1.658788

18 6 0 1.607056 4.670631 0.898695

19 8 0 1.763026 5.836934 0.574922

20 6 0 2.404387 2.572357 1.288844

21 8 0 3.304485 1.747911 1.314876

22 1 0 -0.355594 4.364336 1.937676

23 1 0 0.564567 1.839881 2.375214

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.395279 0.000000

3 C 2.393504 2.691046 0.000000

4 C 1.398092 2.389257 1.402231 0.000000

5 H 1.100141 2.188092 3.387285 2.161219 0.000000

6 H 2.180786 3.395251 2.173124 1.098555 2.506925

7 C 2.512471 1.495467 2.507261 2.899671 3.502609

8 H 3.403161 2.157659 3.266596 3.836193 4.332344

9 H 3.014329 2.129038 3.271805 3.501285 3.874045

10 C 2.898626 2.517461 1.487274 2.499872 3.995611

11 H 3.861344 3.311642 2.152854 3.409965 4.958345

12 H 3.444553 3.237160 2.114454 2.950955 4.477767

13 H 3.387935 3.780387 1.100501 2.164929 4.288801

14 H 2.175272 1.102430 3.774001 3.391988 2.542372

15 O 4.542386 3.707656 3.673784 4.535893 5.408287

16 C 2.972863 2.906415 2.115711 2.612469 3.741908

17 C 2.638632 2.165819 2.896705 2.989259 3.257606

18 C 4.187162 3.766000 2.803094 3.782837 5.079060

19 O 5.181807 4.848564 3.369884 4.539542 6.107931

20 C 3.795690 2.838471 3.740635 4.189874 4.501385

21 O 4.546005 3.390403 4.816094 5.178289 5.141659

22 H 3.283215 3.628722 2.400627 2.643122 3.871706

23 H 2.604650 2.375772 3.590372 3.256037 2.843927

6 7 8 9 10

6 H 0.000000

7 C 3.995157 0.000000

8 H 4.929563 1.123611 0.000000

9 H 4.539722 1.126174 1.794979 0.000000

10 C 3.470003 1.519547 2.180652 2.169683 0.000000

11 H 4.313839 2.178806 2.296166 2.883511 1.124043

12 H 3.782201 2.170609 2.925298 2.265906 1.125917

13 H 2.493004 3.496033 4.142615 4.228396 2.205789

14 H 4.313551 2.210286 2.482612 2.612584 3.502992

15 O 5.393229 3.320698 2.707897 4.350273 3.340942

16 C 3.227422 3.163498 3.359580 4.257328 2.815415

17 C 3.764799 2.818533 2.848588 3.874027 3.193147

18 C 4.471287 3.471497 3.290105 4.556497 2.952126

19 O 5.105512 4.345707 4.160900 5.348414 3.505786

20 C 5.087159 2.929207 2.370909 3.940207 3.488159

21 O 6.116662 3.465904 2.664016 4.272181 4.345667

22 H 2.872347 4.049400 4.393055 5.083853 3.516569

23 H 3.872179 3.470256 3.599325 4.392629 4.034916

11 12 13 14 15

11 H 0.000000

12 H 1.804226 0.000000

13 H 2.486668 2.599825 0.000000

14 H 4.177765 4.204007 4.851308 0.000000

15 O 2.780541 4.395311 4.068977 4.070204 0.000000

16 C 2.902990 3.860886 2.501038 3.627158 2.370578

17 C 3.435353 4.271753 3.639869 2.513328 2.363158

18 C 2.452774 3.983517 2.922691 4.423783 1.408598

19 O 2.750422 4.351355 3.102388 5.577400 2.229888

20 C 3.356871 4.577152 4.428572 2.921448 1.407844

21 O 4.205441 5.352666 5.574281 3.090982 2.232678

22 H 3.683370 4.428247 2.464253 4.379701 3.342493

23 H 4.439545 5.037910 4.371951 2.411339 3.356083

16 17 18 19 20

16 C 0.000000

17 C 1.425833 0.000000

18 C 1.490975 2.332493 0.000000

19 O 2.502668 3.541289 1.220417 0.000000

20 C 2.346533 1.492548 2.278313 3.402719 0.000000

21 O 3.555984 2.507302 3.405402 4.432126 1.220886

22 H 1.092432 2.247057 2.241716 2.917908 3.354053

23 H 2.257052 1.091473 3.358577 4.544643 2.258685

21 22 23

21 O 0.000000

22 H 4.541997 0.000000

23 H 2.939374 2.722317 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.320735 -0.690116 -0.666106

2 6 0 1.381597 -1.349763 0.127423

3 6 0 1.348383 1.341021 0.144989

4 6 0 2.314142 0.707872 -0.650425

5 1 0 2.918611 -1.217386 -1.424289

6 1 0 2.900050 1.288997 -1.375567

7 6 0 0.946636 -0.770575 1.435770

8 1 0 -0.075853 -1.150136 1.705865

9 1 0 1.640155 -1.161519 2.232301

10 6 0 0.966492 0.748724 1.454695

11 1 0 -0.032512 1.144261 1.784866

12 1 0 1.719713 1.102907 2.212918

13 1 0 1.189107 2.424661 0.037943

14 1 0 1.187409 -2.426426 -0.008374

15 8 0 -2.068861 -0.001220 0.277364

16 6 0 -0.263083 0.721351 -1.077884

17 6 0 -0.281934 -0.704185 -1.100041

18 6 0 -1.421221 1.139059 -0.236906

19 8 0 -1.905840 2.213795 0.078536

20 6 0 -1.424581 -1.139241 -0.244013

21 8 0 -1.895312 -2.218318 0.079355

22 1 0 0.075287 1.368859 -1.890069

23 1 0 0.115149 -1.353155 -1.882649

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2238812 0.8799517 0.6753574

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.7593878659 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.495796722059E-01 A.U. after 15 cycles

Convg = 0.9479D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.006987447 0.009404138 -0.000782177

2 6 0.009977171 0.003004873 0.002411413

3 6 0.000294111 0.002578705 0.006057309

4 6 0.004725899 -0.006114793 0.002045860

5 1 0.001535876 -0.001924706 -0.001977239

6 1 -0.000891713 -0.001325676 -0.000785923

7 6 -0.003268507 -0.004793680 0.001342765

8 1 0.000132004 0.000034028 0.000035182

9 1 -0.000646110 -0.000049392 0.000406675

10 6 0.000081606 -0.000065242 -0.000914797

11 1 -0.000053345 -0.000074706 0.000086234

12 1 0.000497947 -0.000012425 -0.000420937

13 1 -0.000259121 0.002147768 -0.001500359

14 1 -0.001399418 -0.001831760 -0.002266358

15 8 -0.000695047 0.000220763 0.000942699

16 6 0.005594417 -0.007953737 -0.001677671

17 6 -0.002908940 0.002950142 -0.010654294

18 6 -0.000753945 0.000389147 -0.000183458

19 8 -0.000338356 0.000771342 -0.000734161

20 6 -0.005661981 0.000245371 0.003605718

21 8 -0.000579565 -0.000090408 -0.000148454

22 1 -0.000068313 -0.000513353 0.001585924

23 1 0.001672776 0.003003603 0.003526050

-------------------------------------------------------------------

Cartesian Forces: Max 0.010654294 RMS 0.003255945

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.007000586 RMS 0.001340599

Search for a saddle point.

Step number 26 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 25 26

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0

Eigenvalues --- -0.06508 0.00074 0.00225 0.00434 0.00606

Eigenvalues --- 0.00987 0.01023 0.01439 0.02004 0.02115

Eigenvalues --- 0.02275 0.02344 0.02545 0.02900 0.03007

Eigenvalues --- 0.03123 0.03153 0.03416 0.03615 0.03721

Eigenvalues --- 0.03844 0.03884 0.04125 0.04351 0.04600

Eigenvalues --- 0.05232 0.05595 0.05794 0.06051 0.06480

Eigenvalues --- 0.07349 0.08400 0.08742 0.09137 0.09832

Eigenvalues --- 0.11883 0.13687 0.14281 0.15864 0.20617

Eigenvalues --- 0.22648 0.25725 0.26812 0.27016 0.28505

Eigenvalues --- 0.30360 0.30822 0.31249 0.31571 0.31959

Eigenvalues --- 0.31999 0.32431 0.32943 0.34504 0.36012

Eigenvalues --- 0.37513 0.39581 0.40395 0.43274 0.46861

Eigenvalues --- 0.50504 1.08431 1.10834

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D73

1 0.58720 0.44548 -0.19069 0.17743 -0.15334

D79 D71 D80 D86 D85

1 0.14479 0.12778 0.12716 -0.12609 -0.12089

RFO step: Lambda0=4.487125114D-04 Lambda=-3.49829480D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.739

Iteration 1 RMS(Cart)= 0.03581235 RMS(Int)= 0.00134340

Iteration 2 RMS(Cart)= 0.00111059 RMS(Int)= 0.00074755

Iteration 3 RMS(Cart)= 0.00000120 RMS(Int)= 0.00074755

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00074755

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63669 0.00190 0.00000 0.03100 0.03100 2.66770

R2 2.64201 -0.00700 0.00000 -0.03731 -0.03686 2.60515

R3 2.07897 -0.00073 0.00000 -0.00150 -0.00150 2.07747

R4 2.82602 -0.00460 0.00000 -0.02426 -0.02440 2.80163

R5 2.08329 0.00013 0.00000 0.00219 0.00219 2.08548

R6 4.09280 -0.00124 0.00000 -0.13984 -0.14052 3.95229

R7 2.64983 0.00059 0.00000 -0.00824 -0.00782 2.64201

R8 2.81054 0.00170 0.00000 0.00353 0.00348 2.81402

R9 2.07965 0.00219 0.00000 -0.00148 -0.00148 2.07817

R10 3.99811 -0.00291 0.00000 0.17558 0.17611 4.17423

R11 2.07597 0.00010 0.00000 0.00377 0.00377 2.07974

R12 2.12332 0.00014 0.00000 0.00090 0.00090 2.12421

R13 2.12816 -0.00019 0.00000 -0.00006 -0.00006 2.12810

R14 2.87153 0.00123 0.00000 0.00759 0.00735 2.87888

R15 2.12413 -0.00009 0.00000 -0.00152 -0.00152 2.12261

R16 2.12767 0.00015 0.00000 0.00104 0.00104 2.12871

R17 2.66186 -0.00122 0.00000 0.00822 0.00817 2.67003

R18 2.66044 0.00014 0.00000 0.00297 0.00271 2.66315

R19 2.69443 -0.00684 0.00000 -0.03880 -0.03884 2.65559

R20 2.81753 -0.00110 0.00000 -0.01444 -0.01425 2.80329

R21 2.06440 0.00061 0.00000 -0.00416 -0.00416 2.06023

R22 2.82051 -0.00634 0.00000 -0.00917 -0.00926 2.81125

R23 2.06259 -0.00028 0.00000 0.00589 0.00589 2.06848

R24 2.30625 0.00089 0.00000 0.00070 0.00070 2.30696

R25 2.30714 -0.00037 0.00000 -0.00010 -0.00010 2.30704

A1 2.05238 0.00127 0.00000 0.01721 0.01698 2.06936

A2 2.13075 -0.00293 0.00000 -0.05654 -0.05650 2.07425

A3 2.08235 0.00170 0.00000 0.03339 0.03303 2.11538

A4 2.10625 -0.00057 0.00000 -0.04685 -0.04783 2.05842

A5 2.10624 0.00014 0.00000 0.01445 0.01282 2.11907

A6 1.62456 -0.00070 0.00000 0.03271 0.03335 1.65792

A7 2.02059 -0.00015 0.00000 0.00407 0.00240 2.02299

A8 1.72844 0.00048 0.00000 0.02864 0.02905 1.75749

A9 1.65691 0.00201 0.00000 0.02352 0.02346 1.68036

A10 2.09042 -0.00143 0.00000 -0.02406 -0.02549 2.06493

A11 2.08187 0.00101 0.00000 0.04467 0.04441 2.12629

A12 1.63531 0.00041 0.00000 -0.00495 -0.00633 1.62898

A13 2.02710 0.00015 0.00000 0.01294 0.01136 2.03847

A14 1.76886 -0.00043 0.00000 -0.05250 -0.05224 1.71662

A15 1.69304 0.00069 0.00000 -0.01895 -0.01867 1.67437

A16 2.05004 0.00053 0.00000 0.01672 0.01704 2.06708

A17 2.11651 -0.00141 0.00000 0.00025 0.00000 2.11652

A18 2.09776 0.00097 0.00000 -0.01997 -0.02019 2.07757

A19 1.92213 -0.00008 0.00000 0.00792 0.00766 1.92979

A20 1.88098 -0.00016 0.00000 -0.00787 -0.00768 1.87330

A21 1.97613 -0.00005 0.00000 0.00902 0.00921 1.98534

A22 1.84742 0.00019 0.00000 0.00409 0.00411 1.85153

A23 1.92479 -0.00012 0.00000 -0.00638 -0.00640 1.91839

A24 1.90734 0.00024 0.00000 -0.00730 -0.00746 1.89988

A25 1.97204 -0.00059 0.00000 0.01231 0.01259 1.98464

A26 1.92489 0.00028 0.00000 -0.00184 -0.00175 1.92314

A27 1.87127 0.00039 0.00000 0.00117 0.00090 1.87217

A28 1.92184 0.00011 0.00000 -0.00114 -0.00126 1.92058

A29 1.90885 0.00003 0.00000 -0.00773 -0.00783 1.90102

A30 1.86091 -0.00019 0.00000 -0.00375 -0.00372 1.85719

A31 1.88467 -0.00107 0.00000 -0.00377 -0.00396 1.88071

A32 1.88797 0.00063 0.00000 -0.02019 -0.02045 1.86752

A33 1.75541 -0.00107 0.00000 -0.01018 -0.00966 1.74575

A34 1.59100 0.00019 0.00000 -0.04991 -0.04972 1.54127

A35 1.85313 0.00157 0.00000 0.01710 0.01670 1.86983

A36 2.19585 -0.00118 0.00000 0.01278 0.01062 2.20647

A37 2.08735 -0.00035 0.00000 0.01795 0.01653 2.10388

A38 1.85360 0.00104 0.00000 0.04136 0.04061 1.89421

A39 1.74781 -0.00103 0.00000 -0.04639 -0.04585 1.70196

A40 1.52048 0.00163 0.00000 0.08549 0.08692 1.60740

A41 1.86778 0.00084 0.00000 0.00116 0.00139 1.86917

A42 2.21529 -0.00123 0.00000 -0.03179 -0.03615 2.17914

A43 2.11349 -0.00046 0.00000 -0.01023 -0.01096 2.10252

A44 1.91376 -0.00187 0.00000 -0.01184 -0.01157 1.90219

A45 2.02188 0.00130 0.00000 0.00338 0.00325 2.02513

A46 2.34753 0.00057 0.00000 0.00844 0.00830 2.35583

A47 1.90406 0.00055 0.00000 -0.00274 -0.00289 1.90118

A48 2.02630 0.00015 0.00000 0.00268 0.00275 2.02905

A49 2.35282 -0.00071 0.00000 0.00007 0.00014 2.35295

D1 -0.58664 -0.00150 0.00000 -0.05234 -0.05188 -0.63852

D2 2.90382 0.00046 0.00000 0.04221 0.04237 2.94620

D3 1.20057 -0.00148 0.00000 -0.00705 -0.00815 1.19242

D4 2.75756 -0.00196 0.00000 -0.02299 -0.02287 2.73469

D5 -0.03516 0.00000 0.00000 0.07155 0.07137 0.03621

D6 -1.73842 -0.00194 0.00000 0.02229 0.02085 -1.71756

D7 -0.01841 0.00014 0.00000 0.03731 0.03767 0.01926

D8 -2.95279 -0.00048 0.00000 0.05591 0.05656 -2.89623

D9 2.92639 0.00003 0.00000 -0.00197 -0.00283 2.92357

D10 -0.00799 -0.00060 0.00000 0.01663 0.01606 0.00807

D11 2.70962 0.00041 0.00000 0.05078 0.04991 2.75952

D12 -1.56608 0.00051 0.00000 0.05543 0.05451 -1.51157

D13 0.54560 0.00067 0.00000 0.04649 0.04557 0.59117

D14 -0.76454 -0.00139 0.00000 -0.03672 -0.03648 -0.80102

D15 1.24295 -0.00130 0.00000 -0.03206 -0.03188 1.21107

D16 -2.92855 -0.00114 0.00000 -0.04100 -0.04082 -2.96937

D17 0.98059 0.00110 0.00000 0.00588 0.00637 0.98695

D18 2.98807 0.00119 0.00000 0.01054 0.01097 2.99905

D19 -1.18343 0.00135 0.00000 0.00160 0.00203 -1.18140

D20 -1.03719 0.00070 0.00000 0.00165 0.00025 -1.03694

D21 -2.97793 -0.00012 0.00000 0.00548 0.00520 -2.97273

D22 1.19194 0.00011 0.00000 0.00289 0.00486 1.19680

D23 1.08742 0.00004 0.00000 -0.03456 -0.03558 1.05184

D24 -0.85331 -0.00079 0.00000 -0.03073 -0.03064 -0.88395

D25 -2.96663 -0.00056 0.00000 -0.03332 -0.03098 -2.99761

D26 3.13126 0.00042 0.00000 -0.02002 -0.02145 3.10981

D27 1.19052 -0.00041 0.00000 -0.01619 -0.01651 1.17402

D28 -0.92279 -0.00017 0.00000 -0.01878 -0.01685 -0.93964

D29 0.64369 0.00018 0.00000 -0.02777 -0.02750 0.61620

D30 -2.70278 0.00050 0.00000 -0.04372 -0.04357 -2.74635

D31 -2.94245 -0.00046 0.00000 0.05965 0.06033 -2.88212

D32 -0.00573 -0.00014 0.00000 0.04370 0.04426 0.03852

D33 -1.19440 0.00075 0.00000 0.04224 0.04179 -1.15261

D34 1.74232 0.00107 0.00000 0.02629 0.02572 1.76803

D35 -0.63468 -0.00009 0.00000 0.02903 0.02860 -0.60607

D36 -2.79394 -0.00001 0.00000 0.02295 0.02235 -2.77159

D37 1.46970 -0.00015 0.00000 0.02770 0.02717 1.49687

D38 2.93799 0.00030 0.00000 -0.06397 -0.06364 2.87435

D39 0.77873 0.00037 0.00000 -0.07005 -0.06989 0.70884

D40 -1.24081 0.00023 0.00000 -0.06530 -0.06507 -1.30589

D41 1.12785 -0.00032 0.00000 -0.01711 -0.01672 1.11113

D42 -1.03141 -0.00024 0.00000 -0.02319 -0.02298 -1.05439

D43 -3.05095 -0.00038 0.00000 -0.01843 -0.01816 -3.06911

D44 1.05063 -0.00155 0.00000 -0.05226 -0.05206 0.99857

D45 2.98925 -0.00007 0.00000 -0.04433 -0.04423 2.94502

D46 -1.19225 -0.00052 0.00000 -0.03866 -0.03868 -1.23093

D47 -1.06757 -0.00008 0.00000 -0.01551 -0.01528 -1.08285

D48 0.87105 0.00139 0.00000 -0.00758 -0.00745 0.86360

D49 2.97273 0.00094 0.00000 -0.00192 -0.00191 2.97083

D50 -3.13613 -0.00034 0.00000 -0.01043 -0.01063 3.13643

D51 -1.19751 0.00114 0.00000 -0.00250 -0.00280 -1.20031

D52 0.90418 0.00069 0.00000 0.00316 0.00275 0.90692

D53 0.05105 -0.00023 0.00000 -0.03931 -0.03980 0.01125

D54 2.21200 -0.00021 0.00000 -0.03365 -0.03384 2.17815

D55 -2.03177 -0.00036 0.00000 -0.04339 -0.04361 -2.07539

D56 -2.11151 0.00000 0.00000 -0.05144 -0.05173 -2.16324

D57 0.04943 0.00003 0.00000 -0.04577 -0.04577 0.00366

D58 2.08885 -0.00013 0.00000 -0.05552 -0.05554 2.03331

D59 2.14777 -0.00029 0.00000 -0.04850 -0.04879 2.09897

D60 -1.97448 -0.00027 0.00000 -0.04284 -0.04284 -2.01731

D61 0.06494 -0.00043 0.00000 -0.05259 -0.05261 0.01234

D62 -0.04960 0.00011 0.00000 -0.00680 -0.00682 -0.05642

D63 3.08639 -0.00030 0.00000 -0.00909 -0.00885 3.07753

D64 0.03214 0.00052 0.00000 0.01673 0.01661 0.04875

D65 -3.10647 0.00044 0.00000 0.01564 0.01571 -3.09076

D66 -0.01066 0.00096 0.00000 0.03724 0.03718 0.02652

D67 1.84466 0.00055 0.00000 0.00258 0.00266 1.84732

D68 -1.73493 -0.00152 0.00000 -0.09558 -0.09363 -1.82856

D69 -1.88236 0.00123 0.00000 0.04950 0.04937 -1.83299

D70 -0.02704 0.00083 0.00000 0.01484 0.01484 -0.01220

D71 2.67655 -0.00124 0.00000 -0.08332 -0.08144 2.59511

D72 1.82634 0.00111 0.00000 -0.03995 -0.04067 1.78567

D73 -2.60153 0.00070 0.00000 -0.07461 -0.07520 -2.67672

D74 0.10207 -0.00137 0.00000 -0.17277 -0.17148 -0.06942

D75 -1.91747 -0.00135 0.00000 0.01511 0.01551 -1.90196

D76 1.23120 -0.00083 0.00000 0.01805 0.01814 1.24934

D77 0.04802 -0.00058 0.00000 -0.00537 -0.00533 0.04269

D78 -3.08651 -0.00006 0.00000 -0.00243 -0.00270 -3.08920

D79 2.66486 -0.00085 0.00000 0.07536 0.07602 2.74088

D80 -0.46967 -0.00033 0.00000 0.07830 0.07865 -0.39101

D81 1.92766 0.00010 0.00000 0.00685 0.00638 1.93405

D82 -1.21771 0.00021 0.00000 0.00823 0.00752 -1.21018

D83 -0.00199 -0.00088 0.00000 -0.02029 -0.02019 -0.02217

D84 3.13583 -0.00078 0.00000 -0.01891 -0.01904 3.11678

D85 -2.73649 0.00131 0.00000 0.07773 0.07887 -2.65763

D86 0.40133 0.00141 0.00000 0.07910 0.08001 0.48133

Item Value Threshold Converged?

Maximum Force 0.007001 0.000450 NO

RMS Force 0.001341 0.000300 NO

Maximum Displacement 0.121630 0.001800 NO

RMS Displacement 0.035840 0.001200 NO

Predicted change in Energy=-1.858828D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.142990 1.569539 0.414207

2 6 0 0.218578 1.316293 0.140614

3 6 0 -0.785961 3.787385 -0.388513

4 6 0 -1.644515 2.827304 0.155353

5 1 0 -1.705498 0.845945 1.021304

6 1 0 -2.618935 3.147046 0.554706

7 6 0 0.818058 1.957863 -1.053952

8 1 0 1.935916 2.016713 -0.951494

9 1 0 0.620434 1.281767 -1.932605

10 6 0 0.251408 3.338889 -1.358141

11 1 0 1.082534 4.092481 -1.412824

12 1 0 -0.228876 3.320345 -2.376919

13 1 0 -1.042128 4.856827 -0.395869

14 1 0 0.714739 0.395962 0.493774

15 8 0 2.745761 3.801100 0.773771

16 6 0 0.479030 3.867993 1.420510

17 6 0 0.943502 2.562694 1.655598

18 6 0 1.625164 4.652465 0.899392

19 8 0 1.799467 5.818019 0.580914

20 6 0 2.378137 2.531704 1.263215

21 8 0 3.256116 1.683547 1.278005

22 1 0 -0.344148 4.364558 1.934710

23 1 0 0.567806 1.896564 2.438703

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.411684 0.000000

3 C 2.385512 2.719442 0.000000

4 C 1.378588 2.398851 1.398092 0.000000

5 H 1.099350 2.167696 3.388982 2.163186 0.000000

6 H 2.164875 3.402147 2.158585 1.100551 2.519354

7 C 2.480321 1.482557 2.522466 2.877953 3.451286

8 H 3.397759 2.152333 3.295579 3.834274 4.303780

9 H 2.949577 2.112089 3.261946 3.446484 3.784901

10 C 2.866385 2.517586 1.489114 2.479296 3.963081

11 H 3.828346 3.296484 2.152573 3.390671 4.923220

12 H 3.419256 3.248756 2.117128 2.942707 4.455445

13 H 3.387131 3.796389 1.099719 2.187619 4.305300

14 H 2.198811 1.103588 3.812123 3.404707 2.517602

15 O 4.497948 3.600251 3.718084 4.539300 5.348637

16 C 2.987723 2.866556 2.208906 2.681996 3.750240

17 C 2.623139 2.091461 2.944367 3.003096 3.219745

18 C 4.171631 3.699225 2.867156 3.817801 5.059423

19 O 5.170631 4.791515 3.427492 4.581102 6.099200

20 C 3.747653 2.720506 3.783709 4.182877 4.424520

21 O 4.484560 3.264226 4.851989 5.156036 5.038361

22 H 3.280580 3.581530 2.434274 2.687046 3.881780

23 H 2.670646 2.395806 3.660743 3.312752 2.877625

6 7 8 9 10

6 H 0.000000

7 C 3.976790 0.000000

8 H 4.928789 1.124085 0.000000

9 H 4.489933 1.126141 1.798115 0.000000

10 C 3.454658 1.523436 2.179697 2.167473 0.000000

11 H 4.297197 2.180673 2.291265 2.895483 1.123237

12 H 3.786402 2.168565 2.901314 2.252675 1.126466

13 H 2.512621 3.506759 4.152555 4.231633 2.214348

14 H 4.322680 2.201286 2.491366 2.584736 3.507861

15 O 5.408858 3.233285 2.610828 4.264801 3.313682

16 C 3.296479 3.144280 3.343076 4.236973 2.837722

17 C 3.774174 2.779067 2.842518 3.823657 3.188118

18 C 4.516356 3.424595 3.235665 4.515672 2.951126

19 O 5.163048 4.305434 4.100832 5.318410 3.507493

20 C 5.084423 2.851736 2.316400 3.855532 3.470739

21 O 6.097640 3.384877 2.612391 4.173279 4.326395

22 H 2.925987 4.009364 4.363626 5.038863 3.499936

23 H 3.907488 3.502145 3.657813 4.414644 4.073872

11 12 13 14 15

11 H 0.000000

12 H 1.801519 0.000000

13 H 2.476411 2.635662 0.000000

14 H 4.175481 4.205152 4.876204 0.000000

15 O 2.762684 4.359638 4.102526 3.974722 0.000000

16 C 2.905580 3.901477 2.567285 3.601305 2.358138

17 C 3.431442 4.267283 3.662553 2.469189 2.357839

18 C 2.440158 3.993272 2.972190 4.371637 1.412919

19 O 2.732484 4.370507 3.154784 5.530184 2.236209

20 C 3.357945 4.546322 4.456116 2.814307 1.409280

21 O 4.215208 5.308742 5.598791 2.954910 2.235787

22 H 3.649032 4.437771 2.482157 4.352849 3.348552

23 H 4.463324 5.084493 4.403390 2.460923 3.338076

16 17 18 19 20

16 C 0.000000

17 C 1.405278 0.000000

18 C 1.483436 2.324575 0.000000

19 O 2.500215 3.533378 1.220790 0.000000

20 C 2.327448 1.487649 2.279684 3.405915 0.000000

21 O 3.536144 2.502730 3.408492 4.438651 1.220834

22 H 1.090229 2.232187 2.243426 2.922396 3.349790

23 H 2.220615 1.094592 3.329035 4.510674 2.249994

21 22 23

21 O 0.000000

22 H 4.536626 0.000000

23 H 2.935917 2.678930 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.294263 -0.725205 -0.633603

2 6 0 1.278197 -1.362032 0.111321

3 6 0 1.422345 1.353347 0.147455

4 6 0 2.355788 0.651957 -0.621568

5 1 0 2.861990 -1.314272 -1.367944

6 1 0 2.968765 1.202762 -1.351011

7 6 0 0.891593 -0.763959 1.411637

8 1 0 -0.142219 -1.092948 1.705859

9 1 0 1.586333 -1.182182 2.193058

10 6 0 0.979398 0.756718 1.437918

11 1 0 -0.007491 1.193953 1.748622

12 1 0 1.725750 1.065975 2.222929

13 1 0 1.258857 2.433173 0.018503

14 1 0 1.068712 -2.439264 -0.005276

15 8 0 -2.043053 0.014735 0.300052

16 6 0 -0.281789 0.713331 -1.103773

17 6 0 -0.286039 -0.691941 -1.104553

18 6 0 -1.410423 1.153289 -0.247500

19 8 0 -1.889267 2.232869 0.061599

20 6 0 -1.410197 -1.126345 -0.232394

21 8 0 -1.875117 -2.205606 0.098487

22 1 0 0.098109 1.359916 -1.895104

23 1 0 0.041878 -1.318040 -1.940377

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2268050 0.8912441 0.6799244

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.7310296319 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.487692291040E-01 A.U. after 15 cycles

Convg = 0.7174D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.012402003 -0.015070429 0.007159674

2 6 -0.007387945 0.004357226 0.006787240

3 6 0.009796980 -0.002764937 0.004114026

4 6 -0.004896184 0.014943458 0.003046158

5 1 -0.002610280 -0.000831544 -0.001773699

6 1 -0.001797615 -0.002332530 -0.001391501

7 6 0.002240667 0.001425427 -0.007953889

8 1 0.000122260 -0.000192001 -0.001405633

9 1 0.000096198 -0.000063689 -0.000683800

10 6 -0.000175697 0.001736765 -0.001909188

11 1 0.000508999 0.000157995 0.000075646

12 1 0.000222270 0.000209259 -0.000132821

13 1 -0.001726099 -0.000131979 -0.001157997

14 1 -0.002603759 -0.000737960 -0.000884298

15 8 -0.000071296 0.000527604 0.001630817

16 6 -0.008394705 0.010078124 -0.007968461

17 6 -0.002232925 -0.014197282 -0.000347679

18 6 0.001346900 0.000788657 -0.001228705

19 8 0.000091202 -0.000565642 -0.000646031

20 6 0.004751801 0.002174508 0.002203220

21 8 -0.000137164 0.000119663 -0.000084414

22 1 -0.000393340 0.000445172 0.001703504

23 1 0.000847729 -0.000075865 0.000847832

-------------------------------------------------------------------

Cartesian Forces: Max 0.015070429 RMS 0.004707832

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011503844 RMS 0.001988521

Search for a saddle point.

Step number 27 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0

Eigenvalues --- -0.06333 -0.00319 0.00243 0.00532 0.00609

Eigenvalues --- 0.00994 0.01074 0.01466 0.02081 0.02151

Eigenvalues --- 0.02282 0.02350 0.02590 0.02907 0.03004

Eigenvalues --- 0.03132 0.03231 0.03435 0.03648 0.03762

Eigenvalues --- 0.03843 0.03888 0.04206 0.04409 0.05020

Eigenvalues --- 0.05233 0.05696 0.05808 0.06112 0.06522

Eigenvalues --- 0.07345 0.08418 0.08739 0.09291 0.09834

Eigenvalues --- 0.11902 0.13711 0.14376 0.15898 0.20711

Eigenvalues --- 0.22676 0.25825 0.26919 0.27576 0.28512

Eigenvalues --- 0.30395 0.31253 0.31284 0.31640 0.31963

Eigenvalues --- 0.32057 0.32430 0.32999 0.34626 0.36167

Eigenvalues --- 0.37561 0.39584 0.40394 0.43483 0.47012

Eigenvalues --- 0.50779 1.08432 1.10834

Eigenvectors required to have negative eigenvalues:

R10 R6 D4 D30 D86

1 0.53548 0.49737 0.18215 -0.18032 -0.15157

D71 D85 A40 D73 D1

1 0.14882 -0.14731 -0.13901 -0.13249 0.12159

RFO step: Lambda0=7.368995887D-04 Lambda=-4.68317056D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.796

Iteration 1 RMS(Cart)= 0.06268966 RMS(Int)= 0.00226697

Iteration 2 RMS(Cart)= 0.00245427 RMS(Int)= 0.00082029

Iteration 3 RMS(Cart)= 0.00000356 RMS(Int)= 0.00082028

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00082028

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.66770 -0.00621 0.00000 -0.01973 -0.01971 2.64798

R2 2.60515 0.01150 0.00000 0.05749 0.05835 2.66350

R3 2.07747 0.00090 0.00000 0.00239 0.00239 2.07986

R4 2.80163 0.00982 0.00000 0.03204 0.03214 2.83377

R5 2.08548 -0.00084 0.00000 0.00202 0.00202 2.08750

R6 3.95229 -0.00023 0.00000 -0.03153 -0.03160 3.92069

R7 2.64201 0.00203 0.00000 -0.01080 -0.01003 2.63198

R8 2.81402 0.00127 0.00000 -0.01368 -0.01458 2.79944

R9 2.07817 0.00028 0.00000 0.00008 0.00008 2.07825

R10 4.17423 -0.00592 0.00000 0.15402 0.15417 4.32840

R11 2.07974 0.00041 0.00000 -0.00186 -0.00186 2.07788

R12 2.12421 -0.00002 0.00000 -0.00320 -0.00320 2.12101

R13 2.12810 0.00055 0.00000 0.00075 0.00075 2.12885

R14 2.87888 0.00054 0.00000 -0.00608 -0.00706 2.87182

R15 2.12261 0.00048 0.00000 0.00311 0.00311 2.12572

R16 2.12871 0.00002 0.00000 0.00094 0.00094 2.12965

R17 2.67003 0.00001 0.00000 0.00836 0.00838 2.67841

R18 2.66315 0.00029 0.00000 -0.00517 -0.00532 2.65783

R19 2.65559 0.01124 0.00000 0.01647 0.01665 2.67224

R20 2.80329 0.00161 0.00000 -0.01503 -0.01484 2.78844

R21 2.06023 0.00130 0.00000 -0.00306 -0.00306 2.05718

R22 2.81125 0.00348 0.00000 0.02955 0.02942 2.84066

R23 2.06848 0.00036 0.00000 0.00186 0.00186 2.07034

R24 2.30696 -0.00036 0.00000 -0.00006 -0.00006 2.30690

R25 2.30704 -0.00018 0.00000 -0.00050 -0.00050 2.30655

A1 2.06936 -0.00148 0.00000 -0.02486 -0.02572 2.04363

A2 2.07425 0.00251 0.00000 0.06053 0.06099 2.13524

A3 2.11538 -0.00060 0.00000 -0.03268 -0.03241 2.08297

A4 2.05842 0.00153 0.00000 0.02176 0.02112 2.07953

A5 2.11907 -0.00203 0.00000 -0.04825 -0.04766 2.07141

A6 1.65792 -0.00124 0.00000 -0.02771 -0.03041 1.62751

A7 2.02299 0.00003 0.00000 -0.00593 -0.00889 2.01410

A8 1.75749 0.00156 0.00000 0.08588 0.08674 1.84423

A9 1.68036 0.00076 0.00000 0.01845 0.01815 1.69852

A10 2.06493 0.00137 0.00000 0.04889 0.04803 2.11296

A11 2.12629 -0.00101 0.00000 -0.01427 -0.01751 2.10877

A12 1.62898 -0.00203 0.00000 -0.06256 -0.06222 1.56676

A13 2.03847 -0.00072 0.00000 -0.00254 -0.00345 2.03502

A14 1.71662 0.00357 0.00000 0.01098 0.01136 1.72798

A15 1.67437 -0.00038 0.00000 -0.03930 -0.03965 1.63472

A16 2.06708 -0.00096 0.00000 -0.01090 -0.01098 2.05610

A17 2.11652 -0.00137 0.00000 -0.07051 -0.07048 2.04603

A18 2.07757 0.00273 0.00000 0.08098 0.08100 2.15858

A19 1.92979 0.00095 0.00000 0.01634 0.01701 1.94680

A20 1.87330 0.00022 0.00000 -0.01028 -0.01063 1.86267

A21 1.98534 -0.00051 0.00000 -0.00895 -0.00944 1.97590

A22 1.85153 -0.00046 0.00000 -0.00125 -0.00127 1.85026

A23 1.91839 -0.00055 0.00000 -0.00241 -0.00253 1.91586

A24 1.89988 0.00037 0.00000 0.00676 0.00711 1.90699

A25 1.98464 0.00004 0.00000 -0.00695 -0.00847 1.97617

A26 1.92314 0.00006 0.00000 -0.00156 -0.00157 1.92157

A27 1.87217 0.00007 0.00000 0.00215 0.00311 1.87528

A28 1.92058 0.00023 0.00000 0.00211 0.00279 1.92337

A29 1.90102 -0.00038 0.00000 0.00532 0.00553 1.90655

A30 1.85719 -0.00004 0.00000 -0.00058 -0.00082 1.85637

A31 1.88071 0.00220 0.00000 0.00396 0.00388 1.88460

A32 1.86752 0.00019 0.00000 -0.00666 -0.00726 1.86026

A33 1.74575 0.00088 0.00000 0.01797 0.01899 1.76474

A34 1.54127 -0.00035 0.00000 -0.10427 -0.10382 1.43745

A35 1.86983 -0.00098 0.00000 0.01606 0.01542 1.88525

A36 2.20647 0.00057 0.00000 0.02083 0.01712 2.22359

A37 2.10388 0.00015 0.00000 0.01259 0.01070 2.11458

A38 1.89421 -0.00159 0.00000 -0.01961 -0.01977 1.87445

A39 1.70196 0.00381 0.00000 0.04713 0.04691 1.74887

A40 1.60740 -0.00031 0.00000 0.04976 0.05069 1.65809

A41 1.86917 -0.00238 0.00000 -0.02042 -0.01980 1.84937

A42 2.17914 0.00173 0.00000 0.00264 0.00088 2.18002

A43 2.10252 -0.00021 0.00000 -0.02535 -0.02763 2.07489

A44 1.90219 0.00063 0.00000 -0.00246 -0.00225 1.89994

A45 2.02513 -0.00073 0.00000 -0.00403 -0.00421 2.02092

A46 2.35583 0.00009 0.00000 0.00633 0.00615 2.36199

A47 1.90118 0.00057 0.00000 0.00369 0.00345 1.90463

A48 2.02905 -0.00031 0.00000 0.00704 0.00716 2.03621

A49 2.35295 -0.00026 0.00000 -0.01073 -0.01062 2.34234

D1 -0.63852 0.00025 0.00000 0.00638 0.00618 -0.63234

D2 2.94620 0.00141 0.00000 0.08934 0.08883 3.03503

D3 1.19242 0.00170 0.00000 0.09479 0.09440 1.28682

D4 2.73469 -0.00166 0.00000 -0.00324 -0.00329 2.73140

D5 0.03621 -0.00049 0.00000 0.07972 0.07937 0.11558

D6 -1.71756 -0.00020 0.00000 0.08517 0.08493 -1.63263

D7 0.01926 0.00003 0.00000 -0.01913 -0.01893 0.00033

D8 -2.89623 -0.00233 0.00000 -0.02768 -0.02736 -2.92359

D9 2.92357 0.00240 0.00000 0.00358 0.00315 2.92672

D10 0.00807 0.00004 0.00000 -0.00496 -0.00528 0.00279

D11 2.75952 0.00082 0.00000 0.06666 0.06703 2.82655

D12 -1.51157 0.00089 0.00000 0.06792 0.06831 -1.44326

D13 0.59117 0.00119 0.00000 0.06373 0.06417 0.65534

D14 -0.80102 -0.00083 0.00000 -0.02302 -0.02314 -0.82416

D15 1.21107 -0.00076 0.00000 -0.02175 -0.02186 1.18921

D16 -2.96937 -0.00046 0.00000 -0.02595 -0.02600 -2.99537

D17 0.98695 0.00090 0.00000 0.04275 0.04307 1.03003

D18 2.99905 0.00097 0.00000 0.04402 0.04435 3.04340

D19 -1.18140 0.00127 0.00000 0.03982 0.04022 -1.14118

D20 -1.03694 -0.00269 0.00000 -0.04888 -0.04743 -1.08437

D21 -2.97273 -0.00122 0.00000 -0.04067 -0.03915 -3.01188

D22 1.19680 -0.00142 0.00000 -0.02945 -0.02962 1.16718

D23 1.05184 -0.00110 0.00000 -0.01581 -0.01551 1.03633

D24 -0.88395 0.00037 0.00000 -0.00759 -0.00723 -0.89118

D25 -2.99761 0.00017 0.00000 0.00363 0.00230 -2.99531

D26 3.10981 -0.00051 0.00000 0.00232 0.00386 3.11366

D27 1.17402 0.00095 0.00000 0.01053 0.01214 1.18615

D28 -0.93964 0.00075 0.00000 0.02175 0.02167 -0.91797

D29 0.61620 0.00045 0.00000 -0.01767 -0.01803 0.59817

D30 -2.74635 0.00223 0.00000 -0.02904 -0.02992 -2.77627

D31 -2.88212 -0.00084 0.00000 0.08546 0.08534 -2.79677

D32 0.03852 0.00094 0.00000 0.07409 0.07345 0.11197

D33 -1.15261 -0.00274 0.00000 -0.00337 -0.00133 -1.15394

D34 1.76803 -0.00096 0.00000 -0.01474 -0.01322 1.75481

D35 -0.60607 0.00023 0.00000 0.07791 0.07847 -0.52761

D36 -2.77159 -0.00015 0.00000 0.08148 0.08223 -2.68936

D37 1.49687 -0.00017 0.00000 0.08178 0.08230 1.57917

D38 2.87435 0.00154 0.00000 -0.01696 -0.01726 2.85709

D39 0.70884 0.00116 0.00000 -0.01339 -0.01350 0.69534

D40 -1.30589 0.00114 0.00000 -0.01309 -0.01343 -1.31932

D41 1.11113 0.00021 0.00000 0.02280 0.02289 1.13401

D42 -1.05439 -0.00017 0.00000 0.02637 0.02665 -1.02774

D43 -3.06911 -0.00019 0.00000 0.02667 0.02672 -3.04239

D44 0.99857 0.00170 0.00000 0.03690 0.03653 1.03510

D45 2.94502 0.00103 0.00000 0.05951 0.05867 3.00369

D46 -1.23093 0.00118 0.00000 0.05399 0.05236 -1.17858

D47 -1.08285 0.00017 0.00000 -0.00212 -0.00179 -1.08465

D48 0.86360 -0.00049 0.00000 0.02049 0.02035 0.88394

D49 2.97083 -0.00034 0.00000 0.01497 0.01403 2.98486

D50 3.13643 0.00029 0.00000 0.00708 0.00837 -3.13838

D51 -1.20031 -0.00037 0.00000 0.02969 0.03051 -1.16979

D52 0.90692 -0.00022 0.00000 0.02417 0.02420 0.93112

D53 0.01125 -0.00011 0.00000 -0.09526 -0.09426 -0.08301

D54 2.17815 0.00018 0.00000 -0.10081 -0.10039 2.07776

D55 -2.07539 0.00005 0.00000 -0.09724 -0.09659 -2.17197

D56 -2.16324 -0.00055 0.00000 -0.10831 -0.10771 -2.27095

D57 0.00366 -0.00026 0.00000 -0.11386 -0.11385 -0.11018

D58 2.03331 -0.00040 0.00000 -0.11030 -0.11004 1.92327

D59 2.09897 0.00010 0.00000 -0.10931 -0.10881 1.99016

D60 -2.01731 0.00039 0.00000 -0.11486 -0.11494 -2.13225

D61 0.01234 0.00025 0.00000 -0.11130 -0.11114 -0.09880

D62 -0.05642 0.00068 0.00000 0.01461 0.01475 -0.04167

D63 3.07753 -0.00010 0.00000 -0.00135 -0.00130 3.07624

D64 0.04875 -0.00004 0.00000 -0.00783 -0.00800 0.04075

D65 -3.09076 -0.00044 0.00000 -0.00582 -0.00632 -3.09707

D66 0.02652 -0.00091 0.00000 -0.00193 -0.00124 0.02529

D67 1.84732 0.00173 0.00000 0.03472 0.03536 1.88268

D68 -1.82856 -0.00014 0.00000 -0.05382 -0.05330 -1.88186

D69 -1.83299 -0.00157 0.00000 -0.02598 -0.02596 -1.85895

D70 -0.01220 0.00107 0.00000 0.01067 0.01064 -0.00156

D71 2.59511 -0.00080 0.00000 -0.07787 -0.07802 2.51709

D72 1.78567 -0.00097 0.00000 -0.13579 -0.13646 1.64921

D73 -2.67672 0.00168 0.00000 -0.09915 -0.09986 -2.77658

D74 -0.06942 -0.00019 0.00000 -0.18768 -0.18852 -0.25794

D75 -1.90196 -0.00143 0.00000 -0.02094 -0.02106 -1.92302

D76 1.24934 -0.00044 0.00000 -0.00059 -0.00043 1.24891

D77 0.04269 -0.00118 0.00000 -0.01602 -0.01615 0.02654

D78 -3.08920 -0.00019 0.00000 0.00433 0.00449 -3.08472

D79 2.74088 -0.00158 0.00000 0.08865 0.08808 2.82896

D80 -0.39101 -0.00059 0.00000 0.10900 0.10871 -0.28230

D81 1.93405 -0.00150 0.00000 -0.01064 -0.01111 1.92293

D82 -1.21018 -0.00100 0.00000 -0.01315 -0.01317 -1.22335

D83 -0.02217 -0.00061 0.00000 -0.00218 -0.00198 -0.02415

D84 3.11678 -0.00011 0.00000 -0.00469 -0.00403 3.11275

D85 -2.65763 0.00041 0.00000 0.07148 0.06999 -2.58763

D86 0.48133 0.00090 0.00000 0.06897 0.06794 0.54927

Item Value Threshold Converged?

Maximum Force 0.011504 0.000450 NO

RMS Force 0.001989 0.000300 NO

Maximum Displacement 0.326068 0.001800 NO

RMS Displacement 0.063015 0.001200 NO

Predicted change in Energy=-2.778951D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.108721 1.581037 0.466166

2 6 0 0.231217 1.347330 0.129333

3 6 0 -0.793707 3.771324 -0.461906

4 6 0 -1.637058 2.849967 0.154297

5 1 0 -1.675215 0.908806 1.128389

6 1 0 -2.607745 3.113780 0.598392

7 6 0 0.781368 1.941392 -1.132857

8 1 0 1.903550 1.961260 -1.124041

9 1 0 0.489427 1.248177 -1.971492

10 6 0 0.244861 3.333285 -1.423179

11 1 0 1.088079 4.077446 -1.446948

12 1 0 -0.218651 3.345785 -2.450333

13 1 0 -1.022065 4.846894 -0.439933

14 1 0 0.701908 0.401596 0.452304

15 8 0 2.775551 3.835441 0.890173

16 6 0 0.486374 3.854732 1.435664

17 6 0 0.948982 2.538921 1.668642

18 6 0 1.629253 4.664985 0.972353

19 8 0 1.801451 5.838877 0.684998

20 6 0 2.414625 2.550871 1.334871

21 8 0 3.303470 1.715333 1.375198

22 1 0 -0.407642 4.323246 1.843469

23 1 0 0.594286 1.882522 2.470901

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.401252 0.000000

3 C 2.399564 2.697366 0.000000

4 C 1.409463 2.397706 1.392783 0.000000

5 H 1.100613 2.196565 3.391181 2.172192 0.000000

6 H 2.147989 3.376399 2.201665 1.099568 2.452024

7 C 2.501833 1.499567 2.505931 2.886358 3.494892

8 H 3.427405 2.178200 3.315109 3.867797 4.357597

9 H 2.933777 2.118955 3.208045 3.406853 3.796065

10 C 2.910701 2.520813 1.481401 2.502728 4.009400

11 H 3.836404 3.266866 2.145958 3.390732 4.930358

12 H 3.523141 3.294068 2.113200 3.006960 4.568117

13 H 3.390331 3.760549 1.099763 2.172335 4.288913

14 H 2.160937 1.104659 3.798383 3.399131 2.522908

15 O 4.511063 3.639123 3.817308 4.580807 5.332097

16 C 2.941758 2.838780 2.290489 2.675896 3.666792

17 C 2.568585 2.074740 3.015795 3.012904 3.136169

18 C 4.154932 3.697570 2.954059 3.825218 5.005271

19 O 5.161994 4.790448 3.510699 4.586782 6.048917

20 C 3.756220 2.769314 3.874443 4.230762 4.412006

21 O 4.506862 3.335618 4.938514 5.214098 5.049624

22 H 3.147727 3.493205 2.401753 2.556427 3.711669

23 H 2.647657 2.429236 3.754392 3.358795 2.810889

6 7 8 9 10

6 H 0.000000

7 C 3.982186 0.000000

8 H 4.964560 1.122392 0.000000

9 H 4.435905 1.126536 1.796219 0.000000

10 C 3.503183 1.519702 2.173289 2.169823 0.000000

11 H 4.332572 2.180700 2.290744 2.939097 1.124881

12 H 3.880247 2.169816 2.860017 2.265087 1.126963

13 H 2.568303 3.489191 4.165826 4.192975 2.205195

14 H 4.281482 2.211339 2.522174 2.576166 3.510147

15 O 5.439284 3.414211 2.886174 4.484353 3.465278

16 C 3.289925 3.216394 3.485070 4.289854 2.916028

17 C 3.758484 2.869413 3.007319 3.889445 3.268968

18 C 4.527497 3.545247 3.432234 4.651881 3.070592

19 O 5.184078 4.419904 4.280065 5.463778 3.625655

20 C 5.107197 3.021369 2.579745 4.041711 3.595398

21 O 6.123851 3.564048 2.875144 4.397431 4.450143

22 H 2.802406 3.993181 4.441475 4.981436 3.475165

23 H 3.908361 3.609091 3.826745 4.488679 4.170212

11 12 13 14 15

11 H 0.000000

12 H 1.802679 0.000000

13 H 2.461470 2.634485 0.000000

14 H 4.155498 4.235679 4.850654 0.000000

15 O 2.892795 4.512648 4.148989 4.035222 0.000000

16 C 2.953151 3.982092 2.603390 3.596887 2.353352

17 C 3.477543 4.356644 3.695653 2.471575 2.371357

18 C 2.547762 4.107288 3.009506 4.393962 1.417355

19 O 2.856000 4.486270 3.197146 5.552221 2.237124

20 C 3.439284 4.679081 4.498054 2.886469 1.406466

21 O 4.295585 5.449624 5.640180 3.057084 2.238037

22 H 3.622767 4.407707 2.421910 4.306481 3.358488

23 H 4.517861 5.198129 4.457919 2.505885 3.327238

16 17 18 19 20

16 C 0.000000

17 C 1.414087 0.000000

18 C 1.475581 2.338318 0.000000

19 O 2.495948 3.547388 1.220757 0.000000

20 C 2.329885 1.503215 2.284230 3.407242 0.000000

21 O 3.537897 2.511578 3.415514 4.442528 1.220572

22 H 1.088611 2.248290 2.241555 2.918781 3.371227

23 H 2.230016 1.095577 3.325492 4.505490 2.247418

21 22 23

21 O 0.000000

22 H 4.559917 0.000000

23 H 2.927148 2.711948 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.212783 -0.791013 -0.746602

2 6 0 1.252381 -1.363134 0.098273

3 6 0 1.514700 1.320875 0.153686

4 6 0 2.343842 0.611922 -0.712198

5 1 0 2.699195 -1.358534 -1.554484

6 1 0 2.935194 1.081725 -1.511346

7 6 0 1.022183 -0.764150 1.453606

8 1 0 0.039043 -1.089518 1.886428

9 1 0 1.815626 -1.185569 2.133265

10 6 0 1.110078 0.752992 1.460720

11 1 0 0.130027 1.197322 1.788480

12 1 0 1.875790 1.077000 2.221476

13 1 0 1.332865 2.395426 0.006189

14 1 0 1.055555 -2.447276 0.019732

15 8 0 -2.087126 0.066684 0.313977

16 6 0 -0.304203 0.692803 -1.088672

17 6 0 -0.333778 -0.720907 -1.074838

18 6 0 -1.409449 1.180728 -0.241502

19 8 0 -1.861782 2.276645 0.049374

20 6 0 -1.489244 -1.101568 -0.191859

21 8 0 -1.985497 -2.163020 0.149971

22 1 0 0.162873 1.337175 -1.831437

23 1 0 -0.086689 -1.361518 -1.928566

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2105955 0.8593849 0.6663708

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 468.6885819831 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.465541976923E-01 A.U. after 15 cycles

Convg = 0.8695D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000665254 0.011738077 -0.005926033

2 6 -0.004132685 -0.008019120 -0.002868712

3 6 -0.005709502 -0.002199398 0.009835332

4 6 0.008498239 -0.007722258 0.003928754

5 1 0.001960856 -0.001193584 -0.002562111

6 1 0.000232220 0.004697622 -0.003371811

7 6 -0.001966320 -0.002325244 0.004954094

8 1 0.000074777 -0.000324825 0.003416283

9 1 -0.000183319 0.000149425 0.000195609

10 6 0.001164294 0.000415369 -0.000631484

11 1 -0.000037432 -0.000138449 0.000782834

12 1 0.000280306 0.000159815 0.000066234

13 1 -0.002739441 0.000826665 -0.003001276

14 1 0.001942302 0.000977681 -0.000207997

15 8 -0.001768083 -0.000388233 0.001149429

16 6 -0.002800602 -0.005471821 -0.002436285

17 6 0.006969509 0.011100003 -0.000667995

18 6 0.003352392 -0.002693090 -0.000868926

19 8 -0.000063987 -0.000815700 -0.001316622

20 6 -0.004014877 0.000975249 -0.001255350

21 8 -0.001075161 0.001211017 -0.000419995

22 1 0.000775625 0.000471420 0.004004224

23 1 -0.001424368 -0.001430624 -0.002798197

-------------------------------------------------------------------

Cartesian Forces: Max 0.011738077 RMS 0.003715370

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.008838623 RMS 0.001871458

Search for a saddle point.

Step number 28 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 27 28

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06432 -0.00166 0.00336 0.00605 0.00745

Eigenvalues --- 0.00990 0.01101 0.01510 0.02082 0.02223

Eigenvalues --- 0.02302 0.02417 0.02588 0.02924 0.03004

Eigenvalues --- 0.03170 0.03284 0.03447 0.03644 0.03757

Eigenvalues --- 0.03870 0.03888 0.04163 0.04355 0.05144

Eigenvalues --- 0.05200 0.05691 0.06037 0.06351 0.06998

Eigenvalues --- 0.07349 0.08444 0.08764 0.09418 0.09833

Eigenvalues --- 0.11847 0.13740 0.14452 0.15880 0.20867

Eigenvalues --- 0.22705 0.25842 0.26922 0.27694 0.28604

Eigenvalues --- 0.30413 0.31258 0.31416 0.31714 0.31960

Eigenvalues --- 0.32102 0.32438 0.32974 0.34641 0.36416

Eigenvalues --- 0.37559 0.39587 0.40415 0.43678 0.47039

Eigenvalues --- 0.51205 1.08448 1.10839

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D73

1 0.54452 0.48885 -0.18339 0.17895 -0.14337

D71 D86 D85 A40 D79

1 0.14148 -0.14114 -0.13646 -0.13599 0.12548

RFO step: Lambda0=6.289909252D-06 Lambda=-5.27419201D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.10687285 RMS(Int)= 0.00446469

Iteration 2 RMS(Cart)= 0.00607699 RMS(Int)= 0.00120683

Iteration 3 RMS(Cart)= 0.00001112 RMS(Int)= 0.00120680

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00120680

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64798 -0.00319 0.00000 -0.00266 -0.00218 2.64580

R2 2.66350 -0.00503 0.00000 -0.01622 -0.01477 2.64873

R3 2.07986 -0.00182 0.00000 -0.00208 -0.00208 2.07778

R4 2.83377 -0.00884 0.00000 -0.00423 -0.00471 2.82906

R5 2.08750 -0.00007 0.00000 -0.00068 -0.00068 2.08682

R6 3.92069 0.00012 0.00000 -0.04918 -0.04979 3.87091

R7 2.63198 -0.00728 0.00000 -0.01673 -0.01579 2.61619

R8 2.79944 0.00067 0.00000 0.01857 0.01809 2.81753

R9 2.07825 0.00132 0.00000 0.00524 0.00524 2.08349

R10 4.32840 -0.00232 0.00000 -0.04895 -0.04840 4.28000

R11 2.07788 -0.00044 0.00000 0.00563 0.00563 2.08351

R12 2.12101 0.00010 0.00000 -0.00261 -0.00261 2.11840

R13 2.12885 -0.00019 0.00000 0.00218 0.00218 2.13102

R14 2.87182 0.00016 0.00000 -0.00546 -0.00694 2.86488

R15 2.12572 -0.00014 0.00000 -0.00443 -0.00443 2.12129

R16 2.12965 -0.00017 0.00000 -0.00366 -0.00366 2.12599

R17 2.67841 -0.00269 0.00000 -0.00386 -0.00343 2.67498

R18 2.65783 -0.00221 0.00000 -0.00443 -0.00419 2.65365

R19 2.67224 -0.00678 0.00000 -0.00472 -0.00539 2.66685

R20 2.78844 0.00065 0.00000 0.00802 0.00805 2.79649

R21 2.05718 0.00107 0.00000 0.00098 0.00098 2.05816

R22 2.84066 -0.00455 0.00000 -0.00473 -0.00499 2.83567

R23 2.07034 -0.00073 0.00000 -0.00051 -0.00051 2.06983

R24 2.30690 -0.00048 0.00000 0.00028 0.00028 2.30718

R25 2.30655 -0.00163 0.00000 0.00021 0.00021 2.30675

A1 2.04363 0.00223 0.00000 0.02953 0.02812 2.07175

A2 2.13524 -0.00318 0.00000 -0.03671 -0.03583 2.09941

A3 2.08297 0.00094 0.00000 0.01052 0.01088 2.09385

A4 2.07953 -0.00093 0.00000 -0.04633 -0.04530 2.03423

A5 2.07141 0.00242 0.00000 0.04839 0.04649 2.11790

A6 1.62751 0.00150 0.00000 0.05901 0.05454 1.68205

A7 2.01410 -0.00086 0.00000 -0.01628 -0.01582 1.99828

A8 1.84423 -0.00370 0.00000 -0.06984 -0.06912 1.77511

A9 1.69852 0.00120 0.00000 0.04428 0.04363 1.74215

A10 2.11296 -0.00119 0.00000 -0.01736 -0.01707 2.09589

A11 2.10877 0.00101 0.00000 0.01514 0.01442 2.12320

A12 1.56676 0.00263 0.00000 0.03371 0.03248 1.59923

A13 2.03502 0.00004 0.00000 -0.00689 -0.00719 2.02783

A14 1.72798 -0.00356 0.00000 -0.03510 -0.03554 1.69244

A15 1.63472 0.00153 0.00000 0.03905 0.03976 1.67447

A16 2.05610 0.00081 0.00000 0.00323 0.00197 2.05807

A17 2.04603 0.00538 0.00000 0.10928 0.11003 2.15607

A18 2.15858 -0.00601 0.00000 -0.10249 -0.10301 2.05557

A19 1.94680 -0.00239 0.00000 -0.00619 -0.00586 1.94094

A20 1.86267 -0.00005 0.00000 -0.01816 -0.01735 1.84532

A21 1.97590 0.00095 0.00000 0.00517 0.00298 1.97888

A22 1.85026 0.00086 0.00000 0.01875 0.01846 1.86872

A23 1.91586 0.00142 0.00000 0.01476 0.01511 1.93097

A24 1.90699 -0.00083 0.00000 -0.01479 -0.01391 1.89307

A25 1.97617 -0.00079 0.00000 0.01058 0.00917 1.98534

A26 1.92157 -0.00063 0.00000 -0.00571 -0.00490 1.91667

A27 1.87528 0.00098 0.00000 0.01505 0.01494 1.89022

A28 1.92337 0.00121 0.00000 -0.01644 -0.01720 1.90616

A29 1.90655 -0.00075 0.00000 0.00529 0.00662 1.91317

A30 1.85637 0.00001 0.00000 -0.00904 -0.00920 1.84718

A31 1.88460 -0.00094 0.00000 0.00031 0.00020 1.88480

A32 1.86026 -0.00029 0.00000 -0.03339 -0.03702 1.82324

A33 1.76474 -0.00127 0.00000 -0.04607 -0.04598 1.71876

A34 1.43745 0.00163 0.00000 0.06062 0.06252 1.49997

A35 1.88525 -0.00040 0.00000 -0.01317 -0.01332 1.87192

A36 2.22359 -0.00093 0.00000 -0.01287 -0.01367 2.20992

A37 2.11458 0.00127 0.00000 0.03172 0.03262 2.14720

A38 1.87445 0.00158 0.00000 0.06029 0.05624 1.93068

A39 1.74887 -0.00221 0.00000 0.00083 0.00186 1.75074

A40 1.65809 -0.00076 0.00000 -0.05207 -0.05091 1.60718

A41 1.84937 0.00130 0.00000 0.01199 0.01219 1.86157

A42 2.18002 -0.00130 0.00000 -0.00329 -0.00252 2.17750

A43 2.07489 0.00083 0.00000 -0.01196 -0.01254 2.06235

A44 1.89994 -0.00052 0.00000 0.00566 0.00531 1.90525

A45 2.02092 -0.00015 0.00000 -0.00488 -0.00477 2.01615

A46 2.36199 0.00068 0.00000 -0.00035 -0.00024 2.36174

A47 1.90463 0.00055 0.00000 -0.00361 -0.00434 1.90029

A48 2.03621 -0.00058 0.00000 0.00157 0.00192 2.03813

A49 2.34234 0.00003 0.00000 0.00206 0.00242 2.34476

D1 -0.63234 0.00037 0.00000 -0.01193 -0.01254 -0.64488

D2 3.03503 -0.00068 0.00000 0.02195 0.02202 3.05705

D3 1.28682 -0.00329 0.00000 -0.06993 -0.07287 1.21395

D4 2.73140 0.00026 0.00000 -0.03086 -0.03101 2.70039

D5 0.11558 -0.00080 0.00000 0.00302 0.00355 0.11913

D6 -1.63263 -0.00341 0.00000 -0.08886 -0.09134 -1.72397

D7 0.00033 0.00023 0.00000 -0.02071 -0.02037 -0.02004

D8 -2.92359 0.00017 0.00000 -0.05509 -0.05817 -2.98176

D9 2.92672 -0.00021 0.00000 -0.00877 -0.00817 2.91855

D10 0.00279 -0.00027 0.00000 -0.04314 -0.04597 -0.04318

D11 2.82655 -0.00109 0.00000 0.08801 0.08725 2.91380

D12 -1.44326 -0.00134 0.00000 0.09667 0.09625 -1.34701

D13 0.65534 -0.00183 0.00000 0.06920 0.06939 0.72473

D14 -0.82416 0.00090 0.00000 0.07451 0.07418 -0.74998

D15 1.18921 0.00065 0.00000 0.08317 0.08319 1.27240

D16 -2.99537 0.00015 0.00000 0.05570 0.05632 -2.93905

D17 1.03003 -0.00017 0.00000 0.07985 0.08059 1.11062

D18 3.04340 -0.00042 0.00000 0.08851 0.08959 3.13299

D19 -1.14118 -0.00092 0.00000 0.06105 0.06273 -1.07845

D20 -1.08437 0.00355 0.00000 0.16653 0.16940 -0.91497

D21 -3.01188 0.00253 0.00000 0.13448 0.13655 -2.87533

D22 1.16718 0.00232 0.00000 0.16028 0.16159 1.32877

D23 1.03633 0.00222 0.00000 0.12197 0.12302 1.15935

D24 -0.89118 0.00120 0.00000 0.08992 0.09016 -0.80102

D25 -2.99531 0.00100 0.00000 0.11572 0.11520 -2.88010

D26 3.11366 0.00065 0.00000 0.10059 0.10072 -3.06880

D27 1.18615 -0.00038 0.00000 0.06854 0.06787 1.25402

D28 -0.91797 -0.00058 0.00000 0.09434 0.09291 -0.82507

D29 0.59817 -0.00154 0.00000 -0.00715 -0.00691 0.59126

D30 -2.77627 0.00013 0.00000 0.05924 0.05658 -2.71969

D31 -2.79677 -0.00224 0.00000 -0.05101 -0.05060 -2.84738

D32 0.11197 -0.00057 0.00000 0.01538 0.01289 0.12487

D33 -1.15394 0.00115 0.00000 0.01523 0.01697 -1.13697

D34 1.75481 0.00282 0.00000 0.08162 0.08046 1.83527

D35 -0.52761 0.00094 0.00000 0.07040 0.06917 -0.45844

D36 -2.68936 0.00040 0.00000 0.08857 0.08877 -2.60059

D37 1.57917 0.00018 0.00000 0.09392 0.09401 1.67317

D38 2.85709 0.00146 0.00000 0.10933 0.10742 2.96451

D39 0.69534 0.00092 0.00000 0.12749 0.12702 0.82235

D40 -1.31932 0.00070 0.00000 0.13285 0.13225 -1.18707

D41 1.13401 0.00160 0.00000 0.08496 0.08247 1.21648

D42 -1.02774 0.00106 0.00000 0.10313 0.10206 -0.92567

D43 -3.04239 0.00084 0.00000 0.10848 0.10730 -2.93510

D44 1.03510 -0.00149 0.00000 0.09010 0.08708 1.12218

D45 3.00369 -0.00253 0.00000 0.04568 0.04487 3.04856

D46 -1.17858 -0.00094 0.00000 0.08893 0.08738 -1.09120

D47 -1.08465 -0.00043 0.00000 0.10481 0.10235 -0.98229

D48 0.88394 -0.00147 0.00000 0.06039 0.06014 0.94409

D49 2.98486 0.00012 0.00000 0.10364 0.10265 3.08751

D50 -3.13838 -0.00023 0.00000 0.10902 0.10765 -3.03074

D51 -1.16979 -0.00128 0.00000 0.06460 0.06544 -1.10436

D52 0.93112 0.00031 0.00000 0.10785 0.10795 1.03907

D53 -0.08301 0.00017 0.00000 -0.10110 -0.10147 -0.18448

D54 2.07776 -0.00031 0.00000 -0.11339 -0.11433 1.96343

D55 -2.17197 -0.00005 0.00000 -0.13066 -0.13138 -2.30336

D56 -2.27095 0.00150 0.00000 -0.10832 -0.10792 -2.37888

D57 -0.11018 0.00102 0.00000 -0.12062 -0.12078 -0.23096

D58 1.92327 0.00129 0.00000 -0.13788 -0.13784 1.78543

D59 1.99016 0.00014 0.00000 -0.13076 -0.13064 1.85953

D60 -2.13225 -0.00034 0.00000 -0.14306 -0.14350 -2.27575

D61 -0.09880 -0.00007 0.00000 -0.16032 -0.16055 -0.25935

D62 -0.04167 0.00022 0.00000 0.01450 0.01505 -0.02663

D63 3.07624 0.00064 0.00000 0.02940 0.03001 3.10625

D64 0.04075 -0.00001 0.00000 -0.03765 -0.03815 0.00261

D65 -3.09707 -0.00012 0.00000 -0.04346 -0.04432 -3.14139

D66 0.02529 -0.00012 0.00000 -0.13820 -0.13916 -0.11388

D67 1.88268 -0.00144 0.00000 -0.10880 -0.10825 1.77443

D68 -1.88186 0.00031 0.00000 -0.11726 -0.11637 -1.99824

D69 -1.85895 0.00161 0.00000 -0.06591 -0.06761 -1.92656

D70 -0.00156 0.00029 0.00000 -0.03651 -0.03670 -0.03826

D71 2.51709 0.00204 0.00000 -0.04497 -0.04482 2.47226

D72 1.64921 0.00146 0.00000 -0.08963 -0.09148 1.55774

D73 -2.77658 0.00014 0.00000 -0.06023 -0.06057 -2.83714

D74 -0.25794 0.00189 0.00000 -0.06868 -0.06869 -0.32662

D75 -1.92302 0.00070 0.00000 0.07634 0.07771 -1.84531

D76 1.24891 0.00019 0.00000 0.05732 0.05857 1.30748

D77 0.02654 -0.00030 0.00000 0.01522 0.01490 0.04144

D78 -3.08472 -0.00081 0.00000 -0.00381 -0.00425 -3.08897

D79 2.82896 -0.00069 0.00000 0.02678 0.02657 2.85552

D80 -0.28230 -0.00120 0.00000 0.00775 0.00742 -0.27488

D81 1.92293 0.00108 0.00000 0.11603 0.11343 2.03636

D82 -1.22335 0.00121 0.00000 0.12327 0.12112 -1.10223

D83 -0.02415 -0.00019 0.00000 0.04666 0.04736 0.02321

D84 3.11275 -0.00006 0.00000 0.05390 0.05506 -3.11538

D85 -2.58763 -0.00089 0.00000 0.05154 0.05139 -2.53625

D86 0.54927 -0.00076 0.00000 0.05878 0.05908 0.60835

Item Value Threshold Converged?

Maximum Force 0.008839 0.000450 NO

RMS Force 0.001871 0.000300 NO

Maximum Displacement 0.611720 0.001800 NO

RMS Displacement 0.106824 0.001200 NO

Predicted change in Energy=-3.494276D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.144114 1.589437 0.463068

2 6 0 0.200381 1.302248 0.198259

3 6 0 -0.762444 3.769835 -0.430578

4 6 0 -1.640699 2.856344 0.126955

5 1 0 -1.741747 0.914536 1.092569

6 1 0 -2.637122 3.219582 0.428302

7 6 0 0.771443 1.874805 -1.061620

8 1 0 1.889630 1.796043 -1.072447

9 1 0 0.385541 1.222173 -1.896385

10 6 0 0.333748 3.301927 -1.326363

11 1 0 1.220257 3.983933 -1.231179

12 1 0 -0.014972 3.398590 -2.391600

13 1 0 -0.994135 4.847137 -0.467023

14 1 0 0.657490 0.348553 0.516055

15 8 0 2.715739 3.936808 0.792280

16 6 0 0.458272 3.856955 1.475186

17 6 0 0.984186 2.555046 1.616733

18 6 0 1.556029 4.723609 0.991692

19 8 0 1.679400 5.913507 0.747704

20 6 0 2.412636 2.616225 1.161203

21 8 0 3.309123 1.795046 1.051490

22 1 0 -0.444004 4.247626 1.943676

23 1 0 0.728962 1.863040 2.426478

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.400097 0.000000

3 C 2.387134 2.722399 0.000000

4 C 1.401650 2.410369 1.384428 0.000000

5 H 1.099513 2.173010 3.381086 2.171000 0.000000

6 H 2.210803 3.432275 2.134214 1.102546 2.560504

7 C 2.464847 1.497073 2.518365 2.862615 3.446560

8 H 3.406478 2.170734 3.367692 3.876342 4.318709

9 H 2.835798 2.104336 3.155479 3.296979 3.681554

10 C 2.884226 2.518129 1.490975 2.491810 3.982279

11 H 3.767537 3.205445 2.148931 3.361705 4.857414

12 H 3.563303 3.338922 2.131231 3.046332 4.614294

13 H 3.391191 3.799436 1.102538 2.175802 4.296115

14 H 2.188237 1.104299 3.823284 3.423754 2.531609

15 O 4.529570 3.690636 3.690667 4.537468 5.393838

16 C 2.955277 2.867678 2.264878 2.687867 3.693820

17 C 2.606340 2.048395 2.952611 3.033190 3.224397

18 C 4.170522 3.764709 2.882335 3.801779 5.039300

19 O 5.172121 4.873715 3.456340 4.555726 6.067363

20 C 3.767248 2.747338 3.734396 4.190090 4.489917

21 O 4.496648 3.261155 4.761720 5.146053 5.127210

22 H 3.122230 3.483815 2.442697 2.582290 3.676684

23 H 2.727317 2.357721 3.744721 3.448153 2.963677

6 7 8 9 10

6 H 0.000000

7 C 3.955579 0.000000

8 H 4.976966 1.121009 0.000000

9 H 4.304684 1.127689 1.808448 0.000000

10 C 3.451332 1.516029 2.180121 2.157078 0.000000

11 H 4.268194 2.163008 2.293495 2.960839 1.122538

12 H 3.854810 2.170073 2.817061 2.267695 1.125024

13 H 2.479909 3.507930 4.241676 4.133637 2.211202

14 H 4.370923 2.198065 2.477243 2.580123 3.495959

15 O 5.412948 3.386604 2.956779 4.475264 3.250478

16 C 3.329215 3.234560 3.575832 4.279586 2.858713

17 C 3.868830 2.771563 2.937278 3.804855 3.105272

18 C 4.490214 3.598243 3.597583 4.687333 2.981364

19 O 5.098197 4.517649 4.506735 5.538402 3.596232

20 C 5.138213 2.860796 2.436273 3.924454 3.313600

21 O 6.146177 3.303243 2.554617 4.191119 4.096063

22 H 2.857096 4.017386 4.533553 4.958587 3.491762

23 H 4.142878 3.488377 3.687020 4.383582 4.038615

11 12 13 14 15

11 H 0.000000

12 H 1.793040 0.000000

13 H 2.496516 2.600201 0.000000

14 H 4.072533 4.267246 4.891991 0.000000

15 O 2.516560 4.228895 4.022153 4.145873 0.000000

16 C 2.814455 3.922511 2.619566 3.642596 2.359851

17 C 3.195004 4.216232 3.675524 2.487335 2.363739

18 C 2.366648 3.958584 2.940485 4.491628 1.415538

19 O 2.801794 4.364738 3.124180 5.662745 2.232336

20 C 3.002646 4.373532 4.385679 2.939233 1.404249

21 O 3.790140 5.047358 5.489916 3.067604 2.237507

22 H 3.594302 4.438417 2.544314 4.295830 3.377321

23 H 4.256527 5.111285 4.499584 2.438954 3.304301

16 17 18 19 20

16 C 0.000000

17 C 1.411236 0.000000

18 C 1.479840 2.328164 0.000000

19 O 2.499959 3.538050 1.220905 0.000000

20 C 2.336137 1.500573 2.281135 3.403041 0.000000

21 O 3.543775 2.510464 3.413707 4.439595 1.220681

22 H 1.089132 2.238626 2.265605 2.952009 3.381438

23 H 2.225742 1.095308 3.305376 4.486413 2.236731

21 22 23

21 O 0.000000

22 H 4.571335 0.000000

23 H 2.924457 2.700962 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.330375 -0.460873 -0.744234

2 6 0 1.405963 -1.284354 -0.090313

3 6 0 1.306283 1.401576 0.342470

4 6 0 2.285101 0.920351 -0.510159

5 1 0 2.944609 -0.859069 -1.564652

6 1 0 2.871332 1.655271 -1.086210

7 6 0 1.050319 -0.907599 1.314251

8 1 0 0.146789 -1.468831 1.668248

9 1 0 1.918879 -1.243635 1.950150

10 6 0 0.862390 0.584238 1.507770

11 1 0 -0.217416 0.794692 1.730974

12 1 0 1.435021 0.922488 2.415161

13 1 0 1.031869 2.469196 0.364257

14 1 0 1.350299 -2.366733 -0.302049

15 8 0 -2.067810 -0.092363 0.274180

16 6 0 -0.336965 0.766188 -1.080797

17 6 0 -0.241970 -0.641213 -1.123081

18 6 0 -1.502175 1.102171 -0.232664

19 8 0 -2.063181 2.133375 0.102745

20 6 0 -1.334865 -1.172796 -0.242900

21 8 0 -1.690545 -2.290547 0.095016

22 1 0 0.107195 1.468743 -1.784605

23 1 0 0.036972 -1.221977 -2.008859

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2261481 0.8866599 0.6773000

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.2669462028 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.470891359395E-01 A.U. after 16 cycles

Convg = 0.5813D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.009367790 0.005462540 0.004838848

2 6 0.002477354 0.004376724 -0.005660645

3 6 0.014514757 0.004439245 -0.002051936

4 6 -0.001355034 -0.006051049 0.005399157

5 1 -0.001161852 -0.000795457 -0.001426503

6 1 0.000410025 -0.006532339 0.002340353

7 6 -0.003875138 -0.005480833 -0.002110648

8 1 0.000411626 0.000193208 0.000445739

9 1 0.002205990 -0.000225876 -0.001050591

10 6 0.000433942 0.005205775 0.000763980

11 1 0.001102151 0.002095590 -0.001042624

12 1 -0.001319043 -0.000520350 0.000091362

13 1 -0.001374852 -0.001228510 -0.001549645

14 1 -0.001343161 0.001314082 0.002323475

15 8 -0.000189449 0.000327511 0.000221348

16 6 -0.003491343 -0.001178424 -0.010261533

17 6 0.004090592 -0.006197479 0.001290487

18 6 -0.000192610 0.001043678 0.000981088

19 8 -0.000530603 -0.000377836 -0.000482795

20 6 -0.002263730 0.001651011 0.002660324

21 8 0.000027330 0.001049131 0.000524097

22 1 0.002468523 0.002094743 0.003267228

23 1 -0.001677687 -0.000665085 0.000489435

-------------------------------------------------------------------

Cartesian Forces: Max 0.014514757 RMS 0.003570631

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011086637 RMS 0.001797550

Search for a saddle point.

Step number 29 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 28 29

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06463 -0.00073 0.00325 0.00602 0.00664

Eigenvalues --- 0.00995 0.01127 0.01495 0.02093 0.02228

Eigenvalues --- 0.02300 0.02468 0.02615 0.02930 0.03043

Eigenvalues --- 0.03164 0.03364 0.03473 0.03649 0.03781

Eigenvalues --- 0.03877 0.03905 0.04283 0.04380 0.05110

Eigenvalues --- 0.05287 0.05716 0.06052 0.06381 0.07338

Eigenvalues --- 0.07636 0.08417 0.08768 0.09481 0.09839

Eigenvalues --- 0.11916 0.13752 0.14558 0.15958 0.21079

Eigenvalues --- 0.22709 0.25836 0.26956 0.27730 0.28805

Eigenvalues --- 0.30447 0.31260 0.31422 0.31696 0.32000

Eigenvalues --- 0.32090 0.32433 0.32996 0.34637 0.36444

Eigenvalues --- 0.37547 0.39589 0.40413 0.43772 0.47015

Eigenvalues --- 0.51152 1.08443 1.10839

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D86

1 -0.54454 -0.49207 0.18573 -0.18215 0.14700

D71 D85 D73 A40 D79

1 -0.14678 0.14187 0.13401 0.12854 -0.12317

RFO step: Lambda0=4.337572826D-04 Lambda=-5.10977415D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.782

Iteration 1 RMS(Cart)= 0.08538388 RMS(Int)= 0.00281245

Iteration 2 RMS(Cart)= 0.00344481 RMS(Int)= 0.00105424

Iteration 3 RMS(Cart)= 0.00000482 RMS(Int)= 0.00105423

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00105423

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64580 0.00369 0.00000 0.02741 0.02736 2.67316

R2 2.64873 -0.00948 0.00000 -0.03503 -0.03517 2.61356

R3 2.07778 0.00030 0.00000 0.00366 0.00366 2.08144

R4 2.82906 0.00203 0.00000 -0.02067 -0.02012 2.80894

R5 2.08682 -0.00102 0.00000 -0.00373 -0.00373 2.08309

R6 3.87091 0.00004 0.00000 0.14684 0.14635 4.01726

R7 2.61619 0.01109 0.00000 0.03486 0.03473 2.65092

R8 2.81753 -0.00205 0.00000 -0.00563 -0.00580 2.81173

R9 2.08349 -0.00086 0.00000 -0.00281 -0.00281 2.08069

R10 4.28000 -0.00359 0.00000 -0.08409 -0.08401 4.19599

R11 2.08351 -0.00188 0.00000 -0.00402 -0.00402 2.07949

R12 2.11840 0.00039 0.00000 0.00377 0.00377 2.12217

R13 2.13102 0.00015 0.00000 -0.00099 -0.00099 2.13004

R14 2.86488 0.00341 0.00000 0.01815 0.01893 2.88381

R15 2.12129 0.00206 0.00000 0.00469 0.00469 2.12598

R16 2.12599 0.00028 0.00000 -0.00063 -0.00063 2.12535

R17 2.67498 -0.00107 0.00000 0.00044 0.00081 2.67578

R18 2.65365 0.00043 0.00000 0.01168 0.01177 2.66541

R19 2.66685 0.00226 0.00000 0.00150 0.00089 2.66774

R20 2.79649 -0.00118 0.00000 0.00250 0.00263 2.79913

R21 2.05816 0.00011 0.00000 0.00397 0.00397 2.06213

R22 2.83567 -0.00202 0.00000 -0.01628 -0.01659 2.81908

R23 2.06983 0.00117 0.00000 0.00004 0.00004 2.06987

R24 2.30718 -0.00033 0.00000 -0.00054 -0.00054 2.30664

R25 2.30675 -0.00073 0.00000 0.00055 0.00055 2.30731

A1 2.07175 -0.00153 0.00000 -0.02413 -0.02468 2.04707

A2 2.09941 0.00137 0.00000 0.04453 0.04425 2.14366

A3 2.09385 0.00034 0.00000 -0.01091 -0.01140 2.08246

A4 2.03423 0.00191 0.00000 0.03939 0.03887 2.07310

A5 2.11790 -0.00192 0.00000 -0.03226 -0.03446 2.08344

A6 1.68205 -0.00065 0.00000 -0.01810 -0.01816 1.66388

A7 1.99828 0.00013 0.00000 0.03487 0.03407 2.03235

A8 1.77511 0.00146 0.00000 -0.02743 -0.02819 1.74692

A9 1.74215 -0.00098 0.00000 -0.03373 -0.03243 1.70972

A10 2.09589 0.00089 0.00000 0.01272 0.01240 2.10828

A11 2.12320 -0.00027 0.00000 -0.02578 -0.02583 2.09737

A12 1.59923 -0.00246 0.00000 -0.02083 -0.02149 1.57774

A13 2.02783 -0.00075 0.00000 -0.00100 -0.00178 2.02604

A14 1.69244 0.00286 0.00000 0.02389 0.02291 1.71536

A15 1.67447 0.00021 0.00000 0.04685 0.04796 1.72243

A16 2.05807 0.00133 0.00000 0.01293 0.01244 2.07052

A17 2.15607 -0.00741 0.00000 -0.10262 -0.10261 2.05345

A18 2.05557 0.00620 0.00000 0.09029 0.09066 2.14623

A19 1.94094 0.00024 0.00000 -0.00595 -0.00552 1.93542

A20 1.84532 0.00051 0.00000 0.02637 0.02624 1.87155

A21 1.97888 -0.00030 0.00000 -0.01412 -0.01481 1.96408

A22 1.86872 -0.00059 0.00000 -0.00792 -0.00798 1.86073

A23 1.93097 -0.00054 0.00000 -0.00237 -0.00299 1.92798

A24 1.89307 0.00073 0.00000 0.00592 0.00684 1.89992

A25 1.98534 -0.00220 0.00000 -0.00599 -0.00690 1.97844

A26 1.91667 0.00004 0.00000 0.00212 0.00203 1.91870

A27 1.89022 0.00063 0.00000 -0.00280 -0.00218 1.88804

A28 1.90616 0.00206 0.00000 -0.00560 -0.00538 1.90078

A29 1.91317 -0.00006 0.00000 0.01216 0.01248 1.92565

A30 1.84718 -0.00037 0.00000 0.00071 0.00058 1.84776

A31 1.88480 0.00011 0.00000 -0.00007 -0.00028 1.88452

A32 1.82324 0.00040 0.00000 0.01320 0.00968 1.83291

A33 1.71876 0.00014 0.00000 -0.02623 -0.02350 1.69526

A34 1.49997 0.00056 0.00000 0.06953 0.07001 1.56998

A35 1.87192 0.00121 0.00000 0.00947 0.00846 1.88039

A36 2.20992 -0.00024 0.00000 -0.00127 -0.00233 2.20760

A37 2.14720 -0.00144 0.00000 -0.03203 -0.03229 2.11491

A38 1.93068 -0.00156 0.00000 -0.03617 -0.03899 1.89169

A39 1.75074 0.00296 0.00000 0.05481 0.05577 1.80651

A40 1.60718 -0.00010 0.00000 -0.08263 -0.08077 1.52641

A41 1.86157 -0.00180 0.00000 -0.00627 -0.00616 1.85541

A42 2.17750 0.00062 0.00000 0.02492 0.02153 2.19903

A43 2.06235 0.00063 0.00000 0.03031 0.03034 2.09269

A44 1.90525 -0.00066 0.00000 -0.01048 -0.01066 1.89459

A45 2.01615 0.00070 0.00000 0.01422 0.01432 2.03047

A46 2.36174 -0.00004 0.00000 -0.00372 -0.00364 2.35810

A47 1.90029 0.00116 0.00000 0.00483 0.00407 1.90437

A48 2.03813 -0.00126 0.00000 -0.01137 -0.01101 2.02712

A49 2.34476 0.00010 0.00000 0.00653 0.00690 2.35166

D1 -0.64488 -0.00030 0.00000 0.04968 0.04944 -0.59544

D2 3.05705 -0.00063 0.00000 -0.04334 -0.04231 3.01473

D3 1.21395 0.00153 0.00000 0.01856 0.01622 1.23017

D4 2.70039 -0.00127 0.00000 -0.00138 -0.00148 2.69891

D5 0.11913 -0.00161 0.00000 -0.09440 -0.09323 0.02589

D6 -1.72397 0.00055 0.00000 -0.03250 -0.03470 -1.75867

D7 -0.02004 0.00015 0.00000 -0.06518 -0.06466 -0.08469

D8 -2.98176 -0.00133 0.00000 -0.07904 -0.07727 -3.05903

D9 2.91855 0.00124 0.00000 -0.00765 -0.00883 2.90972

D10 -0.04318 -0.00023 0.00000 -0.02150 -0.02144 -0.06462

D11 2.91380 0.00042 0.00000 0.00071 -0.00035 2.91345

D12 -1.34701 0.00013 0.00000 0.00332 0.00232 -1.34469

D13 0.72473 0.00118 0.00000 0.01975 0.01927 0.74400

D14 -0.74998 0.00001 0.00000 0.06558 0.06673 -0.68324

D15 1.27240 -0.00028 0.00000 0.06819 0.06939 1.34179

D16 -2.93905 0.00078 0.00000 0.08462 0.08635 -2.85270

D17 1.11062 -0.00028 0.00000 0.02420 0.02509 1.13571

D18 3.13299 -0.00057 0.00000 0.02681 0.02775 -3.12244

D19 -1.07845 0.00049 0.00000 0.04325 0.04470 -1.03375

D20 -0.91497 -0.00214 0.00000 0.08723 0.08526 -0.82970

D21 -2.87533 -0.00099 0.00000 0.08060 0.08056 -2.79477

D22 1.32877 -0.00204 0.00000 0.06053 0.06232 1.39109

D23 1.15935 0.00002 0.00000 0.11654 0.11432 1.27367

D24 -0.80102 0.00117 0.00000 0.10990 0.10962 -0.69140

D25 -2.88010 0.00012 0.00000 0.08984 0.09137 -2.78873

D26 -3.06880 0.00029 0.00000 0.13438 0.13258 -2.93622

D27 1.25402 0.00144 0.00000 0.12774 0.12788 1.38190

D28 -0.82507 0.00039 0.00000 0.10768 0.10964 -0.71543

D29 0.59126 0.00020 0.00000 0.00134 0.00165 0.59291

D30 -2.71969 0.00019 0.00000 -0.00539 -0.00568 -2.72537

D31 -2.84738 -0.00045 0.00000 -0.05491 -0.05374 -2.90112

D32 0.12487 -0.00046 0.00000 -0.06165 -0.06108 0.06379

D33 -1.13697 -0.00177 0.00000 -0.01564 -0.01362 -1.15059

D34 1.83527 -0.00179 0.00000 -0.02237 -0.02096 1.81432

D35 -0.45844 0.00115 0.00000 0.06538 0.06561 -0.39282

D36 -2.60059 0.00000 0.00000 0.07534 0.07595 -2.52464

D37 1.67317 0.00006 0.00000 0.07492 0.07539 1.74857

D38 2.96451 0.00170 0.00000 0.12295 0.12296 3.08747

D39 0.82235 0.00055 0.00000 0.13291 0.13330 0.95566

D40 -1.18707 0.00061 0.00000 0.13249 0.13274 -1.05432

D41 1.21648 0.00014 0.00000 0.05756 0.05657 1.27305

D42 -0.92567 -0.00101 0.00000 0.06752 0.06691 -0.85876

D43 -2.93510 -0.00095 0.00000 0.06710 0.06635 -2.86875

D44 1.12218 -0.00023 0.00000 0.10949 0.11084 1.23303

D45 3.04856 0.00120 0.00000 0.11426 0.11440 -3.12022

D46 -1.09120 -0.00018 0.00000 0.09071 0.09049 -1.00071

D47 -0.98229 -0.00104 0.00000 0.09740 0.09955 -0.88275

D48 0.94409 0.00039 0.00000 0.10217 0.10310 1.04719

D49 3.08751 -0.00099 0.00000 0.07863 0.07919 -3.11648

D50 -3.03074 -0.00083 0.00000 0.08514 0.08595 -2.94478

D51 -1.10436 0.00060 0.00000 0.08991 0.08951 -1.01484

D52 1.03907 -0.00078 0.00000 0.06637 0.06560 1.10467

D53 -0.18448 -0.00003 0.00000 -0.05881 -0.05825 -0.24273

D54 1.96343 0.00003 0.00000 -0.06447 -0.06440 1.89903

D55 -2.30336 0.00071 0.00000 -0.06000 -0.05981 -2.36316

D56 -2.37888 0.00031 0.00000 -0.03801 -0.03740 -2.41628

D57 -0.23096 0.00037 0.00000 -0.04367 -0.04356 -0.27453

D58 1.78543 0.00105 0.00000 -0.03920 -0.03896 1.74647

D59 1.85953 0.00090 0.00000 -0.03059 -0.03009 1.82944

D60 -2.27575 0.00096 0.00000 -0.03626 -0.03624 -2.31199

D61 -0.25935 0.00164 0.00000 -0.03179 -0.03165 -0.29100

D62 -0.02663 0.00006 0.00000 -0.01437 -0.01350 -0.04013

D63 3.10625 -0.00039 0.00000 -0.01263 -0.01128 3.09497

D64 0.00261 0.00023 0.00000 -0.02322 -0.02402 -0.02141

D65 -3.14139 0.00003 0.00000 -0.02826 -0.02929 3.11250

D66 -0.11388 -0.00066 0.00000 -0.12541 -0.12377 -0.23765

D67 1.77443 0.00119 0.00000 -0.08107 -0.07980 1.69463

D68 -1.99824 0.00043 0.00000 0.00282 0.00510 -1.99314

D69 -1.92656 -0.00138 0.00000 -0.10482 -0.10448 -2.03105

D70 -0.03826 0.00047 0.00000 -0.06048 -0.06052 -0.09877

D71 2.47226 -0.00029 0.00000 0.02341 0.02438 2.49665

D72 1.55774 0.00029 0.00000 -0.02594 -0.02591 1.53183

D73 -2.83714 0.00213 0.00000 0.01840 0.01806 -2.81908

D74 -0.32662 0.00137 0.00000 0.10230 0.10296 -0.22366

D75 -1.84531 -0.00112 0.00000 0.04175 0.04431 -1.80100

D76 1.30748 -0.00055 0.00000 0.03939 0.04137 1.34885

D77 0.04144 -0.00033 0.00000 0.04858 0.04798 0.08941

D78 -3.08897 0.00024 0.00000 0.04622 0.04504 -3.04393

D79 2.85552 -0.00166 0.00000 -0.01978 -0.01894 2.83658

D80 -0.27488 -0.00108 0.00000 -0.02214 -0.02188 -0.29676

D81 2.03636 -0.00157 0.00000 0.03442 0.03183 2.06818

D82 -1.10223 -0.00132 0.00000 0.04074 0.03852 -1.06371

D83 0.02321 -0.00047 0.00000 0.05344 0.05365 0.07686

D84 -3.11538 -0.00022 0.00000 0.05976 0.06034 -3.05504

D85 -2.53625 0.00015 0.00000 -0.02284 -0.02238 -2.55862

D86 0.60835 0.00040 0.00000 -0.01651 -0.01568 0.59267

Item Value Threshold Converged?

Maximum Force 0.011087 0.000450 NO

RMS Force 0.001798 0.000300 NO

Maximum Displacement 0.319473 0.001800 NO

RMS Displacement 0.085644 0.001200 NO

Predicted change in Energy=-2.972541D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.193335 1.620564 0.495063

2 6 0 0.137040 1.262321 0.174452

3 6 0 -0.682207 3.767846 -0.436563

4 6 0 -1.614880 2.886047 0.129489

5 1 0 -1.841449 0.999732 1.133583

6 1 0 -2.620972 3.200393 0.445532

7 6 0 0.737908 1.789489 -1.078748

8 1 0 1.849041 1.626985 -1.089346

9 1 0 0.315707 1.185197 -1.931439

10 6 0 0.411864 3.262389 -1.309137

11 1 0 1.343750 3.871630 -1.147635

12 1 0 0.114107 3.433846 -2.380056

13 1 0 -0.918468 4.839357 -0.527987

14 1 0 0.547530 0.312239 0.553876

15 8 0 2.677762 4.063716 0.788860

16 6 0 0.440370 3.834073 1.478042

17 6 0 1.039261 2.561073 1.595170

18 6 0 1.487775 4.787375 1.044209

19 8 0 1.542043 5.995255 0.876891

20 6 0 2.436862 2.708013 1.094606

21 8 0 3.364131 1.938797 0.896476

22 1 0 -0.458589 4.178035 1.992195

23 1 0 0.808348 1.808637 2.356923

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.414577 0.000000

3 C 2.395829 2.705949 0.000000

4 C 1.383038 2.389086 1.402805 0.000000

5 H 1.101450 2.214341 3.386983 2.148889 0.000000

6 H 2.129897 3.381751 2.204293 1.100417 2.433923

7 C 2.497022 1.486425 2.518536 2.863196 3.488726

8 H 3.430225 2.158961 3.378850 3.881951 4.353685

9 H 2.890444 2.114863 3.146516 3.296587 3.752610

10 C 2.920170 2.505361 1.487905 2.513756 4.020437

11 H 3.768628 3.164262 2.149627 3.369853 4.857700

12 H 3.641937 3.352843 2.126696 3.096336 4.700508

13 H 3.388630 3.795090 1.101051 2.175473 4.284324

14 H 2.178483 1.102325 3.799269 3.388306 2.552632

15 O 4.587014 3.831524 3.588675 4.499828 5.470841

16 C 2.921449 2.899184 2.220423 2.634654 3.654975

17 C 2.660692 2.125842 2.923644 3.049311 3.308979

18 C 4.185524 3.873884 2.817969 3.752097 5.043607

19 O 5.173588 4.986795 3.410836 4.493545 6.038970

20 C 3.836708 2.868082 3.632673 4.168904 4.606918

21 O 4.586164 3.375360 4.636298 5.126022 5.294915

22 H 3.053182 3.487170 2.473283 2.544782 3.570873

23 H 2.740189 2.347829 3.723415 3.463281 3.028583

6 7 8 9 10

6 H 0.000000

7 C 3.949197 0.000000

8 H 4.981213 1.123003 0.000000

9 H 4.281950 1.127167 1.804276 0.000000

10 C 3.504398 1.526047 2.188226 2.170538 0.000000

11 H 4.325247 2.169586 2.301554 2.981299 1.125019

12 H 3.939430 2.187794 2.817921 2.301809 1.124689

13 H 2.555868 3.514060 4.277098 4.104358 2.206084

14 H 4.288658 2.209971 2.474402 2.644351 3.491792

15 O 5.379571 3.524642 3.186235 4.611421 3.190299

16 C 3.292331 3.287252 3.667025 4.319334 2.845347

17 C 3.889435 2.799285 2.955485 3.854029 3.052945

18 C 4.445080 3.749210 3.830227 4.817045 3.003565

19 O 5.032695 4.707401 4.800221 5.703269 3.677578

20 C 5.123029 2.907508 2.506751 3.996901 3.191540

21 O 6.133224 3.289506 2.517183 4.225862 3.915674

22 H 2.832640 4.070314 4.618323 4.995150 3.534811

23 H 4.165410 3.436447 3.604554 4.361356 3.963659

11 12 13 14 15

11 H 0.000000

12 H 1.795143 0.000000

13 H 2.537339 2.543979 0.000000

14 H 4.024720 4.305839 4.879998 0.000000

15 O 2.359342 4.124450 3.907503 4.320496 0.000000

16 C 2.776992 3.892499 2.623202 3.642648 2.352367

17 C 3.055037 4.173736 3.678462 2.526529 2.364901

18 C 2.379814 3.929962 2.874807 4.599058 1.415964

19 O 2.940715 4.382639 3.060049 5.778414 2.242421

20 C 2.752552 4.242087 4.293446 3.098661 1.410476

21 O 3.463549 4.851133 5.364979 3.270521 2.235612

22 H 3.633296 4.471955 2.645780 4.245636 3.361217

23 H 4.101771 5.055913 4.526574 2.357586 3.322486

16 17 18 19 20

16 C 0.000000

17 C 1.411707 0.000000

18 C 1.481234 2.336909 0.000000

19 O 2.499155 3.544336 1.220620 0.000000

20 C 2.324008 1.491792 2.286275 3.413804 0.000000

21 O 3.532516 2.506077 3.414225 4.446936 1.220974

22 H 1.091234 2.239587 2.249068 2.923819 3.369016

23 H 2.238355 1.095331 3.325316 4.500731 2.248195

21 22 23

21 O 0.000000

22 H 4.563768 0.000000

23 H 2.946502 2.711495 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.381948 -0.161583 -0.813009

2 6 0 1.598614 -1.169853 -0.204071

3 6 0 1.126006 1.399683 0.500405

4 6 0 2.166234 1.142124 -0.404831

5 1 0 3.036811 -0.354733 -1.677324

6 1 0 2.714283 1.938984 -0.929783

7 6 0 1.211501 -1.011658 1.222314

8 1 0 0.410137 -1.746377 1.503633

9 1 0 2.116083 -1.267637 1.844174

10 6 0 0.771232 0.411252 1.554446

11 1 0 -0.340319 0.417803 1.727882

12 1 0 1.235420 0.748166 2.521888

13 1 0 0.782537 2.432033 0.669506

14 1 0 1.654409 -2.202399 -0.585984

15 8 0 -2.078657 -0.196851 0.255849

16 6 0 -0.370937 0.793517 -1.023406

17 6 0 -0.220075 -0.604519 -1.148514

18 6 0 -1.579272 1.045552 -0.204589

19 8 0 -2.204130 2.038626 0.131965

20 6 0 -1.268002 -1.218110 -0.282027

21 8 0 -1.550176 -2.359167 0.048342

22 1 0 0.017554 1.551685 -1.705350

23 1 0 0.133290 -1.136813 -2.038202

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2284509 0.8778472 0.6733410

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6681727012 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.465201994012E-01 A.U. after 16 cycles

Convg = 0.5210D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.017810492 -0.012554180 -0.004315344

2 6 -0.013211569 0.000161670 0.009082593

3 6 -0.005136898 -0.004261169 0.007634293

4 6 0.000153752 0.012316964 -0.003289615

5 1 0.004060184 -0.002190394 -0.001763245

6 1 0.001189775 0.005915708 -0.001636945

7 6 -0.004082707 0.003016161 -0.004055963

8 1 -0.000228890 0.000749413 0.000636423

9 1 0.000750389 -0.000046894 0.000017030

10 6 0.001763974 -0.001841096 0.000993891

11 1 -0.000267367 0.001036850 -0.001692747

12 1 -0.000744839 -0.002020453 0.000076390

13 1 -0.000137592 0.000379022 0.000045024

14 1 0.000587451 0.000342921 -0.000360402

15 8 -0.001386248 0.000862185 0.001274859

16 6 -0.004906812 0.000969393 -0.003870549

17 6 -0.002427514 -0.003389669 -0.001865236

18 6 0.002943463 -0.002462008 -0.000865856

19 8 0.000613665 -0.001709510 -0.000685533

20 6 0.001260907 0.001715718 0.001252397

21 8 -0.000203738 0.001080148 0.000932065

22 1 0.001300389 0.000429072 0.002020827

23 1 0.000299733 0.001500148 0.000435642

-------------------------------------------------------------------

Cartesian Forces: Max 0.017810492 RMS 0.004241164

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.016546549 RMS 0.002267079

Search for a saddle point.

Step number 30 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 29 30

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06411 -0.00267 0.00301 0.00568 0.00620

Eigenvalues --- 0.01002 0.01094 0.01544 0.02131 0.02243

Eigenvalues --- 0.02299 0.02489 0.02637 0.02927 0.03087

Eigenvalues --- 0.03173 0.03322 0.03525 0.03653 0.03775

Eigenvalues --- 0.03885 0.03943 0.04394 0.04479 0.05134

Eigenvalues --- 0.05288 0.05739 0.06067 0.06434 0.07340

Eigenvalues --- 0.07816 0.08390 0.08786 0.09586 0.09844

Eigenvalues --- 0.11905 0.13742 0.14514 0.15901 0.21093

Eigenvalues --- 0.22723 0.25861 0.26992 0.27882 0.29378

Eigenvalues --- 0.30649 0.31249 0.31426 0.31747 0.32015

Eigenvalues --- 0.32205 0.32443 0.33175 0.34775 0.36432

Eigenvalues --- 0.37575 0.39589 0.40413 0.43718 0.46972

Eigenvalues --- 0.51170 1.08439 1.10843

Eigenvectors required to have negative eigenvalues:

R10 R6 D30 D4 D71

1 -0.55200 -0.48406 0.18769 -0.18223 -0.14871

D86 D85 D73 D68 D79

1 0.14589 0.14000 0.13411 -0.12792 -0.12471

RFO step: Lambda0=1.766850514D-04 Lambda=-4.94944373D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.641

Iteration 1 RMS(Cart)= 0.06904177 RMS(Int)= 0.00219419

Iteration 2 RMS(Cart)= 0.00247840 RMS(Int)= 0.00058720

Iteration 3 RMS(Cart)= 0.00000280 RMS(Int)= 0.00058719

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00058719

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.67316 -0.01655 0.00000 -0.04981 -0.04999 2.62317

R2 2.61356 0.01366 0.00000 0.04069 0.04044 2.65400

R3 2.08144 -0.00218 0.00000 -0.00578 -0.00578 2.07566

R4 2.80894 0.00199 0.00000 0.00229 0.00269 2.81163

R5 2.08309 -0.00020 0.00000 -0.00089 -0.00089 2.08220

R6 4.01726 -0.00020 0.00000 0.16648 0.16647 4.18373

R7 2.65092 -0.01044 0.00000 -0.02672 -0.02685 2.62407

R8 2.81173 0.00047 0.00000 0.00536 0.00532 2.81705

R9 2.08069 0.00039 0.00000 0.00296 0.00296 2.08364

R10 4.19599 -0.00232 0.00000 -0.08743 -0.08772 4.10828

R11 2.07949 0.00013 0.00000 -0.00298 -0.00298 2.07651

R12 2.12217 -0.00034 0.00000 -0.00006 -0.00006 2.12211

R13 2.13004 -0.00027 0.00000 -0.00110 -0.00110 2.12894

R14 2.88381 -0.00249 0.00000 -0.01382 -0.01313 2.87068

R15 2.12598 0.00010 0.00000 0.00180 0.00180 2.12777

R16 2.12535 -0.00018 0.00000 -0.00010 -0.00010 2.12526

R17 2.67578 -0.00317 0.00000 -0.00833 -0.00811 2.66767

R18 2.66541 -0.00195 0.00000 0.00331 0.00318 2.66860

R19 2.66774 0.00105 0.00000 -0.01440 -0.01454 2.65321

R20 2.79913 0.00061 0.00000 0.00626 0.00650 2.80563

R21 2.06213 0.00002 0.00000 0.00493 0.00493 2.06706

R22 2.81908 0.00063 0.00000 0.00381 0.00349 2.82257

R23 2.06987 -0.00079 0.00000 -0.00198 -0.00198 2.06789

R24 2.30664 -0.00157 0.00000 -0.00098 -0.00098 2.30565

R25 2.30731 -0.00099 0.00000 -0.00052 -0.00052 2.30678

A1 2.04707 0.00208 0.00000 0.02423 0.02433 2.07140

A2 2.14366 -0.00558 0.00000 -0.08164 -0.08188 2.06178

A3 2.08246 0.00342 0.00000 0.05886 0.05891 2.14137

A4 2.07310 -0.00129 0.00000 0.01221 0.01133 2.08443

A5 2.08344 0.00049 0.00000 -0.00558 -0.00659 2.07684

A6 1.66388 -0.00084 0.00000 -0.02815 -0.02812 1.63576

A7 2.03235 0.00058 0.00000 0.02227 0.02192 2.05427

A8 1.74692 0.00117 0.00000 -0.02856 -0.02892 1.71800

A9 1.70972 0.00015 0.00000 -0.00706 -0.00648 1.70325

A10 2.10828 -0.00054 0.00000 0.02267 0.02237 2.13065

A11 2.09737 0.00029 0.00000 0.00112 0.00109 2.09845

A12 1.57774 -0.00100 0.00000 -0.01984 -0.01987 1.55787

A13 2.02604 0.00003 0.00000 -0.03049 -0.03028 1.99576

A14 1.71536 0.00166 0.00000 0.01507 0.01463 1.72999

A15 1.72243 0.00001 0.00000 0.02729 0.02807 1.75050

A16 2.07052 -0.00197 0.00000 -0.02955 -0.02947 2.04105

A17 2.05345 0.00738 0.00000 0.10248 0.10214 2.15559

A18 2.14623 -0.00538 0.00000 -0.07444 -0.07423 2.07200

A19 1.93542 -0.00010 0.00000 0.00485 0.00503 1.94046

A20 1.87155 -0.00024 0.00000 0.00286 0.00277 1.87432

A21 1.96408 0.00076 0.00000 -0.00882 -0.00900 1.95507

A22 1.86073 0.00017 0.00000 -0.00296 -0.00298 1.85775

A23 1.92798 -0.00099 0.00000 -0.00482 -0.00505 1.92293

A24 1.89992 0.00040 0.00000 0.00962 0.00998 1.90990

A25 1.97844 0.00029 0.00000 0.00691 0.00638 1.98482

A26 1.91870 -0.00014 0.00000 -0.01374 -0.01375 1.90495

A27 1.88804 0.00036 0.00000 0.00515 0.00548 1.89352

A28 1.90078 0.00027 0.00000 0.00957 0.00984 1.91063

A29 1.92565 -0.00083 0.00000 -0.01038 -0.01030 1.91535

A30 1.84776 0.00002 0.00000 0.00194 0.00189 1.84964

A31 1.88452 -0.00026 0.00000 -0.00324 -0.00328 1.88123

A32 1.83291 0.00068 0.00000 0.02562 0.02391 1.85683

A33 1.69526 0.00050 0.00000 0.00729 0.00835 1.70361

A34 1.56998 -0.00022 0.00000 0.02859 0.02892 1.59890

A35 1.88039 -0.00143 0.00000 0.00323 0.00231 1.88269

A36 2.20760 0.00045 0.00000 -0.00286 -0.00351 2.20408

A37 2.11491 0.00063 0.00000 -0.02832 -0.02893 2.08598

A38 1.89169 -0.00042 0.00000 -0.04424 -0.04511 1.84658

A39 1.80651 0.00149 0.00000 0.07976 0.08009 1.88660

A40 1.52641 0.00050 0.00000 -0.05024 -0.04918 1.47722

A41 1.85541 -0.00074 0.00000 -0.00403 -0.00327 1.85214

A42 2.19903 0.00039 0.00000 0.01979 0.01799 2.21702

A43 2.09269 -0.00044 0.00000 -0.00205 -0.00144 2.09126

A44 1.89459 0.00164 0.00000 -0.00043 -0.00014 1.89445

A45 2.03047 -0.00188 0.00000 0.00228 0.00214 2.03261

A46 2.35810 0.00024 0.00000 -0.00189 -0.00204 2.35606

A47 1.90437 0.00089 0.00000 0.00159 0.00104 1.90541

A48 2.02712 -0.00092 0.00000 -0.00361 -0.00337 2.02375

A49 2.35166 0.00004 0.00000 0.00212 0.00236 2.35402

D1 -0.59544 -0.00100 0.00000 0.03159 0.03155 -0.56389

D2 3.01473 -0.00066 0.00000 -0.04168 -0.04162 2.97311

D3 1.23017 -0.00044 0.00000 -0.01544 -0.01633 1.21384

D4 2.69891 -0.00072 0.00000 0.01494 0.01579 2.71470

D5 0.02589 -0.00038 0.00000 -0.05834 -0.05738 -0.03149

D6 -1.75867 -0.00016 0.00000 -0.03210 -0.03209 -1.79076

D7 -0.08469 0.00111 0.00000 -0.01041 -0.01027 -0.09497

D8 -3.05903 0.00143 0.00000 0.00651 0.00761 -3.05142

D9 2.90972 0.00002 0.00000 -0.00708 -0.00669 2.90303

D10 -0.06462 0.00034 0.00000 0.00984 0.01120 -0.05342

D11 2.91345 -0.00021 0.00000 -0.02118 -0.02155 2.89190

D12 -1.34469 -0.00019 0.00000 -0.02049 -0.02082 -1.36552

D13 0.74400 0.00060 0.00000 -0.01197 -0.01206 0.73194

D14 -0.68324 -0.00054 0.00000 0.04271 0.04320 -0.64005

D15 1.34179 -0.00053 0.00000 0.04340 0.04392 1.38572

D16 -2.85270 0.00026 0.00000 0.05191 0.05268 -2.80001

D17 1.13571 0.00047 0.00000 0.02548 0.02572 1.16143

D18 -3.12244 0.00048 0.00000 0.02617 0.02645 -3.09599

D19 -1.03375 0.00127 0.00000 0.03469 0.03521 -0.99854

D20 -0.82970 -0.00060 0.00000 0.06571 0.06385 -0.76586

D21 -2.79477 -0.00028 0.00000 0.05120 0.05093 -2.74384

D22 1.39109 -0.00008 0.00000 0.05894 0.05988 1.45096

D23 1.27367 -0.00191 0.00000 0.06493 0.06346 1.33712

D24 -0.69140 -0.00159 0.00000 0.05041 0.05054 -0.64086

D25 -2.78873 -0.00139 0.00000 0.05815 0.05949 -2.72924

D26 -2.93622 -0.00095 0.00000 0.07893 0.07746 -2.85876

D27 1.38190 -0.00063 0.00000 0.06442 0.06454 1.44644

D28 -0.71543 -0.00043 0.00000 0.07216 0.07349 -0.64194

D29 0.59291 -0.00023 0.00000 -0.03334 -0.03319 0.55972

D30 -2.72537 0.00075 0.00000 -0.03302 -0.03243 -2.75780

D31 -2.90112 -0.00095 0.00000 -0.06155 -0.06142 -2.96254

D32 0.06379 0.00003 0.00000 -0.06123 -0.06067 0.00312

D33 -1.15059 -0.00150 0.00000 -0.04145 -0.04045 -1.19104

D34 1.81432 -0.00052 0.00000 -0.04114 -0.03970 1.77462

D35 -0.39282 -0.00063 0.00000 0.04732 0.04747 -0.34535

D36 -2.52464 -0.00109 0.00000 0.04024 0.04047 -2.48417

D37 1.74857 -0.00123 0.00000 0.04240 0.04255 1.79111

D38 3.08747 0.00000 0.00000 0.06885 0.06884 -3.12687

D39 0.95566 -0.00045 0.00000 0.06177 0.06185 1.01751

D40 -1.05432 -0.00060 0.00000 0.06393 0.06393 -0.99040

D41 1.27305 -0.00091 0.00000 0.03771 0.03767 1.31072

D42 -0.85876 -0.00137 0.00000 0.03063 0.03067 -0.82809

D43 -2.86875 -0.00151 0.00000 0.03279 0.03275 -2.83600

D44 1.23303 0.00019 0.00000 0.09586 0.09665 1.32967

D45 -3.12022 -0.00099 0.00000 0.10772 0.10791 -3.01231

D46 -1.00071 -0.00035 0.00000 0.08383 0.08398 -0.91673

D47 -0.88275 0.00076 0.00000 0.07486 0.07613 -0.80661

D48 1.04719 -0.00043 0.00000 0.08672 0.08740 1.13459

D49 -3.11648 0.00021 0.00000 0.06283 0.06346 -3.05302

D50 -2.94478 0.00031 0.00000 0.09609 0.09661 -2.84817

D51 -1.01484 -0.00088 0.00000 0.10795 0.10787 -0.90697

D52 1.10467 -0.00024 0.00000 0.08406 0.08394 1.18861

D53 -0.24273 0.00000 0.00000 -0.02996 -0.02974 -0.27247

D54 1.89903 0.00022 0.00000 -0.03589 -0.03581 1.86322

D55 -2.36316 -0.00007 0.00000 -0.03384 -0.03370 -2.39686

D56 -2.41628 0.00031 0.00000 -0.02614 -0.02595 -2.44223

D57 -0.27453 0.00054 0.00000 -0.03207 -0.03202 -0.30654

D58 1.74647 0.00025 0.00000 -0.03002 -0.02990 1.71657

D59 1.82944 0.00044 0.00000 -0.02548 -0.02531 1.80412

D60 -2.31199 0.00066 0.00000 -0.03142 -0.03139 -2.34338

D61 -0.29100 0.00037 0.00000 -0.02937 -0.02927 -0.32027

D62 -0.04013 0.00027 0.00000 0.00358 0.00391 -0.03621

D63 3.09497 -0.00029 0.00000 -0.00074 -0.00011 3.09485

D64 -0.02141 0.00020 0.00000 -0.02035 -0.02046 -0.04188

D65 3.11250 0.00032 0.00000 -0.00940 -0.00945 3.10305

D66 -0.23765 0.00014 0.00000 -0.07776 -0.07674 -0.31438

D67 1.69463 0.00130 0.00000 -0.00800 -0.00722 1.68740

D68 -1.99314 -0.00037 0.00000 0.01481 0.01601 -1.97713

D69 -2.03105 -0.00019 0.00000 -0.09690 -0.09635 -2.12740

D70 -0.09877 0.00098 0.00000 -0.02714 -0.02683 -0.12561

D71 2.49665 -0.00069 0.00000 -0.00433 -0.00360 2.49304

D72 1.53183 0.00059 0.00000 -0.02071 -0.02041 1.51142

D73 -2.81908 0.00175 0.00000 0.04905 0.04911 -2.76998

D74 -0.22366 0.00008 0.00000 0.07186 0.07234 -0.15133

D75 -1.80100 -0.00132 0.00000 -0.01503 -0.01389 -1.81489

D76 1.34885 -0.00059 0.00000 -0.00956 -0.00883 1.34002

D77 0.08941 -0.00074 0.00000 0.01607 0.01570 0.10512

D78 -3.04393 -0.00001 0.00000 0.02154 0.02077 -3.02315

D79 2.83658 -0.00148 0.00000 -0.04845 -0.04752 2.78906

D80 -0.29676 -0.00075 0.00000 -0.04298 -0.04245 -0.33921

D81 2.06818 -0.00079 0.00000 0.01342 0.01306 2.08124

D82 -1.06371 -0.00094 0.00000 -0.00038 -0.00088 -1.06459

D83 0.07686 -0.00067 0.00000 0.03016 0.03011 0.10697

D84 -3.05504 -0.00081 0.00000 0.01636 0.01617 -3.03886

D85 -2.55862 0.00056 0.00000 0.00074 0.00152 -2.55711

D86 0.59267 0.00042 0.00000 -0.01306 -0.01242 0.58025

Item Value Threshold Converged?

Maximum Force 0.016547 0.000450 NO

RMS Force 0.002267 0.000300 NO

Maximum Displacement 0.329684 0.001800 NO

RMS Displacement 0.069089 0.001200 NO

Predicted change in Energy=-2.697386D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.200285 1.632683 0.497714

2 6 0 0.073596 1.212118 0.141017

3 6 0 -0.646727 3.752619 -0.433631

4 6 0 -1.603479 2.932015 0.148986

5 1 0 -1.796107 0.982201 1.152182

6 1 0 -2.559416 3.374855 0.461276

7 6 0 0.688874 1.725953 -1.112419

8 1 0 1.791230 1.513542 -1.139983

9 1 0 0.232652 1.155312 -1.969990

10 6 0 0.436668 3.211782 -1.303114

11 1 0 1.387369 3.782118 -1.106410

12 1 0 0.168898 3.417020 -2.375954

13 1 0 -0.848438 4.827481 -0.574155

14 1 0 0.455289 0.261397 0.546633

15 8 0 2.662859 4.169428 0.845748

16 6 0 0.422422 3.802040 1.458664

17 6 0 1.078904 2.566432 1.575133

18 6 0 1.434542 4.822351 1.086051

19 8 0 1.430899 6.036213 0.962902

20 6 0 2.476162 2.792618 1.098203

21 8 0 3.443245 2.076178 0.894337

22 1 0 -0.479756 4.108893 1.995697

23 1 0 0.874198 1.777760 2.305573

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.388121 0.000000

3 C 2.380747 2.702449 0.000000

4 C 1.404436 2.402226 1.388599 0.000000

5 H 1.098390 2.138015 3.392800 2.201201 0.000000

6 H 2.209915 3.422389 2.145214 1.098839 2.604762

7 C 2.483978 1.487849 2.520309 2.881078 3.443358

8 H 3.412536 2.163812 3.384675 3.898403 4.290143

9 H 2.893226 2.117753 3.143200 3.319354 3.727437

10 C 2.901060 2.493189 1.490721 2.519735 3.998099

11 H 3.726826 3.144356 2.142672 3.353187 4.803675

12 H 3.649176 3.347509 2.133187 3.122798 4.715648

13 H 3.388131 3.799009 1.102617 2.164673 4.320243

14 H 2.150289 1.101855 3.789985 3.395416 2.440293

15 O 4.634661 3.993321 3.572660 4.496477 5.489508

16 C 2.874493 2.926700 2.174006 2.564463 3.601013

17 C 2.688386 2.213933 2.901718 3.059856 3.309738

18 C 4.178807 3.972284 2.790240 3.698787 5.018787

19 O 5.150787 5.078353 3.388457 4.416555 5.999370

20 C 3.901576 3.030925 3.608400 4.190932 4.640346

21 O 4.681492 3.559301 4.615390 5.172758 5.358552

22 H 2.982403 3.483869 2.460984 2.461328 3.495784

23 H 2.755519 2.376178 3.703582 3.481674 3.015586

6 7 8 9 10

6 H 0.000000

7 C 3.968221 0.000000

8 H 4.995661 1.122972 0.000000

9 H 4.316604 1.126587 1.801779 0.000000

10 C 3.480831 1.519098 2.178409 2.171501 0.000000

11 H 4.266217 2.171577 2.304488 2.996540 1.125969

12 H 3.936413 2.174075 2.789768 2.298737 1.124637

13 H 2.471778 3.503217 4.274364 4.074547 2.189375

14 H 4.334668 2.225295 2.489434 2.679934 3.482338

15 O 5.296349 3.701568 3.428789 4.787399 3.238922

16 C 3.173110 3.315359 3.723415 4.335534 2.824186

17 C 3.889935 2.842791 2.997972 3.908363 3.018815

18 C 4.293866 3.870009 4.003831 4.922510 3.049228

19 O 4.822559 4.841064 5.000651 5.819008 3.755095

20 C 5.108984 3.036285 2.667329 4.138589 3.178294

21 O 6.156788 3.425827 2.680331 4.400032 3.893314

22 H 2.686679 4.087112 4.661084 4.995782 3.539321

23 H 4.212107 3.423405 3.575279 4.368005 3.907746

11 12 13 14 15

11 H 0.000000

12 H 1.797139 0.000000

13 H 2.524858 2.504167 0.000000

14 H 3.999600 4.310625 4.879036 0.000000

15 O 2.363854 4.143105 3.844264 4.498394 0.000000

16 C 2.740643 3.862228 2.607483 3.656369 2.351637

17 C 2.960357 4.142788 3.666937 2.599980 2.368652

18 C 2.427178 3.944906 2.822819 4.695978 1.411671

19 O 3.060211 4.427277 3.003158 5.871422 2.239718

20 C 2.650452 4.217002 4.241511 3.285611 1.412160

21 O 3.337641 4.818092 5.305156 3.513148 2.234516

22 H 3.635382 4.473340 2.693777 4.216316 3.346950

23 H 3.990291 5.010122 4.534436 2.359812 3.324226

16 17 18 19 20

16 C 0.000000

17 C 1.404016 0.000000

18 C 1.484675 2.335561 0.000000

19 O 2.500867 3.540919 1.220099 0.000000

20 C 2.316617 1.493637 2.281433 3.410541 0.000000

21 O 3.524548 2.508773 3.407801 4.442535 1.220696

22 H 1.093841 2.232818 2.236295 2.903762 3.357905

23 H 2.240328 1.094282 3.327275 4.499679 2.248104

21 22 23

21 O 0.000000

22 H 4.553555 0.000000

23 H 2.946293 2.713558 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.377376 -0.042623 -0.856689

2 6 0 1.732526 -1.122906 -0.270140

3 6 0 1.072605 1.365692 0.551208

4 6 0 2.083894 1.250288 -0.393346

5 1 0 2.993023 -0.228173 -1.747200

6 1 0 2.483927 2.164718 -0.852954

7 6 0 1.363487 -1.060133 1.169848

8 1 0 0.634590 -1.871349 1.437622

9 1 0 2.297937 -1.261567 1.766023

10 6 0 0.801216 0.297504 1.554987

11 1 0 -0.310458 0.212421 1.712306

12 1 0 1.229978 0.619706 2.543500

13 1 0 0.681583 2.358968 0.827376

14 1 0 1.833240 -2.119073 -0.730131

15 8 0 -2.119886 -0.209658 0.250928

16 6 0 -0.372454 0.787476 -0.966610

17 6 0 -0.237974 -0.600091 -1.133443

18 6 0 -1.601880 1.033726 -0.171542

19 8 0 -2.228252 2.025726 0.163473

20 6 0 -1.296666 -1.224366 -0.284676

21 8 0 -1.588640 -2.368355 0.025387

22 1 0 -0.009290 1.559925 -1.650659

23 1 0 0.126904 -1.124684 -2.021766

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2317820 0.8608863 0.6613926

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 469.4711200818 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.458175530394E-01 A.U. after 15 cycles

Convg = 0.7332D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001415176 -0.002921177 -0.000961196

2 6 -0.002248617 -0.003214768 -0.003414355

3 6 -0.002852670 0.002444980 -0.009566990

4 6 0.004456009 -0.001866227 -0.001655838

5 1 -0.004356794 0.003345323 0.000841243

6 1 -0.001175782 -0.004598601 0.002494588

7 6 0.000196287 -0.000003691 0.001425299

8 1 0.000030703 0.000479048 0.001652337

9 1 0.000098813 -0.000147105 0.000190430

10 6 0.001080407 0.001617370 0.000211567

11 1 0.000102844 0.000038538 -0.001791327

12 1 -0.001222920 -0.000817067 0.000231177

13 1 -0.000117012 0.001076176 0.001796635

14 1 0.002408001 0.000361642 -0.001771466

15 8 -0.000988694 -0.000173729 0.000778731

16 6 0.001749319 0.002058814 0.012805686

17 6 0.002383598 0.005759482 0.002581644

18 6 0.003514971 -0.001175974 -0.004395042

19 8 0.000141446 -0.000973494 -0.000374793

20 6 -0.000112725 -0.002232432 0.000106192

21 8 -0.001193995 0.001007762 0.000638562

22 1 0.000403156 -0.000372460 0.000593754

23 1 -0.000881169 0.000307590 -0.002416837

-------------------------------------------------------------------

Cartesian Forces: Max 0.012805686 RMS 0.002759694

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.007987009 RMS 0.001500803

Search for a saddle point.

Step number 31 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 30 31

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06684 -0.00251 0.00316 0.00533 0.00625

Eigenvalues --- 0.01010 0.01151 0.01702 0.02133 0.02249

Eigenvalues --- 0.02351 0.02500 0.02677 0.02931 0.03117

Eigenvalues --- 0.03196 0.03300 0.03652 0.03707 0.03762

Eigenvalues --- 0.03891 0.03972 0.04417 0.05061 0.05253

Eigenvalues --- 0.05720 0.05878 0.06085 0.06628 0.07337

Eigenvalues --- 0.07825 0.08552 0.08807 0.09656 0.09817

Eigenvalues --- 0.11870 0.13719 0.14470 0.15925 0.21080

Eigenvalues --- 0.22726 0.25879 0.26987 0.27941 0.29672

Eigenvalues --- 0.30691 0.31237 0.31419 0.31803 0.32005

Eigenvalues --- 0.32328 0.32498 0.33329 0.35010 0.36418

Eigenvalues --- 0.37671 0.39604 0.40414 0.43700 0.46941

Eigenvalues --- 0.51184 1.08443 1.10844

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D71

1 -0.53002 -0.50205 0.19065 -0.18024 -0.14556

D86 D68 D85 A40 D1

1 0.14217 -0.13171 0.13088 0.12756 -0.12651

RFO step: Lambda0=6.477228120D-04 Lambda=-5.00845047D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.10322227 RMS(Int)= 0.00376492

Iteration 2 RMS(Cart)= 0.00490703 RMS(Int)= 0.00113099

Iteration 3 RMS(Cart)= 0.00000865 RMS(Int)= 0.00113097

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00113097

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62317 0.00185 0.00000 0.01441 0.01436 2.63753

R2 2.65400 -0.00317 0.00000 -0.00587 -0.00588 2.64812

R3 2.07566 0.00088 0.00000 0.00077 0.00077 2.07643

R4 2.81163 -0.00117 0.00000 0.00222 0.00295 2.81458

R5 2.08220 -0.00013 0.00000 0.00189 0.00189 2.08409

R6 4.18373 0.00496 0.00000 -0.08351 -0.08366 4.10007

R7 2.62407 0.00259 0.00000 0.00227 0.00230 2.62637

R8 2.81705 0.00004 0.00000 -0.00490 -0.00493 2.81213

R9 2.08364 0.00084 0.00000 -0.00212 -0.00212 2.08152

R10 4.10828 0.00799 0.00000 0.08213 0.08169 4.18997

R11 2.07651 -0.00012 0.00000 0.00126 0.00126 2.07777

R12 2.12211 -0.00010 0.00000 0.00053 0.00053 2.12264

R13 2.12894 -0.00011 0.00000 -0.00021 -0.00021 2.12873

R14 2.87068 0.00096 0.00000 0.00079 0.00172 2.87240

R15 2.12777 -0.00021 0.00000 -0.00132 -0.00132 2.12645

R16 2.12526 -0.00008 0.00000 0.00146 0.00146 2.12672

R17 2.66767 -0.00122 0.00000 0.00065 0.00117 2.66884

R18 2.66860 -0.00075 0.00000 -0.00637 -0.00623 2.66236

R19 2.65321 -0.00151 0.00000 0.00593 0.00474 2.65794

R20 2.80563 0.00178 0.00000 -0.00367 -0.00349 2.80214

R21 2.06706 -0.00015 0.00000 -0.00405 -0.00405 2.06301

R22 2.82257 -0.00181 0.00000 0.00501 0.00458 2.82714

R23 2.06789 -0.00167 0.00000 0.00048 0.00048 2.06837

R24 2.30565 -0.00093 0.00000 0.00064 0.00064 2.30630

R25 2.30678 -0.00164 0.00000 -0.00005 -0.00005 2.30673

A1 2.07140 -0.00132 0.00000 -0.00540 -0.00599 2.06541

A2 2.06178 0.00628 0.00000 0.01800 0.01789 2.07967

A3 2.14137 -0.00501 0.00000 -0.01744 -0.01753 2.12385

A4 2.08443 -0.00057 0.00000 -0.00315 -0.00351 2.08093

A5 2.07684 0.00125 0.00000 0.00834 0.00798 2.08482

A6 1.63576 0.00120 0.00000 -0.00181 -0.00227 1.63350

A7 2.05427 -0.00071 0.00000 -0.01991 -0.01982 2.03445

A8 1.71800 -0.00108 0.00000 0.03505 0.03361 1.75161

A9 1.70325 -0.00002 0.00000 0.00526 0.00702 1.71026

A10 2.13065 -0.00185 0.00000 -0.01163 -0.01211 2.11854

A11 2.09845 0.00131 0.00000 0.00099 0.00090 2.09936

A12 1.55787 0.00028 0.00000 0.02023 0.01994 1.57781

A13 1.99576 0.00066 0.00000 0.02077 0.02111 2.01687

A14 1.72999 -0.00033 0.00000 -0.00408 -0.00580 1.72419

A15 1.75050 -0.00037 0.00000 -0.04741 -0.04562 1.70488

A16 2.04105 0.00288 0.00000 0.01084 0.01039 2.05144

A17 2.15559 -0.00692 0.00000 -0.02152 -0.02151 2.13409

A18 2.07200 0.00408 0.00000 0.00852 0.00876 2.08076

A19 1.94046 -0.00058 0.00000 -0.00722 -0.00657 1.93388

A20 1.87432 -0.00115 0.00000 -0.00277 -0.00250 1.87182

A21 1.95507 0.00171 0.00000 0.01599 0.01445 1.96952

A22 1.85775 0.00068 0.00000 -0.00159 -0.00185 1.85590

A23 1.92293 -0.00056 0.00000 -0.00051 -0.00062 1.92231

A24 1.90990 -0.00017 0.00000 -0.00492 -0.00387 1.90603

A25 1.98482 -0.00083 0.00000 0.00151 -0.00037 1.98445

A26 1.90495 0.00056 0.00000 0.00649 0.00691 1.91186

A27 1.89352 0.00027 0.00000 -0.00822 -0.00753 1.88599

A28 1.91063 0.00005 0.00000 0.00356 0.00367 1.91430

A29 1.91535 0.00019 0.00000 -0.00552 -0.00457 1.91078

A30 1.84964 -0.00018 0.00000 0.00219 0.00194 1.85158

A31 1.88123 0.00007 0.00000 0.00033 0.00011 1.88134

A32 1.85683 -0.00119 0.00000 0.00678 0.00174 1.85857

A33 1.70361 -0.00103 0.00000 0.01609 0.01913 1.72274

A34 1.59890 0.00114 0.00000 -0.06061 -0.05905 1.53985

A35 1.88269 -0.00071 0.00000 -0.00237 -0.00317 1.87953

A36 2.20408 -0.00050 0.00000 0.01121 0.01170 2.21579

A37 2.08598 0.00175 0.00000 0.01355 0.01308 2.09906

A38 1.84658 0.00117 0.00000 0.03269 0.02811 1.87469

A39 1.88660 -0.00134 0.00000 -0.08174 -0.07997 1.80663

A40 1.47722 -0.00047 0.00000 0.04972 0.05194 1.52916

A41 1.85214 0.00081 0.00000 0.00269 0.00312 1.85526

A42 2.21702 -0.00024 0.00000 -0.00888 -0.00968 2.20734

A43 2.09126 -0.00033 0.00000 0.00037 0.00092 2.09217

A44 1.89445 -0.00025 0.00000 0.00549 0.00529 1.89974

A45 2.03261 -0.00017 0.00000 -0.00611 -0.00600 2.02661

A46 2.35606 0.00041 0.00000 0.00059 0.00067 2.35673

A47 1.90541 0.00025 0.00000 0.00146 0.00044 1.90584

A48 2.02375 -0.00011 0.00000 0.00289 0.00340 2.02715

A49 2.35402 -0.00014 0.00000 -0.00434 -0.00383 2.35019

D1 -0.56389 -0.00038 0.00000 -0.02088 -0.02109 -0.58498

D2 2.97311 -0.00013 0.00000 0.02469 0.02419 2.99730

D3 1.21384 -0.00102 0.00000 0.01823 0.01598 1.22983

D4 2.71470 0.00044 0.00000 0.01867 0.01949 2.73419

D5 -0.03149 0.00069 0.00000 0.06424 0.06477 0.03328

D6 -1.79076 -0.00021 0.00000 0.05778 0.05657 -1.73419

D7 -0.09497 0.00052 0.00000 0.04136 0.04136 -0.05360

D8 -3.05142 -0.00024 0.00000 0.05381 0.05441 -2.99701

D9 2.90303 0.00062 0.00000 0.00289 0.00266 2.90569

D10 -0.05342 -0.00014 0.00000 0.01534 0.01571 -0.03771

D11 2.89190 0.00017 0.00000 -0.04513 -0.04576 2.84614

D12 -1.36552 0.00000 0.00000 -0.05255 -0.05293 -1.41844

D13 0.73194 0.00007 0.00000 -0.05086 -0.05068 0.68126

D14 -0.64005 0.00036 0.00000 -0.08386 -0.08365 -0.72370

D15 1.38572 0.00020 0.00000 -0.09127 -0.09082 1.29490

D16 -2.80001 0.00027 0.00000 -0.08959 -0.08856 -2.88858

D17 1.16143 -0.00047 0.00000 -0.06311 -0.06227 1.09916

D18 -3.09599 -0.00063 0.00000 -0.07053 -0.06943 3.11776

D19 -0.99854 -0.00056 0.00000 -0.06884 -0.06718 -1.06572

D20 -0.76586 0.00056 0.00000 -0.12961 -0.13121 -0.89707

D21 -2.74384 -0.00032 0.00000 -0.11160 -0.11150 -2.85534

D22 1.45096 0.00029 0.00000 -0.12164 -0.12062 1.33034

D23 1.33712 0.00006 0.00000 -0.12751 -0.12956 1.20756

D24 -0.64086 -0.00082 0.00000 -0.10950 -0.10985 -0.75071

D25 -2.72924 -0.00021 0.00000 -0.11954 -0.11897 -2.84821

D26 -2.85876 -0.00094 0.00000 -0.13858 -0.13999 -2.99875

D27 1.44644 -0.00182 0.00000 -0.12056 -0.12029 1.32616

D28 -0.64194 -0.00121 0.00000 -0.13061 -0.12940 -0.77134

D29 0.55972 -0.00012 0.00000 0.01457 0.01467 0.57438

D30 -2.75780 -0.00061 0.00000 -0.00062 -0.00133 -2.75913

D31 -2.96254 0.00040 0.00000 0.05076 0.05146 -2.91109

D32 0.00312 -0.00009 0.00000 0.03557 0.03546 0.03859

D33 -1.19104 0.00028 0.00000 0.00774 0.01033 -1.18071

D34 1.77462 -0.00021 0.00000 -0.00745 -0.00566 1.76896

D35 -0.34535 -0.00013 0.00000 -0.08473 -0.08474 -0.43009

D36 -2.48417 -0.00003 0.00000 -0.09521 -0.09442 -2.57859

D37 1.79111 -0.00025 0.00000 -0.09682 -0.09629 1.69483

D38 -3.12687 -0.00079 0.00000 -0.11546 -0.11623 3.04009

D39 1.01751 -0.00069 0.00000 -0.12594 -0.12591 0.89160

D40 -0.99040 -0.00092 0.00000 -0.12755 -0.12778 -1.11817

D41 1.31072 -0.00040 0.00000 -0.06559 -0.06722 1.24350

D42 -0.82809 -0.00030 0.00000 -0.07606 -0.07690 -0.90499

D43 -2.83600 -0.00053 0.00000 -0.07768 -0.07876 -2.91476

D44 1.32967 -0.00205 0.00000 -0.14180 -0.14077 1.18891

D45 -3.01231 -0.00350 0.00000 -0.13668 -0.13658 3.13430

D46 -0.91673 -0.00164 0.00000 -0.13151 -0.13150 -1.04823

D47 -0.80661 -0.00019 0.00000 -0.13330 -0.13158 -0.93819

D48 1.13459 -0.00164 0.00000 -0.12818 -0.12739 1.00720

D49 -3.05302 0.00022 0.00000 -0.12301 -0.12231 3.10786

D50 -2.84817 -0.00069 0.00000 -0.14106 -0.14034 -2.98851

D51 -0.90697 -0.00214 0.00000 -0.13594 -0.13615 -1.04312

D52 1.18861 -0.00028 0.00000 -0.13077 -0.13107 1.05754

D53 -0.27247 0.00078 0.00000 0.09516 0.09550 -0.17697

D54 1.86322 0.00096 0.00000 0.10728 0.10697 1.97019

D55 -2.39686 0.00087 0.00000 0.10882 0.10880 -2.28806

D56 -2.44223 0.00072 0.00000 0.09338 0.09403 -2.34820

D57 -0.30654 0.00089 0.00000 0.10549 0.10550 -0.20104

D58 1.71657 0.00081 0.00000 0.10704 0.10733 1.82390

D59 1.80412 0.00031 0.00000 0.09850 0.09890 1.90302

D60 -2.34338 0.00049 0.00000 0.11062 0.11037 -2.23301

D61 -0.32027 0.00040 0.00000 0.11216 0.11220 -0.20807

D62 -0.03621 0.00070 0.00000 -0.00405 -0.00296 -0.03917

D63 3.09485 0.00050 0.00000 -0.00681 -0.00524 3.08962

D64 -0.04188 0.00006 0.00000 0.03716 0.03627 -0.00560

D65 3.10305 -0.00013 0.00000 0.03478 0.03347 3.13653

D66 -0.31438 -0.00007 0.00000 0.15011 0.15148 -0.16290

D67 1.68740 -0.00071 0.00000 0.07344 0.07467 1.76208

D68 -1.97713 -0.00030 0.00000 0.06293 0.06492 -1.91221

D69 -2.12740 0.00183 0.00000 0.13028 0.13058 -1.99681

D70 -0.12561 0.00120 0.00000 0.05361 0.05378 -0.07183

D71 2.49304 0.00161 0.00000 0.04310 0.04402 2.53706

D72 1.51142 0.00021 0.00000 0.08037 0.07980 1.59122

D73 -2.76998 -0.00043 0.00000 0.00371 0.00299 -2.76699

D74 -0.15133 -0.00002 0.00000 -0.00681 -0.00677 -0.15809

D75 -1.81489 0.00063 0.00000 -0.04583 -0.04223 -1.85713

D76 1.34002 0.00089 0.00000 -0.04228 -0.03929 1.30074

D77 0.10512 -0.00125 0.00000 -0.03280 -0.03365 0.07147

D78 -3.02315 -0.00099 0.00000 -0.02925 -0.03070 -3.05385

D79 2.78906 -0.00044 0.00000 0.01277 0.01306 2.80212

D80 -0.33921 -0.00019 0.00000 0.01632 0.01601 -0.32320

D81 2.08124 0.00040 0.00000 -0.05570 -0.05885 2.02239

D82 -1.06459 0.00063 0.00000 -0.05265 -0.05529 -1.11988

D83 0.10697 -0.00072 0.00000 -0.05735 -0.05699 0.04998

D84 -3.03886 -0.00049 0.00000 -0.05430 -0.05343 -3.09229

D85 -2.55711 -0.00110 0.00000 -0.04434 -0.04411 -2.60122

D86 0.58025 -0.00086 0.00000 -0.04129 -0.04056 0.53970

Item Value Threshold Converged?

Maximum Force 0.007987 0.000450 NO

RMS Force 0.001501 0.000300 NO

Maximum Displacement 0.372026 0.001800 NO

RMS Displacement 0.103224 0.001200 NO

Predicted change in Energy=-3.813747D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.168767 1.599917 0.478263

2 6 0 0.139515 1.254506 0.136033

3 6 0 -0.716015 3.759624 -0.431090

4 6 0 -1.623675 2.885272 0.154790

5 1 0 -1.745358 0.931174 1.132238

6 1 0 -2.590004 3.272410 0.508691

7 6 0 0.739379 1.817859 -1.105393

8 1 0 1.857406 1.710410 -1.092540

9 1 0 0.370970 1.193386 -1.967513

10 6 0 0.355804 3.269869 -1.339840

11 1 0 1.265614 3.923777 -1.235533

12 1 0 -0.000162 3.397558 -2.399808

13 1 0 -0.948439 4.833715 -0.505907

14 1 0 0.562134 0.303190 0.500281

15 8 0 2.712539 4.019988 0.832228

16 6 0 0.448297 3.838929 1.454174

17 6 0 1.019868 2.565082 1.624254

18 6 0 1.523886 4.760406 1.015112

19 8 0 1.600261 5.959962 0.803682

20 6 0 2.445675 2.682833 1.186755

21 8 0 3.377462 1.901628 1.079373

22 1 0 -0.443181 4.229614 1.948575

23 1 0 0.740392 1.821897 2.377632

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.395719 0.000000

3 C 2.386680 2.707245 0.000000

4 C 1.401326 2.401788 1.389818 0.000000

5 H 1.098798 2.156319 3.391706 2.188312 0.000000

6 H 2.195012 3.414833 2.152301 1.099506 2.565858

7 C 2.489274 1.489410 2.518593 2.882960 3.459353

8 H 3.411356 2.160646 3.355487 3.879956 4.305433

9 H 2.918540 2.117123 3.182406 3.368272 3.762453

10 C 2.901474 2.507323 1.488114 2.510014 3.999443

11 H 3.776722 3.205355 2.144978 3.370383 4.860860

12 H 3.588932 3.323051 2.125885 3.069886 4.648021

13 H 3.387416 3.795586 1.101495 2.165386 4.306788

14 H 2.162869 1.102853 3.801059 3.400628 2.473510

15 O 4.587654 3.840968 3.663161 4.533129 5.431724

16 C 2.929245 2.917548 2.217236 2.625058 3.656611

17 C 2.652350 2.169662 2.943580 3.041408 3.249340

18 C 4.186559 3.870478 2.847846 3.763432 5.036337

19 O 5.175269 4.972007 3.425096 4.502060 6.048952

20 C 3.839122 2.909040 3.711225 4.203040 4.542691

21 O 4.595711 3.434088 4.742384 5.180133 5.214198

22 H 3.098968 3.532154 2.440929 2.533473 3.638926

23 H 2.702178 2.389090 3.710098 3.414762 2.919477

6 7 8 9 10

6 H 0.000000

7 C 3.975649 0.000000

8 H 4.978277 1.123251 0.000000

9 H 4.384210 1.126473 1.800662 0.000000

10 C 3.477766 1.520010 2.178962 2.169328 0.000000

11 H 4.281634 2.174569 2.295573 2.964999 1.125269

12 H 3.896448 2.172068 2.829483 2.276618 1.125410

13 H 2.482301 3.507636 4.239333 4.138735 2.200479

14 H 4.330394 2.214458 2.488991 2.630399 3.497113

15 O 5.364748 3.535125 3.125721 4.616403 3.291619

16 C 3.232052 3.274269 3.605819 4.325831 2.852875

17 C 3.843953 2.843940 2.968654 3.899155 3.118262

18 C 4.403940 3.710873 3.722352 4.790501 3.021906

19 O 4.986810 4.641412 4.660523 5.648975 3.657862

20 C 5.115217 2.985560 2.546930 4.058603 3.331044

21 O 6.149421 3.426325 2.657883 4.338677 4.105495

22 H 2.756512 4.067154 4.570281 5.021680 3.517550

23 H 4.085152 3.483027 3.647224 4.405880 4.008007

11 12 13 14 15

11 H 0.000000

12 H 1.798508 0.000000

13 H 2.502474 2.559031 0.000000

14 H 4.076344 4.278060 4.880564 0.000000

15 O 2.525566 4.265234 3.981899 4.306857 0.000000

16 C 2.812424 3.905010 2.604303 3.663921 2.355078

17 C 3.175662 4.233976 3.682189 2.566903 2.368373

18 C 2.414965 3.980171 2.903665 4.588768 1.412290

19 O 2.901109 4.403364 3.078852 5.759238 2.236398

20 C 2.966474 4.399589 4.360208 3.111538 1.408861

21 O 3.729313 5.074529 5.461105 3.288833 2.233977

22 H 3.626577 4.449384 2.577733 4.304070 3.353915

23 H 4.212923 5.084786 4.498666 2.421299 3.333053

16 17 18 19 20

16 C 0.000000

17 C 1.406523 0.000000

18 C 1.482831 2.333353 0.000000

19 O 2.499789 3.540538 1.220439 0.000000

20 C 2.323271 1.496061 2.279357 3.406031 0.000000

21 O 3.531800 2.509047 3.407709 4.438978 1.220671

22 H 1.091696 2.239724 2.241081 2.912136 3.364282

23 H 2.237523 1.094535 3.332440 4.510019 2.251086

21 22 23

21 O 0.000000

22 H 4.557669 0.000000

23 H 2.940403 2.716990 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.352204 -0.348902 -0.809886

2 6 0 1.551429 -1.251464 -0.108336

3 6 0 1.236330 1.392433 0.381255

4 6 0 2.213837 1.017794 -0.532921

5 1 0 2.938526 -0.707621 -1.667153

6 1 0 2.710473 1.792103 -1.135177

7 6 0 1.181256 -0.950908 1.302685

8 1 0 0.311216 -1.581528 1.629859

9 1 0 2.052961 -1.254167 1.948523

10 6 0 0.876802 0.520489 1.532313

11 1 0 -0.214555 0.648314 1.774865

12 1 0 1.441621 0.884139 2.435246

13 1 0 0.937969 2.448700 0.473838

14 1 0 1.544030 -2.313748 -0.404619

15 8 0 -2.098575 -0.119717 0.278510

16 6 0 -0.350301 0.759052 -1.032097

17 6 0 -0.264849 -0.641692 -1.126545

18 6 0 -1.534297 1.083154 -0.200293

19 8 0 -2.102875 2.111666 0.128876

20 6 0 -1.353095 -1.188267 -0.257538

21 8 0 -1.710935 -2.309529 0.066127

22 1 0 0.038998 1.489803 -1.743610

23 1 0 0.081941 -1.215496 -1.991701

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2213475 0.8656472 0.6666604

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 469.4841224091 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.488824107153E-01 A.U. after 16 cycles

Convg = 0.3671D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.005254851 -0.002802156 -0.000593585

2 6 -0.007621820 -0.002999482 -0.003481413

3 6 -0.002935737 -0.000203781 -0.003735580

4 6 0.004581879 0.002273990 -0.000196973

5 1 -0.002912754 0.001396203 -0.000488834

6 1 -0.000687332 -0.003370028 0.001127399

7 6 -0.000004618 -0.000342904 0.001204404

8 1 0.000044364 0.000292295 0.001251946

9 1 0.000063337 -0.000189833 0.000105985

10 6 0.001151844 0.001698081 0.000507275

11 1 0.000108341 0.000126632 -0.000813428

12 1 -0.000707849 -0.000440077 0.000236889

13 1 -0.000241046 0.000778235 -0.000186682

14 1 0.001527093 0.001246866 -0.000268457

15 8 -0.001029434 -0.000213104 0.000754594

16 6 0.001044297 -0.001769815 0.005849083

17 6 0.002958447 0.006727491 0.002197098

18 6 0.002150271 -0.000320819 -0.002850054

19 8 -0.000161907 -0.000751199 -0.000498829

20 6 -0.001546782 -0.001782837 -0.000082645

21 8 -0.000830196 0.000749127 0.000454961

22 1 0.000376186 -0.000327577 0.001372195

23 1 -0.000581434 0.000224693 -0.001865349

-------------------------------------------------------------------

Cartesian Forces: Max 0.007621820 RMS 0.002177385

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.004437087 RMS 0.001031921

Search for a saddle point.

Step number 32 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 29 30 31 32

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06377 -0.00132 0.00385 0.00423 0.00613

Eigenvalues --- 0.00994 0.01113 0.01723 0.02095 0.02249

Eigenvalues --- 0.02358 0.02467 0.02674 0.02920 0.03114

Eigenvalues --- 0.03192 0.03284 0.03646 0.03730 0.03800

Eigenvalues --- 0.03884 0.04046 0.04403 0.05072 0.05172

Eigenvalues --- 0.05719 0.06056 0.06224 0.07023 0.07341

Eigenvalues --- 0.07831 0.08716 0.08915 0.09662 0.09828

Eigenvalues --- 0.11934 0.13735 0.14527 0.16084 0.21248

Eigenvalues --- 0.22754 0.25947 0.27054 0.28091 0.29823

Eigenvalues --- 0.30814 0.31262 0.31434 0.31824 0.32024

Eigenvalues --- 0.32367 0.32583 0.33478 0.35186 0.36445

Eigenvalues --- 0.37823 0.39611 0.40423 0.43791 0.47060

Eigenvalues --- 0.51372 1.08454 1.10847

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D86

1 -0.52641 -0.51419 0.19429 -0.18215 0.14543

D71 D85 D1 D68 A40

1 -0.14340 0.13361 -0.12428 -0.12399 0.12354

RFO step: Lambda0=2.609838185D-04 Lambda=-5.12357776D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.702

Iteration 1 RMS(Cart)= 0.06018105 RMS(Int)= 0.00227595

Iteration 2 RMS(Cart)= 0.00246241 RMS(Int)= 0.00068466

Iteration 3 RMS(Cart)= 0.00000498 RMS(Int)= 0.00068464

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00068464

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63753 -0.00423 0.00000 -0.05823 -0.05765 2.57988

R2 2.64812 -0.00089 0.00000 0.02508 0.02620 2.67432

R3 2.07643 0.00039 0.00000 0.00218 0.00218 2.07861

R4 2.81458 -0.00122 0.00000 -0.00871 -0.00898 2.80560

R5 2.08409 -0.00058 0.00000 -0.00356 -0.00356 2.08053

R6 4.10007 0.00349 0.00000 0.13982 0.13984 4.23991

R7 2.62637 -0.00081 0.00000 -0.02326 -0.02278 2.60360

R8 2.81213 -0.00038 0.00000 0.01181 0.01139 2.82352

R9 2.08152 0.00082 0.00000 0.00650 0.00650 2.08803

R10 4.18997 0.00338 0.00000 -0.15025 -0.15042 4.03954

R11 2.07777 -0.00022 0.00000 -0.00020 -0.00020 2.07756

R12 2.12264 0.00003 0.00000 0.00079 0.00079 2.12342

R13 2.12873 0.00000 0.00000 0.00018 0.00018 2.12891

R14 2.87240 0.00085 0.00000 0.00286 0.00200 2.87440

R15 2.12645 0.00009 0.00000 -0.00249 -0.00249 2.12396

R16 2.12672 -0.00005 0.00000 0.00124 0.00124 2.12796

R17 2.66884 -0.00102 0.00000 -0.01124 -0.01130 2.65754

R18 2.66236 -0.00050 0.00000 0.00795 0.00791 2.67027

R19 2.65794 -0.00331 0.00000 -0.00005 -0.00027 2.65767

R20 2.80214 0.00107 0.00000 0.02061 0.02063 2.82278

R21 2.06301 0.00020 0.00000 0.00315 0.00315 2.06616

R22 2.82714 -0.00261 0.00000 -0.02933 -0.02930 2.79784

R23 2.06837 -0.00129 0.00000 -0.00634 -0.00634 2.06203

R24 2.30630 -0.00066 0.00000 -0.00055 -0.00055 2.30574

R25 2.30673 -0.00115 0.00000 -0.00005 -0.00005 2.30669

A1 2.06541 -0.00018 0.00000 0.00982 0.00982 2.07523

A2 2.07967 0.00334 0.00000 0.03978 0.03958 2.11925

A3 2.12385 -0.00313 0.00000 -0.04416 -0.04451 2.07934

A4 2.08093 0.00008 0.00000 0.01664 0.01454 2.09547

A5 2.08482 0.00058 0.00000 0.01887 0.01772 2.10254

A6 1.63350 0.00072 0.00000 -0.02306 -0.02329 1.61020

A7 2.03445 -0.00041 0.00000 0.00757 0.00507 2.03952

A8 1.75161 -0.00132 0.00000 -0.04856 -0.04778 1.70383

A9 1.71026 0.00004 0.00000 -0.02838 -0.02806 1.68220

A10 2.11854 -0.00105 0.00000 -0.02523 -0.02669 2.09185

A11 2.09936 0.00109 0.00000 0.02180 0.02051 2.11987

A12 1.57781 -0.00004 0.00000 0.03074 0.03092 1.60872

A13 2.01687 0.00004 0.00000 -0.02287 -0.02395 1.99292

A14 1.72419 -0.00043 0.00000 0.02640 0.02693 1.75112

A15 1.70488 0.00024 0.00000 0.02334 0.02345 1.72833

A16 2.05144 0.00160 0.00000 0.00492 0.00496 2.05640

A17 2.13409 -0.00444 0.00000 -0.08309 -0.08333 2.05076

A18 2.08076 0.00295 0.00000 0.08166 0.08169 2.16245

A19 1.93388 -0.00042 0.00000 0.00218 0.00257 1.93645

A20 1.87182 -0.00077 0.00000 -0.00727 -0.00700 1.86482

A21 1.96952 0.00099 0.00000 0.00780 0.00671 1.97623

A22 1.85590 0.00045 0.00000 0.00079 0.00063 1.85652

A23 1.92231 -0.00026 0.00000 -0.00638 -0.00620 1.91611

A24 1.90603 -0.00002 0.00000 0.00252 0.00300 1.90902

A25 1.98445 -0.00102 0.00000 0.00852 0.00727 1.99171

A26 1.91186 0.00023 0.00000 0.00361 0.00384 1.91570

A27 1.88599 0.00041 0.00000 -0.01228 -0.01190 1.87410

A28 1.91430 0.00060 0.00000 0.00847 0.00858 1.92288

A29 1.91078 -0.00004 0.00000 -0.01236 -0.01184 1.89894

A30 1.85158 -0.00014 0.00000 0.00336 0.00323 1.85481

A31 1.88134 -0.00008 0.00000 0.00061 0.00043 1.88177

A32 1.85857 -0.00028 0.00000 0.02322 0.02235 1.88092

A33 1.72274 -0.00148 0.00000 -0.02352 -0.02275 1.69999

A34 1.53985 0.00110 0.00000 0.07977 0.08077 1.62062

A35 1.87953 -0.00005 0.00000 -0.01914 -0.01915 1.86038

A36 2.21579 -0.00076 0.00000 -0.02698 -0.03009 2.18570

A37 2.09906 0.00106 0.00000 0.00753 0.00611 2.10516

A38 1.87469 0.00055 0.00000 -0.01128 -0.01195 1.86274

A39 1.80663 -0.00121 0.00000 -0.03961 -0.03912 1.76751

A40 1.52916 -0.00012 0.00000 -0.01337 -0.01302 1.51614

A41 1.85526 0.00097 0.00000 0.02041 0.02035 1.87561

A42 2.20734 -0.00046 0.00000 0.00305 0.00196 2.20930

A43 2.09217 -0.00020 0.00000 0.00933 0.00842 2.10059

A44 1.89974 -0.00080 0.00000 0.00392 0.00384 1.90359

A45 2.02661 0.00035 0.00000 0.00446 0.00448 2.03109

A46 2.35673 0.00045 0.00000 -0.00829 -0.00826 2.34847

A47 1.90584 0.00003 0.00000 -0.00372 -0.00377 1.90207

A48 2.02715 0.00007 0.00000 -0.00495 -0.00492 2.02223

A49 2.35019 -0.00010 0.00000 0.00867 0.00868 2.35888

D1 -0.58498 0.00006 0.00000 0.01643 0.01707 -0.56791

D2 2.99730 -0.00046 0.00000 -0.09357 -0.09363 2.90366

D3 1.22983 -0.00103 0.00000 -0.05036 -0.04983 1.18000

D4 2.73419 0.00020 0.00000 -0.01248 -0.01252 2.72167

D5 0.03328 -0.00032 0.00000 -0.12248 -0.12322 -0.08994

D6 -1.73419 -0.00089 0.00000 -0.07927 -0.07941 -1.81360

D7 -0.05360 0.00035 0.00000 0.01632 0.01636 -0.03724

D8 -2.99701 -0.00070 0.00000 -0.01373 -0.01252 -3.00953

D9 2.90569 0.00090 0.00000 0.05513 0.05409 2.95979

D10 -0.03771 -0.00015 0.00000 0.02508 0.02522 -0.01250

D11 2.84614 -0.00021 0.00000 -0.08841 -0.08878 2.75736

D12 -1.41844 -0.00034 0.00000 -0.09047 -0.09068 -1.50912

D13 0.68126 -0.00028 0.00000 -0.08748 -0.08760 0.59366

D14 -0.72370 0.00054 0.00000 0.02119 0.02106 -0.70264

D15 1.29490 0.00041 0.00000 0.01913 0.01917 1.31407

D16 -2.88858 0.00046 0.00000 0.02212 0.02224 -2.86634

D17 1.09916 -0.00029 0.00000 -0.03675 -0.03629 1.06287

D18 3.11776 -0.00041 0.00000 -0.03881 -0.03819 3.07958

D19 -1.06572 -0.00036 0.00000 -0.03582 -0.03511 -1.10083

D20 -0.89707 0.00049 0.00000 -0.03361 -0.03289 -0.92996

D21 -2.85534 -0.00027 0.00000 -0.03475 -0.03459 -2.88994

D22 1.33034 0.00007 0.00000 -0.03736 -0.03746 1.29289

D23 1.20756 0.00052 0.00000 -0.03097 -0.03031 1.17726

D24 -0.75071 -0.00025 0.00000 -0.03211 -0.03201 -0.78272

D25 -2.84821 0.00009 0.00000 -0.03472 -0.03487 -2.88308

D26 -2.99875 -0.00025 0.00000 -0.04388 -0.04302 -3.04177

D27 1.32616 -0.00101 0.00000 -0.04501 -0.04472 1.28144

D28 -0.77134 -0.00067 0.00000 -0.04763 -0.04758 -0.81893

D29 0.57438 -0.00058 0.00000 0.00822 0.00787 0.58226

D30 -2.75913 -0.00042 0.00000 0.01822 0.01873 -2.74040

D31 -2.91109 -0.00028 0.00000 -0.08649 -0.08779 -2.99887

D32 0.03859 -0.00012 0.00000 -0.07649 -0.07693 -0.03834

D33 -1.18071 0.00008 0.00000 -0.03894 -0.03859 -1.21930

D34 1.76896 0.00024 0.00000 -0.02894 -0.02773 1.74123

D35 -0.43009 0.00062 0.00000 -0.07682 -0.07634 -0.50643

D36 -2.57859 0.00039 0.00000 -0.09662 -0.09582 -2.67440

D37 1.69483 0.00020 0.00000 -0.09580 -0.09516 1.59967

D38 3.04009 0.00013 0.00000 0.00528 0.00429 3.04439

D39 0.89160 -0.00011 0.00000 -0.01452 -0.01518 0.87642

D40 -1.11817 -0.00029 0.00000 -0.01370 -0.01452 -1.13270

D41 1.24350 0.00007 0.00000 -0.02909 -0.02951 1.21400

D42 -0.90499 -0.00017 0.00000 -0.04888 -0.04898 -0.95397

D43 -2.91476 -0.00035 0.00000 -0.04807 -0.04833 -2.96309

D44 1.18891 -0.00142 0.00000 -0.04739 -0.04725 1.14165

D45 3.13430 -0.00212 0.00000 -0.07044 -0.07066 3.06364

D46 -1.04823 -0.00095 0.00000 -0.05136 -0.05286 -1.10109

D47 -0.93819 -0.00030 0.00000 -0.03022 -0.02995 -0.96815

D48 1.00720 -0.00100 0.00000 -0.05326 -0.05336 0.95384

D49 3.10786 0.00017 0.00000 -0.03419 -0.03556 3.07230

D50 -2.98851 -0.00030 0.00000 -0.01831 -0.01790 -3.00641

D51 -1.04312 -0.00100 0.00000 -0.04135 -0.04131 -1.08443

D52 1.05754 0.00017 0.00000 -0.02228 -0.02350 1.03403

D53 -0.17697 0.00054 0.00000 0.11314 0.11320 -0.06376

D54 1.97019 0.00057 0.00000 0.13030 0.13017 2.10035

D55 -2.28806 0.00072 0.00000 0.13210 0.13210 -2.15596

D56 -2.34820 0.00056 0.00000 0.10943 0.10966 -2.23854

D57 -0.20104 0.00059 0.00000 0.12659 0.12662 -0.07442

D58 1.82390 0.00074 0.00000 0.12839 0.12856 1.95245

D59 1.90302 0.00018 0.00000 0.11065 0.11070 2.01373

D60 -2.23301 0.00021 0.00000 0.12782 0.12767 -2.10534

D61 -0.20807 0.00036 0.00000 0.12961 0.12960 -0.07847

D62 -0.03917 0.00047 0.00000 0.00680 0.00700 -0.03217

D63 3.08962 0.00039 0.00000 0.01266 0.01274 3.10235

D64 -0.00560 0.00000 0.00000 0.00943 0.00924 0.00364

D65 3.13653 -0.00013 0.00000 0.01313 0.01254 -3.13412

D66 -0.16290 -0.00043 0.00000 0.04243 0.04250 -0.12040

D67 1.76208 -0.00113 0.00000 0.00181 0.00193 1.76401

D68 -1.91221 -0.00051 0.00000 0.06785 0.06839 -1.84382

D69 -1.99681 0.00136 0.00000 0.06678 0.06669 -1.93012

D70 -0.07183 0.00066 0.00000 0.02615 0.02612 -0.04571

D71 2.53706 0.00128 0.00000 0.09220 0.09259 2.62965

D72 1.59122 0.00047 0.00000 0.15543 0.15377 1.74499

D73 -2.76699 -0.00024 0.00000 0.11480 0.11320 -2.65378

D74 -0.15809 0.00039 0.00000 0.18084 0.17966 0.02157

D75 -1.85713 0.00016 0.00000 -0.03259 -0.03224 -1.88936

D76 1.30074 0.00026 0.00000 -0.04021 -0.03962 1.26112

D77 0.07147 -0.00074 0.00000 -0.02212 -0.02195 0.04951

D78 -3.05385 -0.00064 0.00000 -0.02974 -0.02934 -3.08319

D79 2.80212 -0.00044 0.00000 -0.11358 -0.11475 2.68737

D80 -0.32320 -0.00034 0.00000 -0.12120 -0.12214 -0.44534

D81 2.02239 0.00008 0.00000 -0.04338 -0.04440 1.97799

D82 -1.11988 0.00024 0.00000 -0.04806 -0.04862 -1.16850

D83 0.04998 -0.00040 0.00000 -0.02209 -0.02218 0.02779

D84 -3.09229 -0.00023 0.00000 -0.02677 -0.02640 -3.11869

D85 -2.60122 -0.00084 0.00000 -0.08025 -0.08099 -2.68221

D86 0.53970 -0.00068 0.00000 -0.08492 -0.08521 0.45449

Item Value Threshold Converged?

Maximum Force 0.004437 0.000450 NO

RMS Force 0.001032 0.000300 NO

Maximum Displacement 0.311169 0.001800 NO

RMS Displacement 0.059879 0.001200 NO

Predicted change in Energy=-3.502114D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.151678 1.572583 0.438943

2 6 0 0.124897 1.231268 0.095919

3 6 0 -0.701435 3.779818 -0.365101

4 6 0 -1.599901 2.890110 0.182085

5 1 0 -1.787146 0.896240 1.029397

6 1 0 -2.583214 3.178496 0.580338

7 6 0 0.767121 1.850983 -1.090554

8 1 0 1.886907 1.792861 -1.017545

9 1 0 0.474347 1.228488 -1.982711

10 6 0 0.340213 3.292893 -1.319217

11 1 0 1.234946 3.972227 -1.284192

12 1 0 -0.085462 3.385029 -2.357646

13 1 0 -0.942288 4.853358 -0.467015

14 1 0 0.575809 0.301958 0.476956

15 8 0 2.708930 3.962383 0.787224

16 6 0 0.440597 3.862244 1.440017

17 6 0 1.000773 2.589775 1.651980

18 6 0 1.541937 4.733787 0.931343

19 8 0 1.633390 5.914862 0.639018

20 6 0 2.415768 2.649715 1.220425

21 8 0 3.338140 1.852146 1.164852

22 1 0 -0.389145 4.289021 2.009959

23 1 0 0.680094 1.852761 2.389981

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.365212 0.000000

3 C 2.391880 2.718542 0.000000

4 C 1.415188 2.394600 1.377765 0.000000

5 H 1.099953 2.153958 3.382073 2.174515 0.000000

6 H 2.155979 3.370493 2.190100 1.099398 2.458469

7 C 2.469546 1.484660 2.530482 2.881351 3.453984

8 H 3.376814 2.158672 3.327640 3.847193 4.300298

9 H 2.937136 2.107801 3.241667 3.427803 3.781208

10 C 2.876861 2.509834 1.494143 2.485998 3.973108

11 H 3.797822 3.263398 2.152049 3.370060 4.893611

12 H 3.498955 3.271531 2.122620 2.998117 4.534519

13 H 3.409998 3.817763 1.104937 2.169823 4.314141

14 H 2.144795 1.100968 3.799464 3.393994 2.498384

15 O 4.553760 3.822841 3.604410 4.481293 5.447438

16 C 2.963112 2.971246 2.137635 2.586710 3.732108

17 C 2.671924 2.243663 2.895225 3.002382 3.320867

18 C 4.182251 3.869570 2.761076 3.719097 5.081257

19 O 5.162559 4.950410 3.319349 4.451077 6.085970

20 C 3.807571 2.919691 3.675320 4.154701 4.558032

21 O 4.556705 3.442824 4.730205 5.140764 5.215426

22 H 3.229332 3.643850 2.449026 2.600771 3.798272

23 H 2.690806 2.440742 3.634921 3.339053 2.975466

6 7 8 9 10

6 H 0.000000

7 C 3.972268 0.000000

8 H 4.945219 1.123668 0.000000

9 H 4.440769 1.126571 1.801496 0.000000

10 C 3.488241 1.521066 2.175629 2.172552 0.000000

11 H 4.322595 2.180833 2.290369 2.931645 1.123952

12 H 3.861758 2.164651 2.867247 2.259343 1.126065

13 H 2.568025 3.510717 4.204054 4.176586 2.192284

14 H 4.273709 2.212050 2.485016 2.630345 3.496775

15 O 5.353884 3.428510 2.939343 4.487770 3.239773

16 C 3.217140 3.248935 3.523318 4.318898 2.819150

17 C 3.786815 2.849894 2.923468 3.916785 3.123895

18 C 4.422556 3.605408 3.544886 4.681729 2.930074

19 O 5.027016 4.500772 4.449647 5.493536 3.518765

20 C 5.067459 2.949006 2.454058 4.006131 3.342362

21 O 6.096171 3.420088 2.621536 4.300862 4.151375

22 H 2.844472 4.110251 4.536189 5.104302 3.550725

23 H 3.959995 3.481623 3.615414 4.421819 3.993451

11 12 13 14 15

11 H 0.000000

12 H 1.800161 0.000000

13 H 2.486869 2.542564 0.000000

14 H 4.123952 4.239997 4.889882 0.000000

15 O 2.542340 4.246430 3.962114 4.247962 0.000000

16 C 2.839789 3.863511 2.555669 3.690720 2.362521

17 C 3.253785 4.229590 3.659157 2.606795 2.355771

18 C 2.362798 3.909607 2.853257 4.558616 1.406310

19 O 2.762485 4.281881 2.997369 5.713968 2.234038

20 C 3.068629 4.427124 4.356608 3.074111 1.413047

21 O 3.862122 5.145753 5.476525 3.241413 2.234191

22 H 3.686388 4.470504 2.599970 4.379259 3.346617

23 H 4.277796 5.047166 4.449509 2.464860 3.336991

16 17 18 19 20

16 C 0.000000

17 C 1.406380 0.000000

18 C 1.493749 2.325718 0.000000

19 O 2.505513 3.533058 1.220145 0.000000

20 C 2.328036 1.480555 2.278268 3.407540 0.000000

21 O 3.537226 2.498935 3.403635 4.437154 1.220645

22 H 1.093363 2.224289 2.256170 2.934874 3.343385

23 H 2.235579 1.091178 3.342261 4.524965 2.239545

21 22 23

21 O 0.000000

22 H 4.532684 0.000000

23 H 2.926799 2.687573 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.363115 -0.439266 -0.716775

2 6 0 1.563641 -1.275846 0.007642

3 6 0 1.199906 1.405967 0.264627

4 6 0 2.198135 0.958918 -0.573180

5 1 0 3.029996 -0.821872 -1.503400

6 1 0 2.761790 1.609479 -1.257095

7 6 0 1.096634 -0.873618 1.358320

8 1 0 0.170403 -1.439851 1.648329

9 1 0 1.898748 -1.182593 2.086544

10 6 0 0.847395 0.621414 1.486378

11 1 0 -0.224445 0.813206 1.765019

12 1 0 1.470434 1.021867 2.334602

13 1 0 0.929772 2.475934 0.320154

14 1 0 1.507873 -2.347323 -0.239255

15 8 0 -2.068206 -0.114221 0.280459

16 6 0 -0.330805 0.742561 -1.071898

17 6 0 -0.266489 -0.660913 -1.135381

18 6 0 -1.500874 1.077192 -0.205731

19 8 0 -2.040406 2.115271 0.140754

20 6 0 -1.341795 -1.194639 -0.268838

21 8 0 -1.720042 -2.309448 0.053817

22 1 0 -0.011066 1.425084 -1.863966

23 1 0 0.122544 -1.257369 -1.962159

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2228434 0.8834213 0.6762466

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.9026739809 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.487899102911E-01 A.U. after 15 cycles

Convg = 0.4816D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.021778181 0.009194210 0.003930824

2 6 0.015205631 -0.008336589 -0.005041908

3 6 -0.001291167 0.006500867 -0.014462658

4 6 -0.004818798 -0.016083413 0.005848234

5 1 0.000178066 0.000195808 0.001250292

6 1 0.000888127 0.004271342 -0.001070882

7 6 0.002581366 0.001614551 -0.001495811

8 1 0.000043058 -0.000485008 0.000612342

9 1 0.000316592 0.000218120 -0.000403554

10 6 -0.000321514 0.000929591 -0.000879514

11 1 0.000376937 -0.000487911 -0.000999951

12 1 -0.000323321 0.000390414 0.000222226

13 1 -0.000185857 -0.000687745 0.002540593

14 1 0.001438002 -0.001354035 -0.001375515

15 8 0.000918779 -0.000676496 0.000570869

16 6 0.011208687 -0.002801376 0.011305661

17 6 -0.003408259 0.006811717 0.005445781

18 6 -0.001826944 0.000723771 -0.000386019

19 8 -0.000125270 0.000336020 -0.000146572

20 6 0.003338514 -0.000150067 -0.002061192

21 8 0.000023244 0.000372361 0.000269216

22 1 -0.000990538 0.000605199 -0.002318311

23 1 -0.001447153 -0.001101333 -0.001354151

-------------------------------------------------------------------

Cartesian Forces: Max 0.021778181 RMS 0.005250644

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.020313307 RMS 0.002253571

Search for a saddle point.

Step number 33 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 32 33

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06325 -0.00246 0.00397 0.00560 0.00827

Eigenvalues --- 0.01020 0.01092 0.01734 0.02101 0.02248

Eigenvalues --- 0.02369 0.02509 0.02688 0.02918 0.03131

Eigenvalues --- 0.03190 0.03268 0.03651 0.03729 0.03753

Eigenvalues --- 0.03917 0.04120 0.04446 0.05117 0.05221

Eigenvalues --- 0.05814 0.06058 0.06363 0.07095 0.07342

Eigenvalues --- 0.08107 0.08794 0.09169 0.09783 0.09834

Eigenvalues --- 0.11945 0.13736 0.14441 0.16196 0.21316

Eigenvalues --- 0.22757 0.25968 0.27131 0.28110 0.29864

Eigenvalues --- 0.30860 0.31278 0.31446 0.31826 0.32032

Eigenvalues --- 0.32403 0.32587 0.33604 0.35431 0.36449

Eigenvalues --- 0.38031 0.39611 0.40428 0.43815 0.47286

Eigenvalues --- 0.51634 1.08456 1.10848

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D86

1 0.55095 0.48343 -0.19097 0.18190 -0.16344

D71 D85 D68 D12 D11

1 0.16185 -0.15003 0.13876 -0.13780 -0.13438

RFO step: Lambda0=1.065667589D-03 Lambda=-6.19319032D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.09209720 RMS(Int)= 0.00352504

Iteration 2 RMS(Cart)= 0.00436540 RMS(Int)= 0.00088810

Iteration 3 RMS(Cart)= 0.00000906 RMS(Int)= 0.00088806

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00088806

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.57988 0.02031 0.00000 0.08674 0.08688 2.66675

R2 2.67432 -0.00618 0.00000 -0.06054 -0.06015 2.61416

R3 2.07861 0.00045 0.00000 -0.00006 -0.00006 2.07855

R4 2.80560 0.00321 0.00000 0.03157 0.03230 2.83790

R5 2.08053 0.00126 0.00000 0.00106 0.00106 2.08158

R6 4.23991 0.00553 0.00000 -0.08355 -0.08455 4.15536

R7 2.60360 0.00972 0.00000 0.08144 0.08165 2.68525

R8 2.82352 0.00153 0.00000 -0.01929 -0.01947 2.80405

R9 2.08803 -0.00086 0.00000 -0.00477 -0.00477 2.08325

R10 4.03954 0.00978 0.00000 0.01186 0.01221 4.05175

R11 2.07756 -0.00006 0.00000 0.00183 0.00183 2.07939

R12 2.12342 0.00011 0.00000 -0.00130 -0.00130 2.12213

R13 2.12891 0.00012 0.00000 -0.00007 -0.00007 2.12884

R14 2.87440 0.00148 0.00000 0.00129 0.00204 2.87644

R15 2.12396 -0.00003 0.00000 0.00040 0.00040 2.12437

R16 2.12796 -0.00005 0.00000 0.00105 0.00105 2.12900

R17 2.65754 0.00067 0.00000 0.01007 0.01012 2.66766

R18 2.67027 -0.00068 0.00000 -0.00472 -0.00465 2.66562

R19 2.65767 -0.00251 0.00000 -0.01289 -0.01405 2.64362

R20 2.82278 -0.00014 0.00000 -0.00906 -0.00910 2.81368

R21 2.06616 -0.00022 0.00000 0.00318 0.00318 2.06934

R22 2.79784 0.00372 0.00000 0.00929 0.00928 2.80713

R23 2.06203 0.00025 0.00000 0.00108 0.00108 2.06311

R24 2.30574 0.00035 0.00000 0.00088 0.00088 2.30662

R25 2.30669 -0.00024 0.00000 0.00046 0.00046 2.30715

A1 2.07523 -0.00287 0.00000 -0.03064 -0.03104 2.04419

A2 2.11925 0.00130 0.00000 -0.01975 -0.01935 2.09990

A3 2.07934 0.00149 0.00000 0.04805 0.04787 2.12721

A4 2.09547 -0.00013 0.00000 0.00719 0.00624 2.10171

A5 2.10254 0.00053 0.00000 0.01557 0.01545 2.11799

A6 1.61020 -0.00035 0.00000 0.00475 0.00440 1.61460

A7 2.03952 -0.00040 0.00000 -0.03396 -0.03345 2.00607

A8 1.70383 0.00006 0.00000 0.03876 0.03752 1.74135

A9 1.68220 0.00029 0.00000 -0.00710 -0.00567 1.67653

A10 2.09185 0.00160 0.00000 0.00405 0.00237 2.09422

A11 2.11987 -0.00170 0.00000 -0.04861 -0.04839 2.07148

A12 1.60872 -0.00018 0.00000 0.02080 0.02085 1.62957

A13 1.99292 0.00045 0.00000 0.03594 0.03724 2.03016

A14 1.75112 -0.00049 0.00000 0.03470 0.03360 1.78472

A15 1.72833 -0.00020 0.00000 -0.03775 -0.03791 1.69041

A16 2.05640 0.00125 0.00000 -0.00083 -0.00127 2.05513

A17 2.05076 0.00383 0.00000 0.10981 0.11023 2.16099

A18 2.16245 -0.00515 0.00000 -0.10417 -0.10453 2.05793

A19 1.93645 -0.00051 0.00000 -0.02063 -0.02043 1.91603

A20 1.86482 0.00026 0.00000 0.01171 0.01264 1.87746

A21 1.97623 0.00008 0.00000 0.00002 -0.00175 1.97449

A22 1.85652 -0.00002 0.00000 0.00155 0.00136 1.85788

A23 1.91611 0.00052 0.00000 0.01925 0.01997 1.93608

A24 1.90902 -0.00036 0.00000 -0.01222 -0.01186 1.89716

A25 1.99171 0.00032 0.00000 -0.01971 -0.02255 1.96916

A26 1.91570 0.00062 0.00000 0.02173 0.02311 1.93881

A27 1.87410 -0.00050 0.00000 -0.01147 -0.01117 1.86293

A28 1.92288 -0.00094 0.00000 0.00171 0.00222 1.92510

A29 1.89894 0.00063 0.00000 0.00469 0.00568 1.90462

A30 1.85481 -0.00015 0.00000 0.00412 0.00374 1.85855

A31 1.88177 -0.00046 0.00000 0.00146 0.00117 1.88294

A32 1.88092 -0.00041 0.00000 -0.00748 -0.01052 1.87041

A33 1.69999 0.00010 0.00000 0.02921 0.03053 1.73052

A34 1.62062 -0.00097 0.00000 -0.01708 -0.01598 1.60464

A35 1.86038 0.00092 0.00000 0.00914 0.00896 1.86934

A36 2.18570 0.00067 0.00000 0.00085 0.00144 2.18714

A37 2.10516 -0.00092 0.00000 -0.01092 -0.01107 2.09409

A38 1.86274 0.00107 0.00000 0.01489 0.01104 1.87378

A39 1.76751 -0.00007 0.00000 -0.05124 -0.04960 1.71791

A40 1.51614 -0.00115 0.00000 0.04351 0.04494 1.56108

A41 1.87561 -0.00065 0.00000 -0.00072 -0.00080 1.87481

A42 2.20930 0.00055 0.00000 -0.00533 -0.00531 2.20399

A43 2.10059 0.00024 0.00000 -0.00072 -0.00052 2.10007

A44 1.90359 0.00030 0.00000 -0.00450 -0.00481 1.89878

A45 2.03109 0.00000 0.00000 0.00040 0.00053 2.03162

A46 2.34847 -0.00030 0.00000 0.00418 0.00431 2.35278

A47 1.90207 -0.00008 0.00000 -0.00293 -0.00318 1.89889

A48 2.02223 -0.00017 0.00000 0.00283 0.00296 2.02519

A49 2.35888 0.00025 0.00000 0.00011 0.00023 2.35911

D1 -0.56791 0.00045 0.00000 -0.04937 -0.04957 -0.61748

D2 2.90366 0.00048 0.00000 -0.00378 -0.00395 2.89972

D3 1.18000 0.00029 0.00000 -0.00038 -0.00206 1.17794

D4 2.72167 0.00098 0.00000 -0.03508 -0.03557 2.68610

D5 -0.08994 0.00101 0.00000 0.01051 0.01005 -0.07988

D6 -1.81360 0.00082 0.00000 0.01391 0.01194 -1.80166

D7 -0.03724 0.00031 0.00000 0.04734 0.04743 0.01019

D8 -3.00953 0.00127 0.00000 0.02828 0.02637 -2.98315

D9 2.95979 -0.00022 0.00000 0.02773 0.02728 2.98707

D10 -0.01250 0.00074 0.00000 0.00866 0.00623 -0.00627

D11 2.75736 -0.00004 0.00000 -0.01674 -0.01754 2.73982

D12 -1.50912 -0.00018 0.00000 -0.01894 -0.01949 -1.52861

D13 0.59366 -0.00040 0.00000 -0.02621 -0.02679 0.56687

D14 -0.70264 0.00010 0.00000 -0.05193 -0.05189 -0.75453

D15 1.31407 -0.00004 0.00000 -0.05412 -0.05384 1.26022

D16 -2.86634 -0.00026 0.00000 -0.06140 -0.06114 -2.92748

D17 1.06287 0.00036 0.00000 -0.04706 -0.04710 1.01577

D18 3.07958 0.00022 0.00000 -0.04925 -0.04905 3.03053

D19 -1.10083 0.00001 0.00000 -0.05653 -0.05634 -1.15717

D20 -0.92996 -0.00058 0.00000 -0.12823 -0.12915 -1.05911

D21 -2.88994 -0.00020 0.00000 -0.11165 -0.11187 -3.00181

D22 1.29289 -0.00021 0.00000 -0.11684 -0.11633 1.17655

D23 1.17726 -0.00076 0.00000 -0.11521 -0.11659 1.06066

D24 -0.78272 -0.00039 0.00000 -0.09863 -0.09931 -0.88203

D25 -2.88308 -0.00040 0.00000 -0.10381 -0.10378 -2.98686

D26 -3.04177 -0.00110 0.00000 -0.14392 -0.14481 3.09660

D27 1.28144 -0.00072 0.00000 -0.12734 -0.12754 1.15390

D28 -0.81893 -0.00073 0.00000 -0.13253 -0.13200 -0.95092

D29 0.58226 -0.00002 0.00000 0.04808 0.04783 0.63008

D30 -2.74040 -0.00005 0.00000 0.09177 0.08956 -2.65084

D31 -2.99887 0.00101 0.00000 0.03418 0.03483 -2.96405

D32 -0.03834 0.00098 0.00000 0.07787 0.07656 0.03822

D33 -1.21930 0.00037 0.00000 -0.00554 -0.00468 -1.22398

D34 1.74123 0.00034 0.00000 0.03815 0.03706 1.77829

D35 -0.50643 -0.00048 0.00000 -0.12242 -0.12308 -0.62951

D36 -2.67440 0.00004 0.00000 -0.12720 -0.12719 -2.80159

D37 1.59967 0.00017 0.00000 -0.13700 -0.13733 1.46234

D38 3.04439 -0.00089 0.00000 -0.08971 -0.09009 2.95429

D39 0.87642 -0.00038 0.00000 -0.09448 -0.09420 0.78222

D40 -1.13270 -0.00025 0.00000 -0.10428 -0.10434 -1.23704

D41 1.21400 -0.00055 0.00000 -0.07559 -0.07668 1.13732

D42 -0.95397 -0.00003 0.00000 -0.08037 -0.08079 -1.03476

D43 -2.96309 0.00010 0.00000 -0.09017 -0.09093 -3.05401

D44 1.14165 0.00111 0.00000 -0.10475 -0.10424 1.03741

D45 3.06364 0.00204 0.00000 -0.08542 -0.08547 2.97817

D46 -1.10109 0.00094 0.00000 -0.09563 -0.09571 -1.19680

D47 -0.96815 -0.00041 0.00000 -0.11912 -0.11816 -1.08631

D48 0.95384 0.00051 0.00000 -0.09979 -0.09939 0.85445

D49 3.07230 -0.00059 0.00000 -0.11001 -0.10963 2.96267

D50 -3.00641 -0.00070 0.00000 -0.15555 -0.15488 3.12189

D51 -1.08443 0.00023 0.00000 -0.13622 -0.13611 -1.22054

D52 1.03403 -0.00087 0.00000 -0.14644 -0.14635 0.88768

D53 -0.06376 0.00001 0.00000 0.10885 0.10811 0.04434

D54 2.10035 0.00034 0.00000 0.12431 0.12355 2.22390

D55 -2.15596 -0.00001 0.00000 0.13292 0.13263 -2.02333

D56 -2.23854 0.00021 0.00000 0.12108 0.12089 -2.11765

D57 -0.07442 0.00054 0.00000 0.13654 0.13633 0.06191

D58 1.95245 0.00020 0.00000 0.14516 0.14541 2.09786

D59 2.01373 0.00015 0.00000 0.11526 0.11481 2.12853

D60 -2.10534 0.00048 0.00000 0.13072 0.13025 -1.97509

D61 -0.07847 0.00013 0.00000 0.13933 0.13933 0.06086

D62 -0.03217 0.00047 0.00000 0.02490 0.02541 -0.00676

D63 3.10235 0.00046 0.00000 0.03488 0.03570 3.13805

D64 0.00364 -0.00023 0.00000 0.00218 0.00142 0.00505

D65 -3.13412 -0.00002 0.00000 0.00101 0.00002 -3.13410

D66 -0.12040 0.00057 0.00000 0.12821 0.12820 0.00780

D67 1.76401 0.00068 0.00000 0.07646 0.07662 1.84063

D68 -1.84382 0.00099 0.00000 0.06141 0.06225 -1.78157

D69 -1.93012 0.00025 0.00000 0.09474 0.09453 -1.83559

D70 -0.04571 0.00036 0.00000 0.04298 0.04294 -0.00277

D71 2.62965 0.00067 0.00000 0.02794 0.02858 2.65822

D72 1.74499 -0.00070 0.00000 0.09952 0.09894 1.84393

D73 -2.65378 -0.00059 0.00000 0.04776 0.04735 -2.60643

D74 0.02157 -0.00028 0.00000 0.03271 0.03299 0.05456

D75 -1.88936 -0.00030 0.00000 -0.04831 -0.04627 -1.93564

D76 1.26112 -0.00030 0.00000 -0.06082 -0.05923 1.20189

D77 0.04951 -0.00047 0.00000 -0.04322 -0.04355 0.00597

D78 -3.08319 -0.00047 0.00000 -0.05574 -0.05651 -3.13970

D79 2.68737 0.00098 0.00000 -0.04378 -0.04352 2.64385

D80 -0.44534 0.00098 0.00000 -0.05630 -0.05647 -0.50181

D81 1.97799 0.00083 0.00000 -0.03502 -0.03742 1.94056

D82 -1.16850 0.00056 0.00000 -0.03352 -0.03564 -1.20414

D83 0.02779 -0.00010 0.00000 -0.02976 -0.02910 -0.00131

D84 -3.11869 -0.00037 0.00000 -0.02825 -0.02732 3.13718

D85 -2.68221 -0.00051 0.00000 -0.01437 -0.01423 -2.69645

D86 0.45449 -0.00078 0.00000 -0.01286 -0.01245 0.44204

Item Value Threshold Converged?

Maximum Force 0.020313 0.000450 NO

RMS Force 0.002254 0.000300 NO

Maximum Displacement 0.344504 0.001800 NO

RMS Displacement 0.092189 0.001200 NO

Predicted change in Energy=-4.646536D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.157107 1.544485 0.438915

2 6 0 0.185753 1.278691 0.096094

3 6 0 -0.722037 3.769341 -0.351076

4 6 0 -1.623022 2.827656 0.215150

5 1 0 -1.743569 0.803404 1.001669

6 1 0 -2.597273 3.195988 0.570075

7 6 0 0.808915 1.935441 -1.102072

8 1 0 1.925794 1.954993 -0.986796

9 1 0 0.591907 1.286426 -1.996928

10 6 0 0.265285 3.331962 -1.368756

11 1 0 1.109580 4.069040 -1.456111

12 1 0 -0.267765 3.337281 -2.361279

13 1 0 -1.015661 4.831542 -0.379776

14 1 0 0.696309 0.366702 0.443898

15 8 0 2.756841 3.844154 0.830960

16 6 0 0.474302 3.882479 1.424627

17 6 0 0.952366 2.593438 1.683229

18 6 0 1.616575 4.674242 0.890539

19 8 0 1.762740 5.825306 0.511626

20 6 0 2.390103 2.569276 1.310479

21 8 0 3.275934 1.729370 1.331283

22 1 0 -0.327421 4.383049 1.977614

23 1 0 0.565051 1.898739 2.431092

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.411186 0.000000

3 C 2.400699 2.688379 0.000000

4 C 1.383356 2.384352 1.420971 0.000000

5 H 1.099923 2.183632 3.416172 2.175026 0.000000

6 H 2.195163 3.412612 2.166509 1.100366 2.576731

7 C 2.528385 1.501750 2.504197 2.906104 3.496056

8 H 3.421322 2.158188 3.272157 3.847117 4.329477

9 H 3.009813 2.132079 3.255787 3.489211 3.831363

10 C 2.913065 2.523496 1.483839 2.515709 4.005998

11 H 3.886177 3.323980 2.160033 3.435296 4.984528

12 H 3.441821 3.237615 2.105696 2.955406 4.461832

13 H 3.390428 3.780555 1.102410 2.176783 4.320201

14 H 2.195985 1.101526 3.771160 3.389383 2.540634

15 O 4.556442 3.705688 3.674969 4.538247 5.434058

16 C 3.016511 2.937341 2.144096 2.640881 3.818186

17 C 2.664300 2.198921 2.885268 2.973674 3.307085

18 C 4.206264 3.769372 2.798135 3.789593 5.127017

19 O 5.182299 4.830245 3.338468 4.531798 6.144416

20 C 3.793748 2.828339 3.726438 4.167935 4.505653

21 O 4.525744 3.358277 4.793286 5.143127 5.114828

22 H 3.333680 3.666130 2.440319 2.684047 3.971373

23 H 2.657084 2.445515 3.591130 3.249762 2.927924

6 7 8 9 10

6 H 0.000000

7 C 3.998396 0.000000

8 H 4.941867 1.122982 0.000000

9 H 4.517389 1.126535 1.801833 0.000000

10 C 3.460028 1.522145 2.190714 2.164601 0.000000

11 H 4.313746 2.183573 2.314230 2.881564 1.124166

12 H 3.746920 2.170253 2.934557 2.253396 1.126620

13 H 2.465512 3.498313 4.158746 4.215128 2.206274

14 H 4.343784 2.205367 2.466006 2.610445 3.502038

15 O 5.399510 3.342785 2.750238 4.384730 3.362877

16 C 3.261303 3.207355 3.411303 4.296552 2.854776

17 C 3.768569 2.865561 2.912766 3.921960 3.214361

18 C 4.477102 3.481931 3.318783 4.567790 2.955016

19 O 5.091802 4.317969 4.153454 5.316496 3.463376

20 C 5.080835 2.953355 2.422891 3.977204 3.503548

21 O 6.101226 3.471291 2.692076 4.298510 4.350002

22 H 2.922757 4.094693 4.445240 5.121643 3.557286

23 H 3.891855 3.541760 3.679231 4.470236 4.072203

11 12 13 14 15

11 H 0.000000

12 H 1.803297 0.000000

13 H 2.501311 2.592010 0.000000

14 H 4.181882 4.197952 4.852224 0.000000

15 O 2.827497 4.426686 4.083208 4.060577 0.000000

16 C 2.955847 3.896278 2.525190 3.656748 2.358790

17 C 3.472402 4.289530 3.624670 2.561223 2.355161

18 C 2.475900 3.989051 2.926963 4.427334 1.411666

19 O 2.717182 4.308922 3.082480 5.562214 2.239458

20 C 3.397507 4.597380 4.424256 2.910539 1.410585

21 O 4.235175 5.364531 5.564978 3.049391 2.234299

22 H 3.735511 4.463539 2.496420 4.419429 3.334350

23 H 4.485206 5.072456 4.359010 2.512630 3.339013

16 17 18 19 20

16 C 0.000000

17 C 1.398945 0.000000

18 C 1.488934 2.323634 0.000000

19 O 2.503642 3.531902 1.220610 0.000000

20 C 2.325473 1.485468 2.281573 3.410789 0.000000

21 O 3.534647 2.503887 3.408812 4.442779 1.220889

22 H 1.095046 2.219735 2.246251 2.932235 3.334633

23 H 2.226305 1.091750 3.344013 4.531748 2.244150

21 22 23

21 O 0.000000

22 H 4.521495 0.000000

23 H 2.930384 2.678422 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.331145 -0.691031 -0.664049

2 6 0 1.383283 -1.340926 0.154876

3 6 0 1.329736 1.346639 0.115974

4 6 0 2.299943 0.691737 -0.689606

5 1 0 2.951875 -1.271102 -1.362651

6 1 0 2.885227 1.304606 -1.391489

7 6 0 0.964021 -0.732853 1.462439

8 1 0 -0.044934 -1.126980 1.758684

9 1 0 1.688252 -1.086301 2.249613

10 6 0 0.968937 0.789160 1.442933

11 1 0 -0.022652 1.186893 1.792658

12 1 0 1.739868 1.165214 2.173358

13 1 0 1.175090 2.429954 -0.017526

14 1 0 1.191016 -2.421587 0.062334

15 8 0 -2.077535 -0.021405 0.272062

16 6 0 -0.307382 0.701592 -1.109142

17 6 0 -0.295337 -0.697299 -1.111312

18 6 0 -1.437271 1.128469 -0.238480

19 8 0 -1.896557 2.204747 0.108755

20 6 0 -1.410697 -1.152946 -0.242420

21 8 0 -1.852578 -2.237809 0.101651

22 1 0 0.014523 1.338672 -1.939583

23 1 0 0.076828 -1.338888 -1.912421

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2155903 0.8790829 0.6770772

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.2723192532 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.484788319966E-01 A.U. after 16 cycles

Convg = 0.4203D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.015939156 -0.006430284 -0.002687774

2 6 -0.002616188 0.008219297 0.000999437

3 6 -0.012411586 -0.006688354 0.014648075

4 6 0.009499051 0.020450790 -0.011854205

5 1 0.000265475 0.001097306 -0.000317705

6 1 0.000532131 -0.004320952 0.001495328

7 6 -0.006700817 -0.004247225 0.006853036

8 1 -0.000102764 0.000911726 0.000001297

9 1 0.000281992 -0.000505015 0.001111344

10 6 0.000839250 -0.002905472 0.000226229

11 1 -0.000514441 -0.000151069 0.001166776

12 1 0.000782482 0.000089557 -0.000702542

13 1 0.000647489 0.000356413 -0.000700004

14 1 -0.002439480 -0.000890931 -0.000154113

15 8 -0.000879608 0.001962549 -0.000948449

16 6 -0.009741923 0.013305475 -0.006411874

17 6 0.002948533 -0.019691801 -0.002081401

18 6 0.002378259 -0.000413385 -0.000696573

19 8 0.000586803 -0.001061247 0.000330580

20 6 0.001399619 0.001053548 0.000523259

21 8 -0.000399960 0.000104393 -0.000118197

22 1 -0.000060604 -0.000042373 -0.001315175

23 1 -0.000232870 -0.000202947 0.000632650

-------------------------------------------------------------------

Cartesian Forces: Max 0.020450790 RMS 0.005808580

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.017203103 RMS 0.002601736

Search for a saddle point.

Step number 34 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 33 34

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06411 -0.00675 0.00128 0.00449 0.00746

Eigenvalues --- 0.00984 0.01032 0.01384 0.01988 0.02137

Eigenvalues --- 0.02384 0.02539 0.02653 0.02953 0.03085

Eigenvalues --- 0.03205 0.03301 0.03596 0.03676 0.03773

Eigenvalues --- 0.03978 0.04067 0.04237 0.04863 0.05185

Eigenvalues --- 0.05851 0.06050 0.06413 0.07135 0.07367

Eigenvalues --- 0.08487 0.08798 0.09625 0.09838 0.10215

Eigenvalues --- 0.11974 0.13835 0.14442 0.16324 0.21397

Eigenvalues --- 0.22860 0.25995 0.27180 0.28273 0.29850

Eigenvalues --- 0.30915 0.31290 0.31482 0.31841 0.32043

Eigenvalues --- 0.32442 0.32606 0.33997 0.36152 0.36651

Eigenvalues --- 0.38846 0.39612 0.40427 0.44340 0.47660

Eigenvalues --- 0.51858 1.08457 1.10854

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D86

1 -0.54329 -0.51092 0.19998 -0.17298 0.14148

D71 D29 D85 D1 D35

1 -0.13274 0.12993 0.12736 -0.12172 -0.12146

RFO step: Lambda0=5.282057640D-04 Lambda=-7.34126997D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.946

Iteration 1 RMS(Cart)= 0.06487583 RMS(Int)= 0.00340231

Iteration 2 RMS(Cart)= 0.00394565 RMS(Int)= 0.00115238

Iteration 3 RMS(Cart)= 0.00001285 RMS(Int)= 0.00115232

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00115232

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.66675 -0.01364 0.00000 -0.07298 -0.07225 2.59450

R2 2.61416 0.00812 0.00000 0.05921 0.05990 2.67406

R3 2.07855 -0.00104 0.00000 -0.00283 -0.00283 2.07572

R4 2.83790 -0.01039 0.00000 -0.06786 -0.06849 2.76941

R5 2.08158 -0.00044 0.00000 -0.00266 -0.00266 2.07892

R6 4.15536 -0.00664 0.00000 0.08376 0.08427 4.23963

R7 2.68525 -0.01720 0.00000 -0.09765 -0.09766 2.58758

R8 2.80405 0.00078 0.00000 0.01528 0.01607 2.82012

R9 2.08325 0.00019 0.00000 -0.00223 -0.00223 2.08102

R10 4.05175 -0.00644 0.00000 0.11869 0.11760 4.16935

R11 2.07939 -0.00144 0.00000 -0.00532 -0.00532 2.07407

R12 2.12213 -0.00009 0.00000 0.00364 0.00364 2.12577

R13 2.12884 -0.00065 0.00000 0.00078 0.00078 2.12962

R14 2.87644 0.00000 0.00000 0.00841 0.00860 2.88503

R15 2.12437 -0.00058 0.00000 -0.00422 -0.00422 2.12014

R16 2.12900 0.00025 0.00000 0.00427 0.00427 2.13328

R17 2.66766 -0.00038 0.00000 -0.00660 -0.00681 2.66086

R18 2.66562 0.00189 0.00000 0.00717 0.00731 2.67292

R19 2.64362 0.01250 0.00000 0.01882 0.01799 2.66161

R20 2.81368 0.00136 0.00000 -0.00016 -0.00044 2.81324

R21 2.06934 -0.00064 0.00000 -0.00982 -0.00982 2.05952

R22 2.80713 0.00059 0.00000 0.00680 0.00710 2.81423

R23 2.06311 0.00065 0.00000 -0.00187 -0.00187 2.06123

R24 2.30662 -0.00103 0.00000 0.00035 0.00035 2.30697

R25 2.30715 -0.00036 0.00000 0.00000 0.00000 2.30715

A1 2.04419 0.00280 0.00000 0.02547 0.02564 2.06983

A2 2.09990 -0.00083 0.00000 -0.01714 -0.01893 2.08097

A3 2.12721 -0.00188 0.00000 0.00337 0.00201 2.12922

A4 2.10171 -0.00222 0.00000 -0.01828 -0.01780 2.08391

A5 2.11799 0.00098 0.00000 -0.00735 -0.00871 2.10928

A6 1.61460 -0.00043 0.00000 -0.06231 -0.06242 1.55218

A7 2.00607 0.00102 0.00000 0.04095 0.04106 2.04713

A8 1.74135 0.00145 0.00000 0.02499 0.02324 1.76459

A9 1.67653 -0.00036 0.00000 -0.00410 -0.00476 1.67177

A10 2.09422 -0.00324 0.00000 -0.02315 -0.02431 2.06991

A11 2.07148 0.00226 0.00000 0.03654 0.03689 2.10837

A12 1.62957 0.00116 0.00000 -0.00923 -0.01031 1.61926

A13 2.03016 0.00098 0.00000 0.00574 0.00542 2.03558

A14 1.78472 -0.00083 0.00000 -0.03463 -0.03495 1.74977

A15 1.69041 -0.00022 0.00000 0.00260 0.00350 1.69391

A16 2.05513 0.00048 0.00000 0.02069 0.02061 2.07574

A17 2.16099 -0.00462 0.00000 -0.08418 -0.08531 2.07568

A18 2.05793 0.00414 0.00000 0.07089 0.07054 2.12847

A19 1.91603 -0.00055 0.00000 -0.00185 -0.00168 1.91435

A20 1.87746 -0.00059 0.00000 -0.01280 -0.01219 1.86527

A21 1.97449 0.00148 0.00000 0.01651 0.01526 1.98975

A22 1.85788 0.00031 0.00000 0.00994 0.00974 1.86762

A23 1.93608 -0.00043 0.00000 -0.00125 -0.00102 1.93507

A24 1.89716 -0.00030 0.00000 -0.01140 -0.01087 1.88629

A25 1.96916 0.00065 0.00000 0.02383 0.02400 1.99316

A26 1.93881 -0.00059 0.00000 0.00832 0.00819 1.94699

A27 1.86293 0.00020 0.00000 -0.01718 -0.01735 1.84558

A28 1.92510 0.00013 0.00000 -0.00013 -0.00053 1.92457

A29 1.90462 -0.00056 0.00000 -0.00820 -0.00819 1.89643

A30 1.85855 0.00014 0.00000 -0.00957 -0.00951 1.84903

A31 1.88294 0.00230 0.00000 0.00392 -0.00121 1.88173

A32 1.87041 -0.00071 0.00000 -0.03720 -0.03907 1.83134

A33 1.73052 0.00211 0.00000 0.00505 0.00640 1.73693

A34 1.60464 -0.00106 0.00000 -0.06390 -0.06203 1.54261

A35 1.86934 -0.00189 0.00000 -0.00026 -0.00272 1.86662

A36 2.18714 0.00100 0.00000 0.03076 0.02837 2.21551

A37 2.09409 0.00090 0.00000 0.02518 0.02405 2.11814

A38 1.87378 -0.00107 0.00000 0.03919 0.03691 1.91069

A39 1.71791 0.00104 0.00000 -0.07333 -0.07118 1.64674

A40 1.56108 0.00067 0.00000 0.02888 0.02907 1.59015

A41 1.87481 -0.00118 0.00000 -0.00496 -0.00578 1.86903

A42 2.20399 -0.00011 0.00000 -0.00668 -0.00671 2.19728

A43 2.10007 0.00108 0.00000 0.01065 0.01154 2.11161

A44 1.89878 0.00074 0.00000 0.00337 -0.00065 1.89813

A45 2.03162 -0.00118 0.00000 -0.00929 -0.00778 2.02384

A46 2.35278 0.00043 0.00000 0.00577 0.00730 2.36008

A47 1.89889 0.00002 0.00000 -0.00086 -0.00373 1.89516

A48 2.02519 0.00015 0.00000 -0.00845 -0.00710 2.01808

A49 2.35911 -0.00018 0.00000 0.00936 0.01071 2.36981

D1 -0.61748 -0.00003 0.00000 0.01338 0.01381 -0.60367

D2 2.89972 0.00044 0.00000 -0.04338 -0.04310 2.85662

D3 1.17794 0.00101 0.00000 0.00128 0.00136 1.17930

D4 2.68610 -0.00052 0.00000 -0.06615 -0.06457 2.62154

D5 -0.07988 -0.00005 0.00000 -0.12291 -0.12147 -0.20136

D6 -1.80166 0.00051 0.00000 -0.07825 -0.07701 -1.87867

D7 0.01019 -0.00056 0.00000 0.02010 0.02080 0.03099

D8 -2.98315 -0.00092 0.00000 -0.04596 -0.04198 -3.02514

D9 2.98707 0.00005 0.00000 0.09898 0.09946 3.08653

D10 -0.00627 -0.00031 0.00000 0.03292 0.03668 0.03041

D11 2.73982 -0.00058 0.00000 -0.00683 -0.00751 2.73231

D12 -1.52861 -0.00081 0.00000 -0.00306 -0.00354 -1.53215

D13 0.56687 -0.00068 0.00000 -0.01583 -0.01614 0.55074

D14 -0.75453 -0.00097 0.00000 0.03751 0.03774 -0.71679

D15 1.26022 -0.00121 0.00000 0.04128 0.04171 1.30194

D16 -2.92748 -0.00107 0.00000 0.02851 0.02911 -2.89837

D17 1.01577 -0.00037 0.00000 0.05662 0.05682 1.07259

D18 3.03053 -0.00061 0.00000 0.06040 0.06079 3.09132

D19 -1.15717 -0.00047 0.00000 0.04762 0.04819 -1.10898

D20 -1.05911 0.00167 0.00000 -0.07341 -0.07501 -1.13412

D21 -3.00181 0.00285 0.00000 -0.05020 -0.04946 -3.05127

D22 1.17655 0.00156 0.00000 -0.06021 -0.05981 1.11674

D23 1.06066 -0.00047 0.00000 -0.10251 -0.10421 0.95646

D24 -0.88203 0.00070 0.00000 -0.07931 -0.07866 -0.96069

D25 -2.98686 -0.00059 0.00000 -0.08931 -0.08901 -3.07587

D26 3.09660 0.00079 0.00000 -0.05600 -0.05778 3.03883

D27 1.15390 0.00196 0.00000 -0.03279 -0.03223 1.12167

D28 -0.95092 0.00068 0.00000 -0.04279 -0.04258 -0.99350

D29 0.63008 -0.00075 0.00000 -0.07633 -0.07602 0.55406

D30 -2.65084 -0.00116 0.00000 -0.02747 -0.02486 -2.67569

D31 -2.96405 -0.00050 0.00000 -0.02792 -0.02789 -2.99194

D32 0.03822 -0.00091 0.00000 0.02094 0.02327 0.06149

D33 -1.22398 0.00025 0.00000 -0.02455 -0.02425 -1.24823

D34 1.77829 -0.00016 0.00000 0.02431 0.02692 1.80520

D35 -0.62951 0.00060 0.00000 0.07398 0.07399 -0.55553

D36 -2.80159 0.00039 0.00000 0.04967 0.04927 -2.75232

D37 1.46234 0.00042 0.00000 0.06658 0.06629 1.52863

D38 2.95429 0.00000 0.00000 0.01871 0.01950 2.97379

D39 0.78222 -0.00021 0.00000 -0.00559 -0.00521 0.77700

D40 -1.23704 -0.00018 0.00000 0.01131 0.01180 -1.22524

D41 1.13732 0.00038 0.00000 0.03323 0.03327 1.17059

D42 -1.03476 0.00018 0.00000 0.00893 0.00856 -1.02620

D43 -3.05401 0.00020 0.00000 0.02583 0.02557 -3.02845

D44 1.03741 -0.00171 0.00000 -0.09582 -0.09433 0.94308

D45 2.97817 -0.00313 0.00000 -0.10500 -0.10605 2.87211

D46 -1.19680 -0.00215 0.00000 -0.09186 -0.09291 -1.28971

D47 -1.08631 0.00151 0.00000 -0.06194 -0.06013 -1.14643

D48 0.85445 0.00008 0.00000 -0.07112 -0.07185 0.78260

D49 2.96267 0.00107 0.00000 -0.05798 -0.05871 2.90396

D50 3.12189 0.00076 0.00000 -0.05991 -0.05815 3.06374

D51 -1.22054 -0.00067 0.00000 -0.06909 -0.06988 -1.29041

D52 0.88768 0.00032 0.00000 -0.05595 -0.05673 0.83095

D53 0.04434 -0.00029 0.00000 -0.02797 -0.02856 0.01578

D54 2.22390 -0.00048 0.00000 0.00062 0.00037 2.22427

D55 -2.02333 -0.00057 0.00000 -0.01586 -0.01615 -2.03948

D56 -2.11765 -0.00034 0.00000 -0.03691 -0.03708 -2.15473

D57 0.06191 -0.00054 0.00000 -0.00832 -0.00814 0.05377

D58 2.09786 -0.00062 0.00000 -0.02480 -0.02466 2.07320

D59 2.12853 -0.00030 0.00000 -0.04144 -0.04181 2.08672

D60 -1.97509 -0.00049 0.00000 -0.01285 -0.01288 -1.98797

D61 0.06086 -0.00058 0.00000 -0.02933 -0.02940 0.03146

D62 -0.00676 0.00000 0.00000 0.16934 0.16986 0.16310

D63 3.13805 0.00002 0.00000 0.20960 0.20995 -2.93518

D64 0.00505 0.00011 0.00000 -0.14238 -0.14249 -0.13744

D65 -3.13410 -0.00021 0.00000 -0.15903 -0.15932 2.98976

D66 0.00780 0.00125 0.00000 0.10253 0.10206 0.10986

D67 1.84063 0.00150 0.00000 0.03406 0.03414 1.87476

D68 -1.78157 0.00129 0.00000 0.03512 0.03552 -1.74605

D69 -1.83559 -0.00007 0.00000 0.11206 0.11146 -1.72413

D70 -0.00277 0.00019 0.00000 0.04359 0.04354 0.04077

D71 2.65822 -0.00002 0.00000 0.04465 0.04492 2.70315

D72 1.84393 -0.00022 0.00000 0.00298 0.00144 1.84537

D73 -2.60643 0.00003 0.00000 -0.06549 -0.06649 -2.67292

D74 0.05456 -0.00018 0.00000 -0.06443 -0.06510 -0.01054

D75 -1.93564 0.00036 0.00000 -0.09418 -0.09230 -2.02794

D76 1.20189 0.00034 0.00000 -0.14505 -0.14354 1.05835

D77 0.00597 -0.00013 0.00000 -0.13268 -0.13298 -0.12702

D78 -3.13970 -0.00015 0.00000 -0.18355 -0.18422 2.95927

D79 2.64385 0.00012 0.00000 -0.02791 -0.02818 2.61567

D80 -0.50181 0.00009 0.00000 -0.07878 -0.07942 -0.58123

D81 1.94056 -0.00126 0.00000 0.07155 0.07039 2.01095

D82 -1.20414 -0.00086 0.00000 0.09274 0.09210 -1.11204

D83 -0.00131 -0.00018 0.00000 0.05934 0.05903 0.05772

D84 3.13718 0.00022 0.00000 0.08052 0.08074 -3.06527

D85 -2.69645 0.00035 0.00000 0.06370 0.06339 -2.63306

D86 0.44204 0.00076 0.00000 0.08488 0.08510 0.52714

Item Value Threshold Converged?

Maximum Force 0.017203 0.000450 NO

RMS Force 0.002602 0.000300 NO

Maximum Displacement 0.351394 0.001800 NO

RMS Displacement 0.064918 0.001200 NO

Predicted change in Energy=-4.556162D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.071725 1.532802 0.421758

2 6 0 0.228536 1.275458 0.063865

3 6 0 -0.774538 3.787327 -0.340338

4 6 0 -1.581463 2.838671 0.228764

5 1 0 -1.656646 0.747336 0.919202

6 1 0 -2.580635 3.080722 0.613052

7 6 0 0.801528 1.953836 -1.101981

8 1 0 1.922401 1.981928 -1.011043

9 1 0 0.559599 1.319234 -2.001294

10 6 0 0.240277 3.352751 -1.344524

11 1 0 1.075498 4.096377 -1.434830

12 1 0 -0.291218 3.360974 -2.340424

13 1 0 -1.085291 4.843139 -0.377738

14 1 0 0.747304 0.377169 0.430224

15 8 0 2.791100 3.815113 0.954985

16 6 0 0.493843 3.941750 1.458338

17 6 0 0.908082 2.622166 1.724571

18 6 0 1.663295 4.654291 0.874471

19 8 0 1.836452 5.730945 0.325676

20 6 0 2.349094 2.533757 1.359247

21 8 0 3.188059 1.647840 1.316127

22 1 0 -0.316021 4.484819 1.945137

23 1 0 0.476069 1.954600 2.471212

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.372951 0.000000

3 C 2.398331 2.734781 0.000000

4 C 1.415052 2.397274 1.369289 0.000000

5 H 1.098426 2.136451 3.406773 2.203642 0.000000

6 H 2.170129 3.384085 2.161072 1.097548 2.528274

7 C 2.451149 1.465508 2.534911 2.869227 3.403446

8 H 3.349541 2.126901 3.314029 3.814209 4.249664

9 H 2.928824 2.091986 3.260396 3.444705 3.710540

10 C 2.855401 2.509750 1.492345 2.461350 3.938395

11 H 3.824841 3.304697 2.171649 3.377693 4.921601

12 H 3.403094 3.224923 2.101361 2.922029 4.395526

13 H 3.405541 3.827467 1.101229 2.152190 4.334063

14 H 2.155093 1.100119 3.812997 3.394515 2.480947

15 O 4.518262 3.716272 3.793732 4.538737 5.403238

16 C 3.054265 3.020606 2.206325 2.652457 3.888387

17 C 2.608385 2.243513 2.907346 2.912413 3.277414

18 C 4.174802 3.759272 2.858394 3.773839 5.127212

19 O 5.107948 4.743976 3.322423 4.478480 6.114766

20 C 3.685485 2.785336 3.770558 4.101249 4.408049

21 O 4.354181 3.235059 4.798276 5.034757 4.943645

22 H 3.406784 3.759751 2.433131 2.693897 4.101048

23 H 2.602660 2.513528 3.581580 3.169162 2.900809

6 7 8 9 10

6 H 0.000000

7 C 3.956038 0.000000

8 H 4.911453 1.124907 0.000000

9 H 4.449575 1.126949 1.810246 0.000000

10 C 3.444364 1.526693 2.195428 2.160672 0.000000

11 H 4.311924 2.185482 2.316837 2.880895 1.121932

12 H 3.747398 2.169763 2.927307 2.237767 1.128881

13 H 2.514723 3.526002 4.199263 4.214203 2.216543

14 H 4.291597 2.199198 2.456289 2.614384 3.501556

15 O 5.432475 3.413775 2.824973 4.466385 3.465287

16 C 3.302771 3.256027 3.461145 4.341771 2.875283

17 C 3.690108 2.906444 2.987027 3.962467 3.224757

18 C 4.533807 3.455642 3.280826 4.539909 2.939885

19 O 5.159160 4.168432 3.981122 5.148625 3.315592

20 C 5.015796 2.964610 2.470801 3.996323 3.525371

21 O 5.985424 3.411219 2.670062 4.245241 4.321482

22 H 2.978996 4.115789 4.473701 5.134390 3.523196

23 H 3.750246 3.587984 3.770772 4.518183 4.070658

11 12 13 14 15

11 H 0.000000

12 H 1.796895 0.000000

13 H 2.518751 2.584473 0.000000

14 H 4.173566 4.202155 4.894496 0.000000

15 O 2.955269 4.535046 4.226037 4.033849 0.000000

16 C 2.955107 3.922271 2.584055 3.718535 2.355162

17 C 3.490436 4.302132 3.650474 2.596381 2.358207

18 C 2.447375 3.978484 3.026287 4.396608 1.408064

19 O 2.519970 4.153533 3.133620 5.464439 2.231096

20 C 3.445388 4.619859 4.488359 2.842479 1.414451

21 O 4.245705 5.330156 5.598271 2.890799 2.232728

22 H 3.675785 4.430539 2.473038 4.505376 3.329130

23 H 4.494852 5.071336 4.347185 2.593739 3.334640

16 17 18 19 20

16 C 0.000000

17 C 1.408466 0.000000

18 C 1.488701 2.328636 0.000000

19 O 2.507337 3.533169 1.220796 0.000000

20 C 2.331142 1.489225 2.280788 3.398982 0.000000

21 O 3.541334 2.512853 3.399810 4.413567 1.220889

22 H 1.089852 2.239767 2.256710 2.967933 3.354512

23 H 2.230470 1.090758 3.353717 4.551346 2.253911

21 22 23

21 O 0.000000

22 H 4.552217 0.000000

23 H 2.963648 2.702993 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.252202 -0.778786 -0.599577

2 6 0 1.336593 -1.354637 0.246028

3 6 0 1.387836 1.370430 0.021501

4 6 0 2.263124 0.630418 -0.727635

5 1 0 2.896262 -1.423885 -1.212416

6 1 0 2.914723 1.089920 -1.481882

7 6 0 0.958970 -0.658613 1.479182

8 1 0 -0.053653 -1.011774 1.818724

9 1 0 1.698901 -0.969864 2.270154

10 6 0 0.995403 0.863677 1.369200

11 1 0 0.018626 1.301176 1.705701

12 1 0 1.774755 1.258848 2.083917

13 1 0 1.270426 2.451419 -0.152805

14 1 0 1.107832 -2.428849 0.182811

15 8 0 -2.134676 -0.029250 0.180291

16 6 0 -0.351404 0.713901 -1.166727

17 6 0 -0.297895 -0.693317 -1.141219

18 6 0 -1.447262 1.123301 -0.246011

19 8 0 -1.827520 2.179980 0.232712

20 6 0 -1.397111 -1.156932 -0.249828

21 8 0 -1.776327 -2.233028 0.184661

22 1 0 -0.010947 1.367847 -1.969360

23 1 0 0.088524 -1.333105 -1.935641

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2130473 0.8933816 0.6859649

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.0492266542 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.468017406051E-01 A.U. after 15 cycles

Convg = 0.9413D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.011050940 0.000881273 0.000569498

2 6 -0.004542425 -0.010468263 0.005604440

3 6 0.001823887 0.004491951 -0.015294862

4 6 -0.012190683 -0.016346478 0.002609712

5 1 -0.002521490 0.003911163 0.005403221

6 1 -0.000198369 0.001766014 0.003393853

7 6 0.009536288 0.011297282 -0.011035420

8 1 0.000080580 0.001931915 -0.001939270

9 1 0.001758189 -0.000763664 -0.000731463

10 6 0.000860293 0.000936109 -0.001776203

11 1 0.000155242 0.000437767 0.001608299

12 1 0.001106734 -0.000091657 0.000164763

13 1 0.001955739 0.000971892 -0.000024669

14 1 0.001139531 -0.002392430 -0.001134659

15 8 -0.000582610 -0.004116296 -0.004498743

16 6 0.009788263 -0.015868746 0.007826525

17 6 0.006721008 0.020543901 0.008391739

18 6 -0.000230784 0.000098030 -0.000968968

19 8 0.000091351 0.001443239 0.003674452

20 6 0.001060292 0.002882185 0.000168694

21 8 -0.001788297 0.000889536 0.002186609

22 1 -0.001542223 0.000026719 -0.001261569

23 1 -0.001429577 -0.002461443 -0.002935980

-------------------------------------------------------------------

Cartesian Forces: Max 0.020543901 RMS 0.005951477

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.019712495 RMS 0.003100014

Search for a saddle point.

Step number 35 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 34 35

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06949 0.00116 0.00258 0.00507 0.00818

Eigenvalues --- 0.00980 0.01149 0.01563 0.01981 0.02151

Eigenvalues --- 0.02387 0.02550 0.02701 0.02927 0.03080

Eigenvalues --- 0.03209 0.03290 0.03587 0.03679 0.03767

Eigenvalues --- 0.03966 0.04059 0.04220 0.04818 0.05149

Eigenvalues --- 0.05994 0.06045 0.06409 0.07130 0.07357

Eigenvalues --- 0.08475 0.08795 0.09839 0.09947 0.10283

Eigenvalues --- 0.11935 0.13819 0.14444 0.16262 0.21185

Eigenvalues --- 0.23001 0.25865 0.27186 0.28355 0.29757

Eigenvalues --- 0.30907 0.31285 0.31488 0.31844 0.32033

Eigenvalues --- 0.32444 0.32639 0.34026 0.36201 0.36895

Eigenvalues --- 0.39559 0.39621 0.40426 0.44888 0.48344

Eigenvalues --- 0.51875 1.08450 1.10854

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D29 D4

1 0.54486 0.53169 -0.19483 -0.14357 0.14292

D71 D35 D73 D37 D1

1 0.13614 0.13515 -0.12733 0.12093 0.11713

RFO step: Lambda0=1.802146831D-03 Lambda=-7.26069150D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.03483185 RMS(Int)= 0.00107093

Iteration 2 RMS(Cart)= 0.00120497 RMS(Int)= 0.00046615

Iteration 3 RMS(Cart)= 0.00000071 RMS(Int)= 0.00046614

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.59450 0.01368 0.00000 0.03482 0.03521 2.62971

R2 2.67406 -0.00573 0.00000 -0.03210 -0.03202 2.64204

R3 2.07572 0.00099 0.00000 0.00132 0.00132 2.07705

R4 2.76941 0.01971 0.00000 0.05832 0.05809 2.82750

R5 2.07892 0.00211 0.00000 0.00378 0.00378 2.08270

R6 4.23963 0.00799 0.00000 -0.11015 -0.10981 4.12982

R7 2.58758 0.01611 0.00000 0.04629 0.04599 2.63357

R8 2.82012 0.00063 0.00000 -0.00366 -0.00331 2.81681

R9 2.08102 0.00038 0.00000 0.00203 0.00203 2.08306

R10 4.16935 0.00994 0.00000 -0.05293 -0.05342 4.11593

R11 2.07407 0.00176 0.00000 0.00284 0.00284 2.07690

R12 2.12577 -0.00003 0.00000 -0.00295 -0.00295 2.12282

R13 2.12962 0.00064 0.00000 -0.00064 -0.00064 2.12898

R14 2.88503 -0.00225 0.00000 -0.00992 -0.00979 2.87524

R15 2.12014 0.00028 0.00000 0.00245 0.00245 2.12259

R16 2.13328 -0.00067 0.00000 -0.00386 -0.00386 2.12941

R17 2.66086 -0.00043 0.00000 0.00346 0.00333 2.66419

R18 2.67292 -0.00346 0.00000 -0.00903 -0.00919 2.66373

R19 2.66161 -0.01242 0.00000 -0.00396 -0.00399 2.65762

R20 2.81324 0.00046 0.00000 0.00124 0.00132 2.81456

R21 2.05952 0.00060 0.00000 0.00553 0.00553 2.06505

R22 2.81423 -0.00110 0.00000 -0.00400 -0.00398 2.81025

R23 2.06123 0.00006 0.00000 0.00280 0.00280 2.06403

R24 2.30697 -0.00037 0.00000 -0.00064 -0.00064 2.30634

R25 2.30715 -0.00195 0.00000 -0.00045 -0.00045 2.30669

A1 2.06983 -0.00237 0.00000 -0.00863 -0.00832 2.06151

A2 2.08097 0.00598 0.00000 0.03478 0.03342 2.11440

A3 2.12922 -0.00375 0.00000 -0.03090 -0.03163 2.09759

A4 2.08391 0.00148 0.00000 -0.00444 -0.00461 2.07930

A5 2.10928 -0.00069 0.00000 0.01130 0.01002 2.11929

A6 1.55218 0.00205 0.00000 0.04656 0.04675 1.59893

A7 2.04713 -0.00041 0.00000 -0.02284 -0.02286 2.02427

A8 1.76459 -0.00332 0.00000 -0.00176 -0.00211 1.76247

A9 1.67177 0.00001 0.00000 0.00804 0.00760 1.67937

A10 2.06991 0.00456 0.00000 0.00831 0.00800 2.07791

A11 2.10837 -0.00151 0.00000 -0.00134 -0.00121 2.10717

A12 1.61926 -0.00075 0.00000 0.00674 0.00676 1.62602

A13 2.03558 -0.00241 0.00000 -0.01020 -0.01017 2.02541

A14 1.74977 -0.00164 0.00000 -0.00573 -0.00551 1.74426

A15 1.69391 0.00079 0.00000 0.00733 0.00739 1.70130

A16 2.07574 -0.00079 0.00000 -0.00686 -0.00723 2.06851

A17 2.07568 0.00091 0.00000 0.01987 0.01897 2.09465

A18 2.12847 -0.00031 0.00000 -0.01777 -0.01820 2.11027

A19 1.91435 0.00202 0.00000 0.01215 0.01218 1.92653

A20 1.86527 0.00127 0.00000 -0.00127 -0.00108 1.86418

A21 1.98975 -0.00221 0.00000 -0.00518 -0.00556 1.98419

A22 1.86762 -0.00099 0.00000 -0.00983 -0.00985 1.85776

A23 1.93507 -0.00057 0.00000 -0.00971 -0.00966 1.92540

A24 1.88629 0.00056 0.00000 0.01376 0.01398 1.90028

A25 1.99316 0.00045 0.00000 -0.01070 -0.01059 1.98258

A26 1.94699 -0.00068 0.00000 -0.01555 -0.01567 1.93133

A27 1.84558 0.00027 0.00000 0.02102 0.02094 1.86652

A28 1.92457 -0.00021 0.00000 -0.00097 -0.00129 1.92329

A29 1.89643 -0.00008 0.00000 0.00581 0.00574 1.90217

A30 1.84903 0.00029 0.00000 0.00310 0.00324 1.85227

A31 1.88173 -0.00288 0.00000 0.00176 -0.00004 1.88169

A32 1.83134 0.00274 0.00000 0.04256 0.04216 1.87350

A33 1.73693 -0.00100 0.00000 0.01909 0.01881 1.75573

A34 1.54261 -0.00107 0.00000 -0.00747 -0.00690 1.53571

A35 1.86662 0.00087 0.00000 0.00382 0.00251 1.86913

A36 2.21551 -0.00062 0.00000 -0.01003 -0.01025 2.20526

A37 2.11814 -0.00056 0.00000 -0.01675 -0.01687 2.10127

A38 1.91069 -0.00048 0.00000 -0.03343 -0.03358 1.87711

A39 1.64674 0.00069 0.00000 0.05488 0.05539 1.70213

A40 1.59015 -0.00164 0.00000 -0.00081 -0.00134 1.58881

A41 1.86903 0.00098 0.00000 -0.00209 -0.00209 1.86694

A42 2.19728 0.00048 0.00000 -0.00479 -0.00474 2.19254

A43 2.11161 -0.00074 0.00000 -0.00051 -0.00076 2.11085

A44 1.89813 0.00001 0.00000 0.00355 0.00243 1.90056

A45 2.02384 0.00079 0.00000 0.00180 0.00213 2.02598

A46 2.36008 -0.00077 0.00000 -0.00392 -0.00358 2.35650

A47 1.89516 0.00136 0.00000 0.01019 0.00914 1.90431

A48 2.01808 0.00086 0.00000 0.00785 0.00837 2.02645

A49 2.36981 -0.00222 0.00000 -0.01801 -0.01749 2.35233

D1 -0.60367 0.00209 0.00000 -0.01064 -0.01049 -0.61417

D2 2.85662 0.00079 0.00000 0.05128 0.05161 2.90823

D3 1.17930 -0.00041 0.00000 0.01352 0.01338 1.19269

D4 2.62154 0.00407 0.00000 0.05355 0.05473 2.67627

D5 -0.20136 0.00278 0.00000 0.11547 0.11683 -0.08452

D6 -1.87867 0.00157 0.00000 0.07771 0.07861 -1.80006

D7 0.03099 -0.00014 0.00000 -0.01398 -0.01380 0.01719

D8 -3.02514 0.00231 0.00000 0.04840 0.04902 -2.97611

D9 3.08653 -0.00169 0.00000 -0.07670 -0.07511 3.01142

D10 0.03041 0.00076 0.00000 -0.01432 -0.01229 0.01812

D11 2.73231 -0.00142 0.00000 0.01115 0.01090 2.74321

D12 -1.53215 -0.00086 0.00000 0.00506 0.00489 -1.52726

D13 0.55074 -0.00062 0.00000 0.01826 0.01825 0.56899

D14 -0.71679 -0.00023 0.00000 -0.04257 -0.04215 -0.75894

D15 1.30194 0.00032 0.00000 -0.04866 -0.04817 1.25377

D16 -2.89837 0.00057 0.00000 -0.03546 -0.03480 -2.93317

D17 1.07259 -0.00225 0.00000 -0.04139 -0.04162 1.03097

D18 3.09132 -0.00170 0.00000 -0.04748 -0.04764 3.04368

D19 -1.10898 -0.00146 0.00000 -0.03428 -0.03427 -1.14325

D20 -1.13412 -0.00055 0.00000 0.03201 0.03113 -1.10299

D21 -3.05127 -0.00179 0.00000 0.01911 0.01936 -3.03191

D22 1.11674 -0.00093 0.00000 0.01594 0.01559 1.13233

D23 0.95646 0.00111 0.00000 0.03734 0.03681 0.99327

D24 -0.96069 -0.00014 0.00000 0.02443 0.02504 -0.93565

D25 -3.07587 0.00072 0.00000 0.02126 0.02127 -3.05460

D26 3.03883 -0.00008 0.00000 0.01536 0.01460 3.05342

D27 1.12167 -0.00132 0.00000 0.00245 0.00283 1.12451

D28 -0.99350 -0.00046 0.00000 -0.00072 -0.00094 -0.99444

D29 0.55406 0.00056 0.00000 0.04593 0.04614 0.60021

D30 -2.67569 -0.00191 0.00000 -0.01648 -0.01536 -2.69105

D31 -2.99194 0.00182 0.00000 0.03467 0.03451 -2.95742

D32 0.06149 -0.00064 0.00000 -0.02774 -0.02699 0.03450

D33 -1.24823 0.00206 0.00000 0.04721 0.04715 -1.20108

D34 1.80520 -0.00041 0.00000 -0.01520 -0.01436 1.79085

D35 -0.55553 0.00018 0.00000 -0.03623 -0.03619 -0.59172

D36 -2.75232 0.00068 0.00000 -0.01315 -0.01338 -2.76570

D37 1.52863 0.00052 0.00000 -0.02103 -0.02111 1.50752

D38 2.97379 -0.00115 0.00000 -0.02725 -0.02691 2.94688

D39 0.77700 -0.00065 0.00000 -0.00416 -0.00410 0.77290

D40 -1.22524 -0.00081 0.00000 -0.01204 -0.01183 -1.23707

D41 1.17059 -0.00042 0.00000 -0.02945 -0.02935 1.14124

D42 -1.02620 0.00008 0.00000 -0.00636 -0.00654 -1.03275

D43 -3.02845 -0.00008 0.00000 -0.01424 -0.01427 -3.04271

D44 0.94308 0.00168 0.00000 0.02260 0.02247 0.96555

D45 2.87211 0.00304 0.00000 0.04519 0.04506 2.91717

D46 -1.28971 0.00220 0.00000 0.02815 0.02790 -1.26181

D47 -1.14643 -0.00257 0.00000 0.01337 0.01355 -1.13289

D48 0.78260 -0.00122 0.00000 0.03596 0.03614 0.81874

D49 2.90396 -0.00205 0.00000 0.01892 0.01898 2.92294

D50 3.06374 0.00012 0.00000 0.02339 0.02349 3.08723

D51 -1.29041 0.00148 0.00000 0.04598 0.04608 -1.24433

D52 0.83095 0.00064 0.00000 0.02895 0.02892 0.85987

D53 0.01578 -0.00010 0.00000 0.00485 0.00460 0.02038

D54 2.22427 -0.00084 0.00000 -0.02548 -0.02559 2.19869

D55 -2.03948 -0.00066 0.00000 -0.01897 -0.01911 -2.05859

D56 -2.15473 -0.00066 0.00000 0.00036 0.00028 -2.15445

D57 0.05377 -0.00140 0.00000 -0.02997 -0.02991 0.02386

D58 2.07320 -0.00122 0.00000 -0.02346 -0.02343 2.04977

D59 2.08672 0.00052 0.00000 0.00950 0.00939 2.09611

D60 -1.98797 -0.00023 0.00000 -0.02083 -0.02080 -2.00877

D61 0.03146 -0.00005 0.00000 -0.01432 -0.01432 0.01714

D62 0.16310 -0.00233 0.00000 -0.09961 -0.09935 0.06375

D63 -2.93518 -0.00286 0.00000 -0.12693 -0.12677 -3.06194

D64 -0.13744 0.00156 0.00000 0.08411 0.08420 -0.05324

D65 2.98976 0.00142 0.00000 0.08580 0.08586 3.07563

D66 0.10986 -0.00168 0.00000 -0.03293 -0.03311 0.07675

D67 1.87476 -0.00067 0.00000 0.01528 0.01525 1.89001

D68 -1.74605 0.00068 0.00000 -0.00036 -0.00053 -1.74658

D69 -1.72413 -0.00195 0.00000 -0.07188 -0.07208 -1.79620

D70 0.04077 -0.00094 0.00000 -0.02368 -0.02372 0.01705

D71 2.70315 0.00041 0.00000 -0.03931 -0.03950 2.66365

D72 1.84537 -0.00111 0.00000 -0.01236 -0.01255 1.83282

D73 -2.67292 -0.00011 0.00000 0.03584 0.03581 -2.63711

D74 -0.01054 0.00125 0.00000 0.02021 0.02003 0.00948

D75 -2.02794 -0.00102 0.00000 0.02227 0.02253 -2.00541

D76 1.05835 -0.00027 0.00000 0.05743 0.05763 1.11598

D77 -0.12702 0.00182 0.00000 0.07667 0.07660 -0.05042

D78 2.95927 0.00257 0.00000 0.11183 0.11170 3.07097

D79 2.61567 0.00100 0.00000 0.02279 0.02290 2.63857

D80 -0.58123 0.00174 0.00000 0.05795 0.05800 -0.52322

D81 2.01095 -0.00022 0.00000 -0.05211 -0.05206 1.95889

D82 -1.11204 -0.00008 0.00000 -0.05471 -0.05456 -1.16660

D83 0.05772 -0.00016 0.00000 -0.03590 -0.03608 0.02164

D84 -3.06527 -0.00002 0.00000 -0.03850 -0.03858 -3.10385

D85 -2.63306 -0.00181 0.00000 -0.01981 -0.01990 -2.65296

D86 0.52714 -0.00167 0.00000 -0.02240 -0.02240 0.50474

Item Value Threshold Converged?

Maximum Force 0.019712 0.000450 NO

RMS Force 0.003100 0.000300 NO

Maximum Displacement 0.180835 0.001800 NO

RMS Displacement 0.034773 0.001200 NO

Predicted change in Energy=-3.328825D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.109899 1.541170 0.433510

2 6 0 0.216397 1.289184 0.095966

3 6 0 -0.771978 3.782110 -0.354734

4 6 0 -1.613618 2.826292 0.211174

5 1 0 -1.705629 0.802399 0.987949

6 1 0 -2.600571 3.105810 0.605764

7 6 0 0.803331 1.963010 -1.104126

8 1 0 1.922614 2.007367 -1.019592

9 1 0 0.576287 1.305667 -1.990467

10 6 0 0.237653 3.351486 -1.363235

11 1 0 1.070150 4.102018 -1.435932

12 1 0 -0.276772 3.356550 -2.365781

13 1 0 -1.067207 4.843619 -0.388125

14 1 0 0.733984 0.379038 0.440059

15 8 0 2.791099 3.812882 0.901010

16 6 0 0.490382 3.894589 1.416632

17 6 0 0.935749 2.590531 1.697534

18 6 0 1.655525 4.648000 0.875215

19 8 0 1.823662 5.768392 0.421370

20 6 0 2.381640 2.542122 1.353171

21 8 0 3.239844 1.674185 1.365602

22 1 0 -0.325112 4.422441 1.917138

23 1 0 0.516068 1.924144 2.454356

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.391581 0.000000

3 C 2.399444 2.719319 0.000000

4 C 1.398107 2.392683 1.393628 0.000000

5 H 1.099126 2.174116 3.398996 2.169790 0.000000

6 H 2.167918 3.390477 2.173406 1.099049 2.500537

7 C 2.490527 1.496246 2.520379 2.883906 3.466796

8 H 3.394846 2.161349 3.294324 3.832800 4.318138

9 H 2.962153 2.117308 3.259786 3.457630 3.785681

10 C 2.884689 2.526422 1.490592 2.486321 3.975204

11 H 3.847775 3.314761 2.159807 3.397506 4.946477

12 H 3.438857 3.252294 2.114389 2.951106 4.451160

13 H 3.403392 3.809986 1.102306 2.174243 4.316552

14 H 2.179564 1.102116 3.805327 3.398923 2.535968

15 O 4.538394 3.694082 3.778010 4.566264 5.412128

16 C 3.010981 2.933831 2.178059 2.649755 3.816788

17 C 2.623660 2.185405 2.923696 2.960426 3.267691

18 C 4.182710 3.736303 2.855750 3.800903 5.108690

19 O 5.145418 4.769957 3.359315 4.529351 6.118659

20 C 3.746802 2.799767 3.794708 4.164972 4.457106

21 O 4.450478 3.301731 4.847434 5.120170 5.035905

22 H 3.334481 3.664315 2.402315 2.668005 3.984209

23 H 2.621880 2.460687 3.605840 3.222002 2.888702

6 7 8 9 10

6 H 0.000000

7 C 3.976967 0.000000

8 H 4.930270 1.123347 0.000000

9 H 4.480329 1.126609 1.802103 0.000000

10 C 3.463066 1.521511 2.182622 2.166441 0.000000

11 H 4.316845 2.180974 2.299478 2.893266 1.123226

12 H 3.780607 2.168029 2.910295 2.252707 1.126835

13 H 2.521706 3.508487 4.169185 4.217307 2.209063

14 H 4.310685 2.213206 2.488950 2.605947 3.511930

15 O 5.445845 3.375474 2.775403 4.421782 3.443803

16 C 3.291454 3.191106 3.398247 4.279979 2.843676

17 C 3.736715 2.874129 2.949026 3.921917 3.230278

18 C 4.534899 3.442847 3.261069 4.532998 2.949909

19 O 5.166932 4.224825 4.028830 5.223869 3.397304

20 C 5.069397 2.977372 2.475212 3.996002 3.553957

21 O 6.061134 3.481318 2.745042 4.300411 4.390107

22 H 2.937846 4.055888 4.416926 5.078993 3.496354

23 H 3.811439 3.570270 3.748814 4.488049 4.085195

11 12 13 14 15

11 H 0.000000

12 H 1.798483 0.000000

13 H 2.493224 2.597554 0.000000

14 H 4.182455 4.214254 4.884942 0.000000

15 O 2.916602 4.504664 4.196524 4.029328 0.000000

16 C 2.918267 3.896750 2.565909 3.656793 2.359204

17 C 3.481561 4.309005 3.665817 2.551990 2.360279

18 C 2.445845 3.988191 3.007917 4.388921 1.409828

19 O 2.606560 4.242289 3.141275 5.498443 2.233832

20 C 3.454328 4.643388 4.497060 2.868358 1.409588

21 O 4.295409 5.396310 5.627749 2.968731 2.234109

22 H 3.645889 4.413826 2.458117 4.433120 3.333894

23 H 4.492714 5.090589 4.371475 2.547986 3.340057

16 17 18 19 20

16 C 0.000000

17 C 1.406352 0.000000

18 C 1.489402 2.329692 0.000000

19 O 2.505857 3.537765 1.220460 0.000000

20 C 2.325951 1.487121 2.278246 3.404175 0.000000

21 O 3.534451 2.501743 3.405014 4.433923 1.220649

22 H 1.092778 2.234701 2.249312 2.943830 3.343674

23 H 2.227147 1.092237 3.348348 4.541043 2.252745

21 22 23

21 O 0.000000

22 H 4.534976 0.000000

23 H 2.943946 2.690292 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.265754 -0.810544 -0.616254

2 6 0 1.304476 -1.372871 0.218149

3 6 0 1.423006 1.338022 0.040077

4 6 0 2.318537 0.583067 -0.715081

5 1 0 2.871983 -1.435466 -1.287102

6 1 0 2.954371 1.056542 -1.476294

7 6 0 0.938736 -0.668388 1.486491

8 1 0 -0.084440 -0.982598 1.827506

9 1 0 1.660593 -1.022463 2.275669

10 6 0 1.020671 0.847785 1.389024

11 1 0 0.046624 1.309832 1.704272

12 1 0 1.794542 1.220742 2.118261

13 1 0 1.312055 2.420763 -0.134392

14 1 0 1.065721 -2.448024 0.176892

15 8 0 -2.114750 0.025368 0.226036

16 6 0 -0.297228 0.685356 -1.125583

17 6 0 -0.311151 -0.720715 -1.101106

18 6 0 -1.411407 1.149437 -0.252914

19 8 0 -1.812652 2.236594 0.129992

20 6 0 -1.447836 -1.128432 -0.233211

21 8 0 -1.892266 -2.196537 0.156169

22 1 0 0.065178 1.315432 -1.941566

23 1 0 0.049355 -1.374466 -1.898369

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2169780 0.8823069 0.6773403

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4172447846 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.497418826694E-01 A.U. after 15 cycles

Convg = 0.7933D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000140875 -0.000867848 -0.000549353

2 6 0.001450172 0.002339339 -0.003934554

3 6 -0.001318305 -0.002707259 -0.001901927

4 6 -0.000931486 0.001867269 -0.001810907

5 1 0.000644443 0.000117723 0.001392631

6 1 -0.000005823 0.000597932 0.000672589

7 6 -0.001325067 -0.002357460 0.003937137

8 1 -0.000109648 0.000352672 0.000845809

9 1 0.000508474 -0.000111979 0.000223658

10 6 -0.000269876 0.000418393 0.000392301

11 1 0.000153342 0.000264933 0.000764766

12 1 0.000135097 0.000072632 -0.000034240

13 1 0.000325403 -0.000403552 0.000211560

14 1 -0.001006003 -0.000319547 -0.000841669

15 8 -0.000813796 -0.000732390 -0.002323709

16 6 -0.000727118 0.001503892 0.000305762

17 6 0.001834977 0.002172466 0.001339785

18 6 -0.000349669 -0.000535255 0.000010551

19 8 0.000184513 0.000503014 0.001400189

20 6 0.001116739 -0.001085189 -0.000086749

21 8 0.000337041 0.000253372 0.000877000

22 1 0.000202131 -0.000161805 0.000165053

23 1 0.000105334 -0.001181353 -0.001055682

-------------------------------------------------------------------

Cartesian Forces: Max 0.003937137 RMS 0.001221019

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.004860048 RMS 0.000619785

Search for a saddle point.

Step number 36 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 35 36

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06712 0.00105 0.00380 0.00573 0.00721

Eigenvalues --- 0.00966 0.01056 0.01471 0.02055 0.02182

Eigenvalues --- 0.02525 0.02555 0.02656 0.02967 0.03087

Eigenvalues --- 0.03218 0.03311 0.03602 0.03708 0.03780

Eigenvalues --- 0.04001 0.04081 0.04235 0.04839 0.05249

Eigenvalues --- 0.05944 0.06067 0.06424 0.07157 0.07368

Eigenvalues --- 0.08547 0.08808 0.09855 0.09874 0.10226

Eigenvalues --- 0.12004 0.13837 0.14542 0.16335 0.21515

Eigenvalues --- 0.23607 0.25964 0.27324 0.28431 0.29830

Eigenvalues --- 0.30940 0.31294 0.31515 0.31887 0.32084

Eigenvalues --- 0.32453 0.32688 0.34092 0.36242 0.36964

Eigenvalues --- 0.39608 0.39796 0.40432 0.45292 0.48617

Eigenvalues --- 0.51916 1.08464 1.10856

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D29

1 -0.53946 -0.53226 0.20189 -0.14865 0.14181

D35 D71 D73 D37 D1

1 -0.13496 -0.13444 0.12887 -0.12450 -0.11277

RFO step: Lambda0=5.505354767D-05 Lambda=-2.01641395D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.04980937 RMS(Int)= 0.00164641

Iteration 2 RMS(Cart)= 0.00208646 RMS(Int)= 0.00042207

Iteration 3 RMS(Cart)= 0.00000428 RMS(Int)= 0.00042206

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00042206

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62971 0.00049 0.00000 0.00754 0.00772 2.63743

R2 2.64204 0.00135 0.00000 0.00541 0.00579 2.64783

R3 2.07705 0.00027 0.00000 0.00148 0.00148 2.07853

R4 2.82750 -0.00486 0.00000 -0.04042 -0.04061 2.78689

R5 2.08270 -0.00047 0.00000 0.00129 0.00129 2.08398

R6 4.12982 0.00017 0.00000 -0.04802 -0.04800 4.08182

R7 2.63357 -0.00120 0.00000 -0.00062 -0.00046 2.63312

R8 2.81681 -0.00119 0.00000 -0.00633 -0.00643 2.81038

R9 2.08306 -0.00048 0.00000 -0.00188 -0.00188 2.08118

R10 4.11593 0.00102 0.00000 0.00818 0.00815 4.12408

R11 2.07690 0.00040 0.00000 0.00243 0.00243 2.07933

R12 2.12282 -0.00003 0.00000 0.00281 0.00281 2.12562

R13 2.12898 -0.00021 0.00000 -0.00051 -0.00051 2.12847

R14 2.87524 0.00032 0.00000 0.00330 0.00294 2.87817

R15 2.12259 0.00024 0.00000 0.00163 0.00163 2.12422

R16 2.12941 -0.00003 0.00000 -0.00181 -0.00181 2.12760

R17 2.66419 0.00029 0.00000 0.00101 0.00101 2.66520

R18 2.66373 0.00002 0.00000 0.00036 0.00049 2.66422

R19 2.65762 0.00013 0.00000 0.00836 0.00827 2.66589

R20 2.81456 -0.00057 0.00000 -0.00460 -0.00473 2.80984

R21 2.06505 -0.00015 0.00000 -0.00180 -0.00180 2.06326

R22 2.81025 0.00078 0.00000 0.00428 0.00436 2.81461

R23 2.06403 -0.00005 0.00000 0.00091 0.00091 2.06494

R24 2.30634 -0.00003 0.00000 0.00028 0.00028 2.30661

R25 2.30669 0.00007 0.00000 -0.00029 -0.00029 2.30640

A1 2.06151 -0.00015 0.00000 -0.00440 -0.00470 2.05681

A2 2.11440 -0.00036 0.00000 -0.01891 -0.01903 2.09537

A3 2.09759 0.00048 0.00000 0.01820 0.01790 2.11550

A4 2.07930 0.00061 0.00000 0.01529 0.01544 2.09474

A5 2.11929 -0.00028 0.00000 -0.02217 -0.02242 2.09688

A6 1.59893 0.00070 0.00000 0.01948 0.01923 1.61816

A7 2.02427 -0.00026 0.00000 -0.00354 -0.00376 2.02051

A8 1.76247 -0.00096 0.00000 -0.01457 -0.01489 1.74758

A9 1.67937 0.00002 0.00000 0.02183 0.02249 1.70186

A10 2.07791 0.00057 0.00000 0.01457 0.01473 2.09263

A11 2.10717 -0.00050 0.00000 -0.01115 -0.01119 2.09597

A12 1.62602 0.00098 0.00000 -0.00260 -0.00315 1.62287

A13 2.02541 0.00016 0.00000 0.00536 0.00500 2.03041

A14 1.74426 -0.00146 0.00000 -0.00338 -0.00337 1.74089

A15 1.70130 -0.00015 0.00000 -0.01625 -0.01582 1.68548

A16 2.06851 -0.00075 0.00000 -0.01208 -0.01239 2.05611

A17 2.09465 0.00075 0.00000 0.01189 0.01167 2.10632

A18 2.11027 -0.00007 0.00000 -0.00479 -0.00495 2.10532

A19 1.92653 -0.00076 0.00000 -0.00341 -0.00340 1.92312

A20 1.86418 0.00008 0.00000 0.00891 0.00896 1.87314

A21 1.98419 0.00059 0.00000 0.00244 0.00229 1.98648

A22 1.85776 0.00019 0.00000 -0.00384 -0.00384 1.85392

A23 1.92540 0.00026 0.00000 -0.00627 -0.00642 1.91899

A24 1.90028 -0.00038 0.00000 0.00237 0.00255 1.90282

A25 1.98258 -0.00018 0.00000 -0.00781 -0.00789 1.97469

A26 1.93133 -0.00036 0.00000 -0.00790 -0.00790 1.92343

A27 1.86652 0.00021 0.00000 0.01218 0.01216 1.87869

A28 1.92329 0.00037 0.00000 -0.00230 -0.00265 1.92064

A29 1.90217 -0.00015 0.00000 0.00370 0.00399 1.90616

A30 1.85227 0.00012 0.00000 0.00360 0.00362 1.85589

A31 1.88169 0.00036 0.00000 0.00560 0.00328 1.88497

A32 1.87350 -0.00028 0.00000 -0.00937 -0.01038 1.86312

A33 1.75573 0.00024 0.00000 -0.01022 -0.00967 1.74606

A34 1.53571 0.00036 0.00000 0.03530 0.03561 1.57132

A35 1.86913 -0.00031 0.00000 -0.00591 -0.00647 1.86265

A36 2.20526 0.00006 0.00000 -0.00741 -0.00725 2.19801

A37 2.10127 0.00011 0.00000 0.00421 0.00446 2.10573

A38 1.87711 -0.00011 0.00000 0.00701 0.00580 1.88291

A39 1.70213 -0.00022 0.00000 0.03509 0.03577 1.73789

A40 1.58881 -0.00021 0.00000 -0.03451 -0.03405 1.55476

A41 1.86694 0.00055 0.00000 0.00664 0.00588 1.87282

A42 2.19254 0.00000 0.00000 0.01038 0.01052 2.20306

A43 2.11085 -0.00031 0.00000 -0.01895 -0.01834 2.09250

A44 1.90056 0.00026 0.00000 0.00688 0.00497 1.90553

A45 2.02598 0.00002 0.00000 -0.00191 -0.00113 2.02485

A46 2.35650 -0.00028 0.00000 -0.00451 -0.00372 2.35278

A47 1.90431 -0.00081 0.00000 -0.00553 -0.00704 1.89727

A48 2.02645 0.00030 0.00000 0.00090 0.00157 2.02802

A49 2.35233 0.00051 0.00000 0.00489 0.00556 2.35789

D1 -0.61417 0.00070 0.00000 0.02024 0.02033 -0.59384

D2 2.90823 0.00052 0.00000 0.05239 0.05214 2.96037

D3 1.19269 0.00010 0.00000 0.01718 0.01710 1.20978

D4 2.67627 0.00091 0.00000 0.05765 0.05755 2.73381

D5 -0.08452 0.00073 0.00000 0.08980 0.08936 0.00484

D6 -1.80006 0.00031 0.00000 0.05460 0.05431 -1.74575

D7 0.01719 -0.00028 0.00000 -0.02970 -0.02964 -0.01245

D8 -2.97611 0.00016 0.00000 0.00829 0.00876 -2.96736

D9 3.01142 -0.00056 0.00000 -0.07000 -0.07060 2.94082

D10 0.01812 -0.00012 0.00000 -0.03201 -0.03220 -0.01408

D11 2.74321 -0.00033 0.00000 -0.00078 -0.00091 2.74231

D12 -1.52726 -0.00045 0.00000 -0.00212 -0.00225 -1.52951

D13 0.56899 -0.00052 0.00000 0.00839 0.00854 0.57753

D14 -0.75894 -0.00018 0.00000 -0.03552 -0.03563 -0.79457

D15 1.25377 -0.00030 0.00000 -0.03686 -0.03696 1.21680

D16 -2.93317 -0.00037 0.00000 -0.02635 -0.02617 -2.95934

D17 1.03097 -0.00076 0.00000 -0.01932 -0.01891 1.01206

D18 3.04368 -0.00087 0.00000 -0.02066 -0.02025 3.02343

D19 -1.14325 -0.00094 0.00000 -0.01015 -0.00946 -1.15271

D20 -1.10299 0.00026 0.00000 0.05807 0.05834 -1.04465

D21 -3.03191 -0.00023 0.00000 0.03550 0.03595 -2.99596

D22 1.13233 0.00014 0.00000 0.05686 0.05731 1.18964

D23 0.99327 0.00092 0.00000 0.07638 0.07652 1.06979

D24 -0.93565 0.00043 0.00000 0.05381 0.05413 -0.88152

D25 -3.05460 0.00080 0.00000 0.07516 0.07549 -2.97910

D26 3.05342 0.00044 0.00000 0.07545 0.07527 3.12870

D27 1.12451 -0.00005 0.00000 0.05288 0.05289 1.17739

D28 -0.99444 0.00032 0.00000 0.07423 0.07425 -0.92019

D29 0.60021 -0.00063 0.00000 0.00969 0.00973 0.60994

D30 -2.69105 -0.00100 0.00000 -0.02719 -0.02718 -2.71824

D31 -2.95742 0.00005 0.00000 0.03497 0.03495 -2.92247

D32 0.03450 -0.00033 0.00000 -0.00191 -0.00196 0.03254

D33 -1.20108 0.00039 0.00000 0.01240 0.01277 -1.18831

D34 1.79085 0.00002 0.00000 -0.02448 -0.02414 1.76670

D35 -0.59172 0.00032 0.00000 0.01432 0.01425 -0.57747

D36 -2.76570 0.00024 0.00000 0.02954 0.02971 -2.73599

D37 1.50752 0.00017 0.00000 0.02252 0.02272 1.53024

D38 2.94688 -0.00017 0.00000 -0.00579 -0.00615 2.94073

D39 0.77290 -0.00024 0.00000 0.00943 0.00932 0.78221

D40 -1.23707 -0.00032 0.00000 0.00241 0.00232 -1.23474

D41 1.14124 0.00075 0.00000 0.01318 0.01245 1.15369

D42 -1.03275 0.00068 0.00000 0.02840 0.02792 -1.00483

D43 -3.04271 0.00060 0.00000 0.02137 0.02092 -3.02179

D44 0.96555 0.00067 0.00000 0.07249 0.07242 1.03796

D45 2.91717 0.00034 0.00000 0.05874 0.05819 2.97536

D46 -1.26181 0.00053 0.00000 0.06926 0.06907 -1.19274

D47 -1.13289 0.00009 0.00000 0.05867 0.05857 -1.07432

D48 0.81874 -0.00024 0.00000 0.04492 0.04434 0.86308

D49 2.92294 -0.00004 0.00000 0.05544 0.05522 2.97816

D50 3.08723 0.00032 0.00000 0.05827 0.05831 -3.13765

D51 -1.24433 -0.00001 0.00000 0.04452 0.04408 -1.20025

D52 0.85987 0.00019 0.00000 0.05504 0.05496 0.91483

D53 0.02038 -0.00013 0.00000 -0.02421 -0.02429 -0.00391

D54 2.19869 -0.00045 0.00000 -0.04236 -0.04255 2.15614

D55 -2.05859 -0.00018 0.00000 -0.03718 -0.03737 -2.09596

D56 -2.15445 0.00022 0.00000 -0.01658 -0.01647 -2.17092

D57 0.02386 -0.00009 0.00000 -0.03473 -0.03473 -0.01087

D58 2.04977 0.00017 0.00000 -0.02955 -0.02955 2.02022

D59 2.09611 0.00007 0.00000 -0.00979 -0.00969 2.08642

D60 -2.00877 -0.00024 0.00000 -0.02793 -0.02795 -2.03672

D61 0.01714 0.00002 0.00000 -0.02276 -0.02277 -0.00563

D62 0.06375 -0.00072 0.00000 -0.11255 -0.11286 -0.04911

D63 -3.06194 -0.00073 0.00000 -0.13636 -0.13663 3.08461

D64 -0.05324 0.00064 0.00000 0.10665 0.10619 0.05296

D65 3.07563 0.00059 0.00000 0.12366 0.12324 -3.08431

D66 0.07675 -0.00011 0.00000 -0.07326 -0.07331 0.00344

D67 1.89001 -0.00018 0.00000 -0.02855 -0.02825 1.86176

D68 -1.74658 0.00026 0.00000 -0.03835 -0.03796 -1.78454

D69 -1.79620 -0.00014 0.00000 -0.05530 -0.05552 -1.85172

D70 0.01705 -0.00020 0.00000 -0.01059 -0.01046 0.00660

D71 2.66365 0.00023 0.00000 -0.02039 -0.02017 2.64348

D72 1.83282 0.00016 0.00000 -0.03751 -0.03798 1.79483

D73 -2.63711 0.00009 0.00000 0.00720 0.00708 -2.63003

D74 0.00948 0.00053 0.00000 -0.00260 -0.00263 0.00685

D75 -2.00541 0.00091 0.00000 0.09284 0.09349 -1.91192

D76 1.11598 0.00092 0.00000 0.12317 0.12366 1.23964

D77 -0.05042 0.00060 0.00000 0.07648 0.07626 0.02584

D78 3.07097 0.00061 0.00000 0.10681 0.10643 -3.10578

D79 2.63857 0.00032 0.00000 0.05631 0.05615 2.69472

D80 -0.52322 0.00033 0.00000 0.08664 0.08632 -0.43690

D81 1.95889 -0.00032 0.00000 -0.03626 -0.03658 1.92231

D82 -1.16660 -0.00024 0.00000 -0.05770 -0.05818 -1.22478

D83 0.02164 -0.00026 0.00000 -0.05877 -0.05854 -0.03690

D84 -3.10385 -0.00019 0.00000 -0.08021 -0.08014 3.09920

D85 -2.65296 -0.00076 0.00000 -0.05909 -0.05884 -2.71180

D86 0.50474 -0.00069 0.00000 -0.08053 -0.08044 0.42429

Item Value Threshold Converged?

Maximum Force 0.004860 0.000450 NO

RMS Force 0.000620 0.000300 NO

Maximum Displacement 0.271568 0.001800 NO

RMS Displacement 0.049812 0.001200 NO

Predicted change in Energy=-1.250665D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.137556 1.559417 0.442612

2 6 0 0.188807 1.290277 0.101718

3 6 0 -0.760773 3.774989 -0.379330

4 6 0 -1.631350 2.845278 0.185699

5 1 0 -1.706201 0.841779 1.052069

6 1 0 -2.609252 3.160301 0.579660

7 6 0 0.789792 1.928230 -1.084344

8 1 0 1.910143 1.951496 -0.986784

9 1 0 0.564669 1.269455 -1.969768

10 6 0 0.263104 3.330113 -1.361923

11 1 0 1.115181 4.062613 -1.393281

12 1 0 -0.211298 3.352329 -2.382729

13 1 0 -1.034344 4.841403 -0.407795

14 1 0 0.668460 0.356055 0.438353

15 8 0 2.752652 3.841927 0.800302

16 6 0 0.473313 3.881623 1.417443

17 6 0 0.957278 2.578192 1.656180

18 6 0 1.618827 4.674947 0.898493

19 8 0 1.778655 5.838205 0.565078

20 6 0 2.401971 2.568765 1.294012

21 8 0 3.298292 1.741437 1.335788

22 1 0 -0.344945 4.369099 1.951211

23 1 0 0.578177 1.875076 2.401796

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.395666 0.000000

3 C 2.392972 2.703128 0.000000

4 C 1.401169 2.395423 1.393386 0.000000

5 H 1.099909 2.166881 3.398009 2.184081 0.000000

6 H 2.178876 3.399199 2.171262 1.100335 2.532630

7 C 2.486421 1.474758 2.512332 2.883733 3.460436

8 H 3.389007 2.141271 3.290580 3.836109 4.297248

9 H 2.966686 2.105412 3.250229 3.457131 3.804110

10 C 2.890252 2.511711 1.487188 2.493823 3.987145

11 H 3.835533 3.283144 2.151750 3.393894 4.930893

12 H 3.472037 3.253401 2.119946 2.978334 4.509483

13 H 3.391943 3.790277 1.101313 2.166372 4.310405

14 H 2.170206 1.102797 3.794789 3.398410 2.500318

15 O 4.524545 3.684052 3.706773 4.537678 5.380116

16 C 2.989621 2.920128 2.182369 2.649682 3.758249

17 C 2.626591 2.160006 2.920158 2.989088 3.236387

18 C 4.184734 3.759760 2.846973 3.797291 5.076670

19 O 5.179508 4.840037 3.405504 4.552985 6.111109

20 C 3.777819 2.820318 3.775976 4.191956 4.462970

21 O 4.528537 3.375703 4.853141 5.180979 5.092626

22 H 3.286094 3.631068 2.440758 2.663438 3.886318

23 H 2.623316 2.404986 3.624517 3.276338 2.847429

6 7 8 9 10

6 H 0.000000

7 C 3.980001 0.000000

8 H 4.933547 1.124832 0.000000

9 H 4.488726 1.126339 1.800483 0.000000

10 C 3.471169 1.523065 2.180379 2.169499 0.000000

11 H 4.310228 2.181034 2.292165 2.904674 1.124088

12 H 3.816125 2.171645 2.900260 2.260757 1.125876

13 H 2.506293 3.503109 4.166149 4.213718 2.208559

14 H 4.315919 2.192045 2.473504 2.577619 3.500047

15 O 5.409557 3.326702 2.734452 4.367856 3.336917

16 C 3.274812 3.189803 3.401496 4.278430 2.841343

17 C 3.770660 2.821520 2.878534 3.874846 3.186881

18 C 4.502495 3.487606 3.325104 4.575537 2.959061

19 O 5.140535 4.357332 4.187131 5.364017 3.507242

20 C 5.096329 2.943805 2.413492 3.964359 3.494051

21 O 6.122416 3.490632 2.713931 4.315341 4.360493

22 H 2.910228 4.057100 4.422899 5.080282 3.525063

23 H 3.889947 3.492962 3.641764 4.413336 4.047467

11 12 13 14 15

11 H 0.000000

12 H 1.800849 0.000000

13 H 2.489610 2.606744 0.000000

14 H 4.158487 4.208341 4.871741 0.000000

15 O 2.746237 4.376802 4.098755 4.077520 0.000000

16 C 2.888758 3.897455 2.554546 3.664195 2.361741

17 C 3.395240 4.275237 3.653584 2.550375 2.356464

18 C 2.425044 3.983101 2.961995 4.446094 1.410362

19 O 2.725453 4.339246 3.138958 5.594869 2.233635

20 C 3.333009 4.578381 4.457499 2.938248 1.409847

21 O 4.195432 5.360930 5.605499 3.104947 2.235292

22 H 3.662175 4.453619 2.502649 4.406841 3.346283

23 H 4.413197 5.069244 4.392394 2.484087 3.340902

16 17 18 19 20

16 C 0.000000

17 C 1.410726 0.000000

18 C 1.486901 2.325536 0.000000

19 O 2.501730 3.534522 1.220606 0.000000

20 C 2.336354 1.489427 2.281611 3.407213 0.000000

21 O 3.545077 2.506623 3.408417 4.436981 1.220495

22 H 1.091828 2.233870 2.249035 2.930753 3.349427

23 H 2.237449 1.092718 3.343972 4.530019 2.243795

21 22 23

21 O 0.000000

22 H 4.533931 0.000000

23 H 2.924596 2.697283 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.300794 -0.705465 -0.671903

2 6 0 1.362034 -1.350744 0.134467

3 6 0 1.385912 1.352277 0.137419

4 6 0 2.317744 0.695578 -0.663806

5 1 0 2.875370 -1.278105 -1.414699

6 1 0 2.919857 1.254067 -1.396122

7 6 0 0.973184 -0.762343 1.429646

8 1 0 -0.038332 -1.143306 1.741011

9 1 0 1.702305 -1.138534 2.201334

10 6 0 0.980752 0.760665 1.440326

11 1 0 -0.029019 1.148835 1.745712

12 1 0 1.708026 1.122139 2.220074

13 1 0 1.223410 2.435297 0.021011

14 1 0 1.197219 -2.436360 0.032313

15 8 0 -2.061521 -0.000127 0.299807

16 6 0 -0.296146 0.713202 -1.097489

17 6 0 -0.292061 -0.697506 -1.091450

18 6 0 -1.428769 1.141449 -0.234562

19 8 0 -1.907348 2.217824 0.085218

20 6 0 -1.426236 -1.140160 -0.233490

21 8 0 -1.899678 -2.219150 0.084698

22 1 0 0.056988 1.351539 -1.909838

23 1 0 0.069304 -1.345666 -1.893533

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2213921 0.8779816 0.6735617

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4809859777 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.499879071037E-01 A.U. after 15 cycles

Convg = 0.6668D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000090946 0.003077197 -0.000249115

2 6 -0.006085796 -0.005615759 0.008004685

3 6 -0.001941422 0.001359365 0.000851264

4 6 0.001707576 -0.003840440 0.003015758

5 1 -0.001308932 0.001072158 -0.001053837

6 1 0.000500761 -0.000911950 -0.000344989

7 6 0.005241492 0.004491765 -0.009432365

8 1 0.000190417 0.000283758 -0.000574449

9 1 0.000168003 -0.000037982 -0.000781812

10 6 0.001318862 -0.000107290 0.000025387

11 1 0.000081125 -0.000066594 -0.000103059

12 1 -0.000170538 0.000035988 0.000114840

13 1 -0.000043125 0.000749185 -0.001014139

14 1 0.000062881 -0.000347155 0.000548726

15 8 0.000834484 0.000367933 0.001227964

16 6 0.002022131 -0.003415423 0.000297037

17 6 0.000382848 -0.000431202 0.002274206

18 6 0.000296154 0.000705569 -0.000901030

19 8 -0.000081374 -0.000229390 -0.000441248

20 6 -0.001424332 0.001896327 -0.001420650

21 8 -0.000767653 0.000255057 -0.000201008

22 1 -0.000550985 0.000125204 -0.000629024

23 1 -0.000341631 0.000583679 0.000786859

-------------------------------------------------------------------

Cartesian Forces: Max 0.009432365 RMS 0.002276126

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011532174 RMS 0.001133323

Search for a saddle point.

Step number 37 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07230 -0.00481 0.00462 0.00574 0.00906

Eigenvalues --- 0.00999 0.01159 0.01490 0.01933 0.02137

Eigenvalues --- 0.02471 0.02533 0.02696 0.02998 0.03093

Eigenvalues --- 0.03203 0.03324 0.03570 0.03705 0.03807

Eigenvalues --- 0.03895 0.04054 0.04216 0.04816 0.05329

Eigenvalues --- 0.05998 0.06080 0.06421 0.07277 0.07431

Eigenvalues --- 0.08580 0.08817 0.09783 0.09846 0.10153

Eigenvalues --- 0.12026 0.13821 0.14553 0.16335 0.21614

Eigenvalues --- 0.24310 0.26029 0.27380 0.28504 0.29841

Eigenvalues --- 0.30940 0.31297 0.31523 0.31913 0.32135

Eigenvalues --- 0.32449 0.32742 0.34147 0.36330 0.37017

Eigenvalues --- 0.39610 0.39936 0.40433 0.45482 0.48792

Eigenvalues --- 0.51947 1.08477 1.10854

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D35 D29

1 0.54056 0.52637 -0.19394 0.15204 -0.14675

D37 D4 D71 D36 D73

1 0.14488 0.14259 0.13509 0.12549 -0.12330

RFO step: Lambda0=1.201577241D-05 Lambda=-5.20655418D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.06968592 RMS(Int)= 0.00257083

Iteration 2 RMS(Cart)= 0.00294809 RMS(Int)= 0.00079141

Iteration 3 RMS(Cart)= 0.00000420 RMS(Int)= 0.00079141

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00079141

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63743 -0.00001 0.00000 -0.01664 -0.01621 2.62122

R2 2.64783 -0.00373 0.00000 -0.02448 -0.02363 2.62420

R3 2.07853 -0.00061 0.00000 -0.00326 -0.00326 2.07527

R4 2.78689 0.01153 0.00000 0.10075 0.10051 2.88739

R5 2.08398 0.00049 0.00000 -0.00450 -0.00450 2.07949

R6 4.08182 0.00146 0.00000 -0.06439 -0.06539 4.01643

R7 2.63312 0.00121 0.00000 -0.01679 -0.01639 2.61672

R8 2.81038 0.00175 0.00000 0.01141 0.01169 2.82207

R9 2.08118 0.00076 0.00000 0.00483 0.00483 2.08601

R10 4.12408 -0.00014 0.00000 0.02015 0.02057 4.14465

R11 2.07933 -0.00083 0.00000 -0.00072 -0.00072 2.07861

R12 2.12562 0.00015 0.00000 -0.00567 -0.00567 2.11995

R13 2.12847 0.00060 0.00000 -0.00065 -0.00065 2.12782

R14 2.87817 -0.00074 0.00000 -0.00333 -0.00318 2.87499

R15 2.12422 0.00002 0.00000 0.00102 0.00102 2.12524

R16 2.12760 -0.00003 0.00000 -0.00060 -0.00060 2.12700

R17 2.66520 -0.00041 0.00000 -0.00479 -0.00533 2.65987

R18 2.66422 -0.00004 0.00000 -0.00392 -0.00439 2.65984

R19 2.66589 -0.00159 0.00000 0.01235 0.01200 2.67788

R20 2.80984 0.00082 0.00000 -0.00239 -0.00229 2.80755

R21 2.06326 0.00016 0.00000 -0.00154 -0.00154 2.06172

R22 2.81461 -0.00096 0.00000 0.00313 0.00339 2.81800

R23 2.06494 0.00028 0.00000 0.00090 0.00090 2.06584

R24 2.30661 -0.00011 0.00000 -0.00007 -0.00007 2.30654

R25 2.30640 -0.00074 0.00000 -0.00107 -0.00107 2.30533

A1 2.05681 0.00041 0.00000 0.01299 0.01276 2.06957

A2 2.09537 0.00150 0.00000 0.02825 0.02827 2.12364

A3 2.11550 -0.00188 0.00000 -0.03759 -0.03773 2.07776

A4 2.09474 -0.00050 0.00000 -0.04362 -0.04531 2.04943

A5 2.09688 0.00041 0.00000 -0.00569 -0.00756 2.08931

A6 1.61816 -0.00038 0.00000 0.03754 0.03808 1.65624

A7 2.02051 0.00016 0.00000 0.01343 0.01225 2.03276

A8 1.74758 0.00000 0.00000 0.01726 0.01733 1.76491

A9 1.70186 0.00021 0.00000 0.03413 0.03423 1.73609

A10 2.09263 0.00038 0.00000 0.00458 0.00297 2.09561

A11 2.09597 0.00063 0.00000 0.00958 0.01015 2.10612

A12 1.62287 -0.00101 0.00000 -0.02457 -0.02440 1.59847

A13 2.03041 -0.00104 0.00000 -0.00748 -0.00670 2.02371

A14 1.74089 0.00073 0.00000 -0.02149 -0.02123 1.71966

A15 1.68548 0.00042 0.00000 0.02954 0.02931 1.71479

A16 2.05611 0.00131 0.00000 0.01831 0.01746 2.07357

A17 2.10632 -0.00136 0.00000 -0.01713 -0.01791 2.08841

A18 2.10532 0.00013 0.00000 0.01010 0.00956 2.11488

A19 1.92312 0.00120 0.00000 -0.00077 0.00006 1.92318

A20 1.87314 0.00090 0.00000 -0.00365 -0.00297 1.87018

A21 1.98648 -0.00227 0.00000 -0.02129 -0.02382 1.96266

A22 1.85392 -0.00050 0.00000 0.01413 0.01369 1.86760

A23 1.91899 0.00034 0.00000 0.00738 0.00851 1.92749

A24 1.90282 0.00044 0.00000 0.00650 0.00654 1.90937

A25 1.97469 0.00081 0.00000 0.01751 0.01515 1.98984

A26 1.92343 -0.00016 0.00000 -0.00373 -0.00302 1.92041

A27 1.87869 -0.00037 0.00000 0.00175 0.00238 1.88106

A28 1.92064 -0.00014 0.00000 -0.01120 -0.00982 1.91082

A29 1.90616 -0.00033 0.00000 0.00414 0.00402 1.91019

A30 1.85589 0.00014 0.00000 -0.00975 -0.01010 1.84579

A31 1.88497 -0.00073 0.00000 -0.00660 -0.00703 1.87795

A32 1.86312 0.00090 0.00000 0.00769 0.00647 1.86959

A33 1.74606 -0.00072 0.00000 -0.06283 -0.06232 1.68374

A34 1.57132 -0.00049 0.00000 -0.01545 -0.01448 1.55683

A35 1.86265 0.00077 0.00000 0.01710 0.01693 1.87958

A36 2.19801 -0.00053 0.00000 0.00240 0.00203 2.20003

A37 2.10573 -0.00011 0.00000 0.01475 0.01282 2.11854

A38 1.88291 -0.00039 0.00000 0.00097 -0.00085 1.88205

A39 1.73789 0.00029 0.00000 0.02587 0.02665 1.76455

A40 1.55476 0.00029 0.00000 0.05738 0.05833 1.61309

A41 1.87282 -0.00072 0.00000 -0.02825 -0.02841 1.84441

A42 2.20306 -0.00020 0.00000 -0.02284 -0.02346 2.17960

A43 2.09250 0.00089 0.00000 0.00862 0.00533 2.09784

A44 1.90553 -0.00045 0.00000 -0.00449 -0.00434 1.90119

A45 2.02485 0.00015 0.00000 0.00116 0.00108 2.02592

A46 2.35278 0.00030 0.00000 0.00323 0.00312 2.35590

A47 1.89727 0.00116 0.00000 0.02081 0.02112 1.91839

A48 2.02802 -0.00030 0.00000 -0.00661 -0.00691 2.02111

A49 2.35789 -0.00086 0.00000 -0.01432 -0.01463 2.34326

D1 -0.59384 -0.00005 0.00000 -0.05466 -0.05410 -0.64794

D2 2.96037 -0.00029 0.00000 0.04157 0.04031 3.00067

D3 1.20978 -0.00037 0.00000 -0.01986 -0.02125 1.18853

D4 2.73381 -0.00002 0.00000 -0.07215 -0.07116 2.66266

D5 0.00484 -0.00026 0.00000 0.02407 0.02325 0.02809

D6 -1.74575 -0.00034 0.00000 -0.03735 -0.03831 -1.78406

D7 -0.01245 0.00046 0.00000 0.01870 0.01906 0.00660

D8 -2.96736 -0.00004 0.00000 -0.05003 -0.04852 -3.01588

D9 2.94082 0.00081 0.00000 0.04387 0.04290 2.98372

D10 -0.01408 0.00031 0.00000 -0.02486 -0.02469 -0.03877

D11 2.74231 -0.00054 0.00000 0.10434 0.10340 2.84571

D12 -1.52951 -0.00001 0.00000 0.11866 0.11801 -1.41149

D13 0.57753 -0.00025 0.00000 0.11098 0.10960 0.68713

D14 -0.79457 -0.00025 0.00000 0.00854 0.00811 -0.78646

D15 1.21680 0.00028 0.00000 0.02285 0.02272 1.23952

D16 -2.95934 0.00004 0.00000 0.01518 0.01430 -2.94504

D17 1.01206 0.00004 0.00000 0.06113 0.06150 1.07356

D18 3.02343 0.00057 0.00000 0.07545 0.07611 3.09954

D19 -1.15271 0.00033 0.00000 0.06777 0.06769 -1.08502

D20 -1.04465 0.00047 0.00000 0.09283 0.09254 -0.95211

D21 -2.99596 0.00126 0.00000 0.11275 0.11293 -2.88303

D22 1.18964 0.00027 0.00000 0.09126 0.09131 1.28095

D23 1.06979 -0.00014 0.00000 0.05968 0.05863 1.12841

D24 -0.88152 0.00065 0.00000 0.07960 0.07902 -0.80250

D25 -2.97910 -0.00033 0.00000 0.05811 0.05740 -2.92171

D26 3.12870 0.00009 0.00000 0.08721 0.08640 -3.06809

D27 1.17739 0.00088 0.00000 0.10714 0.10679 1.28418

D28 -0.92019 -0.00010 0.00000 0.08564 0.08517 -0.83502

D29 0.60994 0.00018 0.00000 -0.03356 -0.03288 0.57705

D30 -2.71824 0.00051 0.00000 0.03208 0.03271 -2.68552

D31 -2.92247 -0.00011 0.00000 -0.01571 -0.01502 -2.93749

D32 0.03254 0.00022 0.00000 0.04993 0.05058 0.08312

D33 -1.18831 -0.00014 0.00000 0.00549 0.00598 -1.18233

D34 1.76670 0.00019 0.00000 0.07113 0.07158 1.83828

D35 -0.57747 0.00055 0.00000 0.10194 0.10288 -0.47459

D36 -2.73599 0.00026 0.00000 0.10669 0.10704 -2.62895

D37 1.53024 0.00038 0.00000 0.11927 0.11930 1.64954

D38 2.94073 0.00048 0.00000 0.08114 0.08227 3.02300

D39 0.78221 0.00019 0.00000 0.08589 0.08643 0.86864

D40 -1.23474 0.00032 0.00000 0.09847 0.09869 -1.13605

D41 1.15369 -0.00010 0.00000 0.06096 0.06196 1.21565

D42 -1.00483 -0.00039 0.00000 0.06570 0.06612 -0.93870

D43 -3.02179 -0.00027 0.00000 0.07829 0.07838 -2.94340

D44 1.03796 -0.00096 0.00000 0.05149 0.05152 1.08948

D45 2.97536 -0.00014 0.00000 0.04792 0.04780 3.02316

D46 -1.19274 -0.00042 0.00000 0.05301 0.05338 -1.13936

D47 -1.07432 -0.00124 0.00000 0.05600 0.05666 -1.01766

D48 0.86308 -0.00041 0.00000 0.05244 0.05294 0.91602

D49 2.97816 -0.00070 0.00000 0.05752 0.05852 3.03668

D50 -3.13765 -0.00043 0.00000 0.06098 0.06120 -3.07645

D51 -1.20025 0.00040 0.00000 0.05741 0.05748 -1.14277

D52 0.91483 0.00011 0.00000 0.06250 0.06306 0.97789

D53 -0.00391 -0.00003 0.00000 -0.13123 -0.13115 -0.13506

D54 2.15614 0.00024 0.00000 -0.13190 -0.13166 2.02448

D55 -2.09596 0.00014 0.00000 -0.14765 -0.14706 -2.24303

D56 -2.17092 -0.00021 0.00000 -0.12025 -0.12033 -2.29124

D57 -0.01087 0.00006 0.00000 -0.12092 -0.12083 -0.13170

D58 2.02022 -0.00004 0.00000 -0.13667 -0.13624 1.88398

D59 2.08642 -0.00006 0.00000 -0.14511 -0.14565 1.94076

D60 -2.03672 0.00021 0.00000 -0.14578 -0.14616 -2.18288

D61 -0.00563 0.00011 0.00000 -0.16153 -0.16157 -0.16720

D62 -0.04911 0.00039 0.00000 -0.02536 -0.02464 -0.07375

D63 3.08461 0.00024 0.00000 -0.03516 -0.03405 3.05056

D64 0.05296 -0.00043 0.00000 0.02365 0.02315 0.07610

D65 -3.08431 -0.00030 0.00000 0.04609 0.04564 -3.03868

D66 0.00344 -0.00014 0.00000 -0.08187 -0.08222 -0.07877

D67 1.86176 -0.00029 0.00000 -0.06430 -0.06467 1.79709

D68 -1.78454 -0.00011 0.00000 -0.14796 -0.14718 -1.93172

D69 -1.85172 -0.00001 0.00000 -0.02154 -0.02176 -1.87348

D70 0.00660 -0.00016 0.00000 -0.00397 -0.00421 0.00239

D71 2.64348 0.00002 0.00000 -0.08763 -0.08672 2.55676

D72 1.79483 -0.00031 0.00000 -0.09492 -0.09517 1.69966

D73 -2.63003 -0.00046 0.00000 -0.07735 -0.07762 -2.70766

D74 0.00685 -0.00028 0.00000 -0.16102 -0.16014 -0.15329

D75 -1.91192 -0.00105 0.00000 0.02918 0.03058 -1.88134

D76 1.23964 -0.00086 0.00000 0.04162 0.04256 1.28220

D77 0.02584 -0.00011 0.00000 0.01828 0.01814 0.04398

D78 -3.10578 0.00007 0.00000 0.03071 0.03012 -3.07566

D79 2.69472 0.00000 0.00000 0.08258 0.08357 2.77829

D80 -0.43690 0.00019 0.00000 0.09502 0.09554 -0.34136

D81 1.92231 -0.00017 0.00000 -0.00907 -0.01088 1.91142

D82 -1.22478 -0.00033 0.00000 -0.03754 -0.03910 -1.26388

D83 -0.03690 0.00036 0.00000 -0.01187 -0.01142 -0.04832

D84 3.09920 0.00020 0.00000 -0.04034 -0.03964 3.05956

D85 -2.71180 0.00053 0.00000 0.07536 0.07562 -2.63619

D86 0.42429 0.00037 0.00000 0.04689 0.04740 0.47170

Item Value Threshold Converged?

Maximum Force 0.011532 0.000450 NO

RMS Force 0.001133 0.000300 NO

Maximum Displacement 0.260335 0.001800 NO

RMS Displacement 0.069665 0.001200 NO

Predicted change in Energy=-2.863177D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.145398 1.580789 0.453343

2 6 0 0.175988 1.276073 0.161619

3 6 0 -0.736768 3.779314 -0.382404

4 6 0 -1.608186 2.860887 0.178441

5 1 0 -1.780694 0.896947 1.031935

6 1 0 -2.613757 3.158961 0.509923

7 6 0 0.775887 1.886082 -1.104327

8 1 0 1.895626 1.827199 -1.069402

9 1 0 0.439555 1.250484 -1.970791

10 6 0 0.326119 3.322352 -1.326661

11 1 0 1.215792 4.007627 -1.266084

12 1 0 -0.073535 3.432122 -2.373138

13 1 0 -1.004587 4.848784 -0.437490

14 1 0 0.599870 0.315713 0.491695

15 8 0 2.705019 3.901863 0.725857

16 6 0 0.465162 3.849888 1.450829

17 6 0 0.989973 2.549644 1.655866

18 6 0 1.556552 4.696094 0.903035

19 8 0 1.668917 5.875184 0.608228

20 6 0 2.416801 2.618917 1.227959

21 8 0 3.351624 1.835464 1.251200

22 1 0 -0.385959 4.288600 1.973740

23 1 0 0.689595 1.874020 2.461085

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.387089 0.000000

3 C 2.387250 2.719430 0.000000

4 C 1.388667 2.386461 1.384711 0.000000

5 H 1.098185 2.174808 3.376118 2.148319 0.000000

6 H 2.156364 3.383676 2.168910 1.099955 2.466414

7 C 2.492163 1.527943 2.528562 2.877420 3.475358

8 H 3.409881 2.185476 3.348465 3.860352 4.335471

9 H 2.915065 2.148789 3.209625 3.377254 3.751114

10 C 2.892545 2.534714 1.493374 2.493957 3.985502

11 H 3.797524 3.252833 2.155344 3.372910 4.892459

12 H 3.544759 3.337035 2.126839 3.031834 4.575590

13 H 3.390162 3.810112 1.103870 2.166896 4.287023

14 H 2.155887 1.100417 3.814077 3.384014 2.509338

15 O 4.504149 3.689056 3.617894 4.470686 5.407849

16 C 2.955959 2.893131 2.193253 2.625998 3.733525

17 C 2.635251 2.125401 2.940793 3.005010 3.285924

18 C 4.148238 3.761941 2.784269 3.729422 5.058394

19 O 5.136748 4.855937 3.340859 4.473266 6.071424

20 C 3.790383 2.821623 3.726230 4.166600 4.541208

21 O 4.574345 3.403640 4.812708 5.177066 5.222028

22 H 3.196966 3.560181 2.435949 2.599095 3.786237

23 H 2.735729 2.430818 3.708110 3.385877 3.016533

6 7 8 9 10

6 H 0.000000

7 C 3.964305 0.000000

8 H 4.960080 1.121829 0.000000

9 H 4.372521 1.125995 1.806999 0.000000

10 C 3.470246 1.521379 2.182891 2.172650 0.000000

11 H 4.305796 2.172703 2.292406 2.949746 1.124629

12 H 3.852192 2.172933 2.855363 2.276992 1.125560

13 H 2.518436 3.520279 4.235625 4.169451 2.211651

14 H 4.290897 2.245958 2.529940 2.638813 3.524377

15 O 5.374748 3.336839 2.860472 4.408407 3.194969

16 C 3.292784 3.237578 3.533986 4.297097 2.830562

17 C 3.830316 2.846895 2.961286 3.891454 3.151705

18 C 4.461927 3.540495 3.498004 4.623720 2.893558

19 O 5.072359 4.432074 4.387713 5.436039 3.473306

20 C 5.110160 2.944351 2.485218 4.001764 3.375182

21 O 6.155234 3.490772 2.739560 4.382188 4.243805

22 H 2.895155 4.073877 4.530434 5.046875 3.511885

23 H 4.046015 3.566476 3.731090 4.482504 4.071461

11 12 13 14 15

11 H 0.000000

12 H 1.794196 0.000000

13 H 2.514796 2.573037 0.000000

14 H 4.135140 4.286344 4.897591 0.000000

15 O 2.489340 4.188650 4.001402 4.164967 0.000000

16 C 2.823109 3.884256 2.593011 3.664488 2.354835

17 C 3.273301 4.259423 3.694111 2.549102 2.373772

18 C 2.301126 3.871449 2.894781 4.502463 1.407541

19 O 2.684424 4.230039 3.048712 5.662522 2.231892

20 C 3.096964 4.453198 4.410434 3.024578 1.407525

21 O 3.951808 5.236110 5.559527 3.233981 2.228023

22 H 3.625053 4.441453 2.551575 4.353406 3.355731

23 H 4.326771 5.136123 4.485667 2.512940 3.344413

16 17 18 19 20

16 C 0.000000

17 C 1.417075 0.000000

18 C 1.485690 2.344145 0.000000

19 O 2.502165 3.552144 1.220570 0.000000

20 C 2.318158 1.491221 2.271622 3.398040 0.000000

21 O 3.525537 2.500240 3.395100 4.423150 1.219931

22 H 1.091014 2.240135 2.255174 2.933324 3.346565

23 H 2.230480 1.093193 3.338148 4.516798 2.249158

21 22 23

21 O 0.000000

22 H 4.528738 0.000000

23 H 2.924329 2.687846 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.323554 -0.598220 -0.689290

2 6 0 1.402357 -1.342285 0.033053

3 6 0 1.317469 1.369887 0.212548

4 6 0 2.275732 0.786701 -0.599271

5 1 0 2.976737 -1.061457 -1.440804

6 1 0 2.916327 1.397035 -1.252747

7 6 0 1.017919 -0.831094 1.420678

8 1 0 0.069684 -1.321755 1.765065

9 1 0 1.831311 -1.152225 2.129997

10 6 0 0.878535 0.683268 1.463969

11 1 0 -0.187059 0.955275 1.699155

12 1 0 1.493007 1.091978 2.313832

13 1 0 1.122643 2.455312 0.163327

14 1 0 1.334902 -2.429157 -0.125299

15 8 0 -2.025157 -0.009701 0.325462

16 6 0 -0.298623 0.699762 -1.110153

17 6 0 -0.274642 -0.717107 -1.113312

18 6 0 -1.419995 1.130405 -0.235884

19 8 0 -1.914216 2.204444 0.067395

20 6 0 -1.399661 -1.141121 -0.231107

21 8 0 -1.886332 -2.218617 0.069533

22 1 0 0.093327 1.350329 -1.893383

23 1 0 0.018883 -1.335514 -1.965654

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2214655 0.8867757 0.6805921

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.1358314372 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.477267436292E-01 A.U. after 15 cycles

Convg = 0.4379D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.009720957 -0.002141517 0.005334689

2 6 0.018683158 0.006424158 -0.021496953

3 6 0.011204744 0.006371498 -0.002784173

4 6 -0.012203890 -0.001394460 -0.000449768

5 1 0.000419807 -0.002624097 0.001109199

6 1 0.000146245 0.001764813 0.001279311

7 6 -0.009377215 -0.007964091 0.019535606

8 1 -0.000679222 0.000138306 0.001098065

9 1 0.000415590 0.000232787 0.001989734

10 6 0.000026171 0.000143469 0.000170537

11 1 -0.000239807 0.000333737 -0.001723448

12 1 -0.000887093 -0.000692577 0.000210052

13 1 0.000599350 -0.000957575 -0.000279405

14 1 0.003196132 0.000992357 -0.000422361

15 8 0.001060863 -0.000318806 0.001848603

16 6 -0.003851223 -0.001178791 -0.004894488

17 6 -0.000201085 0.006394662 -0.004078805

18 6 -0.002055281 0.000784486 0.004229797

19 8 -0.000606156 0.000889688 -0.001166126

20 6 0.002029292 -0.004412210 0.001398021

21 8 0.001384036 -0.002185146 -0.001270668

22 1 0.001140561 0.000838516 0.001700172

23 1 -0.000484020 -0.001439206 -0.001337590

-------------------------------------------------------------------

Cartesian Forces: Max 0.021496953 RMS 0.005443531

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.022043658 RMS 0.002522978

Search for a saddle point.

Step number 38 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 37 38

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07239 -0.00265 0.00477 0.00618 0.00931

Eigenvalues --- 0.01002 0.01165 0.01598 0.01964 0.02159

Eigenvalues --- 0.02528 0.02606 0.02763 0.03014 0.03103

Eigenvalues --- 0.03223 0.03374 0.03594 0.03702 0.03822

Eigenvalues --- 0.03998 0.04102 0.04220 0.04793 0.05424

Eigenvalues --- 0.05998 0.06100 0.06425 0.07278 0.07436

Eigenvalues --- 0.08689 0.08810 0.09824 0.09876 0.10218

Eigenvalues --- 0.12073 0.13830 0.14691 0.16446 0.21634

Eigenvalues --- 0.25203 0.26059 0.27577 0.28623 0.29850

Eigenvalues --- 0.30956 0.31302 0.31540 0.31950 0.32188

Eigenvalues --- 0.32453 0.32922 0.34409 0.36342 0.37045

Eigenvalues --- 0.39612 0.39959 0.40430 0.45565 0.48776

Eigenvalues --- 0.51996 1.08488 1.10858

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D35 D4

1 -0.54647 -0.52123 0.19617 -0.14546 -0.14532

D29 D71 D37 D36 D1

1 0.14531 -0.13995 -0.13591 -0.11800 -0.11789

RFO step: Lambda0=1.195165645D-04 Lambda=-5.69706019D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.963

Iteration 1 RMS(Cart)= 0.08729100 RMS(Int)= 0.00360538

Iteration 2 RMS(Cart)= 0.00482393 RMS(Int)= 0.00103184

Iteration 3 RMS(Cart)= 0.00001256 RMS(Int)= 0.00103180

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00103180

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62122 0.01160 0.00000 0.05086 0.05188 2.67310

R2 2.62420 0.00435 0.00000 0.03936 0.04156 2.66576

R3 2.07527 0.00198 0.00000 0.00539 0.00539 2.08066

R4 2.88739 -0.02204 0.00000 -0.08337 -0.08420 2.80320

R5 2.07949 0.00024 0.00000 0.00411 0.00411 2.08360

R6 4.01643 -0.00296 0.00000 -0.17496 -0.17390 3.84252

R7 2.61672 0.00942 0.00000 0.05657 0.05757 2.67430

R8 2.82207 -0.00189 0.00000 -0.01458 -0.01545 2.80662

R9 2.08601 -0.00106 0.00000 -0.00598 -0.00598 2.08003

R10 4.14465 -0.00045 0.00000 0.12851 0.12749 4.27214

R11 2.07861 0.00073 0.00000 -0.00427 -0.00427 2.07434

R12 2.11995 -0.00065 0.00000 0.00254 0.00254 2.12249

R13 2.12782 -0.00179 0.00000 -0.00146 -0.00146 2.12636

R14 2.87499 0.00168 0.00000 -0.00369 -0.00592 2.86907

R15 2.12524 -0.00008 0.00000 0.00369 0.00369 2.12893

R16 2.12700 0.00005 0.00000 -0.00028 -0.00028 2.12672

R17 2.65987 0.00236 0.00000 0.01967 0.02071 2.68058

R18 2.65984 0.00006 0.00000 -0.00415 -0.00322 2.65661

R19 2.67788 0.00147 0.00000 -0.01890 -0.02003 2.65786

R20 2.80755 -0.00144 0.00000 -0.00983 -0.01009 2.79746

R21 2.06172 0.00026 0.00000 0.00002 0.00002 2.06174

R22 2.81800 0.00157 0.00000 0.02560 0.02515 2.84315

R23 2.06584 0.00004 0.00000 0.00343 0.00343 2.06926

R24 2.30654 0.00109 0.00000 -0.00065 -0.00065 2.30589

R25 2.30533 0.00244 0.00000 0.00013 0.00013 2.30547

A1 2.06957 -0.00210 0.00000 -0.02783 -0.02840 2.04117

A2 2.12364 -0.00106 0.00000 0.01274 0.01288 2.13651

A3 2.07776 0.00317 0.00000 0.01731 0.01762 2.09538

A4 2.04943 0.00193 0.00000 0.01620 0.01603 2.06546

A5 2.08931 -0.00076 0.00000 0.00960 0.01073 2.10004

A6 1.65624 0.00026 0.00000 0.02542 0.02289 1.67913

A7 2.03276 -0.00084 0.00000 -0.03435 -0.03532 1.99744

A8 1.76491 -0.00039 0.00000 0.01361 0.01439 1.77930

A9 1.73609 -0.00052 0.00000 -0.01998 -0.01917 1.71692

A10 2.09561 -0.00017 0.00000 0.01903 0.01828 2.11388

A11 2.10612 -0.00133 0.00000 0.01261 0.01398 2.12010

A12 1.59847 0.00138 0.00000 -0.05201 -0.05297 1.54550

A13 2.02371 0.00139 0.00000 -0.01931 -0.02050 2.00321

A14 1.71966 -0.00170 0.00000 -0.01791 -0.01808 1.70158

A15 1.71479 0.00047 0.00000 0.03823 0.03996 1.75475

A16 2.07357 -0.00336 0.00000 -0.01321 -0.01410 2.05947

A17 2.08841 0.00301 0.00000 0.02076 0.02058 2.10900

A18 2.11488 0.00026 0.00000 -0.01218 -0.01201 2.10287

A19 1.92318 -0.00178 0.00000 0.01049 0.01096 1.93414

A20 1.87018 -0.00242 0.00000 -0.00854 -0.00812 1.86206

A21 1.96266 0.00511 0.00000 0.01533 0.01400 1.97666

A22 1.86760 0.00105 0.00000 -0.00267 -0.00289 1.86471

A23 1.92749 -0.00183 0.00000 -0.01653 -0.01692 1.91058

A24 1.90937 -0.00031 0.00000 0.00128 0.00239 1.91176

A25 1.98984 -0.00139 0.00000 -0.00695 -0.00726 1.98258

A26 1.92041 0.00088 0.00000 -0.00119 -0.00100 1.91941

A27 1.88106 0.00008 0.00000 0.00386 0.00388 1.88495

A28 1.91082 -0.00024 0.00000 0.00378 0.00294 1.91375

A29 1.91019 0.00113 0.00000 0.00346 0.00450 1.91469

A30 1.84579 -0.00037 0.00000 -0.00265 -0.00270 1.84309

A31 1.87795 0.00081 0.00000 0.01230 0.01164 1.88958

A32 1.86959 -0.00096 0.00000 -0.04379 -0.04621 1.82338

A33 1.68374 0.00166 0.00000 0.01772 0.01936 1.70310

A34 1.55683 0.00033 0.00000 -0.00316 -0.00199 1.55484

A35 1.87958 -0.00124 0.00000 -0.00334 -0.00292 1.87666

A36 2.20003 0.00178 0.00000 0.01870 0.01744 2.21747

A37 2.11854 -0.00100 0.00000 -0.00226 -0.00192 2.11662

A38 1.88205 0.00136 0.00000 0.04384 0.04096 1.92301

A39 1.76455 -0.00120 0.00000 0.02354 0.02396 1.78851

A40 1.61309 -0.00143 0.00000 -0.04653 -0.04585 1.56724

A41 1.84441 0.00187 0.00000 0.02059 0.01953 1.86394

A42 2.17960 0.00082 0.00000 0.01024 0.01027 2.18987

A43 2.09784 -0.00206 0.00000 -0.04175 -0.04083 2.05700

A44 1.90119 0.00062 0.00000 -0.00051 -0.00208 1.89910

A45 2.02592 0.00015 0.00000 -0.00538 -0.00459 2.02133

A46 2.35590 -0.00076 0.00000 0.00580 0.00656 2.36246

A47 1.91839 -0.00201 0.00000 -0.02314 -0.02495 1.89343

A48 2.02111 0.00120 0.00000 0.01819 0.01910 2.04022

A49 2.34326 0.00080 0.00000 0.00494 0.00585 2.34911

D1 -0.64794 0.00030 0.00000 0.00228 0.00203 -0.64591

D2 3.00067 -0.00018 0.00000 0.03013 0.03017 3.03084

D3 1.18853 0.00044 0.00000 0.03591 0.03606 1.22459

D4 2.66266 -0.00006 0.00000 -0.01450 -0.01441 2.64824

D5 0.02809 -0.00054 0.00000 0.01336 0.01373 0.04181

D6 -1.78406 0.00008 0.00000 0.01914 0.01962 -1.76444

D7 0.00660 -0.00076 0.00000 -0.02090 -0.02038 -0.01378

D8 -3.01588 0.00003 0.00000 0.02345 0.02450 -2.99138

D9 2.98372 -0.00081 0.00000 -0.00487 -0.00467 2.97904

D10 -0.03877 -0.00001 0.00000 0.03948 0.04020 0.00143

D11 2.84571 0.00062 0.00000 0.06673 0.06618 2.91189

D12 -1.41149 -0.00042 0.00000 0.06426 0.06387 -1.34762

D13 0.68713 0.00065 0.00000 0.06940 0.06982 0.75695

D14 -0.78646 0.00108 0.00000 0.05201 0.05205 -0.73442

D15 1.23952 0.00003 0.00000 0.04954 0.04974 1.28926

D16 -2.94504 0.00111 0.00000 0.05468 0.05569 -2.88935

D17 1.07356 -0.00005 0.00000 0.02433 0.02548 1.09904

D18 3.09954 -0.00110 0.00000 0.02186 0.02318 3.12272

D19 -1.08502 -0.00002 0.00000 0.02700 0.02913 -1.05589

D20 -0.95211 -0.00220 0.00000 0.06843 0.07043 -0.88168

D21 -2.88303 -0.00421 0.00000 0.02141 0.02273 -2.86030

D22 1.28095 -0.00152 0.00000 0.07246 0.07300 1.35395

D23 1.12841 -0.00020 0.00000 0.09505 0.09719 1.22560

D24 -0.80250 -0.00221 0.00000 0.04804 0.04949 -0.75302

D25 -2.92171 0.00048 0.00000 0.09908 0.09976 -2.82195

D26 -3.06809 -0.00138 0.00000 0.05625 0.05779 -3.01029

D27 1.28418 -0.00339 0.00000 0.00923 0.01009 1.29428

D28 -0.83502 -0.00069 0.00000 0.06028 0.06036 -0.77466

D29 0.57705 -0.00080 0.00000 -0.02895 -0.02956 0.54749

D30 -2.68552 -0.00142 0.00000 -0.07167 -0.07197 -2.75749

D31 -2.93749 -0.00083 0.00000 0.00532 0.00545 -2.93203

D32 0.08312 -0.00145 0.00000 -0.03740 -0.03695 0.04617

D33 -1.18233 0.00038 0.00000 0.02019 0.02148 -1.16085

D34 1.83828 -0.00024 0.00000 -0.02254 -0.02092 1.81736

D35 -0.47459 -0.00184 0.00000 0.07810 0.07743 -0.39717

D36 -2.62895 -0.00119 0.00000 0.07913 0.07961 -2.54933

D37 1.64954 -0.00125 0.00000 0.08077 0.08121 1.73075

D38 3.02300 -0.00126 0.00000 0.03926 0.03812 3.06112

D39 0.86864 -0.00061 0.00000 0.04028 0.04031 0.90895

D40 -1.13605 -0.00067 0.00000 0.04192 0.04190 -1.09415

D41 1.21565 -0.00127 0.00000 0.01035 0.00760 1.22325

D42 -0.93870 -0.00062 0.00000 0.01138 0.00979 -0.92892

D43 -2.94340 -0.00068 0.00000 0.01302 0.01138 -2.93202

D44 1.08948 0.00284 0.00000 0.11601 0.11456 1.20405

D45 3.02316 0.00189 0.00000 0.10859 0.10720 3.13036

D46 -1.13936 0.00101 0.00000 0.10686 0.10611 -1.03325

D47 -1.01766 0.00295 0.00000 0.10873 0.10632 -0.91135

D48 0.91602 0.00201 0.00000 0.10131 0.09895 1.01497

D49 3.03668 0.00113 0.00000 0.09958 0.09786 3.13454

D50 -3.07645 0.00180 0.00000 0.12375 0.12260 -2.95384

D51 -1.14277 0.00086 0.00000 0.11633 0.11524 -1.02753

D52 0.97789 -0.00002 0.00000 0.11460 0.11415 1.09204

D53 -0.13506 0.00033 0.00000 -0.09363 -0.09371 -0.22877

D54 2.02448 0.00029 0.00000 -0.09730 -0.09799 1.92648

D55 -2.24303 0.00034 0.00000 -0.09642 -0.09705 -2.34008

D56 -2.29124 0.00032 0.00000 -0.10605 -0.10536 -2.39660

D57 -0.13170 0.00028 0.00000 -0.10972 -0.10964 -0.24135

D58 1.88398 0.00034 0.00000 -0.10885 -0.10870 1.77528

D59 1.94076 0.00031 0.00000 -0.09380 -0.09338 1.84738

D60 -2.18288 0.00027 0.00000 -0.09747 -0.09767 -2.28055

D61 -0.16720 0.00033 0.00000 -0.09659 -0.09673 -0.26393

D62 -0.07375 0.00023 0.00000 0.04493 0.04625 -0.02750

D63 3.05056 0.00078 0.00000 0.04057 0.04164 3.09220

D64 0.07610 -0.00086 0.00000 -0.08647 -0.08583 -0.00973

D65 -3.03868 -0.00056 0.00000 -0.08595 -0.08590 -3.12457

D66 -0.07877 0.00024 0.00000 -0.11369 -0.11390 -0.19268

D67 1.79709 0.00024 0.00000 -0.06116 -0.06000 1.73709

D68 -1.93172 0.00060 0.00000 -0.09312 -0.09190 -2.02362

D69 -1.87348 -0.00075 0.00000 -0.11482 -0.11630 -1.98978

D70 0.00239 -0.00076 0.00000 -0.06229 -0.06239 -0.06000

D71 2.55676 -0.00039 0.00000 -0.09425 -0.09429 2.46246

D72 1.69966 0.00074 0.00000 -0.14454 -0.14645 1.55322

D73 -2.70766 0.00073 0.00000 -0.09200 -0.09254 -2.80020

D74 -0.15329 0.00110 0.00000 -0.12396 -0.12444 -0.27773

D75 -1.88134 0.00099 0.00000 0.05397 0.05534 -1.82601

D76 1.28220 0.00027 0.00000 0.05970 0.06144 1.34364

D77 0.04398 0.00030 0.00000 0.01280 0.01222 0.05620

D78 -3.07566 -0.00043 0.00000 0.01853 0.01832 -3.05734

D79 2.77829 -0.00028 0.00000 0.04710 0.04606 2.82435

D80 -0.34136 -0.00100 0.00000 0.05283 0.05216 -0.28920

D81 1.91142 0.00263 0.00000 0.15687 0.15515 2.06657

D82 -1.26388 0.00225 0.00000 0.15635 0.15536 -1.10852

D83 -0.04832 0.00100 0.00000 0.09336 0.09314 0.04481

D84 3.05956 0.00061 0.00000 0.09284 0.09334 -3.13028

D85 -2.63619 -0.00044 0.00000 0.10362 0.10341 -2.53278

D86 0.47170 -0.00082 0.00000 0.10310 0.10362 0.57531

Item Value Threshold Converged?

Maximum Force 0.022044 0.000450 NO

RMS Force 0.002523 0.000300 NO

Maximum Displacement 0.488694 0.001800 NO

RMS Displacement 0.087840 0.001200 NO

Predicted change in Energy=-4.296727D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.168828 1.603704 0.505932

2 6 0 0.178987 1.304345 0.198177

3 6 0 -0.724752 3.779252 -0.461977

4 6 0 -1.635333 2.887319 0.152859

5 1 0 -1.795632 0.938836 1.120218

6 1 0 -2.621133 3.238539 0.484180

7 6 0 0.747043 1.833706 -1.065758

8 1 0 1.865520 1.731445 -1.074395

9 1 0 0.353728 1.182220 -1.894609

10 6 0 0.369036 3.279542 -1.333599

11 1 0 1.278457 3.935399 -1.224116

12 1 0 0.040533 3.393819 -2.403917

13 1 0 -0.960487 4.847443 -0.584231

14 1 0 0.631693 0.359358 0.541350

15 8 0 2.695483 3.996885 0.802253

16 6 0 0.441697 3.832111 1.473858

17 6 0 1.001594 2.546428 1.582069

18 6 0 1.515114 4.749860 1.030067

19 8 0 1.609500 5.953114 0.850560

20 6 0 2.428169 2.652862 1.116053

21 8 0 3.350085 1.863409 0.992594

22 1 0 -0.449488 4.205785 1.980312

23 1 0 0.772610 1.817625 2.366579

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.414544 0.000000

3 C 2.422201 2.716194 0.000000

4 C 1.410657 2.408239 1.415176 0.000000

5 H 1.101036 2.209723 3.423168 2.181299 0.000000

6 H 2.186858 3.415198 2.187200 1.097693 2.524802

7 C 2.488709 1.483389 2.513142 2.875907 3.470515

8 H 3.423598 2.155516 3.358286 3.885637 4.341496

9 H 2.873748 2.103617 3.155968 3.325035 3.710548

10 C 2.925292 2.506763 1.485197 2.526043 4.023171

11 H 3.797245 3.186565 2.148973 3.388909 4.891350

12 H 3.624125 3.340054 2.122581 3.098737 4.670970

13 H 3.428367 3.803171 1.100704 2.200183 4.345091

14 H 2.188956 1.102593 3.813434 3.417736 2.561794

15 O 4.555000 3.734627 3.652897 4.517612 5.442690

16 C 2.914870 2.843586 2.260720 2.636612 3.674472

17 C 2.599525 2.033374 2.945887 3.018648 3.259161

18 C 4.168519 3.787987 2.860992 3.763491 5.049065

19 O 5.172546 4.907446 3.449226 4.518277 6.067175

20 C 3.796231 2.778456 3.701331 4.182674 4.558333

21 O 4.552456 3.316552 4.731863 5.158288 5.229677

22 H 3.076048 3.462563 2.494490 2.546403 3.636595

23 H 2.697582 2.306038 3.753771 3.441364 2.986897

6 7 8 9 10

6 H 0.000000

7 C 3.964905 0.000000

8 H 4.983026 1.123176 0.000000

9 H 4.328613 1.125223 1.805523 0.000000

10 C 3.499588 1.518246 2.168699 2.171112 0.000000

11 H 4.314011 2.173612 2.285711 2.980718 1.126579

12 H 3.930608 2.173425 2.803871 2.290995 1.125412

13 H 2.547120 3.497162 4.235095 4.108299 2.188036

14 H 4.344402 2.183988 2.452669 2.586168 3.480215

15 O 5.379839 3.459079 3.056610 4.547442 3.238642

16 C 3.273029 3.245999 3.596341 4.286751 2.862242

17 C 3.848185 2.753862 2.909875 3.790526 3.072248

18 C 4.437411 3.672379 3.696265 4.757163 3.010356

19 O 5.039981 4.624459 4.646879 5.645737 3.668417

20 C 5.122278 2.873587 2.442058 3.940835 3.260913

21 O 6.148570 3.318663 2.548292 4.216411 4.037729

22 H 2.808918 4.041904 4.562112 4.980173 3.536937

23 H 4.132785 3.432469 3.611396 4.328617 3.998923

11 12 13 14 15

11 H 0.000000

12 H 1.793794 0.000000

13 H 2.500830 2.535019 0.000000

14 H 4.040203 4.269897 4.893351 0.000000

15 O 2.473442 4.206183 4.001488 4.190335 0.000000

16 C 2.826641 3.923031 2.689378 3.600789 2.357489

17 C 3.143337 4.186860 3.719852 2.450142 2.362457

18 C 2.408462 3.975610 2.957039 4.505084 1.418500

19 O 2.912909 4.427557 3.144196 5.686987 2.237973

20 C 2.905706 4.317408 4.380656 2.969473 1.405819

21 O 3.674042 4.983129 5.474657 3.139338 2.239744

22 H 3.650652 4.485630 2.692533 4.246712 3.364863

23 H 4.199277 5.077199 4.570635 2.340483 3.300565

16 17 18 19 20

16 C 0.000000

17 C 1.406477 0.000000

18 C 1.480350 2.328846 0.000000

19 O 2.500183 3.536971 1.220226 0.000000

20 C 2.337675 1.504532 2.288769 3.410626 0.000000

21 O 3.544872 2.515831 3.420544 4.446964 1.220002

22 H 1.091027 2.240023 2.249143 2.927273 3.382222

23 H 2.228140 1.095007 3.306898 4.483410 2.236585

21 22 23

21 O 0.000000

22 H 4.571549 0.000000

23 H 2.921182 2.710356 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.346211 -0.345816 -0.810458

2 6 0 1.464925 -1.236785 -0.154376

3 6 0 1.240879 1.401514 0.451342

4 6 0 2.231390 1.022090 -0.485487

5 1 0 2.994534 -0.662510 -1.642120

6 1 0 2.781361 1.783473 -1.053605

7 6 0 1.125167 -0.973333 1.265342

8 1 0 0.250299 -1.598863 1.589135

9 1 0 2.008858 -1.307611 1.876467

10 6 0 0.834636 0.489278 1.550706

11 1 0 -0.261523 0.621050 1.774878

12 1 0 1.375098 0.808237 2.484900

13 1 0 0.967398 2.456881 0.602860

14 1 0 1.433913 -2.301007 -0.441046

15 8 0 -2.074387 -0.120917 0.264606

16 6 0 -0.333190 0.777373 -1.046526

17 6 0 -0.220895 -0.623109 -1.111467

18 6 0 -1.522266 1.091494 -0.222595

19 8 0 -2.115673 2.110055 0.092609

20 6 0 -1.311698 -1.187482 -0.242416

21 8 0 -1.664066 -2.313843 0.066702

22 1 0 0.075047 1.502998 -1.751614

23 1 0 0.077064 -1.196355 -1.995576

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2219888 0.8820289 0.6753043

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.7563986788 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.465086124741E-01 A.U. after 16 cycles

Convg = 0.3165D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001798284 0.020478319 -0.009752157

2 6 -0.008815703 0.002341706 0.011069650

3 6 -0.007071729 -0.014374526 0.018686555

4 6 0.021328258 -0.006968574 -0.004914983

5 1 0.003265914 0.000660637 -0.001649263

6 1 0.000213851 -0.000301235 -0.000334039

7 6 0.001049400 0.001893855 -0.007008279

8 1 0.000383121 -0.000938896 -0.000003311

9 1 0.000594627 0.000119236 -0.001843281

10 6 -0.000489771 0.001120682 -0.001894065

11 1 -0.000678754 0.000172873 -0.000254000

12 1 -0.000736192 -0.000983771 -0.000369872

13 1 -0.002158246 -0.000193260 0.002788516

14 1 -0.001516026 -0.001847869 0.001234418

15 8 -0.000686543 0.000994863 -0.001106766

16 6 -0.007453671 0.011382797 -0.012395847

17 6 0.006470193 -0.017614781 -0.003949508

18 6 0.002590508 -0.003384474 0.001822660

19 8 0.000081611 -0.000302708 -0.001504281

20 6 -0.005676565 0.005945737 0.006502862

21 8 -0.000225201 0.000609970 -0.000769346

22 1 0.001781344 0.000147589 0.001942590

23 1 -0.000452144 0.001041829 0.003701749

-------------------------------------------------------------------

Cartesian Forces: Max 0.021328258 RMS 0.006395688

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.018922310 RMS 0.002929378

Search for a saddle point.

Step number 39 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 29 30 32 38 39

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07704 -0.00777 -0.00013 0.00445 0.00758

Eigenvalues --- 0.00962 0.01091 0.01688 0.01888 0.02165

Eigenvalues --- 0.02563 0.02668 0.02817 0.03011 0.03156

Eigenvalues --- 0.03303 0.03352 0.03604 0.03683 0.03826

Eigenvalues --- 0.03906 0.04128 0.04408 0.04694 0.05594

Eigenvalues --- 0.06029 0.06097 0.06382 0.07212 0.07362

Eigenvalues --- 0.08713 0.08816 0.09806 0.09845 0.10401

Eigenvalues --- 0.12029 0.13840 0.14728 0.16793 0.21598

Eigenvalues --- 0.25950 0.26646 0.28162 0.28933 0.29887

Eigenvalues --- 0.30905 0.31299 0.31687 0.31960 0.32209

Eigenvalues --- 0.32447 0.32966 0.35045 0.36940 0.37468

Eigenvalues --- 0.39627 0.40393 0.40445 0.46071 0.49024

Eigenvalues --- 0.51988 1.08481 1.10860

Eigenvectors required to have negative eigenvalues:

R6 R10 D4 D71 D30

1 -0.60032 -0.47707 -0.16343 -0.16290 0.15415

D68 D1 D85 D13 D86

1 -0.14023 -0.12869 0.12493 0.12208 0.11651

RFO step: Lambda0=9.377107154D-04 Lambda=-7.78261379D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.786

Iteration 1 RMS(Cart)= 0.06257749 RMS(Int)= 0.00194912

Iteration 2 RMS(Cart)= 0.00248965 RMS(Int)= 0.00074309

Iteration 3 RMS(Cart)= 0.00000373 RMS(Int)= 0.00074309

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00074309

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.67310 -0.00876 0.00000 -0.02745 -0.02658 2.64652

R2 2.66576 -0.01812 0.00000 0.00005 0.00147 2.66722

R3 2.08066 -0.00318 0.00000 -0.00132 -0.00132 2.07934

R4 2.80320 0.00633 0.00000 -0.00947 -0.00976 2.79343

R5 2.08360 0.00135 0.00000 -0.00260 -0.00260 2.08100

R6 3.84252 -0.00155 0.00000 0.17930 0.17926 4.02178

R7 2.67430 -0.01892 0.00000 -0.00767 -0.00724 2.66706

R8 2.80662 0.00062 0.00000 0.00923 0.00876 2.81537

R9 2.08003 -0.00004 0.00000 0.00262 0.00262 2.08265

R10 4.27214 -0.00824 0.00000 -0.16430 -0.16455 4.10759

R11 2.07434 -0.00039 0.00000 0.00287 0.00287 2.07721

R12 2.12249 0.00047 0.00000 -0.00064 -0.00064 2.12186

R13 2.12636 0.00108 0.00000 0.00303 0.00303 2.12939

R14 2.86907 -0.00221 0.00000 0.01155 0.01063 2.87970

R15 2.12893 -0.00047 0.00000 -0.00349 -0.00349 2.12544

R16 2.12672 0.00047 0.00000 -0.00120 -0.00120 2.12552

R17 2.68058 -0.00197 0.00000 -0.01252 -0.01284 2.66773

R18 2.65661 0.00049 0.00000 0.00768 0.00760 2.66421

R19 2.65786 0.00555 0.00000 0.00485 0.00462 2.66248

R20 2.79746 -0.00109 0.00000 0.01070 0.01058 2.80804

R21 2.06174 -0.00050 0.00000 0.00335 0.00335 2.06509

R22 2.84315 -0.00553 0.00000 -0.02603 -0.02576 2.81739

R23 2.06926 0.00205 0.00000 -0.00499 -0.00499 2.06428

R24 2.30589 -0.00007 0.00000 0.00027 0.00027 2.30617

R25 2.30547 -0.00049 0.00000 0.00109 0.00109 2.30655

A1 2.04117 0.00342 0.00000 0.00614 0.00541 2.04658

A2 2.13651 -0.00369 0.00000 -0.02029 -0.02006 2.11645

A3 2.09538 0.00025 0.00000 0.01064 0.01082 2.10620

A4 2.06546 -0.00339 0.00000 0.01946 0.01774 2.08320

A5 2.10004 0.00227 0.00000 -0.00939 -0.01026 2.08978

A6 1.67913 -0.00183 0.00000 -0.03943 -0.04008 1.63905

A7 1.99744 0.00045 0.00000 0.02947 0.02858 2.02601

A8 1.77930 0.00410 0.00000 -0.02281 -0.02189 1.75741

A9 1.71692 -0.00075 0.00000 -0.01529 -0.01489 1.70202

A10 2.11388 -0.00028 0.00000 -0.02570 -0.02846 2.08542

A11 2.12010 0.00008 0.00000 -0.01867 -0.01702 2.10308

A12 1.54550 -0.00049 0.00000 0.06795 0.06802 1.61352

A13 2.00321 -0.00019 0.00000 0.02970 0.02967 2.03288

A14 1.70158 0.00428 0.00000 0.03279 0.03378 1.73537

A15 1.75475 -0.00253 0.00000 -0.06085 -0.06042 1.69434

A16 2.05947 0.00432 0.00000 -0.00120 -0.00241 2.05706

A17 2.10900 -0.00225 0.00000 0.00227 0.00271 2.11170

A18 2.10287 -0.00201 0.00000 0.00259 0.00307 2.10594

A19 1.93414 0.00082 0.00000 0.00034 0.00080 1.93494

A20 1.86206 0.00216 0.00000 -0.00741 -0.00717 1.85489

A21 1.97666 -0.00404 0.00000 0.01305 0.01159 1.98825

A22 1.86471 -0.00103 0.00000 -0.00135 -0.00151 1.86320

A23 1.91058 0.00252 0.00000 0.01069 0.01076 1.92134

A24 1.91176 -0.00033 0.00000 -0.01704 -0.01632 1.89544

A25 1.98258 -0.00114 0.00000 -0.00578 -0.00727 1.97531

A26 1.91941 -0.00012 0.00000 0.00470 0.00495 1.92435

A27 1.88495 0.00068 0.00000 0.00015 0.00075 1.88570

A28 1.91375 0.00137 0.00000 -0.00230 -0.00185 1.91190

A29 1.91469 -0.00078 0.00000 -0.00462 -0.00419 1.91050

A30 1.84309 0.00004 0.00000 0.00894 0.00871 1.85180

A31 1.88958 0.00012 0.00000 -0.00410 -0.00417 1.88542

A32 1.82338 -0.00035 0.00000 0.04610 0.04435 1.86772

A33 1.70310 0.00218 0.00000 0.01538 0.01601 1.71911

A34 1.55484 -0.00059 0.00000 -0.00933 -0.00851 1.54633

A35 1.87666 -0.00006 0.00000 -0.00609 -0.00572 1.87094

A36 2.21747 -0.00143 0.00000 -0.00322 -0.00443 2.21304

A37 2.11662 0.00112 0.00000 -0.01108 -0.01162 2.10500

A38 1.92301 -0.00339 0.00000 -0.03399 -0.03634 1.88667

A39 1.78851 0.00343 0.00000 -0.04575 -0.04548 1.74303

A40 1.56724 0.00259 0.00000 0.00087 0.00255 1.56979

A41 1.86394 -0.00160 0.00000 0.00193 0.00144 1.86537

A42 2.18987 -0.00132 0.00000 0.00906 0.00734 2.19721

A43 2.05700 0.00159 0.00000 0.03728 0.03626 2.09327

A44 1.89910 -0.00034 0.00000 0.00075 0.00061 1.89972

A45 2.02133 -0.00045 0.00000 0.00737 0.00741 2.02874

A46 2.36246 0.00079 0.00000 -0.00783 -0.00780 2.35466

A47 1.89343 0.00193 0.00000 0.00694 0.00712 1.90055

A48 2.04022 -0.00160 0.00000 -0.01176 -0.01236 2.02786

A49 2.34911 -0.00029 0.00000 0.00613 0.00554 2.35465

D1 -0.64591 -0.00160 0.00000 0.05523 0.05507 -0.59084

D2 3.03084 -0.00032 0.00000 -0.03484 -0.03427 2.99658

D3 1.22459 0.00115 0.00000 0.01040 0.00993 1.23452

D4 2.64824 -0.00150 0.00000 0.08038 0.08016 2.72841

D5 0.04181 -0.00022 0.00000 -0.00969 -0.00917 0.03264

D6 -1.76444 0.00125 0.00000 0.03556 0.03502 -1.72942

D7 -0.01378 0.00043 0.00000 -0.06173 -0.06154 -0.07532

D8 -2.99138 0.00013 0.00000 -0.08717 -0.08682 -3.07821

D9 2.97904 -0.00004 0.00000 -0.08910 -0.08932 2.88972

D10 0.00143 -0.00034 0.00000 -0.11455 -0.11460 -0.11317

D11 2.91189 -0.00036 0.00000 -0.06091 -0.06166 2.85023

D12 -1.34762 0.00007 0.00000 -0.06655 -0.06710 -1.41472

D13 0.75695 -0.00132 0.00000 -0.08489 -0.08534 0.67162

D14 -0.73442 -0.00093 0.00000 0.01259 0.01305 -0.72137

D15 1.28926 -0.00050 0.00000 0.00694 0.00761 1.29687

D16 -2.88935 -0.00189 0.00000 -0.01140 -0.01063 -2.89998

D17 1.09904 0.00052 0.00000 -0.00698 -0.00654 1.09250

D18 3.12272 0.00095 0.00000 -0.01263 -0.01198 3.11074

D19 -1.05589 -0.00044 0.00000 -0.03097 -0.03022 -1.08611

D20 -0.88168 0.00336 0.00000 -0.08728 -0.08540 -0.96708

D21 -2.86030 0.00484 0.00000 -0.05321 -0.05323 -2.91353

D22 1.35395 0.00215 0.00000 -0.08653 -0.08603 1.26792

D23 1.22560 0.00026 0.00000 -0.08481 -0.08320 1.14240

D24 -0.75302 0.00173 0.00000 -0.05073 -0.05104 -0.80405

D25 -2.82195 -0.00095 0.00000 -0.08406 -0.08384 -2.90579

D26 -3.01029 0.00163 0.00000 -0.06469 -0.06334 -3.07363

D27 1.29428 0.00310 0.00000 -0.03062 -0.03118 1.26310

D28 -0.77466 0.00041 0.00000 -0.06394 -0.06398 -0.83863

D29 0.54749 0.00198 0.00000 0.09561 0.09495 0.64244

D30 -2.75749 0.00225 0.00000 0.12093 0.12011 -2.63738

D31 -2.93203 0.00055 0.00000 0.04892 0.04957 -2.88246

D32 0.04617 0.00082 0.00000 0.07424 0.07474 0.12091

D33 -1.16085 -0.00271 0.00000 0.01758 0.01831 -1.14254

D34 1.81736 -0.00244 0.00000 0.04291 0.04347 1.86083

D35 -0.39717 -0.00013 0.00000 -0.12015 -0.11973 -0.51690

D36 -2.54933 -0.00101 0.00000 -0.11654 -0.11581 -2.66515

D37 1.73075 -0.00137 0.00000 -0.12971 -0.12922 1.60152

D38 3.06112 0.00115 0.00000 -0.06836 -0.06815 2.99297

D39 0.90895 0.00027 0.00000 -0.06475 -0.06423 0.84472

D40 -1.09415 -0.00009 0.00000 -0.07792 -0.07765 -1.17180

D41 1.22325 0.00187 0.00000 -0.02414 -0.02521 1.19804

D42 -0.92892 0.00098 0.00000 -0.02053 -0.02130 -0.95021

D43 -2.93202 0.00062 0.00000 -0.03370 -0.03471 -2.96673

D44 1.20405 -0.00272 0.00000 -0.08929 -0.09001 1.11403

D45 3.13036 -0.00215 0.00000 -0.07979 -0.07904 3.05132

D46 -1.03325 -0.00097 0.00000 -0.09139 -0.09111 -1.12437

D47 -0.91135 -0.00258 0.00000 -0.07439 -0.07655 -0.98789

D48 1.01497 -0.00201 0.00000 -0.06489 -0.06558 0.94939

D49 3.13454 -0.00083 0.00000 -0.07649 -0.07764 3.05690

D50 -2.95384 -0.00295 0.00000 -0.09974 -0.10096 -3.05481

D51 -1.02753 -0.00238 0.00000 -0.09024 -0.08999 -1.11752

D52 1.09204 -0.00120 0.00000 -0.10184 -0.10206 0.98998

D53 -0.22877 0.00014 0.00000 0.11371 0.11416 -0.11462

D54 1.92648 0.00021 0.00000 0.11395 0.11402 2.04050

D55 -2.34008 0.00060 0.00000 0.12080 0.12107 -2.21901

D56 -2.39660 0.00006 0.00000 0.09576 0.09613 -2.30047

D57 -0.24135 0.00013 0.00000 0.09600 0.09599 -0.14536

D58 1.77528 0.00051 0.00000 0.10284 0.10305 1.87832

D59 1.84738 0.00004 0.00000 0.10103 0.10124 1.94862

D60 -2.28055 0.00011 0.00000 0.10127 0.10111 -2.17945

D61 -0.26393 0.00049 0.00000 0.10812 0.10816 -0.15577

D62 -0.02750 -0.00033 0.00000 -0.01772 -0.01719 -0.04469

D63 3.09220 -0.00041 0.00000 -0.00674 -0.00597 3.08623

D64 -0.00973 0.00082 0.00000 0.01380 0.01333 0.00360

D65 -3.12457 -0.00043 0.00000 -0.02744 -0.02776 3.13085

D66 -0.19268 0.00158 0.00000 0.09442 0.09444 -0.09824

D67 1.73709 0.00319 0.00000 0.02666 0.02716 1.76426

D68 -2.02362 0.00166 0.00000 0.11647 0.11718 -1.90644

D69 -1.98978 -0.00068 0.00000 0.06186 0.06138 -1.92839

D70 -0.06000 0.00094 0.00000 -0.00590 -0.00590 -0.06590

D71 2.46246 -0.00059 0.00000 0.08391 0.08412 2.54658

D72 1.55322 -0.00005 0.00000 0.11834 0.11757 1.67079

D73 -2.80020 0.00156 0.00000 0.05058 0.05029 -2.74991

D74 -0.27773 0.00003 0.00000 0.14039 0.14031 -0.13742

D75 -1.82601 -0.00087 0.00000 -0.03934 -0.03818 -1.86418

D76 1.34364 -0.00075 0.00000 -0.05374 -0.05270 1.29094

D77 0.05620 -0.00045 0.00000 0.01456 0.01431 0.07051

D78 -3.05734 -0.00032 0.00000 0.00016 -0.00021 -3.05756

D79 2.82435 -0.00171 0.00000 -0.03589 -0.03583 2.78852

D80 -0.28920 -0.00159 0.00000 -0.05029 -0.05035 -0.33955

D81 2.06657 -0.00405 0.00000 -0.06191 -0.06286 2.00371

D82 -1.10852 -0.00249 0.00000 -0.01065 -0.01118 -1.11971

D83 0.04481 -0.00116 0.00000 -0.00450 -0.00417 0.04064

D84 -3.13028 0.00040 0.00000 0.04676 0.04751 -3.08277

D85 -2.53278 0.00133 0.00000 -0.07584 -0.07675 -2.60953

D86 0.57531 0.00289 0.00000 -0.02459 -0.02507 0.55024

Item Value Threshold Converged?

Maximum Force 0.018922 0.000450 NO

RMS Force 0.002929 0.000300 NO

Maximum Displacement 0.280790 0.001800 NO

RMS Displacement 0.062544 0.001200 NO

Predicted change in Energy=-4.142976D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.148687 1.571421 0.480181

2 6 0 0.180742 1.281083 0.149029

3 6 0 -0.716616 3.784810 -0.391668

4 6 0 -1.629763 2.857881 0.155016

5 1 0 -1.739380 0.895453 1.116491

6 1 0 -2.644069 3.171527 0.439748

7 6 0 0.769224 1.871972 -1.071495

8 1 0 1.889829 1.805281 -1.047808

9 1 0 0.423759 1.230540 -1.931116

10 6 0 0.335939 3.309391 -1.332787

11 1 0 1.232778 3.986686 -1.288370

12 1 0 -0.067917 3.394788 -2.379080

13 1 0 -0.967020 4.857175 -0.435644

14 1 0 0.640154 0.345296 0.503879

15 8 0 2.714485 3.934068 0.789408

16 6 0 0.450399 3.857185 1.440700

17 6 0 0.986223 2.569352 1.639312

18 6 0 1.557685 4.724663 0.961697

19 8 0 1.674381 5.913370 0.711377

20 6 0 2.407976 2.618539 1.193239

21 8 0 3.308754 1.800897 1.093905

22 1 0 -0.417370 4.289969 1.944567

23 1 0 0.682094 1.861661 2.413874

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.400478 0.000000

3 C 2.417829 2.714084 0.000000

4 C 1.411435 2.400887 1.411346 0.000000

5 H 1.100337 2.184390 3.415988 2.188053 0.000000

6 H 2.190466 3.411430 2.186880 1.099210 2.541054

7 C 2.485239 1.478222 2.515717 2.869057 3.469001

8 H 3.409108 2.151321 3.338055 3.865525 4.322399

9 H 2.898817 2.094902 3.192906 3.349200 3.752248

10 C 2.917448 2.516723 1.489831 2.506272 4.016591

11 H 3.825265 3.239318 2.155218 3.398780 4.916584

12 H 3.559228 3.304680 2.126672 3.024777 4.610800

13 H 3.415834 3.801005 1.102091 2.187529 4.324455

14 H 2.168846 1.101215 3.804350 3.404014 2.517965

15 O 4.538923 3.724013 3.631758 4.520301 5.401581

16 C 2.950320 2.894379 2.173646 2.641717 3.697580

17 C 2.626269 2.128235 2.915797 3.021550 3.241017

18 C 4.183209 3.796662 2.808445 3.780930 5.055437

19 O 5.184177 4.899519 3.385904 4.534636 6.082547

20 C 3.775547 2.799953 3.692586 4.175947 4.491712

21 O 4.505341 3.308694 4.727202 5.136894 5.128742

22 H 3.173288 3.554587 2.408885 2.592927 3.735794

23 H 2.678650 2.391224 3.677765 3.382245 2.912095

6 7 8 9 10

6 H 0.000000

7 C 3.952628 0.000000

8 H 4.963435 1.122838 0.000000

9 H 4.335896 1.126824 1.805526 0.000000

10 C 3.470062 1.523871 2.181315 2.165025 0.000000

11 H 4.322131 2.175760 2.290877 2.943463 1.124732

12 H 3.825206 2.174753 2.851594 2.264152 1.124776

13 H 2.533814 3.511451 4.224973 4.162114 2.213189

14 H 4.333338 2.197545 2.470015 2.599939 3.500249

15 O 5.423821 3.391052 2.930385 4.467409 3.248294

16 C 3.323818 3.217739 3.531988 4.274239 2.829383

17 C 3.870476 2.807472 2.936141 3.854445 3.131117

18 C 4.509922 3.590735 3.559666 4.675794 2.959783

19 O 5.122549 4.508973 4.474098 5.520483 3.570818

20 C 5.137773 2.893422 2.439704 3.952880 3.339374

21 O 6.143505 3.338146 2.569105 4.218917 4.123350

22 H 2.910942 4.043679 4.522295 5.008845 3.502864

23 H 4.083661 3.486473 3.666749 4.398181 4.031527

11 12 13 14 15

11 H 0.000000

12 H 1.797720 0.000000

13 H 2.514758 2.593050 0.000000

14 H 4.101595 4.255845 4.880857 0.000000

15 O 2.552525 4.251105 3.988278 4.154956 0.000000

16 C 2.841956 3.882420 2.555333 3.639644 2.357154

17 C 3.262046 4.235567 3.654413 2.520992 2.360440

18 C 2.390183 3.946130 2.888643 4.497812 1.411705

19 O 2.811782 4.350837 3.067280 5.667110 2.237307

20 C 3.067785 4.415209 4.365244 2.961089 1.409838

21 O 3.842211 5.099414 5.473811 3.096503 2.235239

22 H 3.642369 4.429152 2.507837 4.330633 3.357018

23 H 4.304137 5.087770 4.451116 2.439099 3.326315

16 17 18 19 20

16 C 0.000000

17 C 1.408923 0.000000

18 C 1.485949 2.330471 0.000000

19 O 2.501588 3.537949 1.220371 0.000000

20 C 2.329718 1.490900 2.283060 3.409731 0.000000

21 O 3.538189 2.506421 3.410591 4.441840 1.220576

22 H 1.092798 2.241377 2.248518 2.920892 3.367603

23 H 2.232233 1.092368 3.327500 4.505494 2.245324

21 22 23

21 O 0.000000

22 H 4.561042 0.000000

23 H 2.940298 2.706611 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.346679 -0.457728 -0.747180

2 6 0 1.464406 -1.271694 -0.025799

3 6 0 1.231053 1.412164 0.303906

4 6 0 2.257626 0.935453 -0.539180

5 1 0 2.961553 -0.865260 -1.563629

6 1 0 2.879049 1.634752 -1.116309

7 6 0 1.064235 -0.873976 1.340519

8 1 0 0.148905 -1.435524 1.668545

9 1 0 1.903159 -1.194345 2.021182

10 6 0 0.847029 0.624893 1.509031

11 1 0 -0.227568 0.821625 1.776540

12 1 0 1.457731 0.996815 2.377269

13 1 0 0.963049 2.481158 0.309438

14 1 0 1.402252 -2.347042 -0.254794

15 8 0 -2.063311 -0.116157 0.271218

16 6 0 -0.325215 0.752929 -1.062906

17 6 0 -0.243726 -0.651853 -1.133709

18 6 0 -1.507363 1.082766 -0.225185

19 8 0 -2.074744 2.114275 0.096329

20 6 0 -1.324555 -1.192687 -0.260730

21 8 0 -1.675352 -2.309558 0.084736

22 1 0 0.053678 1.468409 -1.796893

23 1 0 0.104440 -1.230669 -1.992207

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2226804 0.8870757 0.6782421

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.1000414337 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.485143717414E-01 A.U. after 15 cycles

Convg = 0.7170D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.005707910 0.020574228 -0.006778401

2 6 -0.004780140 -0.000599523 0.011693755

3 6 -0.006469958 -0.012336853 0.008367944

4 6 0.014132710 -0.008571820 -0.001261436

5 1 0.000101677 0.000681016 -0.002670761

6 1 0.002018599 -0.000029910 0.002138101

7 6 0.000254881 0.002614193 -0.009829476

8 1 0.000402837 0.000073830 0.000085420

9 1 0.001359862 -0.000183816 -0.001604310

10 6 0.000863850 0.000121076 0.002386431

11 1 -0.000423307 0.000433159 -0.000494456

12 1 -0.000745651 -0.000447896 0.000045434

13 1 -0.000920402 -0.001008332 -0.001191259

14 1 0.001015116 -0.001178858 0.000379837

15 8 0.000496503 0.000342855 0.000509788

16 6 -0.005006672 0.006004977 -0.004736354

17 6 0.000935713 -0.007053403 -0.002276715

18 6 0.000758554 -0.001524964 0.000503189

19 8 0.000153622 -0.000363331 -0.000863294

20 6 -0.000224704 0.002391236 0.000801759

21 8 0.000269200 0.000434455 0.000914600

22 1 0.001972766 -0.000225025 0.002783402

23 1 -0.000457147 -0.000147295 0.001096799

-------------------------------------------------------------------

Cartesian Forces: Max 0.020574228 RMS 0.004667833

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.018067907 RMS 0.002236611

Search for a saddle point.

Step number 40 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 29 32 38 39 40

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07569 0.00000 0.00095 0.00578 0.00740

Eigenvalues --- 0.01060 0.01292 0.01624 0.01892 0.02159

Eigenvalues --- 0.02568 0.02714 0.02781 0.03050 0.03160

Eigenvalues --- 0.03312 0.03340 0.03605 0.03688 0.03840

Eigenvalues --- 0.03903 0.04103 0.04341 0.04762 0.05522

Eigenvalues --- 0.06033 0.06101 0.06384 0.07230 0.07376

Eigenvalues --- 0.08703 0.08826 0.09850 0.09910 0.10361

Eigenvalues --- 0.12092 0.13887 0.14710 0.16903 0.21656

Eigenvalues --- 0.25970 0.27167 0.28478 0.29222 0.29915

Eigenvalues --- 0.30913 0.31300 0.31699 0.31969 0.32277

Eigenvalues --- 0.32448 0.33043 0.35296 0.37059 0.38253

Eigenvalues --- 0.39626 0.40426 0.41187 0.46564 0.49242

Eigenvalues --- 0.52160 1.08482 1.10860

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D71 D4

1 0.59400 0.48916 -0.16232 0.16114 0.15303

D68 D85 D86 D29 D1

1 0.12925 -0.12915 -0.12871 -0.12455 0.12155

RFO step: Lambda0=2.169724811D-04 Lambda=-4.44952709D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.04482101 RMS(Int)= 0.00120627

Iteration 2 RMS(Cart)= 0.00133447 RMS(Int)= 0.00032518

Iteration 3 RMS(Cart)= 0.00000081 RMS(Int)= 0.00032518

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64652 -0.00112 0.00000 -0.00094 -0.00096 2.64556

R2 2.66722 -0.01807 0.00000 -0.05231 -0.05224 2.61499

R3 2.07934 -0.00202 0.00000 -0.00131 -0.00131 2.07803

R4 2.79343 0.00774 0.00000 0.03853 0.03849 2.83192

R5 2.08100 0.00155 0.00000 0.00270 0.00270 2.08370

R6 4.02178 -0.00160 0.00000 0.03533 0.03538 4.05716

R7 2.66706 -0.01247 0.00000 -0.03821 -0.03810 2.62896

R8 2.81537 -0.00092 0.00000 -0.00396 -0.00393 2.81144

R9 2.08265 -0.00072 0.00000 0.00046 0.00046 2.08311

R10 4.10759 -0.00189 0.00000 -0.01667 -0.01674 4.09086

R11 2.07721 -0.00132 0.00000 -0.00125 -0.00125 2.07595

R12 2.12186 0.00040 0.00000 0.00164 0.00164 2.12350

R13 2.12939 0.00091 0.00000 -0.00121 -0.00121 2.12818

R14 2.87970 -0.00348 0.00000 -0.00996 -0.01002 2.86968

R15 2.12544 -0.00010 0.00000 -0.00072 -0.00072 2.12472

R16 2.12552 0.00019 0.00000 0.00317 0.00317 2.12869

R17 2.66773 0.00001 0.00000 0.00187 0.00179 2.66953

R18 2.66421 0.00008 0.00000 -0.00251 -0.00245 2.66176

R19 2.66248 0.00142 0.00000 0.00305 0.00300 2.66548

R20 2.80804 -0.00005 0.00000 0.00662 0.00650 2.81454

R21 2.06509 -0.00037 0.00000 0.00068 0.00068 2.06577

R22 2.81739 -0.00019 0.00000 0.00548 0.00560 2.82299

R23 2.06428 0.00100 0.00000 0.00051 0.00051 2.06478

R24 2.30617 -0.00016 0.00000 -0.00070 -0.00070 2.30547

R25 2.30655 -0.00017 0.00000 -0.00044 -0.00044 2.30612

A1 2.04658 0.00230 0.00000 0.01632 0.01605 2.06263

A2 2.11645 -0.00080 0.00000 0.00656 0.00671 2.12316

A3 2.10620 -0.00147 0.00000 -0.02381 -0.02370 2.08250

A4 2.08320 -0.00276 0.00000 -0.00259 -0.00296 2.08024

A5 2.08978 0.00282 0.00000 0.04291 0.04284 2.13262

A6 1.63905 -0.00164 0.00000 -0.01299 -0.01314 1.62592

A7 2.02601 -0.00035 0.00000 -0.02139 -0.02192 2.00410

A8 1.75741 0.00341 0.00000 -0.01353 -0.01371 1.74370

A9 1.70202 -0.00096 0.00000 -0.01525 -0.01517 1.68686

A10 2.08542 0.00095 0.00000 0.01303 0.01273 2.09815

A11 2.10308 0.00017 0.00000 0.00254 0.00244 2.10552

A12 1.61352 -0.00086 0.00000 0.00378 0.00372 1.61724

A13 2.03288 -0.00149 0.00000 -0.02712 -0.02722 2.00567

A14 1.73537 0.00297 0.00000 0.01882 0.01845 1.75381

A15 1.69434 -0.00101 0.00000 0.00966 0.01006 1.70440

A16 2.05706 0.00330 0.00000 0.00172 0.00149 2.05855

A17 2.11170 -0.00208 0.00000 -0.01540 -0.01539 2.09631

A18 2.10594 -0.00120 0.00000 0.01019 0.01009 2.11603

A19 1.93494 0.00118 0.00000 -0.01027 -0.01044 1.92450

A20 1.85489 0.00230 0.00000 0.02382 0.02421 1.87910

A21 1.98825 -0.00446 0.00000 -0.01310 -0.01358 1.97467

A22 1.86320 -0.00110 0.00000 -0.01182 -0.01180 1.85140

A23 1.92134 0.00192 0.00000 0.00122 0.00124 1.92258

A24 1.89544 0.00032 0.00000 0.01141 0.01146 1.90690

A25 1.97531 0.00027 0.00000 0.00268 0.00229 1.97760

A26 1.92435 -0.00029 0.00000 0.00107 0.00129 1.92565

A27 1.88570 -0.00026 0.00000 -0.01712 -0.01734 1.86836

A28 1.91190 0.00102 0.00000 0.01602 0.01575 1.92765

A29 1.91050 -0.00089 0.00000 -0.00915 -0.00881 1.90169

A30 1.85180 0.00010 0.00000 0.00612 0.00611 1.85791

A31 1.88542 0.00006 0.00000 0.00263 0.00205 1.88746

A32 1.86772 -0.00125 0.00000 -0.01359 -0.01358 1.85414

A33 1.71911 0.00190 0.00000 0.02550 0.02551 1.74463

A34 1.54633 0.00047 0.00000 0.05987 0.06027 1.60660

A35 1.87094 -0.00022 0.00000 -0.00734 -0.00777 1.86317

A36 2.21304 -0.00093 0.00000 -0.02778 -0.02836 2.18468

A37 2.10500 0.00074 0.00000 0.00111 -0.00116 2.10385

A38 1.88667 -0.00172 0.00000 0.00568 0.00518 1.89185

A39 1.74303 0.00213 0.00000 0.01757 0.01787 1.76090

A40 1.56979 0.00098 0.00000 -0.04239 -0.04239 1.52740

A41 1.86537 -0.00019 0.00000 0.00767 0.00739 1.87277

A42 2.19721 -0.00092 0.00000 0.00487 0.00472 2.20193

A43 2.09327 0.00047 0.00000 0.00000 0.00012 2.09339

A44 1.89972 0.00020 0.00000 0.00503 0.00446 1.90417

A45 2.02874 -0.00058 0.00000 -0.00494 -0.00467 2.02407

A46 2.35466 0.00038 0.00000 -0.00019 0.00008 2.35473

A47 1.90055 0.00022 0.00000 -0.00400 -0.00420 1.89635

A48 2.02786 -0.00029 0.00000 0.00447 0.00456 2.03242

A49 2.35465 0.00008 0.00000 -0.00040 -0.00030 2.35435

D1 -0.59084 -0.00144 0.00000 -0.00520 -0.00488 -0.59572

D2 2.99658 -0.00063 0.00000 -0.04712 -0.04785 2.94872

D3 1.23452 0.00096 0.00000 -0.02934 -0.02923 1.20529

D4 2.72841 -0.00147 0.00000 0.00310 0.00346 2.73187

D5 0.03264 -0.00066 0.00000 -0.03882 -0.03951 -0.00688

D6 -1.72942 0.00093 0.00000 -0.02104 -0.02089 -1.75030

D7 -0.07532 0.00108 0.00000 0.04172 0.04179 -0.03353

D8 -3.07821 0.00098 0.00000 0.06919 0.06888 -3.00933

D9 2.88972 0.00118 0.00000 0.03671 0.03680 2.92652

D10 -0.11317 0.00109 0.00000 0.06417 0.06389 -0.04928

D11 2.85023 -0.00098 0.00000 -0.07368 -0.07363 2.77660

D12 -1.41472 -0.00039 0.00000 -0.07948 -0.07945 -1.49417

D13 0.67162 -0.00106 0.00000 -0.05692 -0.05688 0.61474

D14 -0.72137 -0.00094 0.00000 -0.01742 -0.01786 -0.73922

D15 1.29687 -0.00035 0.00000 -0.02321 -0.02367 1.27319

D16 -2.89998 -0.00102 0.00000 -0.00065 -0.00111 -2.90109

D17 1.09250 -0.00029 0.00000 -0.04928 -0.04903 1.04348

D18 3.11074 0.00030 0.00000 -0.05508 -0.05485 3.05589

D19 -1.08611 -0.00036 0.00000 -0.03252 -0.03228 -1.11839

D20 -0.96708 0.00325 0.00000 -0.00683 -0.00687 -0.97394

D21 -2.91353 0.00311 0.00000 -0.02442 -0.02442 -2.93795

D22 1.26792 0.00222 0.00000 -0.01767 -0.01755 1.25036

D23 1.14240 0.00063 0.00000 -0.01550 -0.01563 1.12677

D24 -0.80405 0.00048 0.00000 -0.03309 -0.03319 -0.83724

D25 -2.90579 -0.00040 0.00000 -0.02634 -0.02632 -2.93211

D26 -3.07363 0.00085 0.00000 -0.04571 -0.04582 -3.11945

D27 1.26310 0.00070 0.00000 -0.06330 -0.06337 1.19973

D28 -0.83863 -0.00018 0.00000 -0.05655 -0.05651 -0.89514

D29 0.64244 0.00070 0.00000 -0.01739 -0.01753 0.62491

D30 -2.63738 0.00072 0.00000 -0.04689 -0.04707 -2.68445

D31 -2.88246 -0.00073 0.00000 -0.05759 -0.05798 -2.94044

D32 0.12091 -0.00071 0.00000 -0.08709 -0.08752 0.03339

D33 -1.14254 -0.00240 0.00000 -0.04364 -0.04356 -1.18610

D34 1.86083 -0.00238 0.00000 -0.07314 -0.07310 1.78773

D35 -0.51690 0.00052 0.00000 -0.03348 -0.03390 -0.55080

D36 -2.66515 -0.00080 0.00000 -0.05710 -0.05722 -2.72237

D37 1.60152 -0.00062 0.00000 -0.05531 -0.05545 1.54607

D38 2.99297 0.00156 0.00000 -0.00081 -0.00144 2.99153

D39 0.84472 0.00024 0.00000 -0.02443 -0.02476 0.81996

D40 -1.17180 0.00042 0.00000 -0.02264 -0.02299 -1.19479

D41 1.19804 0.00151 0.00000 -0.01457 -0.01489 1.18315

D42 -0.95021 0.00020 0.00000 -0.03819 -0.03820 -0.98842

D43 -2.96673 0.00038 0.00000 -0.03640 -0.03644 -3.00316

D44 1.11403 -0.00092 0.00000 -0.01736 -0.01740 1.09663

D45 3.05132 -0.00077 0.00000 -0.01925 -0.01999 3.03133

D46 -1.12437 0.00016 0.00000 -0.00705 -0.00684 -1.13121

D47 -0.98789 -0.00214 0.00000 -0.03430 -0.03424 -1.02213

D48 0.94939 -0.00199 0.00000 -0.03619 -0.03683 0.91257

D49 3.05690 -0.00106 0.00000 -0.02399 -0.02368 3.03321

D50 -3.05481 -0.00102 0.00000 -0.01293 -0.01294 -3.06775

D51 -1.11752 -0.00087 0.00000 -0.01482 -0.01553 -1.13305

D52 0.98998 0.00007 0.00000 -0.00262 -0.00239 0.98760

D53 -0.11462 -0.00052 0.00000 0.06093 0.06053 -0.05409

D54 2.04050 0.00006 0.00000 0.07619 0.07589 2.11639

D55 -2.21901 0.00026 0.00000 0.08743 0.08712 -2.13188

D56 -2.30047 -0.00024 0.00000 0.08360 0.08347 -2.21701

D57 -0.14536 0.00035 0.00000 0.09887 0.09883 -0.04653

D58 1.87832 0.00054 0.00000 0.11011 0.11006 1.98839

D59 1.94862 -0.00017 0.00000 0.09055 0.09036 2.03898

D60 -2.17945 0.00042 0.00000 0.10582 0.10572 -2.07372

D61 -0.15577 0.00061 0.00000 0.11706 0.11695 -0.03881

D62 -0.04469 0.00040 0.00000 0.05916 0.05941 0.01472

D63 3.08623 0.00000 0.00000 0.05150 0.05170 3.13792

D64 0.00360 0.00012 0.00000 -0.03706 -0.03700 -0.03340

D65 3.13085 0.00012 0.00000 -0.03291 -0.03300 3.09785

D66 -0.09824 0.00080 0.00000 0.03037 0.02999 -0.06824

D67 1.76426 0.00240 0.00000 0.05591 0.05577 1.82002

D68 -1.90644 0.00138 0.00000 0.07984 0.07988 -1.82656

D69 -1.92839 -0.00074 0.00000 0.01019 0.00997 -1.91843

D70 -0.06590 0.00087 0.00000 0.03572 0.03574 -0.03016

D71 2.54658 -0.00016 0.00000 0.05965 0.05986 2.60644

D72 1.67079 -0.00004 0.00000 0.08605 0.08528 1.75607

D73 -2.74991 0.00156 0.00000 0.11159 0.11106 -2.63885

D74 -0.13742 0.00054 0.00000 0.13552 0.13517 -0.00225

D75 -1.86418 -0.00014 0.00000 -0.05303 -0.05276 -1.91694

D76 1.29094 0.00038 0.00000 -0.04329 -0.04294 1.24799

D77 0.07051 -0.00082 0.00000 -0.05989 -0.05985 0.01066

D78 -3.05756 -0.00030 0.00000 -0.05015 -0.05004 -3.10759

D79 2.78852 -0.00197 0.00000 -0.13902 -0.13940 2.64912

D80 -0.33955 -0.00145 0.00000 -0.12928 -0.12959 -0.46913

D81 2.00371 -0.00173 0.00000 0.01543 0.01510 2.01881

D82 -1.11971 -0.00173 0.00000 0.01013 0.00999 -1.10972

D83 0.04064 -0.00064 0.00000 -0.00021 -0.00037 0.04028

D84 -3.08277 -0.00064 0.00000 -0.00551 -0.00547 -3.08825

D85 -2.60953 0.00080 0.00000 -0.02399 -0.02416 -2.63369

D86 0.55024 0.00080 0.00000 -0.02930 -0.02927 0.52097

Item Value Threshold Converged?

Maximum Force 0.018068 0.000450 NO

RMS Force 0.002237 0.000300 NO

Maximum Displacement 0.180988 0.001800 NO

RMS Displacement 0.044827 0.001200 NO

Predicted change in Energy=-2.776388D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.154187 1.581108 0.458237

2 6 0 0.171470 1.273784 0.129452

3 6 0 -0.728637 3.764172 -0.383065

4 6 0 -1.619651 2.853125 0.175044

5 1 0 -1.764966 0.910160 1.079523

6 1 0 -2.610142 3.169176 0.529788

7 6 0 0.782453 1.888131 -1.093270

8 1 0 1.903624 1.866301 -1.021040

9 1 0 0.513878 1.238166 -1.972875

10 6 0 0.302306 3.305266 -1.352583

11 1 0 1.171527 4.018330 -1.365279

12 1 0 -0.163692 3.352086 -2.377063

13 1 0 -0.988114 4.833286 -0.452385

14 1 0 0.665498 0.352819 0.481002

15 8 0 2.748758 3.920554 0.863202

16 6 0 0.453123 3.871062 1.427550

17 6 0 0.972157 2.576303 1.636690

18 6 0 1.583300 4.714336 0.948104

19 8 0 1.714428 5.889693 0.648527

20 6 0 2.413776 2.607151 1.246289

21 8 0 3.306754 1.777845 1.182401

22 1 0 -0.373475 4.316162 1.987567

23 1 0 0.623409 1.853990 2.378642

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.399969 0.000000

3 C 2.377950 2.697201 0.000000

4 C 1.383792 2.388411 1.391186 0.000000

5 H 1.099645 2.187382 3.370241 2.148095 0.000000

6 H 2.155663 3.389711 2.174254 1.098546 2.473800

7 C 2.500402 1.498590 2.511436 2.882696 3.488094

8 H 3.408783 2.162190 3.307223 3.849403 4.334181

9 H 2.968224 2.130327 3.232962 3.431267 3.823330

10 C 2.893642 2.518028 1.487751 2.496396 3.990650

11 H 3.830692 3.281290 2.154057 3.394255 4.925522

12 H 3.486599 3.273269 2.113056 2.980273 4.524939

13 H 3.381342 3.788564 1.102333 2.171069 4.282658

14 H 2.195556 1.102646 3.785175 3.401036 2.564374

15 O 4.568367 3.766456 3.697284 4.549281 5.429822

16 C 2.960896 2.917231 2.164789 2.627044 3.715910

17 C 2.626881 2.146957 2.895366 2.988396 3.252432

18 C 4.189382 3.807998 2.831939 3.784260 5.069509

19 O 5.179678 4.894565 3.398616 4.534425 6.089966

20 C 3.795280 2.837804 3.724010 4.180502 4.513255

21 O 4.523617 3.345562 4.762410 5.142028 5.146436

22 H 3.229377 3.606330 2.459823 2.641718 3.789675

23 H 2.631020 2.366377 3.619923 3.299308 2.877996

6 7 8 9 10

6 H 0.000000

7 C 3.973046 0.000000

8 H 4.947387 1.123707 0.000000

9 H 4.444280 1.126185 1.797760 0.000000

10 C 3.470475 1.518571 2.178248 2.168509 0.000000

11 H 4.314320 2.182456 2.299064 2.920786 1.124352

12 H 3.803729 2.164828 2.884467 2.256353 1.126456

13 H 2.522875 3.495651 4.181927 4.182434 2.193259

14 H 4.320193 2.202088 2.465707 2.613109 3.494408

15 O 5.421581 3.438732 2.912829 4.498136 3.357590

16 C 3.268366 3.224129 3.481179 4.301014 2.841129

17 C 3.795998 2.821746 2.904352 3.876802 3.148944

18 C 4.488593 3.577149 3.477274 4.664712 2.986568

19 O 5.110501 4.462614 4.360152 5.472639 3.560589

20 C 5.105781 2.941384 2.439240 3.980798 3.420498

21 O 6.113212 3.400431 2.613761 4.248196 4.217329

22 H 2.905749 4.089383 4.498745 5.093776 3.554602

23 H 3.950168 3.475720 3.632758 4.396241 4.016385

11 12 13 14 15

11 H 0.000000

12 H 1.802886 0.000000

13 H 2.482252 2.564763 0.000000

14 H 4.135310 4.225127 4.866233 0.000000

15 O 2.731912 4.393726 4.065472 4.149070 0.000000

16 C 2.887505 3.889071 2.556794 3.649533 2.364503

17 C 3.336316 4.242901 3.647036 2.524587 2.358305

18 C 2.450657 3.995552 2.930476 4.481448 1.412653

19 O 2.802169 4.372754 3.103504 5.637844 2.234598

20 C 3.217902 4.508541 4.406135 2.953668 1.408544

21 O 4.008695 5.214595 5.518526 3.082027 2.237063

22 H 3.703688 4.474756 2.568768 4.365465 3.342011

23 H 4.359098 5.047826 4.414513 2.419984 3.329317

16 17 18 19 20

16 C 0.000000

17 C 1.410509 0.000000

18 C 1.489389 2.327838 0.000000

19 O 2.504523 3.536380 1.220002 0.000000

20 C 2.339761 1.493864 2.284476 3.409030 0.000000

21 O 3.547515 2.508835 3.412941 4.441600 1.220344

22 H 1.093159 2.227318 2.251221 2.937408 3.352458

23 H 2.236549 1.092636 3.339073 4.524435 2.248307

21 22 23

21 O 0.000000

22 H 4.542623 0.000000

23 H 2.938899 2.684959 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.335312 -0.525671 -0.733182

2 6 0 1.448263 -1.305887 0.018030

3 6 0 1.293205 1.377750 0.239265

4 6 0 2.267610 0.850221 -0.601951

5 1 0 2.949092 -0.960508 -1.535310

6 1 0 2.859110 1.496772 -1.264449

7 6 0 1.045803 -0.843171 1.385397

8 1 0 0.083748 -1.334383 1.695038

9 1 0 1.827592 -1.202976 2.111785

10 6 0 0.920385 0.666477 1.491662

11 1 0 -0.119615 0.952843 1.808773

12 1 0 1.613186 1.035294 2.299687

13 1 0 1.072329 2.457720 0.235181

14 1 0 1.318803 -2.386014 -0.161955

15 8 0 -2.105425 -0.078006 0.241210

16 6 0 -0.316365 0.749293 -1.064820

17 6 0 -0.261151 -0.659453 -1.108670

18 6 0 -1.488384 1.106824 -0.218166

19 8 0 -2.014206 2.151857 0.127986

20 6 0 -1.373354 -1.174463 -0.254622

21 8 0 -1.750932 -2.281792 0.092505

22 1 0 0.016796 1.417693 -1.863095

23 1 0 0.115506 -1.264436 -1.936908

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2229334 0.8765771 0.6733275

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.3755787994 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.494789443085E-01 A.U. after 13 cycles

Convg = 0.7885D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.004403700 -0.012000406 0.002267451

2 6 0.005143348 0.004835075 -0.002757706

3 6 0.005312878 0.010626956 0.000383034

4 6 -0.007087202 0.004173756 0.000476355

5 1 0.001274099 -0.002659658 -0.000959278

6 1 -0.000750381 0.001623316 0.000356272

7 6 -0.001675303 -0.003736200 0.003674313

8 1 -0.000068930 -0.000085998 0.000699411

9 1 -0.000385717 -0.000193210 0.000698398

10 6 -0.000223118 -0.000071634 -0.001470952

11 1 -0.000117259 -0.000413556 0.000423584

12 1 0.000421694 0.000423071 -0.000403951

13 1 -0.000943443 0.000602925 0.000732169

14 1 -0.003002117 -0.000540626 0.000140984

15 8 -0.001247404 0.000241503 -0.001901655

16 6 0.000114276 0.002091985 -0.004330155

17 6 0.002755841 -0.008459456 -0.002523491

18 6 0.000791441 -0.001721237 0.002286765

19 8 -0.000143911 0.000004676 -0.000872049

20 6 -0.005257113 0.002841650 0.001133892

21 8 0.000168139 0.000573192 0.000831129

22 1 -0.000040698 0.000617384 -0.001300640

23 1 0.000557181 0.001226493 0.002416117

-------------------------------------------------------------------

Cartesian Forces: Max 0.012000406 RMS 0.003104533

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.012348992 RMS 0.001631842

Search for a saddle point.

Step number 41 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 33 34 37 40

41

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0

Eigenvalues --- -0.07746 -0.00208 0.00416 0.00473 0.00746

Eigenvalues --- 0.01074 0.01182 0.01587 0.01974 0.02157

Eigenvalues --- 0.02538 0.02715 0.02858 0.03119 0.03220

Eigenvalues --- 0.03271 0.03475 0.03593 0.03691 0.03856

Eigenvalues --- 0.04008 0.04191 0.04528 0.04781 0.05761

Eigenvalues --- 0.06104 0.06343 0.06553 0.07273 0.07433

Eigenvalues --- 0.08723 0.08853 0.09855 0.09932 0.10456

Eigenvalues --- 0.12144 0.13898 0.14657 0.17072 0.21683

Eigenvalues --- 0.25966 0.27404 0.28566 0.29486 0.29913

Eigenvalues --- 0.30988 0.31303 0.31722 0.31974 0.32276

Eigenvalues --- 0.32462 0.33105 0.35384 0.37084 0.38599

Eigenvalues --- 0.39652 0.40435 0.42626 0.46996 0.49770

Eigenvalues --- 0.52600 1.08483 1.10865

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D71

1 -0.57858 -0.51011 0.16485 -0.15011 -0.14869

D35 D29 D37 D73 D1

1 -0.13074 0.12824 -0.12693 0.12367 -0.12197

RFO step: Lambda0=1.748273022D-04 Lambda=-3.26141536D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.08650559 RMS(Int)= 0.00352647

Iteration 2 RMS(Cart)= 0.00452093 RMS(Int)= 0.00077504

Iteration 3 RMS(Cart)= 0.00001295 RMS(Int)= 0.00077496

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00077496

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64556 -0.00215 0.00000 -0.00747 -0.00682 2.63874

R2 2.61499 0.01235 0.00000 0.05366 0.05484 2.66983

R3 2.07803 0.00037 0.00000 -0.00175 -0.00175 2.07627

R4 2.83192 -0.00443 0.00000 -0.01663 -0.01711 2.81482

R5 2.08370 -0.00085 0.00000 0.00053 0.00053 2.08423

R6 4.05716 -0.00065 0.00000 0.07101 0.07087 4.12803

R7 2.62896 0.00706 0.00000 0.02851 0.02900 2.65796

R8 2.81144 0.00154 0.00000 0.00579 0.00546 2.81690

R9 2.08311 0.00076 0.00000 -0.00327 -0.00327 2.07983

R10 4.09086 -0.00426 0.00000 0.01179 0.01184 4.10269

R11 2.07595 0.00126 0.00000 -0.00110 -0.00110 2.07485

R12 2.12350 -0.00002 0.00000 0.00314 0.00314 2.12664

R13 2.12818 -0.00034 0.00000 -0.00124 -0.00124 2.12694

R14 2.86968 0.00345 0.00000 0.00909 0.00804 2.87773

R15 2.12472 -0.00036 0.00000 -0.00236 -0.00236 2.12235

R16 2.12869 0.00021 0.00000 0.00094 0.00094 2.12964

R17 2.66953 -0.00227 0.00000 -0.00877 -0.00855 2.66098

R18 2.66176 -0.00039 0.00000 -0.00159 -0.00106 2.66070

R19 2.66548 0.00417 0.00000 0.01174 0.01109 2.67656

R20 2.81454 -0.00154 0.00000 -0.00501 -0.00540 2.80914

R21 2.06577 -0.00038 0.00000 -0.00189 -0.00189 2.06388

R22 2.82299 -0.00434 0.00000 -0.02142 -0.02130 2.80170

R23 2.06478 0.00065 0.00000 0.00221 0.00221 2.06700

R24 2.30547 0.00020 0.00000 0.00161 0.00161 2.30708

R25 2.30612 -0.00031 0.00000 0.00111 0.00111 2.30722

A1 2.06263 -0.00040 0.00000 0.00079 -0.00056 2.06207

A2 2.12316 -0.00254 0.00000 -0.00938 -0.00887 2.11429

A3 2.08250 0.00293 0.00000 0.00495 0.00550 2.08800

A4 2.08024 0.00108 0.00000 -0.00173 -0.00215 2.07809

A5 2.13262 -0.00227 0.00000 -0.01516 -0.01507 2.11756

A6 1.62592 0.00115 0.00000 0.01527 0.01439 1.64031

A7 2.00410 0.00088 0.00000 0.00444 0.00425 2.00834

A8 1.74370 -0.00161 0.00000 -0.02278 -0.02288 1.72082

A9 1.68686 0.00112 0.00000 0.03815 0.03927 1.72613

A10 2.09815 -0.00168 0.00000 -0.03031 -0.03016 2.06799

A11 2.10552 0.00029 0.00000 0.00861 0.00922 2.11474

A12 1.61724 0.00058 0.00000 0.02356 0.02153 1.63877

A13 2.00567 0.00157 0.00000 0.02860 0.02800 2.03366

A14 1.75381 -0.00157 0.00000 -0.03523 -0.03513 1.71868

A15 1.70440 0.00045 0.00000 -0.00734 -0.00605 1.69835

A16 2.05855 -0.00191 0.00000 0.00830 0.00685 2.06540

A17 2.09631 0.00221 0.00000 0.00997 0.01047 2.10678

A18 2.11603 -0.00033 0.00000 -0.02084 -0.02011 2.09591

A19 1.92450 -0.00108 0.00000 -0.01285 -0.01184 1.91266

A20 1.87910 -0.00127 0.00000 -0.00876 -0.00904 1.87006

A21 1.97467 0.00255 0.00000 0.02016 0.01870 1.99337

A22 1.85140 0.00065 0.00000 0.00117 0.00089 1.85229

A23 1.92258 -0.00086 0.00000 -0.00809 -0.00832 1.91427

A24 1.90690 -0.00011 0.00000 0.00744 0.00863 1.91553

A25 1.97760 0.00013 0.00000 0.01251 0.01113 1.98873

A26 1.92565 -0.00028 0.00000 -0.00152 -0.00156 1.92408

A27 1.86836 0.00035 0.00000 -0.00085 0.00002 1.86838

A28 1.92765 -0.00044 0.00000 -0.00833 -0.00786 1.91979

A29 1.90169 0.00031 0.00000 0.00154 0.00185 1.90354

A30 1.85791 -0.00005 0.00000 -0.00405 -0.00427 1.85364

A31 1.88746 -0.00013 0.00000 -0.00718 -0.00863 1.87884

A32 1.85414 0.00166 0.00000 0.04537 0.04280 1.89695

A33 1.74463 -0.00108 0.00000 0.00910 0.01013 1.75476

A34 1.60660 -0.00086 0.00000 -0.05232 -0.05158 1.55502

A35 1.86317 -0.00010 0.00000 0.00539 0.00474 1.86791

A36 2.18468 0.00038 0.00000 -0.00291 -0.00223 2.18245

A37 2.10385 -0.00013 0.00000 -0.00068 -0.00056 2.10329

A38 1.89185 0.00003 0.00000 -0.02795 -0.03068 1.86117

A39 1.76090 0.00019 0.00000 -0.02283 -0.02234 1.73856

A40 1.52740 0.00109 0.00000 0.06563 0.06666 1.59406

A41 1.87277 -0.00168 0.00000 -0.01333 -0.01364 1.85912

A42 2.20193 0.00030 0.00000 -0.02556 -0.02546 2.17646

A43 2.09339 0.00078 0.00000 0.03006 0.03016 2.12354

A44 1.90417 0.00012 0.00000 -0.00108 -0.00314 1.90103

A45 2.02407 -0.00011 0.00000 -0.00308 -0.00254 2.02153

A46 2.35473 0.00000 0.00000 0.00505 0.00559 2.36033

A47 1.89635 0.00182 0.00000 0.01514 0.01402 1.91038

A48 2.03242 -0.00119 0.00000 -0.01123 -0.01077 2.02165

A49 2.35435 -0.00063 0.00000 -0.00411 -0.00362 2.35072

D1 -0.59572 -0.00043 0.00000 -0.02031 -0.02006 -0.61578

D2 2.94872 0.00028 0.00000 0.01479 0.01462 2.96334

D3 1.20529 -0.00143 0.00000 -0.03812 -0.03859 1.16670

D4 2.73187 -0.00070 0.00000 0.00160 0.00204 2.73391

D5 -0.00688 0.00001 0.00000 0.03671 0.03672 0.02984

D6 -1.75030 -0.00169 0.00000 -0.01621 -0.01649 -1.76680

D7 -0.03353 0.00024 0.00000 0.06704 0.06711 0.03358

D8 -3.00933 0.00051 0.00000 0.08623 0.08697 -2.92236

D9 2.92652 -0.00009 0.00000 0.04409 0.04379 2.97030

D10 -0.04928 0.00018 0.00000 0.06328 0.06365 0.01437

D11 2.77660 0.00105 0.00000 -0.07086 -0.07100 2.70560

D12 -1.49417 0.00054 0.00000 -0.08114 -0.08099 -1.57515

D13 0.61474 0.00114 0.00000 -0.06520 -0.06460 0.55014

D14 -0.73922 -0.00032 0.00000 -0.10777 -0.10782 -0.84704

D15 1.27319 -0.00083 0.00000 -0.11805 -0.11780 1.15539

D16 -2.90109 -0.00024 0.00000 -0.10211 -0.10142 -3.00251

D17 1.04348 0.00037 0.00000 -0.07481 -0.07380 0.96968

D18 3.05589 -0.00014 0.00000 -0.08509 -0.08378 2.97211

D19 -1.11839 0.00045 0.00000 -0.06915 -0.06740 -1.18579

D20 -0.97394 -0.00216 0.00000 -0.09547 -0.09366 -1.06761

D21 -2.93795 -0.00040 0.00000 -0.06096 -0.05973 -2.99769

D22 1.25036 -0.00142 0.00000 -0.10317 -0.10205 1.14831

D23 1.12677 -0.00106 0.00000 -0.09745 -0.09646 1.03031

D24 -0.83724 0.00071 0.00000 -0.06294 -0.06253 -0.89977

D25 -2.93211 -0.00031 0.00000 -0.10515 -0.10484 -3.03695

D26 -3.11945 -0.00022 0.00000 -0.08811 -0.08754 3.07620

D27 1.19973 0.00155 0.00000 -0.05361 -0.05360 1.14612

D28 -0.89514 0.00053 0.00000 -0.09582 -0.09592 -0.99106

D29 0.62491 -0.00095 0.00000 -0.03669 -0.03644 0.58847

D30 -2.68445 -0.00097 0.00000 -0.05299 -0.05314 -2.73759

D31 -2.94044 -0.00007 0.00000 -0.01113 -0.01047 -2.95091

D32 0.03339 -0.00010 0.00000 -0.02743 -0.02717 0.00622

D33 -1.18610 0.00085 0.00000 -0.00399 -0.00267 -1.18877

D34 1.78773 0.00083 0.00000 -0.02029 -0.01937 1.76836

D35 -0.55080 -0.00009 0.00000 -0.05585 -0.05545 -0.60625

D36 -2.72237 0.00061 0.00000 -0.05300 -0.05215 -2.77452

D37 1.54607 0.00062 0.00000 -0.04694 -0.04631 1.49977

D38 2.99153 -0.00067 0.00000 -0.07639 -0.07670 2.91483

D39 0.81996 0.00002 0.00000 -0.07353 -0.07340 0.74656

D40 -1.19479 0.00003 0.00000 -0.06748 -0.06755 -1.26234

D41 1.18315 -0.00084 0.00000 -0.05824 -0.05896 1.12419

D42 -0.98842 -0.00015 0.00000 -0.05539 -0.05566 -1.04407

D43 -3.00316 -0.00014 0.00000 -0.04933 -0.04981 -3.05298

D44 1.09663 -0.00069 0.00000 -0.11618 -0.11731 0.97932

D45 3.03133 -0.00071 0.00000 -0.09334 -0.09434 2.93699

D46 -1.13121 -0.00120 0.00000 -0.10460 -0.10491 -1.23612

D47 -1.02213 0.00116 0.00000 -0.08482 -0.08543 -1.10757

D48 0.91257 0.00114 0.00000 -0.06198 -0.06247 0.85010

D49 3.03321 0.00065 0.00000 -0.07324 -0.07303 2.96018

D50 -3.06775 -0.00023 0.00000 -0.10404 -0.10472 3.11072

D51 -1.13305 -0.00025 0.00000 -0.08120 -0.08175 -1.21480

D52 0.98760 -0.00074 0.00000 -0.09246 -0.09232 0.89528

D53 -0.05409 0.00045 0.00000 0.10179 0.10268 0.04860

D54 2.11639 -0.00016 0.00000 0.10265 0.10278 2.21917

D55 -2.13188 -0.00029 0.00000 0.09390 0.09424 -2.03764

D56 -2.21701 0.00066 0.00000 0.11007 0.11100 -2.10600

D57 -0.04653 0.00005 0.00000 0.11093 0.11109 0.06457

D58 1.98839 -0.00008 0.00000 0.10218 0.10256 2.09094

D59 2.03898 0.00043 0.00000 0.10895 0.10970 2.14869

D60 -2.07372 -0.00018 0.00000 0.10981 0.10979 -1.96393

D61 -0.03881 -0.00031 0.00000 0.10106 0.10126 0.06245

D62 0.01472 -0.00077 0.00000 0.10177 0.10163 0.11635

D63 3.13792 -0.00037 0.00000 0.14215 0.14208 -3.00318

D64 -0.03340 0.00086 0.00000 -0.07546 -0.07601 -0.10941

D65 3.09785 0.00070 0.00000 -0.09207 -0.09258 3.00527

D66 -0.06824 0.00023 0.00000 0.11670 0.11695 0.04871

D67 1.82002 -0.00030 0.00000 0.07241 0.07329 1.89332

D68 -1.82656 -0.00138 0.00000 0.06435 0.06576 -1.76080

D69 -1.91843 0.00081 0.00000 0.08647 0.08586 -1.83256

D70 -0.03016 0.00028 0.00000 0.04217 0.04220 0.01204

D71 2.60644 -0.00080 0.00000 0.03412 0.03467 2.64111

D72 1.75607 0.00061 0.00000 0.08292 0.08205 1.83812

D73 -2.63885 0.00008 0.00000 0.03863 0.03840 -2.60046

D74 -0.00225 -0.00100 0.00000 0.03057 0.03086 0.02861

D75 -1.91694 -0.00108 0.00000 -0.14421 -0.14257 -2.05951

D76 1.24799 -0.00159 0.00000 -0.19533 -0.19410 1.05389

D77 0.01066 0.00028 0.00000 -0.08978 -0.09025 -0.07960

D78 -3.10759 -0.00024 0.00000 -0.14090 -0.14179 3.03380

D79 2.64912 0.00065 0.00000 -0.08738 -0.08738 2.56174

D80 -0.46913 0.00014 0.00000 -0.13850 -0.13891 -0.60805

D81 2.01881 -0.00121 0.00000 -0.02626 -0.02768 1.99113

D82 -1.10972 -0.00101 0.00000 -0.00526 -0.00668 -1.11640

D83 0.04028 -0.00075 0.00000 0.01878 0.01915 0.05943

D84 -3.08825 -0.00054 0.00000 0.03979 0.04015 -3.04810

D85 -2.63369 0.00036 0.00000 0.04432 0.04501 -2.58868

D86 0.52097 0.00056 0.00000 0.06533 0.06600 0.58697

Item Value Threshold Converged?

Maximum Force 0.012349 0.000450 NO

RMS Force 0.001632 0.000300 NO

Maximum Displacement 0.505266 0.001800 NO

RMS Displacement 0.086341 0.001200 NO

Predicted change in Energy=-2.464118D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.146068 1.529567 0.410702

2 6 0 0.191853 1.275929 0.101742

3 6 0 -0.780093 3.795370 -0.359439

4 6 0 -1.644537 2.833611 0.193818

5 1 0 -1.742824 0.808616 0.986281

6 1 0 -2.615646 3.138380 0.605631

7 6 0 0.806802 1.961739 -1.068823

8 1 0 1.920854 2.028703 -0.924406

9 1 0 0.646863 1.298249 -1.963818

10 6 0 0.241677 3.347936 -1.348276

11 1 0 1.075889 4.097267 -1.411105

12 1 0 -0.255851 3.345640 -2.359457

13 1 0 -1.054855 4.860824 -0.384631

14 1 0 0.680967 0.333919 0.401464

15 8 0 2.799630 3.848047 0.928766

16 6 0 0.491260 3.879519 1.398415

17 6 0 0.961058 2.573684 1.681621

18 6 0 1.644262 4.650352 0.863460

19 8 0 1.795077 5.761713 0.381152

20 6 0 2.402227 2.559497 1.333893

21 8 0 3.268229 1.699625 1.297400

22 1 0 -0.313617 4.386546 1.934981

23 1 0 0.550443 1.918275 2.455085

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.396361 0.000000

3 C 2.420933 2.739517 0.000000

4 C 1.412813 2.409809 1.406534 0.000000

5 H 1.098717 2.178019 3.414456 2.176755 0.000000

6 H 2.187678 3.406564 2.175374 1.097965 2.516846

7 C 2.487865 1.489537 2.526592 2.891969 3.471849

8 H 3.381961 2.146880 3.276494 3.822344 4.308349

9 H 2.984369 2.115200 3.293304 3.501891 3.827979

10 C 2.885534 2.529476 1.490641 2.490057 3.979515

11 H 3.853461 3.321171 2.154486 3.401958 4.950538

12 H 3.429925 3.246790 2.115930 2.951243 4.454384

13 H 3.426098 3.826528 1.100601 2.189046 4.332793

14 H 2.183511 1.102927 3.833447 3.420460 2.538132

15 O 4.605678 3.755031 3.804820 4.617342 5.465833

16 C 3.029636 2.923985 2.171052 2.665822 3.819873

17 C 2.673088 2.184459 2.947889 3.011685 3.303020

18 C 4.210728 3.751858 2.846748 3.816434 5.123122

19 O 5.153860 4.771861 3.323624 4.521042 6.116870

20 C 3.808338 2.837516 3.810763 4.213218 4.513078

21 O 4.505683 3.327643 4.850379 5.161307 5.099151

22 H 3.343461 3.645848 2.414840 2.686001 3.967903

23 H 2.684911 2.465648 3.635293 3.281631 2.940714

6 7 8 9 10

6 H 0.000000

7 C 3.987660 0.000000

8 H 4.914491 1.125367 0.000000

9 H 4.542259 1.125529 1.799164 0.000000

10 C 3.467847 1.522827 2.177079 2.178138 0.000000

11 H 4.314408 2.179460 2.286876 2.885145 1.123100

12 H 3.795172 2.170288 2.920914 2.272275 1.126955

13 H 2.526560 3.512632 4.143321 4.252248 2.213241

14 H 4.332937 2.197129 2.483454 2.554536 3.512672

15 O 5.471129 3.394094 2.741624 4.416210 3.460946

16 C 3.290997 3.140813 3.296172 4.241671 2.808769

17 C 3.777493 2.821917 2.830122 3.874878 3.208933

18 C 4.527622 3.415215 3.185280 4.497210 2.924946

19 O 5.136803 4.185560 3.956724 5.171053 3.351163

20 C 5.103383 2.945461 2.369257 3.942962 3.533220

21 O 6.096601 3.424374 2.619186 4.203357 4.344715

22 H 2.936738 4.019685 4.327630 5.065643 3.488100

23 H 3.864357 3.533488 3.648449 4.463231 4.074902

11 12 13 14 15

11 H 0.000000

12 H 1.799402 0.000000

13 H 2.485304 2.614216 0.000000

14 H 4.195731 4.191751 4.911608 0.000000

15 O 2.916914 4.516723 4.196163 4.137133 0.000000

16 C 2.877951 3.868436 2.555912 3.687977 2.355871

17 C 3.449557 4.290349 3.682977 2.594957 2.360326

18 C 2.408858 3.962310 2.981152 4.446681 1.408131

19 O 2.549469 4.189827 3.085472 5.540992 2.229602

20 C 3.414516 4.617817 4.494535 2.964010 1.407983

21 O 4.229781 5.338643 5.613508 3.059702 2.229617

22 H 3.634653 4.419165 2.480922 4.445746 3.315835

23 H 4.468952 5.085990 4.393128 2.597033 3.333544

16 17 18 19 20

16 C 0.000000

17 C 1.416376 0.000000

18 C 1.486531 2.334246 0.000000

19 O 2.505477 3.542645 1.220856 0.000000

20 C 2.323449 1.482594 2.273211 3.395664 0.000000

21 O 3.531812 2.496927 3.395933 4.417041 1.220931

22 H 1.092158 2.230574 2.247453 2.958388 3.327946

23 H 2.228572 1.093807 3.345738 4.541182 2.257730

21 22 23

21 O 0.000000

22 H 4.522796 0.000000

23 H 2.962162 2.666360 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.312587 -0.806431 -0.591915

2 6 0 1.321196 -1.387280 0.201547

3 6 0 1.423242 1.346976 0.065976

4 6 0 2.354540 0.602967 -0.680665

5 1 0 2.915359 -1.412421 -1.282292

6 1 0 2.972568 1.098780 -1.440756

7 6 0 0.900672 -0.698733 1.453657

8 1 0 -0.149362 -1.005090 1.718281

9 1 0 1.557378 -1.085734 2.281777

10 6 0 0.991581 0.820124 1.391911

11 1 0 0.009507 1.276088 1.690211

12 1 0 1.746222 1.174843 2.150013

13 1 0 1.293373 2.427283 -0.099530

14 1 0 1.132600 -2.473744 0.179719

15 8 0 -2.150156 0.044026 0.165000

16 6 0 -0.275134 0.681114 -1.111145

17 6 0 -0.311905 -0.734683 -1.094200

18 6 0 -1.398221 1.155837 -0.260798

19 8 0 -1.776528 2.242038 0.148519

20 6 0 -1.467452 -1.116280 -0.247336

21 8 0 -1.912263 -2.172850 0.172754

22 1 0 0.085477 1.289181 -1.943624

23 1 0 0.041809 -1.376558 -1.906171

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2266048 0.8789754 0.6728127

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.3586542179 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.482355440191E-01 A.U. after 16 cycles

Convg = 0.4474D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000576680 0.018244012 0.001241250

2 6 -0.005875367 0.003069114 -0.001772261

3 6 -0.003988119 -0.016411132 0.006254320

4 6 0.015803108 -0.003870629 -0.001802491

5 1 -0.000082223 -0.000580249 -0.000840171

6 1 -0.000727659 -0.001455668 -0.000491248

7 6 0.002307206 0.000994423 0.000367201

8 1 -0.000108510 -0.000119039 -0.001344015

9 1 -0.000583248 0.000898606 -0.000749131

10 6 -0.001799234 -0.000494536 -0.001498003

11 1 0.000381127 0.000200969 -0.000280066

12 1 0.000289550 -0.000154863 0.000063720

13 1 -0.000568789 -0.000409060 -0.000106351

14 1 -0.000959640 0.001162456 0.002049122

15 8 -0.000022230 -0.000890500 -0.004263634

16 6 -0.002065931 -0.004593596 0.002445858

17 6 -0.007174979 0.006644386 -0.001477804

18 6 0.000246993 0.002345885 0.000261984

19 8 -0.000361788 0.001171655 0.002045263

20 6 0.004204608 -0.004853346 0.000778553

21 8 0.001230951 -0.000322925 0.002108487

22 1 -0.000755276 0.000633299 -0.000604663

23 1 0.001186130 -0.001209261 -0.002385919

-------------------------------------------------------------------

Cartesian Forces: Max 0.018244012 RMS 0.004202095

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.017265350 RMS 0.002266468

Search for a saddle point.

Step number 42 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 34 36 41 42

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0

Eigenvalues --- -0.07707 -0.00079 0.00224 0.00583 0.00703

Eigenvalues --- 0.01047 0.01183 0.01433 0.01977 0.02179

Eigenvalues --- 0.02553 0.02727 0.02910 0.03136 0.03233

Eigenvalues --- 0.03309 0.03479 0.03601 0.03694 0.03864

Eigenvalues --- 0.04037 0.04193 0.04548 0.04796 0.05974

Eigenvalues --- 0.06216 0.06361 0.06607 0.07321 0.07826

Eigenvalues --- 0.08788 0.08868 0.09816 0.09938 0.10443

Eigenvalues --- 0.12170 0.13926 0.14639 0.17141 0.21660

Eigenvalues --- 0.25915 0.27456 0.28567 0.29676 0.29897

Eigenvalues --- 0.31019 0.31307 0.31739 0.31977 0.32302

Eigenvalues --- 0.32468 0.33106 0.35351 0.37060 0.38677

Eigenvalues --- 0.39669 0.40437 0.42964 0.47157 0.49945

Eigenvalues --- 0.53128 1.08479 1.10867

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D71 D4

1 -0.58127 -0.50765 0.15502 -0.15121 -0.14165

D86 D85 D35 D73 D29

1 0.14020 0.13451 -0.12927 0.12610 0.12485

RFO step: Lambda0=5.182226862D-05 Lambda=-3.61055492D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.06892327 RMS(Int)= 0.00886033

Iteration 2 RMS(Cart)= 0.00876529 RMS(Int)= 0.00111206

Iteration 3 RMS(Cart)= 0.00017224 RMS(Int)= 0.00110111

Iteration 4 RMS(Cart)= 0.00000006 RMS(Int)= 0.00110111

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63874 -0.00531 0.00000 0.00691 0.00724 2.64597

R2 2.66983 -0.01727 0.00000 -0.01153 -0.01052 2.65930

R3 2.07627 -0.00001 0.00000 -0.00241 -0.00241 2.07387

R4 2.81482 0.00068 0.00000 -0.00108 -0.00139 2.81342

R5 2.08423 -0.00086 0.00000 -0.00026 -0.00026 2.08397

R6 4.12803 -0.00334 0.00000 0.05476 0.05432 4.18235

R7 2.65796 -0.01361 0.00000 0.00082 0.00144 2.65940

R8 2.81690 -0.00077 0.00000 -0.00051 -0.00066 2.81625

R9 2.07983 -0.00025 0.00000 0.00255 0.00255 2.08239

R10 4.10269 -0.00121 0.00000 -0.05129 -0.05110 4.05159

R11 2.07485 0.00006 0.00000 -0.00235 -0.00235 2.07251

R12 2.12664 -0.00029 0.00000 -0.00369 -0.00369 2.12295

R13 2.12694 0.00015 0.00000 0.00274 0.00274 2.12968

R14 2.87773 -0.00413 0.00000 0.00198 0.00141 2.87914

R15 2.12235 0.00043 0.00000 -0.00140 -0.00140 2.12095

R16 2.12964 -0.00018 0.00000 0.00110 0.00110 2.13074

R17 2.66098 0.00245 0.00000 -0.00143 -0.00165 2.65933

R18 2.66070 0.00192 0.00000 0.00179 0.00173 2.66243

R19 2.67656 -0.00576 0.00000 0.00651 0.00626 2.68282

R20 2.80914 0.00122 0.00000 0.00119 0.00112 2.81026

R21 2.06388 0.00055 0.00000 0.00046 0.00046 2.06434

R22 2.80170 0.00393 0.00000 0.00696 0.00713 2.80882

R23 2.06700 -0.00141 0.00000 -0.00303 -0.00303 2.06396

R24 2.30708 0.00021 0.00000 -0.00052 -0.00052 2.30657

R25 2.30722 0.00104 0.00000 0.00005 0.00005 2.30728

A1 2.06207 0.00130 0.00000 -0.00207 -0.00279 2.05928

A2 2.11429 -0.00084 0.00000 0.00549 0.00487 2.11916

A3 2.08800 -0.00023 0.00000 0.00877 0.00813 2.09612

A4 2.07809 0.00037 0.00000 -0.01013 -0.01058 2.06751

A5 2.11756 0.00011 0.00000 0.02662 0.02628 2.14384

A6 1.64031 -0.00325 0.00000 0.00173 0.00136 1.64166

A7 2.00834 -0.00020 0.00000 0.00896 0.00783 2.01617

A8 1.72082 0.00418 0.00000 0.00126 0.00130 1.72212

A9 1.72613 -0.00138 0.00000 -0.06380 -0.06308 1.66305

A10 2.06799 0.00176 0.00000 0.00308 0.00240 2.07040

A11 2.11474 -0.00060 0.00000 -0.02106 -0.02103 2.09371

A12 1.63877 -0.00218 0.00000 0.01504 0.01439 1.65315

A13 2.03366 -0.00143 0.00000 -0.00237 -0.00324 2.03042

A14 1.71868 0.00385 0.00000 0.03330 0.03349 1.75217

A15 1.69835 -0.00082 0.00000 0.00447 0.00476 1.70310

A16 2.06540 0.00230 0.00000 -0.00397 -0.00394 2.06146

A17 2.10678 -0.00239 0.00000 0.01166 0.01135 2.11812

A18 2.09591 0.00024 0.00000 -0.00147 -0.00183 2.09408

A19 1.91266 0.00163 0.00000 0.00706 0.00719 1.91985

A20 1.87006 0.00177 0.00000 -0.00835 -0.00869 1.86137

A21 1.99337 -0.00352 0.00000 -0.00390 -0.00437 1.98901

A22 1.85229 -0.00065 0.00000 0.00936 0.00950 1.86179

A23 1.91427 0.00147 0.00000 0.01927 0.01912 1.93338

A24 1.91553 -0.00051 0.00000 -0.02327 -0.02308 1.89245

A25 1.98873 -0.00180 0.00000 -0.00401 -0.00416 1.98457

A26 1.92408 0.00096 0.00000 0.01269 0.01259 1.93667

A27 1.86838 0.00045 0.00000 -0.00949 -0.00945 1.85893

A28 1.91979 0.00063 0.00000 0.00682 0.00678 1.92657

A29 1.90354 0.00017 0.00000 -0.00981 -0.00984 1.89370

A30 1.85364 -0.00034 0.00000 0.00351 0.00356 1.85720

A31 1.87884 0.00018 0.00000 0.01004 0.00203 1.88087

A32 1.89695 -0.00193 0.00000 -0.02475 -0.02601 1.87094

A33 1.75476 0.00161 0.00000 -0.05010 -0.04904 1.70572

A34 1.55502 0.00034 0.00000 0.03722 0.03729 1.59231

A35 1.86791 0.00061 0.00000 0.00166 -0.00149 1.86642

A36 2.18245 -0.00011 0.00000 0.01326 0.01427 2.19672

A37 2.10329 -0.00051 0.00000 0.00170 0.00314 2.10643

A38 1.86117 -0.00081 0.00000 0.01957 0.01851 1.87968

A39 1.73856 0.00044 0.00000 -0.01949 -0.01828 1.72028

A40 1.59406 -0.00027 0.00000 -0.03924 -0.03924 1.55482

A41 1.85912 0.00241 0.00000 0.00117 -0.00047 1.85865

A42 2.17646 -0.00054 0.00000 0.02825 0.02901 2.20547

A43 2.12354 -0.00161 0.00000 -0.00823 -0.00837 2.11518

A44 1.90103 -0.00042 0.00000 0.00946 0.00358 1.90462

A45 2.02153 0.00114 0.00000 0.00112 0.00327 2.02481

A46 2.36033 -0.00072 0.00000 -0.00923 -0.00706 2.35326

A47 1.91038 -0.00263 0.00000 0.00469 -0.00090 1.90947

A48 2.02165 0.00138 0.00000 -0.00200 -0.00017 2.02148

A49 2.35072 0.00125 0.00000 -0.00086 0.00096 2.35168

D1 -0.61578 0.00002 0.00000 -0.01955 -0.01936 -0.63514

D2 2.96334 -0.00066 0.00000 -0.08817 -0.08858 2.87476

D3 1.16670 0.00304 0.00000 -0.01900 -0.01909 1.14761

D4 2.73391 -0.00121 0.00000 -0.08702 -0.08679 2.64712

D5 0.02984 -0.00189 0.00000 -0.15564 -0.15600 -0.12616

D6 -1.76680 0.00181 0.00000 -0.08648 -0.08651 -1.85331

D7 0.03358 -0.00040 0.00000 -0.02428 -0.02437 0.00920

D8 -2.92236 -0.00135 0.00000 -0.06194 -0.06210 -2.98446

D9 2.97030 0.00074 0.00000 0.04176 0.04175 3.01206

D10 0.01437 -0.00021 0.00000 0.00411 0.00402 0.01839

D11 2.70560 -0.00104 0.00000 0.09121 0.09114 2.79674

D12 -1.57515 -0.00005 0.00000 0.10131 0.10124 -1.47391

D13 0.55014 -0.00168 0.00000 0.06324 0.06343 0.61357

D14 -0.84704 -0.00034 0.00000 0.16039 0.16034 -0.68670

D15 1.15539 0.00066 0.00000 0.17049 0.17045 1.32584

D16 -3.00251 -0.00097 0.00000 0.13243 0.13263 -2.86987

D17 0.96968 0.00021 0.00000 0.09093 0.09140 1.06107

D18 2.97211 0.00121 0.00000 0.10103 0.10150 3.07361

D19 -1.18579 -0.00042 0.00000 0.06297 0.06369 -1.12210

D20 -1.06761 0.00127 0.00000 0.06240 0.06248 -1.00512

D21 -2.99769 -0.00127 0.00000 0.06285 0.06482 -2.93287

D22 1.14831 0.00038 0.00000 0.08236 0.08273 1.23104

D23 1.03031 0.00165 0.00000 0.05260 0.05214 1.08246

D24 -0.89977 -0.00089 0.00000 0.05304 0.05448 -0.84529

D25 -3.03695 0.00076 0.00000 0.07255 0.07239 -2.96456

D26 3.07620 0.00215 0.00000 0.04628 0.04577 3.12197

D27 1.14612 -0.00039 0.00000 0.04673 0.04811 1.19423

D28 -0.99106 0.00126 0.00000 0.06623 0.06602 -0.92504

D29 0.58847 0.00106 0.00000 0.02580 0.02582 0.61429

D30 -2.73759 0.00171 0.00000 0.06466 0.06446 -2.67313

D31 -2.95091 0.00000 0.00000 -0.03253 -0.03211 -2.98301

D32 0.00622 0.00065 0.00000 0.00633 0.00654 0.01276

D33 -1.18877 -0.00246 0.00000 -0.02170 -0.02171 -1.21048

D34 1.76836 -0.00181 0.00000 0.01716 0.01693 1.78529

D35 -0.60625 0.00006 0.00000 0.02065 0.02062 -0.58563

D36 -2.77452 -0.00019 0.00000 0.00460 0.00472 -2.76980

D37 1.49977 -0.00053 0.00000 -0.00080 -0.00066 1.49911

D38 2.91483 0.00093 0.00000 0.08062 0.08057 2.99540

D39 0.74656 0.00068 0.00000 0.06457 0.06467 0.81124

D40 -1.26234 0.00034 0.00000 0.05917 0.05930 -1.20304

D41 1.12419 0.00016 0.00000 0.05797 0.05761 1.18180

D42 -1.04407 -0.00009 0.00000 0.04192 0.04171 -1.00237

D43 -3.05298 -0.00043 0.00000 0.03652 0.03633 -3.01664

D44 0.97932 0.00041 0.00000 0.06682 0.06697 1.04629

D45 2.93699 0.00114 0.00000 0.03818 0.03744 2.97442

D46 -1.23612 0.00084 0.00000 0.04298 0.04279 -1.19333

D47 -1.10757 -0.00157 0.00000 0.05509 0.05500 -1.05257

D48 0.85010 -0.00084 0.00000 0.02645 0.02547 0.87557

D49 2.96018 -0.00114 0.00000 0.03125 0.03082 2.99100

D50 3.11072 -0.00077 0.00000 0.04896 0.04914 -3.12333

D51 -1.21480 -0.00003 0.00000 0.02032 0.01961 -1.19519

D52 0.89528 -0.00034 0.00000 0.02511 0.02496 0.92024

D53 0.04860 -0.00010 0.00000 -0.06215 -0.06198 -0.01338

D54 2.21917 0.00033 0.00000 -0.04298 -0.04300 2.17617

D55 -2.03764 0.00038 0.00000 -0.04055 -0.04060 -2.07824

D56 -2.10600 -0.00082 0.00000 -0.08354 -0.08334 -2.18934

D57 0.06457 -0.00039 0.00000 -0.06437 -0.06436 0.00021

D58 2.09094 -0.00034 0.00000 -0.06194 -0.06196 2.02898

D59 2.14869 -0.00059 0.00000 -0.09258 -0.09224 2.05644

D60 -1.96393 -0.00016 0.00000 -0.07340 -0.07327 -2.03720

D61 0.06245 -0.00011 0.00000 -0.07098 -0.07087 -0.00842

D62 0.11635 -0.00112 0.00000 -0.20847 -0.20845 -0.09209

D63 -3.00318 -0.00094 0.00000 -0.25904 -0.25945 3.02056

D64 -0.10941 0.00122 0.00000 0.19803 0.19754 0.08812

D65 3.00527 0.00129 0.00000 0.25497 0.25469 -3.02322

D66 0.04871 0.00009 0.00000 -0.07227 -0.07204 -0.02333

D67 1.89332 0.00121 0.00000 -0.08586 -0.08541 1.80791

D68 -1.76080 0.00133 0.00000 -0.04984 -0.04912 -1.80992

D69 -1.83256 -0.00120 0.00000 -0.00527 -0.00543 -1.83799

D70 0.01204 -0.00008 0.00000 -0.01886 -0.01879 -0.00675

D71 2.64111 0.00005 0.00000 0.01716 0.01750 2.65860

D72 1.83812 -0.00105 0.00000 -0.03609 -0.03642 1.80171

D73 -2.60046 0.00007 0.00000 -0.04968 -0.04978 -2.65024

D74 0.02861 0.00019 0.00000 -0.01366 -0.01349 0.01512

D75 -2.05951 0.00200 0.00000 0.18832 0.18881 -1.87070

D76 1.05389 0.00180 0.00000 0.25326 0.25368 1.30757

D77 -0.07960 0.00075 0.00000 0.14093 0.14073 0.06113

D78 3.03380 0.00055 0.00000 0.20587 0.20560 -3.04378

D79 2.56174 0.00074 0.00000 0.17428 0.17394 2.73568

D80 -0.60805 0.00054 0.00000 0.23922 0.23881 -0.36923

D81 1.99113 -0.00065 0.00000 -0.09548 -0.09619 1.89494

D82 -1.11640 -0.00072 0.00000 -0.16758 -0.16859 -1.28499

D83 0.05943 -0.00065 0.00000 -0.10960 -0.10914 -0.04971

D84 -3.04810 -0.00072 0.00000 -0.18170 -0.18154 3.05355

D85 -2.58868 -0.00110 0.00000 -0.15729 -0.15642 -2.74510

D86 0.58697 -0.00117 0.00000 -0.22939 -0.22882 0.35816

Item Value Threshold Converged?

Maximum Force 0.017265 0.000450 NO

RMS Force 0.002266 0.000300 NO

Maximum Displacement 0.404279 0.001800 NO

RMS Displacement 0.071592 0.001200 NO

Predicted change in Energy=-2.863745D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.162817 1.535020 0.412502

2 6 0 0.174944 1.251028 0.112046

3 6 0 -0.723206 3.786687 -0.338440

4 6 0 -1.626907 2.844149 0.186369

5 1 0 -1.799382 0.807475 0.931965

6 1 0 -2.615257 3.167483 0.534824

7 6 0 0.790056 1.906307 -1.074870

8 1 0 1.909976 1.882387 -0.989631

9 1 0 0.520230 1.274734 -1.968396

10 6 0 0.297138 3.326537 -1.322378

11 1 0 1.163283 4.039010 -1.365563

12 1 0 -0.195849 3.362648 -2.335791

13 1 0 -1.004799 4.850911 -0.387740

14 1 0 0.690435 0.346515 0.475740

15 8 0 2.717492 3.858152 0.714830

16 6 0 0.472659 3.892530 1.437929

17 6 0 0.975735 2.587894 1.683602

18 6 0 1.594658 4.690916 0.876467

19 8 0 1.749313 5.862977 0.572863

20 6 0 2.400531 2.598423 1.260370

21 8 0 3.319164 1.795983 1.314644

22 1 0 -0.339114 4.378714 1.983812

23 1 0 0.615315 1.886525 2.439304

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.400190 0.000000

3 C 2.413953 2.727485 0.000000

4 C 1.407243 2.406289 1.407294 0.000000

5 H 1.097443 2.183340 3.412885 2.175708 0.000000

6 H 2.188488 3.411271 2.173905 1.096724 2.528441

7 C 2.482709 1.488799 2.523513 2.883050 3.455432

8 H 3.395394 2.150033 3.314220 3.849351 4.313619

9 H 2.927297 2.109033 3.242344 3.422904 3.743130

10 C 2.889777 2.525914 1.490293 2.492180 3.977830

11 H 3.852560 3.306506 2.162751 3.409010 4.949631

12 H 3.439238 3.253971 2.108868 2.945854 4.447298

13 H 3.414745 3.821091 1.101952 2.178006 4.326934

14 H 2.202519 1.102791 3.807368 3.419355 2.572901

15 O 4.532675 3.691205 3.599012 4.492357 5.454900

16 C 3.046988 2.970545 2.144011 2.659640 3.864679

17 C 2.701415 2.213202 2.900371 3.013489 3.381734

18 C 4.216469 3.799046 2.768776 3.776938 5.157878

19 O 5.218948 4.895003 3.354818 4.545498 6.187107

20 C 3.814073 2.843828 3.704847 4.175418 4.577621

21 O 4.579314 3.410181 4.799619 5.180278 5.227151

22 H 3.351730 3.681057 2.427112 2.691487 3.999064

23 H 2.719051 2.452328 3.621893 3.319687 3.044205

6 7 8 9 10

6 H 0.000000

7 C 3.972133 0.000000

8 H 4.945015 1.123414 0.000000

9 H 4.436202 1.126978 1.805164 0.000000

10 C 3.457824 1.523575 2.190328 2.162639 0.000000

11 H 4.318379 2.184541 2.312985 2.901405 1.122359

12 H 3.759263 2.163991 2.904792 2.237662 1.127539

13 H 2.505719 3.516297 4.203608 4.196812 2.211855

14 H 4.346143 2.201651 2.448162 2.619992 3.502634

15 O 5.380301 3.275322 2.731468 4.324548 3.207951

16 C 3.297957 3.218693 3.464045 4.296298 2.823200

17 C 3.814556 2.847491 2.918342 3.907552 3.168912

18 C 4.490095 3.494159 3.386677 4.573614 2.894825

19 O 5.129971 4.392087 4.279286 5.387078 3.483429

20 C 5.099841 2.919931 2.411609 3.963914 3.409546

21 O 6.140561 3.481140 2.702399 4.345582 4.292916

22 H 2.957613 4.091864 4.486805 5.098344 3.527433

23 H 3.962890 3.518571 3.665209 4.450971 4.040436

11 12 13 14 15

11 H 0.000000

12 H 1.801679 0.000000

13 H 2.513146 2.581517 0.000000

14 H 4.153132 4.217495 4.889683 0.000000

15 O 2.603135 4.247278 4.007079 4.061738 0.000000

16 C 2.891019 3.868933 2.536620 3.680687 2.358671

17 C 3.382059 4.257742 3.651604 2.562051 2.363428

18 C 2.374398 3.910091 2.894995 4.455560 1.407259

19 O 2.725396 4.300647 3.087420 5.618007 2.230885

20 C 3.240617 4.500844 4.402980 2.934478 1.408898

21 O 4.106398 5.304284 5.561236 3.116879 2.230320

22 H 3.686585 4.439806 2.508059 4.426385 3.350245

23 H 4.405732 5.063443 4.405057 2.496569 3.358611

16 17 18 19 20

16 C 0.000000

17 C 1.419688 0.000000

18 C 1.487125 2.336072 0.000000

19 O 2.502168 3.543773 1.220582 0.000000

20 C 2.328718 1.486365 2.274936 3.399126 0.000000

21 O 3.537414 2.500983 3.398022 4.422116 1.220960

22 H 1.092400 2.241872 2.250146 2.924951 3.346410

23 H 2.246588 1.092202 3.356512 4.536708 2.254701

21 22 23

21 O 0.000000

22 H 4.527835 0.000000

23 H 2.929822 2.707289 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.374504 -0.613840 -0.644880

2 6 0 1.439002 -1.337009 0.105049

3 6 0 1.279897 1.385461 0.149980

4 6 0 2.290746 0.790806 -0.627867

5 1 0 3.068056 -1.115547 -1.331653

6 1 0 2.896121 1.406887 -1.303713

7 6 0 0.995478 -0.780726 1.412856

8 1 0 0.021008 -1.248573 1.718776

9 1 0 1.761017 -1.099947 2.175829

10 6 0 0.896232 0.739421 1.436995

11 1 0 -0.131215 1.059095 1.756137

12 1 0 1.608838 1.132144 2.217576

13 1 0 1.089314 2.467890 0.070460

14 1 0 1.267488 -2.417420 -0.034386

15 8 0 -2.013485 -0.053015 0.343131

16 6 0 -0.324172 0.722617 -1.108744

17 6 0 -0.281569 -0.696260 -1.130807

18 6 0 -1.450371 1.108447 -0.217480

19 8 0 -1.982972 2.163118 0.088830

20 6 0 -1.378125 -1.165191 -0.243705

21 8 0 -1.844271 -2.256586 0.043186

22 1 0 0.002147 1.385273 -1.913568

23 1 0 0.093321 -1.320298 -1.945018

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2233706 0.8805960 0.6748774

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5747129899 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.485611374639E-01 A.U. after 16 cycles

Convg = 0.4725D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.003388215 0.011251051 -0.001753520

2 6 -0.005059321 0.007759901 0.003521891

3 6 -0.006587253 -0.010014374 0.005159751

4 6 0.013793288 -0.004214276 -0.003876587

5 1 0.000716372 -0.000158728 0.001888865

6 1 -0.000872257 -0.001280330 0.001364914

7 6 -0.000052277 0.000039535 -0.000611702

8 1 0.000008014 0.001279261 -0.000757984

9 1 0.001172472 -0.000335748 -0.000291526

10 6 -0.001793912 -0.001405655 -0.001260769

11 1 0.000273113 0.000000071 0.000139605

12 1 0.000885513 0.000490452 -0.000282808

13 1 0.000739011 0.000015302 0.000186971

14 1 -0.004155099 -0.000447031 -0.000455504

15 8 0.001741553 0.000711472 0.001563917

16 6 -0.000374403 -0.010933339 -0.000444338

17 6 -0.003848403 0.008071313 -0.005035542

18 6 0.000649817 0.001960703 0.001941610

19 8 -0.000966060 0.000356284 -0.001593026

20 6 0.000475441 -0.002499092 0.002836703

21 8 -0.000301905 -0.001193352 -0.001517694

22 1 0.000045511 -0.000225773 0.000218297

23 1 0.000122569 0.000772352 -0.000941523

-------------------------------------------------------------------

Cartesian Forces: Max 0.013793288 RMS 0.003679583

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.013534029 RMS 0.002058424

Search for a saddle point.

Step number 43 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 34 37 42 43

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0

Eigenvalues --- -0.07644 -0.00098 0.00528 0.00678 0.00784

Eigenvalues --- 0.01086 0.01137 0.01423 0.01988 0.02175

Eigenvalues --- 0.02545 0.02769 0.02926 0.03109 0.03207

Eigenvalues --- 0.03378 0.03462 0.03652 0.03693 0.03868

Eigenvalues --- 0.04046 0.04180 0.04509 0.04818 0.05978

Eigenvalues --- 0.06249 0.06353 0.06577 0.07329 0.08136

Eigenvalues --- 0.08824 0.08927 0.09863 0.09883 0.10534

Eigenvalues --- 0.12145 0.13842 0.14642 0.17136 0.21837

Eigenvalues --- 0.26027 0.27394 0.28592 0.29781 0.29959

Eigenvalues --- 0.31028 0.31304 0.31751 0.31981 0.32366

Eigenvalues --- 0.32491 0.33150 0.35417 0.37078 0.38775

Eigenvalues --- 0.39684 0.40434 0.43053 0.47199 0.50111

Eigenvalues --- 0.54030 1.08498 1.10864

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D71 D4

1 -0.57577 -0.50673 0.15828 -0.15388 -0.14595

D86 D85 D35 D73 D1

1 0.13700 0.13292 -0.12867 0.12556 -0.12477

RFO step: Lambda0=1.768926530D-05 Lambda=-4.52098725D-03.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.823

Iteration 1 RMS(Cart)= 0.06504859 RMS(Int)= 0.00276003

Iteration 2 RMS(Cart)= 0.00315432 RMS(Int)= 0.00083027

Iteration 3 RMS(Cart)= 0.00000544 RMS(Int)= 0.00083026

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00083026

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64597 -0.00915 0.00000 -0.01904 -0.01832 2.62765

R2 2.65930 -0.01353 0.00000 -0.04054 -0.03872 2.62059

R3 2.07387 0.00058 0.00000 0.00677 0.00677 2.08063

R4 2.81342 0.00068 0.00000 0.00859 0.00872 2.82214

R5 2.08397 -0.00173 0.00000 -0.00489 -0.00489 2.07908

R6 4.18235 -0.00384 0.00000 -0.17699 -0.17663 4.00571

R7 2.65940 -0.01076 0.00000 -0.04153 -0.04052 2.61888

R8 2.81625 -0.00032 0.00000 0.00220 0.00135 2.81760

R9 2.08239 -0.00018 0.00000 -0.00041 -0.00041 2.08198

R10 4.05159 -0.00146 0.00000 0.12721 0.12627 4.17786

R11 2.07251 0.00084 0.00000 0.00904 0.00904 2.08154

R12 2.12295 -0.00008 0.00000 -0.00193 -0.00193 2.12101

R13 2.12968 0.00014 0.00000 -0.00063 -0.00063 2.12905

R14 2.87914 -0.00328 0.00000 -0.00018 -0.00106 2.87808

R15 2.12095 0.00021 0.00000 0.00419 0.00419 2.12514

R16 2.13074 -0.00012 0.00000 -0.00346 -0.00346 2.12728

R17 2.65933 0.00136 0.00000 0.00928 0.00912 2.66846

R18 2.66243 0.00096 0.00000 0.00028 0.00009 2.66252

R19 2.68282 -0.00994 0.00000 -0.03756 -0.03820 2.64462

R20 2.81026 0.00128 0.00000 -0.00028 -0.00019 2.81007

R21 2.06434 -0.00003 0.00000 -0.00162 -0.00162 2.06272

R22 2.80882 -0.00008 0.00000 0.00191 0.00193 2.81076

R23 2.06396 -0.00119 0.00000 0.00294 0.00294 2.06691

R24 2.30657 0.00062 0.00000 0.00008 0.00008 2.30665

R25 2.30728 0.00049 0.00000 -0.00102 -0.00102 2.30626

A1 2.05928 0.00117 0.00000 -0.00708 -0.00771 2.05156

A2 2.11916 -0.00127 0.00000 -0.00984 -0.00983 2.10934

A3 2.09612 0.00008 0.00000 0.02142 0.02148 2.11760

A4 2.06751 0.00124 0.00000 0.00280 0.00028 2.06779

A5 2.14384 -0.00166 0.00000 -0.05839 -0.05746 2.08638

A6 1.64166 -0.00239 0.00000 -0.00466 -0.00498 1.63668

A7 2.01617 0.00031 0.00000 0.02650 0.02408 2.04026

A8 1.72212 0.00327 0.00000 0.06950 0.07030 1.79242

A9 1.66305 -0.00042 0.00000 0.01818 0.01632 1.67937

A10 2.07040 0.00112 0.00000 0.03870 0.03553 2.10593

A11 2.09371 0.00034 0.00000 0.00910 0.00904 2.10276

A12 1.65315 -0.00254 0.00000 -0.08095 -0.07994 1.57321

A13 2.03042 -0.00127 0.00000 -0.01237 -0.01274 2.01768

A14 1.75217 0.00268 0.00000 -0.02467 -0.02413 1.72803

A15 1.70310 -0.00047 0.00000 0.02711 0.02719 1.73029

A16 2.06146 0.00181 0.00000 0.01363 0.01343 2.07489

A17 2.11812 -0.00273 0.00000 -0.03051 -0.03041 2.08771

A18 2.09408 0.00086 0.00000 0.01685 0.01693 2.11102

A19 1.91985 0.00165 0.00000 0.01691 0.01795 1.93780

A20 1.86137 0.00124 0.00000 0.00113 0.00097 1.86234

A21 1.98901 -0.00299 0.00000 -0.01953 -0.02121 1.96779

A22 1.86179 -0.00074 0.00000 0.00383 0.00354 1.86533

A23 1.93338 0.00058 0.00000 -0.00691 -0.00630 1.92709

A24 1.89245 0.00038 0.00000 0.00618 0.00661 1.89906

A25 1.98457 -0.00198 0.00000 -0.00394 -0.00704 1.97754

A26 1.93667 0.00070 0.00000 -0.00998 -0.00974 1.92693

A27 1.85893 0.00085 0.00000 0.02236 0.02373 1.88266

A28 1.92657 0.00055 0.00000 -0.00852 -0.00718 1.91939

A29 1.89370 0.00051 0.00000 0.01617 0.01634 1.91004

A30 1.85720 -0.00053 0.00000 -0.01498 -0.01528 1.84192

A31 1.88087 -0.00144 0.00000 0.00112 -0.00023 1.88064

A32 1.87094 -0.00037 0.00000 -0.01574 -0.01714 1.85380

A33 1.70572 0.00108 0.00000 0.00674 0.00781 1.71353

A34 1.59231 -0.00039 0.00000 -0.05007 -0.04949 1.54282

A35 1.86642 0.00083 0.00000 0.00595 0.00578 1.87220

A36 2.19672 -0.00053 0.00000 0.01981 0.01855 2.21527

A37 2.10643 -0.00041 0.00000 0.00635 0.00556 2.11199

A38 1.87968 -0.00073 0.00000 0.01618 0.01535 1.89503

A39 1.72028 0.00024 0.00000 0.02765 0.02753 1.74781

A40 1.55482 -0.00014 0.00000 0.03720 0.03855 1.59337

A41 1.85865 0.00260 0.00000 0.01128 0.01072 1.86937

A42 2.20547 -0.00115 0.00000 -0.02761 -0.02927 2.17620

A43 2.11518 -0.00123 0.00000 -0.02432 -0.02599 2.08919

A44 1.90462 -0.00076 0.00000 -0.00446 -0.00512 1.89949

A45 2.02481 0.00101 0.00000 0.00231 0.00259 2.02739

A46 2.35326 -0.00024 0.00000 0.00264 0.00291 2.35617

A47 1.90947 -0.00116 0.00000 -0.00601 -0.00681 1.90266

A48 2.02148 0.00095 0.00000 0.00794 0.00823 2.02971

A49 2.35168 0.00022 0.00000 -0.00123 -0.00094 2.35074

D1 -0.63514 -0.00028 0.00000 -0.02284 -0.02239 -0.65753

D2 2.87476 -0.00001 0.00000 0.06382 0.06270 2.93746

D3 1.14761 0.00237 0.00000 0.05518 0.05612 1.20373

D4 2.64712 -0.00019 0.00000 -0.06104 -0.06056 2.58656

D5 -0.12616 0.00008 0.00000 0.02563 0.02453 -0.10163

D6 -1.85331 0.00245 0.00000 0.01699 0.01795 -1.83536

D7 0.00920 -0.00043 0.00000 0.00411 0.00353 0.01274

D8 -2.98446 -0.00005 0.00000 0.00272 0.00237 -2.98209

D9 3.01206 -0.00063 0.00000 0.03920 0.03926 3.05132

D10 0.01839 -0.00025 0.00000 0.03781 0.03810 0.05649

D11 2.79674 -0.00109 0.00000 0.08544 0.08609 2.88283

D12 -1.47391 -0.00046 0.00000 0.09907 0.10002 -1.37389

D13 0.61357 -0.00092 0.00000 0.09590 0.09636 0.70993

D14 -0.68670 -0.00177 0.00000 -0.01237 -0.01359 -0.70029

D15 1.32584 -0.00114 0.00000 0.00126 0.00035 1.32618

D16 -2.86987 -0.00160 0.00000 -0.00191 -0.00331 -2.87318

D17 1.06107 -0.00049 0.00000 0.05022 0.05062 1.11169

D18 3.07361 0.00014 0.00000 0.06385 0.06456 3.13817

D19 -1.12210 -0.00033 0.00000 0.06068 0.06090 -1.06120

D20 -1.00512 0.00041 0.00000 0.03034 0.03158 -0.97354

D21 -2.93287 -0.00230 0.00000 0.00259 0.00373 -2.92914

D22 1.23104 -0.00104 0.00000 0.01902 0.01990 1.25095

D23 1.08246 0.00172 0.00000 0.04391 0.04380 1.12626

D24 -0.84529 -0.00099 0.00000 0.01615 0.01594 -0.82934

D25 -2.96456 0.00026 0.00000 0.03258 0.03212 -2.93244

D26 3.12197 0.00254 0.00000 0.08768 0.08838 -3.07283

D27 1.19423 -0.00018 0.00000 0.05992 0.06052 1.25475

D28 -0.92504 0.00108 0.00000 0.07635 0.07670 -0.84834

D29 0.61429 0.00086 0.00000 -0.05993 -0.06109 0.55320

D30 -2.67313 0.00016 0.00000 -0.06272 -0.06406 -2.73719

D31 -2.98301 0.00100 0.00000 0.02271 0.02331 -2.95970

D32 0.01276 0.00030 0.00000 0.01992 0.02034 0.03310

D33 -1.21048 -0.00102 0.00000 0.00733 0.00836 -1.20211

D34 1.78529 -0.00172 0.00000 0.00454 0.00539 1.79068

D35 -0.58563 0.00060 0.00000 0.13963 0.14080 -0.44484

D36 -2.76980 0.00084 0.00000 0.16216 0.16332 -2.60648

D37 1.49911 0.00063 0.00000 0.17239 0.17319 1.67230

D38 2.99540 0.00007 0.00000 0.05502 0.05545 3.05086

D39 0.81124 0.00031 0.00000 0.07756 0.07798 0.88922

D40 -1.20304 0.00011 0.00000 0.08778 0.08785 -1.11519

D41 1.18180 -0.00047 0.00000 0.04116 0.04114 1.22294

D42 -1.00237 -0.00023 0.00000 0.06370 0.06367 -0.93870

D43 -3.01664 -0.00044 0.00000 0.07392 0.07354 -2.94310

D44 1.04629 -0.00047 0.00000 0.05649 0.05704 1.10333

D45 2.97442 0.00074 0.00000 0.06137 0.06168 3.03610

D46 -1.19333 0.00037 0.00000 0.05994 0.05996 -1.13337

D47 -1.05257 -0.00151 0.00000 0.04245 0.04210 -1.01047

D48 0.87557 -0.00030 0.00000 0.04734 0.04674 0.92231

D49 2.99100 -0.00067 0.00000 0.04591 0.04502 3.03602

D50 -3.12333 -0.00072 0.00000 0.05398 0.05427 -3.06906

D51 -1.19519 0.00049 0.00000 0.05887 0.05890 -1.13629

D52 0.92024 0.00012 0.00000 0.05744 0.05718 0.97742

D53 -0.01338 0.00007 0.00000 -0.14826 -0.14695 -0.16033

D54 2.17617 -0.00008 0.00000 -0.17146 -0.17074 2.00542

D55 -2.07824 -0.00011 0.00000 -0.18486 -0.18376 -2.26201

D56 -2.18934 -0.00031 0.00000 -0.15033 -0.14975 -2.33909

D57 0.00021 -0.00046 0.00000 -0.17353 -0.17354 -0.17333

D58 2.02898 -0.00050 0.00000 -0.18692 -0.18656 1.84242

D59 2.05644 0.00004 0.00000 -0.15472 -0.15436 1.90208

D60 -2.03720 -0.00011 0.00000 -0.17792 -0.17816 -2.21535

D61 -0.00842 -0.00015 0.00000 -0.19132 -0.19117 -0.19960

D62 -0.09209 0.00055 0.00000 0.07117 0.07146 -0.02064

D63 3.02056 0.00088 0.00000 0.08522 0.08548 3.10603

D64 0.08812 -0.00076 0.00000 -0.08208 -0.08192 0.00620

D65 -3.02322 -0.00095 0.00000 -0.10124 -0.10124 -3.12446

D66 -0.02333 0.00003 0.00000 -0.05491 -0.05430 -0.07763

D67 1.80791 0.00108 0.00000 -0.01298 -0.01234 1.79557

D68 -1.80992 0.00138 0.00000 -0.10440 -0.10316 -1.91308

D69 -1.83799 -0.00135 0.00000 -0.05864 -0.05851 -1.89651

D70 -0.00675 -0.00030 0.00000 -0.01671 -0.01656 -0.02331

D71 2.65860 0.00000 0.00000 -0.10813 -0.10737 2.55123

D72 1.80171 -0.00107 0.00000 -0.12468 -0.12541 1.67630

D73 -2.65024 -0.00002 0.00000 -0.08275 -0.08345 -2.73369

D74 0.01512 0.00029 0.00000 -0.17417 -0.17427 -0.15915

D75 -1.87070 -0.00029 0.00000 -0.01998 -0.01917 -1.88987

D76 1.30757 -0.00073 0.00000 -0.03773 -0.03691 1.27066

D77 0.06113 -0.00007 0.00000 -0.03285 -0.03318 0.02795

D78 -3.04378 -0.00051 0.00000 -0.05060 -0.05092 -3.09470

D79 2.73568 -0.00040 0.00000 0.03371 0.03340 2.76908

D80 -0.36923 -0.00085 0.00000 0.01595 0.01566 -0.35357

D81 1.89494 0.00060 0.00000 0.09202 0.09186 1.98680

D82 -1.28499 0.00086 0.00000 0.11650 0.11641 -1.16858

D83 -0.04971 0.00058 0.00000 0.06100 0.06108 0.01137

D84 3.05355 0.00083 0.00000 0.08547 0.08563 3.13918

D85 -2.74510 0.00034 0.00000 0.14846 0.14831 -2.59679

D86 0.35816 0.00060 0.00000 0.17294 0.17286 0.53101

Item Value Threshold Converged?

Maximum Force 0.013534 0.000450 NO

RMS Force 0.002058 0.000300 NO

Maximum Displacement 0.250240 0.001800 NO

RMS Displacement 0.065211 0.001200 NO

Predicted change in Energy=-3.696777D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.130485 1.583501 0.466665

2 6 0 0.192344 1.297018 0.148039

3 6 0 -0.735807 3.770379 -0.406273

4 6 0 -1.596085 2.859129 0.185449

5 1 0 -1.750658 0.854864 1.011390

6 1 0 -2.584386 3.172241 0.557651

7 6 0 0.763314 1.872443 -1.106218

8 1 0 1.883057 1.795536 -1.111297

9 1 0 0.387809 1.234393 -1.955465

10 6 0 0.328655 3.312526 -1.344570

11 1 0 1.219606 3.996612 -1.290680

12 1 0 -0.067554 3.415555 -2.393197

13 1 0 -1.015864 4.832948 -0.485894

14 1 0 0.653502 0.372606 0.526516

15 8 0 2.726563 3.921294 0.816373

16 6 0 0.456827 3.859978 1.453126

17 6 0 0.976699 2.575079 1.646241

18 6 0 1.566042 4.714251 0.952018

19 8 0 1.684262 5.894737 0.664958

20 6 0 2.405519 2.614809 1.234880

21 8 0 3.311224 1.797615 1.198598

22 1 0 -0.409656 4.298543 1.951460

23 1 0 0.658672 1.886948 2.434686

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.390493 0.000000

3 C 2.387515 2.699303 0.000000

4 C 1.386755 2.374882 1.385854 0.000000

5 H 1.101023 2.171666 3.397045 2.173280 0.000000

6 H 2.155504 3.375570 2.168909 1.101505 2.504239

7 C 2.478694 1.493412 2.517826 2.865086 3.440899

8 H 3.408278 2.166323 3.354923 3.862280 4.312140

9 H 2.879897 2.113493 3.177064 3.340525 3.676861

10 C 2.898135 2.511719 1.491009 2.500230 3.989259

11 H 3.799250 3.226916 2.158008 3.376528 4.898222

12 H 3.558800 3.318678 2.126106 3.048841 4.580523

13 H 3.388128 3.790044 1.101737 2.164098 4.313575

14 H 2.156956 1.100204 3.787497 3.370424 2.499532

15 O 4.523759 3.708876 3.675002 4.495725 5.430151

16 C 2.945338 2.888247 2.210830 2.612117 3.754841

17 C 2.610527 2.119732 2.928178 2.972173 3.286434

18 C 4.160339 3.769736 2.834493 3.745417 5.089095

19 O 5.152561 4.861281 3.393695 4.495056 6.108929

20 C 3.762589 2.795700 3.727821 4.144132 4.518978

21 O 4.506701 3.328917 4.779735 5.122008 5.152328

22 H 3.177367 3.553010 2.438080 2.568720 3.813259

23 H 2.676989 2.407122 3.682789 3.329885 2.982590

6 7 8 9 10

6 H 0.000000

7 C 3.957908 0.000000

8 H 4.963744 1.122392 0.000000

9 H 4.347982 1.126646 1.806452 0.000000

10 C 3.481944 1.523017 2.184455 2.166871 0.000000

11 H 4.308860 2.180441 2.305880 2.960352 1.124576

12 H 3.886020 2.174363 2.841235 2.270779 1.125707

13 H 2.511413 3.509255 4.245085 4.132740 2.203801

14 H 4.280519 2.219772 2.493785 2.640738 3.499945

15 O 5.369749 3.427608 2.991030 4.513568 3.284849

16 C 3.244047 3.254916 3.587802 4.303133 2.853635

17 C 3.771333 2.848730 3.005526 3.887996 3.147814

18 C 4.445152 3.599525 3.588407 4.685200 2.961464

19 O 5.064076 4.490441 4.471919 5.501475 3.541707

20 C 5.066411 2.954434 2.539433 4.019328 3.384336

21 O 6.087580 3.436514 2.715747 4.337245 4.202187

22 H 2.817927 4.075686 4.571877 5.028820 3.518685

23 H 3.961397 3.542480 3.752528 4.446642 4.052648

11 12 13 14 15

11 H 0.000000

12 H 1.791634 0.000000

13 H 2.518823 2.558535 0.000000

14 H 4.093421 4.278339 4.868923 0.000000

15 O 2.591575 4.285347 4.066051 4.120047 0.000000

16 C 2.851136 3.907261 2.622077 3.613731 2.358159

17 C 3.271890 4.256046 3.689753 2.491812 2.358602

18 C 2.380066 3.942804 2.957688 4.456867 1.412087

19 O 2.764653 4.309004 3.121304 5.619214 2.236916

20 C 3.113554 4.463208 4.425728 2.932374 1.408944

21 O 3.925170 5.189882 5.547473 3.089633 2.235607

22 H 3.641034 4.446656 2.567834 4.309727 3.356577

23 H 4.317833 5.115907 4.473564 2.436056 3.321698

16 17 18 19 20

16 C 0.000000

17 C 1.399473 0.000000

18 C 1.487027 2.324936 0.000000

19 O 2.503608 3.533227 1.220626 0.000000

20 C 2.322817 1.487388 2.278682 3.406311 0.000000

21 O 3.530681 2.500969 3.407819 4.440517 1.220420

22 H 1.091544 2.232815 2.252793 2.930429 3.357626

23 H 2.212928 1.093760 3.318926 4.499572 2.240712

21 22 23

21 O 0.000000

22 H 4.546030 0.000000

23 H 2.927785 2.681534 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.312673 -0.526355 -0.739646

2 6 0 1.422528 -1.291674 0.005605

3 6 0 1.298399 1.393362 0.253409

4 6 0 2.236153 0.852370 -0.611769

5 1 0 2.982968 -0.996711 -1.475663

6 1 0 2.815830 1.495254 -1.292937

7 6 0 1.083204 -0.843425 1.389156

8 1 0 0.174370 -1.377832 1.774117

9 1 0 1.944899 -1.147057 2.048414

10 6 0 0.895311 0.664579 1.490140

11 1 0 -0.171575 0.901869 1.754945

12 1 0 1.513257 1.062818 2.342645

13 1 0 1.095295 2.476215 0.251301

14 1 0 1.318854 -2.365732 -0.209106

15 8 0 -2.070062 -0.075657 0.286460

16 6 0 -0.329456 0.728178 -1.086512

17 6 0 -0.267006 -0.669645 -1.113242

18 6 0 -1.480613 1.102186 -0.222681

19 8 0 -2.005940 2.153203 0.107957

20 6 0 -1.359929 -1.173239 -0.239036

21 8 0 -1.755129 -2.280186 0.089460

22 1 0 0.053151 1.416276 -1.842556

23 1 0 0.054415 -1.262000 -1.974704

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2198839 0.8842846 0.6793463

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.9503974180 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.486112663177E-01 A.U. after 15 cycles

Convg = 0.9394D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.006163511 -0.009937887 0.000682882

2 6 0.008212363 -0.004650981 -0.002104293

3 6 0.006563804 0.005499747 -0.002753462

4 6 -0.013813307 0.003967474 -0.000254184

5 1 0.001136363 0.002258206 0.002385211

6 1 0.000429404 0.001113636 -0.000374957

7 6 -0.001152668 0.001369218 0.001975786

8 1 -0.000173655 0.000499924 0.001253028

9 1 0.001078477 -0.000363875 0.000048171

10 6 0.000295234 0.000161298 0.000064149

11 1 -0.000233976 0.000180190 0.000361523

12 1 -0.000845110 -0.000804160 0.000214096

13 1 0.000575961 0.000652383 0.000851266

14 1 0.002060091 -0.002163499 -0.001794283

15 8 -0.000495985 0.000408894 -0.000482429

16 6 -0.004201928 0.012794953 -0.005984991

17 6 0.001927401 -0.009696051 0.004523673

18 6 0.000140262 0.000515843 0.001241690

19 8 0.000020948 -0.000845955 -0.000565220

20 6 0.003920264 0.000357815 0.000083558

21 8 0.000202695 0.000144221 -0.000528703

22 1 0.001093778 0.000574870 0.001595139

23 1 -0.000576906 -0.002036264 -0.000437649

-------------------------------------------------------------------

Cartesian Forces: Max 0.013813307 RMS 0.003653444

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.012509399 RMS 0.001995254

Search for a saddle point.

Step number 44 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 32 38 40 43 44

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0

Eigenvalues --- -0.07144 -0.00232 0.00211 0.00689 0.00757

Eigenvalues --- 0.00937 0.01122 0.01463 0.02023 0.02179

Eigenvalues --- 0.02569 0.02792 0.02946 0.03116 0.03262

Eigenvalues --- 0.03470 0.03500 0.03641 0.03693 0.03858

Eigenvalues --- 0.04074 0.04172 0.04528 0.04786 0.05993

Eigenvalues --- 0.06294 0.06400 0.06531 0.07332 0.08199

Eigenvalues --- 0.08829 0.09055 0.09913 0.10002 0.10555

Eigenvalues --- 0.12113 0.13860 0.14715 0.17018 0.21747

Eigenvalues --- 0.25987 0.27491 0.28632 0.29763 0.30102

Eigenvalues --- 0.31102 0.31305 0.31775 0.31984 0.32361

Eigenvalues --- 0.32512 0.33171 0.35474 0.37117 0.38940

Eigenvalues --- 0.39698 0.40438 0.43160 0.47239 0.50140

Eigenvalues --- 0.55304 1.08493 1.10869

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D30 D4

1 -0.57467 -0.51092 -0.15410 0.14994 -0.13358

D85 D86 D73 D35 D29

1 0.12947 0.12928 0.12911 -0.12910 0.12487

RFO step: Lambda0=3.989250098D-07 Lambda=-2.90895581D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.05173970 RMS(Int)= 0.00213535

Iteration 2 RMS(Cart)= 0.00240984 RMS(Int)= 0.00055706

Iteration 3 RMS(Cart)= 0.00000274 RMS(Int)= 0.00055705

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00055705

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62765 0.01053 0.00000 -0.00205 -0.00200 2.62565

R2 2.62059 0.01159 0.00000 0.00407 0.00439 2.62498

R3 2.08063 -0.00095 0.00000 0.00126 0.00126 2.08189

R4 2.82214 -0.00146 0.00000 -0.01117 -0.01127 2.81087

R5 2.07908 0.00206 0.00000 0.00432 0.00432 2.08341

R6 4.00571 0.00126 0.00000 0.11415 0.11388 4.11959

R7 2.61888 0.00905 0.00000 0.00035 0.00060 2.61948

R8 2.81760 -0.00023 0.00000 0.00045 0.00053 2.81813

R9 2.08198 0.00042 0.00000 0.00201 0.00201 2.08399

R10 4.17786 -0.00001 0.00000 -0.07033 -0.07023 4.10763

R11 2.08154 -0.00020 0.00000 0.00034 0.00034 2.08188

R12 2.12101 -0.00021 0.00000 0.00375 0.00375 2.12477

R13 2.12905 -0.00019 0.00000 -0.00169 -0.00169 2.12736

R14 2.87808 0.00168 0.00000 -0.00100 -0.00102 2.87706

R15 2.12514 -0.00006 0.00000 -0.00008 -0.00008 2.12506

R16 2.12728 0.00002 0.00000 0.00047 0.00047 2.12775

R17 2.66846 0.00043 0.00000 -0.00094 -0.00108 2.66738

R18 2.66252 0.00079 0.00000 0.00166 0.00145 2.66397

R19 2.64462 0.01251 0.00000 0.00579 0.00573 2.65035

R20 2.81007 -0.00041 0.00000 -0.00015 -0.00004 2.81003

R21 2.06272 0.00009 0.00000 0.00181 0.00181 2.06453

R22 2.81076 0.00358 0.00000 0.00062 0.00063 2.81139

R23 2.06691 0.00113 0.00000 -0.00180 -0.00180 2.06511

R24 2.30665 -0.00068 0.00000 -0.00028 -0.00028 2.30637

R25 2.30626 0.00007 0.00000 0.00019 0.00019 2.30645

A1 2.05156 -0.00103 0.00000 0.01435 0.01259 2.06415

A2 2.10934 0.00110 0.00000 -0.00957 -0.01074 2.09859

A3 2.11760 -0.00016 0.00000 -0.01346 -0.01446 2.10314

A4 2.06779 -0.00077 0.00000 0.03137 0.02976 2.09755

A5 2.08638 0.00107 0.00000 -0.00022 -0.00012 2.08626

A6 1.63668 0.00169 0.00000 -0.01348 -0.01235 1.62433

A7 2.04026 -0.00010 0.00000 -0.01970 -0.01855 2.02171

A8 1.79242 -0.00289 0.00000 -0.05663 -0.05660 1.73582

A9 1.67937 0.00082 0.00000 0.04462 0.04407 1.72344

A10 2.10593 -0.00034 0.00000 -0.00796 -0.00927 2.09666

A11 2.10276 -0.00059 0.00000 0.00737 0.00768 2.11044

A12 1.57321 0.00283 0.00000 0.02211 0.02279 1.59600

A13 2.01768 0.00092 0.00000 -0.00439 -0.00354 2.01414

A14 1.72803 -0.00244 0.00000 0.02286 0.02259 1.75063

A15 1.73029 -0.00051 0.00000 -0.03147 -0.03169 1.69860

A16 2.07489 -0.00233 0.00000 -0.01388 -0.01409 2.06080

A17 2.08771 0.00247 0.00000 0.00493 0.00505 2.09276

A18 2.11102 -0.00021 0.00000 0.00805 0.00817 2.11919

A19 1.93780 -0.00133 0.00000 -0.01271 -0.01171 1.92609

A20 1.86234 -0.00051 0.00000 0.01256 0.01311 1.87545

A21 1.96779 0.00240 0.00000 0.01064 0.00762 1.97541

A22 1.86533 0.00039 0.00000 -0.01101 -0.01134 1.85399

A23 1.92709 -0.00069 0.00000 -0.01168 -0.01078 1.91631

A24 1.89906 -0.00033 0.00000 0.01253 0.01313 1.91219

A25 1.97754 0.00229 0.00000 0.00375 0.00107 1.97861

A26 1.92693 -0.00113 0.00000 -0.00562 -0.00483 1.92210

A27 1.88266 -0.00067 0.00000 -0.00695 -0.00611 1.87655

A28 1.91939 -0.00070 0.00000 0.00201 0.00293 1.92232

A29 1.91004 -0.00064 0.00000 -0.00507 -0.00441 1.90563

A30 1.84192 0.00075 0.00000 0.01231 0.01190 1.85381

A31 1.88064 0.00243 0.00000 0.00024 -0.00017 1.88047

A32 1.85380 -0.00032 0.00000 0.03667 0.03646 1.89025

A33 1.71353 0.00044 0.00000 -0.00323 -0.00328 1.71025

A34 1.54282 0.00041 0.00000 0.01049 0.01074 1.55356

A35 1.87220 -0.00098 0.00000 0.00070 0.00027 1.87247

A36 2.21527 0.00074 0.00000 -0.01164 -0.01204 2.20323

A37 2.11199 0.00002 0.00000 -0.00894 -0.00927 2.10271

A38 1.89503 0.00042 0.00000 -0.04102 -0.04122 1.85382

A39 1.74781 0.00056 0.00000 0.03093 0.03105 1.77885

A40 1.59337 -0.00083 0.00000 -0.03035 -0.02976 1.56361

A41 1.86937 -0.00224 0.00000 -0.00256 -0.00247 1.86690

A42 2.17620 0.00171 0.00000 0.02621 0.02530 2.20150

A43 2.08919 0.00056 0.00000 0.00192 0.00166 2.09085

A44 1.89949 0.00094 0.00000 -0.00016 -0.00015 1.89935

A45 2.02739 -0.00080 0.00000 0.00209 0.00208 2.02947

A46 2.35617 -0.00014 0.00000 -0.00186 -0.00188 2.35429

A47 1.90266 -0.00015 0.00000 0.00113 0.00091 1.90358

A48 2.02971 -0.00040 0.00000 0.00056 0.00055 2.03026

A49 2.35074 0.00056 0.00000 -0.00195 -0.00196 2.34878

D1 -0.65753 0.00134 0.00000 0.08077 0.08170 -0.57583

D2 2.93746 0.00091 0.00000 0.05824 0.05847 2.99593

D3 1.20373 -0.00121 0.00000 0.01439 0.01456 1.21829

D4 2.58656 0.00231 0.00000 0.17628 0.17697 2.76353

D5 -0.10163 0.00188 0.00000 0.15374 0.15374 0.05211

D6 -1.83536 -0.00023 0.00000 0.10989 0.10983 -1.72553

D7 0.01274 -0.00034 0.00000 -0.04493 -0.04477 -0.03203

D8 -2.98209 0.00020 0.00000 -0.03880 -0.03901 -3.02109

D9 3.05132 -0.00123 0.00000 -0.14065 -0.14006 2.91126

D10 0.05649 -0.00069 0.00000 -0.13452 -0.13430 -0.07781

D11 2.88283 -0.00042 0.00000 -0.14746 -0.14792 2.73491

D12 -1.37389 -0.00094 0.00000 -0.16000 -0.16011 -1.53399

D13 0.70993 -0.00028 0.00000 -0.13024 -0.13042 0.57951

D14 -0.70029 0.00031 0.00000 -0.12093 -0.12133 -0.82162

D15 1.32618 -0.00021 0.00000 -0.13348 -0.13352 1.19267

D16 -2.87318 0.00044 0.00000 -0.10371 -0.10383 -2.97702

D17 1.11169 -0.00043 0.00000 -0.10818 -0.10788 1.00382

D18 3.13817 -0.00095 0.00000 -0.12072 -0.12006 3.01811

D19 -1.06120 -0.00030 0.00000 -0.09096 -0.09038 -1.15158

D20 -0.97354 -0.00076 0.00000 0.00900 0.00810 -0.96544

D21 -2.92914 0.00132 0.00000 0.01187 0.01176 -2.91738

D22 1.25095 0.00086 0.00000 0.01254 0.01308 1.26403

D23 1.12626 -0.00167 0.00000 0.02599 0.02514 1.15140

D24 -0.82934 0.00042 0.00000 0.02886 0.02880 -0.80054

D25 -2.93244 -0.00004 0.00000 0.02953 0.03012 -2.90232

D26 -3.07283 -0.00224 0.00000 0.00520 0.00408 -3.06875

D27 1.25475 -0.00015 0.00000 0.00807 0.00774 1.26250

D28 -0.84834 -0.00061 0.00000 0.00874 0.00907 -0.83927

D29 0.55320 -0.00043 0.00000 0.05520 0.05473 0.60793

D30 -2.73719 -0.00075 0.00000 0.04868 0.04857 -2.68862

D31 -2.95970 -0.00028 0.00000 0.03866 0.03823 -2.92148

D32 0.03310 -0.00059 0.00000 0.03214 0.03207 0.06516

D33 -1.20211 0.00075 0.00000 0.01606 0.01590 -1.18622

D34 1.79068 0.00044 0.00000 0.00955 0.00973 1.80042

D35 -0.44484 -0.00107 0.00000 -0.10566 -0.10560 -0.55043

D36 -2.60648 -0.00097 0.00000 -0.10674 -0.10652 -2.71300

D37 1.67230 -0.00089 0.00000 -0.11453 -0.11472 1.55758

D38 3.05086 -0.00093 0.00000 -0.09234 -0.09235 2.95851

D39 0.88922 -0.00082 0.00000 -0.09342 -0.09327 0.79595

D40 -1.11519 -0.00074 0.00000 -0.10121 -0.10147 -1.21666

D41 1.22294 0.00071 0.00000 -0.06727 -0.06704 1.15590

D42 -0.93870 0.00081 0.00000 -0.06836 -0.06797 -1.00667

D43 -2.94310 0.00089 0.00000 -0.07615 -0.07617 -3.01927

D44 1.10333 0.00104 0.00000 0.00903 0.00949 1.11281

D45 3.03610 0.00006 0.00000 0.01827 0.01841 3.05451

D46 -1.13337 0.00017 0.00000 0.01063 0.01046 -1.12291

D47 -1.01047 0.00110 0.00000 0.01075 0.01156 -0.99891

D48 0.92231 0.00012 0.00000 0.01999 0.02048 0.94279

D49 3.03602 0.00023 0.00000 0.01235 0.01254 3.04855

D50 -3.06906 0.00093 0.00000 0.01759 0.01805 -3.05102

D51 -1.13629 -0.00005 0.00000 0.02683 0.02697 -1.10932

D52 0.97742 0.00006 0.00000 0.01919 0.01902 0.99645

D53 -0.16033 0.00001 0.00000 0.13237 0.13241 -0.02792

D54 2.00542 -0.00034 0.00000 0.12928 0.12910 2.13453

D55 -2.26201 -0.00020 0.00000 0.14233 0.14257 -2.11943

D56 -2.33909 0.00051 0.00000 0.15015 0.15040 -2.18869

D57 -0.17333 0.00016 0.00000 0.14706 0.14709 -0.02624

D58 1.84242 0.00030 0.00000 0.16011 0.16056 2.00298

D59 1.90208 0.00062 0.00000 0.16275 0.16262 2.06469

D60 -2.21535 0.00027 0.00000 0.15966 0.15931 -2.05604

D61 -0.19960 0.00041 0.00000 0.17271 0.17278 -0.02682

D62 -0.02064 -0.00015 0.00000 -0.04059 -0.04054 -0.06118

D63 3.10603 0.00016 0.00000 -0.03688 -0.03676 3.06928

D64 0.00620 0.00014 0.00000 0.04005 0.04003 0.04623

D65 -3.12446 -0.00027 0.00000 0.05986 0.05992 -3.06454

D66 -0.07763 0.00027 0.00000 -0.00635 -0.00646 -0.08409

D67 1.79557 0.00008 0.00000 0.01019 0.01015 1.80572

D68 -1.91308 0.00011 0.00000 0.05309 0.05368 -1.85940

D69 -1.89651 0.00027 0.00000 -0.01748 -0.01754 -1.91405

D70 -0.02331 0.00009 0.00000 -0.00094 -0.00093 -0.02424

D71 2.55123 0.00011 0.00000 0.04196 0.04259 2.59382

D72 1.67630 0.00088 0.00000 0.03249 0.03214 1.70844

D73 -2.73369 0.00069 0.00000 0.04902 0.04875 -2.68494

D74 -0.15915 0.00072 0.00000 0.09193 0.09227 -0.06688

D75 -1.88987 0.00045 0.00000 -0.01290 -0.01262 -1.90250

D76 1.27066 0.00006 0.00000 -0.01767 -0.01747 1.25319

D77 0.02795 0.00001 0.00000 0.02566 0.02562 0.05357

D78 -3.09470 -0.00038 0.00000 0.02089 0.02078 -3.07393

D79 2.76908 -0.00032 0.00000 -0.02174 -0.02165 2.74743

D80 -0.35357 -0.00070 0.00000 -0.02651 -0.02649 -0.38006

D81 1.98680 -0.00019 0.00000 -0.05720 -0.05746 1.92935

D82 -1.16858 0.00030 0.00000 -0.08215 -0.08246 -1.25103

D83 0.01137 -0.00015 0.00000 -0.02413 -0.02410 -0.01272

D84 3.13918 0.00034 0.00000 -0.04909 -0.04910 3.09008

D85 -2.59679 -0.00069 0.00000 -0.07398 -0.07358 -2.67038

D86 0.53101 -0.00019 0.00000 -0.09894 -0.09858 0.43243

Item Value Threshold Converged?

Maximum Force 0.012509 0.000450 NO

RMS Force 0.001995 0.000300 NO

Maximum Displacement 0.270635 0.001800 NO

RMS Displacement 0.051561 0.001200 NO

Predicted change in Energy=-2.398632D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.156842 1.593449 0.451959

2 6 0 0.150709 1.273749 0.107532

3 6 0 -0.726815 3.778560 -0.386951

4 6 0 -1.614068 2.876425 0.179094

5 1 0 -1.744234 0.914512 1.090499

6 1 0 -2.604328 3.195320 0.541587

7 6 0 0.779152 1.887392 -1.092886

8 1 0 1.899412 1.874595 -0.997606

9 1 0 0.531022 1.233862 -1.975297

10 6 0 0.300569 3.307795 -1.359988

11 1 0 1.174754 4.015065 -1.372251

12 1 0 -0.157918 3.356743 -2.387201

13 1 0 -0.965383 4.854207 -0.434233

14 1 0 0.579927 0.312973 0.436426

15 8 0 2.726657 3.914051 0.789900

16 6 0 0.459861 3.837714 1.433248

17 6 0 0.995841 2.560146 1.651328

18 6 0 1.563041 4.700140 0.932846

19 8 0 1.670896 5.881947 0.647782

20 6 0 2.428378 2.616734 1.253889

21 8 0 3.356186 1.824127 1.278689

22 1 0 -0.394492 4.277030 1.953484

23 1 0 0.671275 1.846468 2.412608

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.389434 0.000000

3 C 2.379790 2.699748 0.000000

4 C 1.389077 2.384979 1.386171 0.000000

5 H 1.101689 2.164736 3.379463 2.167188 0.000000

6 H 2.160842 3.386896 2.174259 1.101685 2.498630

7 C 2.494198 1.487448 2.518492 2.885068 3.475794

8 H 3.394256 2.154138 3.300766 3.838336 4.307912

9 H 2.978214 2.117642 3.252766 3.455549 3.831172

10 C 2.888975 2.512651 1.491288 2.494130 3.989224

11 H 3.824697 3.279213 2.154696 3.388318 4.919254

12 H 3.488249 3.264630 2.121927 2.989473 4.535999

13 H 3.384455 3.789307 1.102800 2.169928 4.295651

14 H 2.157829 1.102493 3.794182 3.383950 2.488249

15 O 4.536624 3.751310 3.651001 4.504625 5.392259

16 C 2.934856 2.902932 2.173666 2.607328 3.677040

17 C 2.647080 2.179993 2.933711 3.013160 3.245097

18 C 4.156987 3.796838 2.799038 3.740067 5.029304

19 O 5.140590 4.882451 3.353197 4.477033 6.044380

20 C 3.813661 2.881930 3.741316 4.190942 4.509429

21 O 4.593922 3.456821 4.823388 5.198064 5.184313

22 H 3.168179 3.567138 2.415894 2.568564 3.724658

23 H 2.692615 2.431536 3.677658 3.357408 2.907094

6 7 8 9 10

6 H 0.000000

7 C 3.978708 0.000000

8 H 4.939342 1.124378 0.000000

9 H 4.473527 1.125752 1.799697 0.000000

10 C 3.473768 1.522475 2.177540 2.175525 0.000000

11 H 4.314651 2.182096 2.290655 2.917729 1.124536

12 H 3.819525 2.170794 2.891426 2.269565 1.125954

13 H 2.527898 3.504172 4.171634 4.209633 2.202510

14 H 4.296331 2.203923 2.497229 2.582021 3.503441

15 O 5.384945 3.383047 2.835294 4.432893 3.297798

16 C 3.255300 3.207345 3.440232 4.289905 2.847518

17 C 3.820496 2.833772 2.881540 3.889408 3.179687

18 C 4.447980 3.553819 3.438531 4.640844 2.964717

19 O 5.050424 4.447652 4.338017 5.457522 3.540508

20 C 5.115689 2.959602 2.428952 3.992485 3.440566

21 O 6.160456 3.502782 2.703009 4.349527 4.301243

22 H 2.836710 4.045761 4.443267 5.054974 3.521594

23 H 4.006207 3.507392 3.624731 4.432681 4.062681

11 12 13 14 15

11 H 0.000000

12 H 1.799868 0.000000

13 H 2.482786 2.590074 0.000000

14 H 4.163006 4.216849 4.875329 0.000000

15 O 2.663364 4.327278 4.001694 4.207274 0.000000

16 C 2.900578 3.899848 2.559700 3.664951 2.357560

17 C 3.360183 4.274979 3.668608 2.588196 2.360263

18 C 2.435891 3.973553 2.878466 4.523293 1.411514

19 O 2.794985 4.351131 3.029352 5.678764 2.237732

20 C 3.228547 4.527039 4.401552 3.064691 1.409711

21 O 4.072634 5.304394 5.549005 3.271178 2.236740

22 H 3.686688 4.443471 2.521952 4.354848 3.350709

23 H 4.391066 5.099672 4.453049 2.503047 3.336567

16 17 18 19 20

16 C 0.000000

17 C 1.402503 0.000000

18 C 1.487006 2.327554 0.000000

19 O 2.502489 3.535134 1.220476 0.000000

20 C 2.323365 1.487724 2.278696 3.406283 0.000000

21 O 3.530882 2.500362 3.406821 4.438936 1.220520

22 H 1.092502 2.229802 2.247811 2.923430 3.348822

23 H 2.229104 1.092807 3.335924 4.516519 2.241284

21 22 23

21 O 0.000000

22 H 4.532071 0.000000

23 H 2.914622 2.693378 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.314117 -0.599713 -0.727277

2 6 0 1.432476 -1.340899 0.049819

3 6 0 1.330129 1.351894 0.214209

4 6 0 2.274594 0.785206 -0.627409

5 1 0 2.888197 -1.086148 -1.531971

6 1 0 2.878820 1.402678 -1.311038

7 6 0 1.028954 -0.851939 1.395400

8 1 0 0.043452 -1.302206 1.695853

9 1 0 1.787457 -1.233252 2.134718

10 6 0 0.950353 0.665993 1.482771

11 1 0 -0.080922 0.982689 1.800191

12 1 0 1.651468 1.027154 2.286372

13 1 0 1.114967 2.432900 0.178167

14 1 0 1.347896 -2.428237 -0.111530

15 8 0 -2.060523 0.001510 0.312920

16 6 0 -0.291990 0.703266 -1.079171

17 6 0 -0.304672 -0.699022 -1.100261

18 6 0 -1.426447 1.142552 -0.224056

19 8 0 -1.905560 2.222063 0.083627

20 6 0 -1.428613 -1.136138 -0.229050

21 8 0 -1.911471 -2.216844 0.068594

22 1 0 0.096715 1.357427 -1.863098

23 1 0 0.018983 -1.334030 -1.928656

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2204633 0.8765030 0.6737560

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4075309129 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.495312424303E-01 A.U. after 15 cycles

Convg = 0.6722D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001577651 -0.010736319 0.004705962

2 6 0.001972995 -0.006289937 -0.001270015

3 6 0.002820105 0.005986496 -0.006827013

4 6 -0.010693589 0.005253730 0.000320986

5 1 -0.000710378 0.000065613 -0.002014986

6 1 0.001508576 0.001270749 0.000554641

7 6 0.001209896 0.001690064 -0.000251913

8 1 -0.000117860 -0.000310042 0.000186800

9 1 -0.000332621 0.000327212 -0.000236738

10 6 0.000122146 -0.000044811 0.000674210

11 1 -0.000079104 -0.000386461 0.000248114

12 1 -0.000329602 0.000067581 0.000265090

13 1 -0.000745519 -0.000115572 -0.000210786

14 1 0.001811503 0.000768289 0.000949620

15 8 -0.000114764 0.000859073 0.000917038

16 6 -0.000427577 0.006532371 0.002874799

17 6 0.000142712 -0.003127152 0.002123309

18 6 0.001380876 -0.000159902 -0.001540552

19 8 0.000061113 -0.000901098 -0.000562230

20 6 0.001853357 -0.000474494 0.000821378

21 8 -0.000197746 0.000330038 -0.001555336

22 1 0.000338159 0.000401703 0.000986832

23 1 -0.001050329 -0.001007131 -0.001159211

-------------------------------------------------------------------

Cartesian Forces: Max 0.010736319 RMS 0.002748722

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011789136 RMS 0.001447037

Search for a saddle point.

Step number 45 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 27 33 37 38 40

41 44 45

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0

Eigenvalues --- -0.07112 0.00139 0.00339 0.00757 0.00836

Eigenvalues --- 0.00968 0.01089 0.01482 0.01991 0.02234

Eigenvalues --- 0.02573 0.02791 0.03036 0.03106 0.03232

Eigenvalues --- 0.03460 0.03529 0.03636 0.03716 0.03851

Eigenvalues --- 0.04121 0.04176 0.04503 0.04822 0.05996

Eigenvalues --- 0.06322 0.06380 0.06638 0.07341 0.08306

Eigenvalues --- 0.08827 0.09121 0.09894 0.10001 0.10453

Eigenvalues --- 0.12111 0.13844 0.14628 0.17018 0.21814

Eigenvalues --- 0.26010 0.27513 0.28680 0.29854 0.30173

Eigenvalues --- 0.31108 0.31302 0.31776 0.31984 0.32383

Eigenvalues --- 0.32531 0.33191 0.35533 0.37138 0.38961

Eigenvalues --- 0.39700 0.40438 0.43414 0.47524 0.50219

Eigenvalues --- 0.56104 1.08498 1.10871

Eigenvectors required to have negative eigenvalues:

R6 R10 D4 D71 D30

1 0.57858 0.50981 0.15070 0.14547 -0.14008

D73 D1 D86 D35 R19

1 -0.13843 0.13319 -0.12915 0.12856 -0.12554

RFO step: Lambda0=1.148615252D-04 Lambda=-1.78277611D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.02920895 RMS(Int)= 0.00043462

Iteration 2 RMS(Cart)= 0.00054590 RMS(Int)= 0.00012293

Iteration 3 RMS(Cart)= 0.00000015 RMS(Int)= 0.00012293

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62565 0.00398 0.00000 0.01217 0.01203 2.63768

R2 2.62498 0.01179 0.00000 0.01871 0.01856 2.64353

R3 2.08189 -0.00083 0.00000 -0.00431 -0.00431 2.07758

R4 2.81087 0.00178 0.00000 0.00696 0.00704 2.81791

R5 2.08341 0.00032 0.00000 -0.00035 -0.00035 2.08306

R6 4.11959 0.00117 0.00000 -0.02986 -0.02990 4.08969

R7 2.61948 0.00654 0.00000 0.01990 0.01990 2.63938

R8 2.81813 -0.00012 0.00000 -0.00325 -0.00323 2.81490

R9 2.08399 0.00006 0.00000 -0.00100 -0.00100 2.08299

R10 4.10763 0.00375 0.00000 0.00677 0.00682 4.11445

R11 2.08188 -0.00081 0.00000 -0.00456 -0.00456 2.07733

R12 2.12477 -0.00010 0.00000 -0.00062 -0.00062 2.12414

R13 2.12736 0.00007 0.00000 0.00033 0.00033 2.12769

R14 2.87706 0.00159 0.00000 -0.00067 -0.00054 2.87652

R15 2.12506 -0.00031 0.00000 -0.00078 -0.00078 2.12429

R16 2.12775 -0.00010 0.00000 0.00056 0.00056 2.12830

R17 2.66738 -0.00063 0.00000 -0.00336 -0.00335 2.66403

R18 2.66397 0.00028 0.00000 0.00019 0.00024 2.66421

R19 2.65035 0.00618 0.00000 0.01881 0.01879 2.66914

R20 2.81003 0.00099 0.00000 0.00133 0.00129 2.81132

R21 2.06453 0.00037 0.00000 -0.00099 -0.00099 2.06354

R22 2.81139 0.00194 0.00000 0.00250 0.00252 2.81391

R23 2.06511 0.00016 0.00000 0.00021 0.00021 2.06532

R24 2.30637 -0.00074 0.00000 0.00002 0.00002 2.30638

R25 2.30645 -0.00040 0.00000 -0.00008 -0.00008 2.30637

A1 2.06415 -0.00090 0.00000 -0.00244 -0.00263 2.06152

A2 2.09859 0.00100 0.00000 0.00848 0.00846 2.10705

A3 2.10314 -0.00005 0.00000 -0.00196 -0.00201 2.10113

A4 2.09755 -0.00040 0.00000 -0.00952 -0.00952 2.08803

A5 2.08626 0.00009 0.00000 0.00926 0.00922 2.09548

A6 1.62433 0.00115 0.00000 0.00548 0.00547 1.62980

A7 2.02171 0.00061 0.00000 0.00463 0.00465 2.02636

A8 1.73582 -0.00202 0.00000 0.00263 0.00247 1.73829

A9 1.72344 0.00010 0.00000 -0.01901 -0.01883 1.70461

A10 2.09666 -0.00047 0.00000 -0.00598 -0.00597 2.09069

A11 2.11044 -0.00020 0.00000 -0.00690 -0.00707 2.10337

A12 1.59600 0.00099 0.00000 0.01276 0.01282 1.60882

A13 2.01414 0.00071 0.00000 0.00792 0.00798 2.02213

A14 1.75063 -0.00160 0.00000 -0.00445 -0.00464 1.74599

A15 1.69860 0.00043 0.00000 0.00403 0.00419 1.70279

A16 2.06080 -0.00151 0.00000 -0.00147 -0.00149 2.05931

A17 2.09276 0.00200 0.00000 0.01225 0.01216 2.10492

A18 2.11919 -0.00053 0.00000 -0.01288 -0.01290 2.10629

A19 1.92609 -0.00056 0.00000 -0.00356 -0.00349 1.92260

A20 1.87545 -0.00042 0.00000 0.00136 0.00135 1.87681

A21 1.97541 0.00155 0.00000 0.00328 0.00319 1.97860

A22 1.85399 0.00033 0.00000 0.00072 0.00071 1.85470

A23 1.91631 -0.00054 0.00000 0.00247 0.00245 1.91875

A24 1.91219 -0.00043 0.00000 -0.00452 -0.00443 1.90776

A25 1.97861 0.00191 0.00000 0.00580 0.00566 1.98427

A26 1.92210 -0.00066 0.00000 0.00110 0.00111 1.92321

A27 1.87655 -0.00067 0.00000 -0.00509 -0.00501 1.87154

A28 1.92232 -0.00086 0.00000 -0.00307 -0.00302 1.91930

A29 1.90563 -0.00024 0.00000 -0.00094 -0.00090 1.90473

A30 1.85381 0.00044 0.00000 0.00191 0.00188 1.85570

A31 1.88047 0.00119 0.00000 0.00344 0.00321 1.88368

A32 1.89025 -0.00075 0.00000 -0.01829 -0.01853 1.87172

A33 1.71025 -0.00042 0.00000 0.01158 0.01182 1.72208

A34 1.55356 0.00073 0.00000 0.01679 0.01670 1.57026

A35 1.87247 -0.00063 0.00000 -0.00418 -0.00442 1.86805

A36 2.20323 0.00044 0.00000 -0.00602 -0.00570 2.19753

A37 2.10271 0.00038 0.00000 0.00557 0.00542 2.10813

A38 1.85382 0.00163 0.00000 0.02361 0.02334 1.87715

A39 1.77885 -0.00059 0.00000 -0.02382 -0.02371 1.75514

A40 1.56361 -0.00120 0.00000 -0.00484 -0.00468 1.55893

A41 1.86690 -0.00139 0.00000 -0.00193 -0.00188 1.86502

A42 2.20150 0.00103 0.00000 -0.00109 -0.00100 2.20050

A43 2.09085 0.00053 0.00000 0.00506 0.00493 2.09578

A44 1.89935 0.00054 0.00000 0.00447 0.00421 1.90356

A45 2.02947 -0.00064 0.00000 -0.00390 -0.00379 2.02568

A46 2.35429 0.00010 0.00000 -0.00047 -0.00035 2.35394

A47 1.90358 0.00033 0.00000 0.00098 0.00071 1.90428

A48 2.03026 -0.00098 0.00000 -0.00573 -0.00577 2.02449

A49 2.34878 0.00066 0.00000 0.00565 0.00561 2.35439

D1 -0.57583 0.00066 0.00000 -0.02695 -0.02692 -0.60276

D2 2.99593 -0.00028 0.00000 -0.03958 -0.03964 2.95629

D3 1.21829 -0.00108 0.00000 -0.02232 -0.02255 1.19574

D4 2.76353 0.00035 0.00000 -0.04973 -0.04966 2.71388

D5 0.05211 -0.00059 0.00000 -0.06236 -0.06238 -0.01027

D6 -1.72553 -0.00140 0.00000 -0.04510 -0.04528 -1.77081

D7 -0.03203 0.00025 0.00000 0.02823 0.02824 -0.00378

D8 -3.02109 0.00059 0.00000 0.04461 0.04487 -2.97623

D9 2.91126 0.00069 0.00000 0.05230 0.05213 2.96339

D10 -0.07781 0.00103 0.00000 0.06869 0.06875 -0.00906

D11 2.73491 0.00016 0.00000 0.01174 0.01169 2.74660

D12 -1.53399 0.00002 0.00000 0.01149 0.01146 -1.52254

D13 0.57951 0.00016 0.00000 0.00881 0.00882 0.58833

D14 -0.82162 0.00095 0.00000 0.02518 0.02518 -0.79644

D15 1.19267 0.00081 0.00000 0.02493 0.02495 1.21762

D16 -2.97702 0.00095 0.00000 0.02226 0.02232 -2.95470

D17 1.00382 0.00014 0.00000 0.00612 0.00623 1.01005

D18 3.01811 0.00000 0.00000 0.00587 0.00600 3.02410

D19 -1.15158 0.00014 0.00000 0.00320 0.00337 -1.14821

D20 -0.96544 -0.00106 0.00000 -0.03106 -0.03132 -0.99676

D21 -2.91738 0.00014 0.00000 -0.02759 -0.02745 -2.94483

D22 1.26403 -0.00005 0.00000 -0.02887 -0.02894 1.23509

D23 1.15140 -0.00154 0.00000 -0.03917 -0.03943 1.11196

D24 -0.80054 -0.00034 0.00000 -0.03569 -0.03556 -0.83610

D25 -2.90232 -0.00053 0.00000 -0.03697 -0.03705 -2.93937

D26 -3.06875 -0.00140 0.00000 -0.03878 -0.03899 -3.10774

D27 1.26250 -0.00020 0.00000 -0.03530 -0.03511 1.22738

D28 -0.83927 -0.00039 0.00000 -0.03658 -0.03661 -0.87588

D29 0.60793 -0.00077 0.00000 -0.00945 -0.00946 0.59847

D30 -2.68862 -0.00088 0.00000 -0.02377 -0.02380 -2.71241

D31 -2.92148 -0.00051 0.00000 -0.02264 -0.02250 -2.94398

D32 0.06516 -0.00062 0.00000 -0.03696 -0.03683 0.02833

D33 -1.18622 0.00058 0.00000 -0.01098 -0.01075 -1.19697

D34 1.80042 0.00047 0.00000 -0.02530 -0.02508 1.77533

D35 -0.55043 -0.00026 0.00000 -0.01155 -0.01154 -0.56198

D36 -2.71300 -0.00003 0.00000 -0.01261 -0.01259 -2.72559

D37 1.55758 0.00016 0.00000 -0.01263 -0.01262 1.54496

D38 2.95851 -0.00033 0.00000 0.00391 0.00396 2.96247

D39 0.79595 -0.00010 0.00000 0.00285 0.00291 0.79886

D40 -1.21666 0.00009 0.00000 0.00284 0.00288 -1.21378

D41 1.15590 -0.00019 0.00000 -0.00071 -0.00075 1.15515

D42 -1.00667 0.00005 0.00000 -0.00177 -0.00180 -1.00846

D43 -3.01927 0.00024 0.00000 -0.00179 -0.00183 -3.02110

D44 1.11281 0.00040 0.00000 -0.03596 -0.03567 1.07715

D45 3.05451 -0.00067 0.00000 -0.04088 -0.04095 3.01356

D46 -1.12291 -0.00020 0.00000 -0.03195 -0.03178 -1.15468

D47 -0.99891 0.00089 0.00000 -0.03211 -0.03179 -1.03070

D48 0.94279 -0.00018 0.00000 -0.03703 -0.03707 0.90572

D49 3.04855 0.00029 0.00000 -0.02809 -0.02790 3.02065

D50 -3.05102 0.00041 0.00000 -0.04041 -0.04015 -3.09116

D51 -1.10932 -0.00066 0.00000 -0.04533 -0.04542 -1.15475

D52 0.99645 -0.00019 0.00000 -0.03639 -0.03626 0.96019

D53 -0.02792 0.00020 0.00000 0.01021 0.01027 -0.01765

D54 2.13453 0.00008 0.00000 0.01355 0.01356 2.14808

D55 -2.11943 -0.00002 0.00000 0.01355 0.01359 -2.10584

D56 -2.18869 0.00022 0.00000 0.01062 0.01068 -2.17801

D57 -0.02624 0.00010 0.00000 0.01396 0.01396 -0.01228

D58 2.00298 0.00000 0.00000 0.01396 0.01400 2.01698

D59 2.06469 0.00038 0.00000 0.01094 0.01098 2.07568

D60 -2.05604 0.00026 0.00000 0.01427 0.01427 -2.04178

D61 -0.02682 0.00016 0.00000 0.01428 0.01430 -0.01252

D62 -0.06118 0.00046 0.00000 0.04207 0.04226 -0.01891

D63 3.06928 0.00058 0.00000 0.05023 0.05043 3.11971

D64 0.04623 -0.00020 0.00000 -0.03195 -0.03201 0.01421

D65 -3.06454 -0.00068 0.00000 -0.05660 -0.05657 -3.12111

D66 -0.08409 -0.00002 0.00000 0.03824 0.03843 -0.04565

D67 1.80572 -0.00057 0.00000 0.02058 0.02070 1.82642

D68 -1.85940 -0.00022 0.00000 0.02607 0.02617 -1.83323

D69 -1.91405 0.00103 0.00000 0.03442 0.03447 -1.87958

D70 -0.02424 0.00048 0.00000 0.01676 0.01673 -0.00751

D71 2.59382 0.00083 0.00000 0.02224 0.02220 2.61603

D72 1.70844 0.00057 0.00000 0.04257 0.04267 1.75111

D73 -2.68494 0.00002 0.00000 0.02491 0.02493 -2.66001

D74 -0.06688 0.00037 0.00000 0.03039 0.03041 -0.03647

D75 -1.90250 0.00052 0.00000 -0.02056 -0.02033 -1.92283

D76 1.25319 0.00038 0.00000 -0.03088 -0.03066 1.22253

D77 0.05357 -0.00063 0.00000 -0.03699 -0.03703 0.01654

D78 -3.07393 -0.00077 0.00000 -0.04731 -0.04736 -3.12129

D79 2.74743 -0.00015 0.00000 -0.04819 -0.04820 2.69924

D80 -0.38006 -0.00030 0.00000 -0.05851 -0.05853 -0.43859

D81 1.92935 0.00092 0.00000 0.02447 0.02423 1.95358

D82 -1.25103 0.00148 0.00000 0.05518 0.05506 -1.19597

D83 -0.01272 -0.00015 0.00000 0.00889 0.00888 -0.00384

D84 3.09008 0.00041 0.00000 0.03960 0.03971 3.12979

D85 -2.67038 -0.00070 0.00000 0.00584 0.00575 -2.66462

D86 0.43243 -0.00015 0.00000 0.03655 0.03658 0.46901

Item Value Threshold Converged?

Maximum Force 0.011789 0.000450 NO

RMS Force 0.001447 0.000300 NO

Maximum Displacement 0.123248 0.001800 NO

RMS Displacement 0.029166 0.001200 NO

Predicted change in Energy=-9.139658D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.152076 1.569509 0.443775

2 6 0 0.172411 1.275675 0.115663

3 6 0 -0.739511 3.781319 -0.380427

4 6 0 -1.624160 2.860890 0.186123

5 1 0 -1.753126 0.865788 1.037250

6 1 0 -2.603628 3.184798 0.565767

7 6 0 0.791822 1.906191 -1.085327

8 1 0 1.911475 1.911213 -0.986151

9 1 0 0.556608 1.252188 -1.971140

10 6 0 0.288199 3.317349 -1.353769

11 1 0 1.152694 4.035514 -1.377123

12 1 0 -0.181027 3.353430 -2.376982

13 1 0 -1.000881 4.850981 -0.430521

14 1 0 0.630714 0.334102 0.459871

15 8 0 2.742730 3.889408 0.815316

16 6 0 0.464523 3.865100 1.431702

17 6 0 0.974913 2.567266 1.655603

18 6 0 1.588382 4.692336 0.916107

19 8 0 1.716149 5.859388 0.582562

20 6 0 2.412014 2.595377 1.266708

21 8 0 3.319529 1.779310 1.262858

22 1 0 -0.370102 4.325755 1.964257

23 1 0 0.625949 1.860120 2.412334

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.395801 0.000000

3 C 2.396169 2.712187 0.000000

4 C 1.398897 2.396985 1.396700 0.000000

5 H 1.099408 2.173712 3.396697 2.172898 0.000000

6 H 2.175096 3.399078 2.173948 1.099274 2.514649

7 C 2.496046 1.491173 2.521502 2.892232 3.473404

8 H 3.398057 2.154587 3.300292 3.844063 4.314669

9 H 2.975249 2.122006 3.256808 3.463734 3.812426

10 C 2.891454 2.518149 1.489581 2.497346 3.986745

11 H 3.835208 3.287260 2.153708 3.396233 4.931547

12 H 3.475915 3.264240 2.116891 2.982405 4.507421

13 H 3.399311 3.802334 1.102270 2.174669 4.313003

14 H 2.169062 1.102307 3.803541 3.397654 2.509731

15 O 4.548570 3.731977 3.683407 4.530282 5.422569

16 C 2.976430 2.919317 2.177276 2.631064 3.750925

17 C 2.643508 2.164170 2.925508 3.000128 3.274078

18 C 4.181538 3.784080 2.816033 3.769283 5.081617

19 O 5.162271 4.859171 3.357973 4.506197 6.097431

20 C 3.798995 2.842945 3.748549 4.186748 4.515808

21 O 4.550843 3.387338 4.815001 5.173899 5.159191

22 H 3.243493 3.607576 2.435244 2.623023 3.839723

23 H 2.668531 2.412876 3.654450 3.319721 2.922251

6 7 8 9 10

6 H 0.000000

7 C 3.986230 0.000000

8 H 4.941317 1.124048 0.000000

9 H 4.489763 1.125927 1.800051 0.000000

10 C 3.473450 1.522191 2.178850 2.172115 0.000000

11 H 4.313756 2.179310 2.289381 2.907762 1.124125

12 H 3.815391 2.170095 2.897062 2.263633 1.126250

13 H 2.517450 3.509180 4.175258 4.213145 2.205933

14 H 4.312615 2.210216 2.493713 2.599652 3.508044

15 O 5.398360 3.369219 2.801700 4.415699 3.325192

16 C 3.259786 3.206226 3.428900 4.291285 2.844288

17 C 3.791444 2.825463 2.878613 3.880422 3.176559

18 C 4.468597 3.521768 3.384911 4.608186 2.955234

19 O 5.080766 4.389078 4.252893 5.393721 3.500055

20 C 5.098568 2.938038 2.407071 3.966150 3.449454

21 O 6.127407 3.452445 2.656700 4.286063 4.289670

22 H 2.871619 4.062551 4.443030 5.078677 3.529808

23 H 3.949019 3.501895 3.633853 4.425973 4.052299

11 12 13 14 15

11 H 0.000000

12 H 1.801046 0.000000

13 H 2.489765 2.589118 0.000000

14 H 4.165029 4.221730 4.884373 0.000000

15 O 2.712259 4.361926 4.060955 4.150560 0.000000

16 C 2.896916 3.896745 2.566563 3.666063 2.360243

17 C 3.374135 4.268021 3.670290 2.556417 2.362058

18 C 2.424901 3.970884 2.922817 4.485475 1.409741

19 O 2.735757 4.317176 3.070093 5.632229 2.233576

20 C 3.263392 4.535965 4.429016 2.989545 1.409838

21 O 4.093304 5.289630 5.564947 3.156444 2.232825

22 H 3.683472 4.452811 2.531542 4.381564 3.346668

23 H 4.401112 5.081214 4.435499 2.478077 3.339048

16 17 18 19 20

16 C 0.000000

17 C 1.412446 0.000000

18 C 1.487689 2.332193 0.000000

19 O 2.502956 3.541034 1.220486 0.000000

20 C 2.330695 1.489056 2.280028 3.406766 0.000000

21 O 3.539786 2.504465 3.406293 4.436290 1.220477

22 H 1.091979 2.235312 2.251369 2.934886 3.349769

23 H 2.237776 1.092919 3.344611 4.531087 2.245683

21 22 23

21 O 0.000000

22 H 4.537590 0.000000

23 H 2.929710 2.696711 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.324760 -0.632397 -0.690988

2 6 0 1.405075 -1.343601 0.081429

3 6 0 1.336620 1.365614 0.188305

4 6 0 2.291891 0.764985 -0.634782

5 1 0 2.940326 -1.144322 -1.444453

6 1 0 2.886416 1.367418 -1.336221

7 6 0 0.992481 -0.811961 1.412114

8 1 0 -0.004272 -1.239201 1.707801

9 1 0 1.734133 -1.186678 2.171884

10 6 0 0.941938 0.708454 1.465497

11 1 0 -0.083893 1.047789 1.775627

12 1 0 1.650220 1.073628 2.261377

13 1 0 1.146882 2.449685 0.126746

14 1 0 1.282097 -2.428988 -0.066535

15 8 0 -2.077111 -0.015149 0.274429

16 6 0 -0.298285 0.715281 -1.094146

17 6 0 -0.285278 -0.697061 -1.105299

18 6 0 -1.437862 1.133762 -0.234230

19 8 0 -1.913424 2.205852 0.103482

20 6 0 -1.412484 -1.146111 -0.242138

21 8 0 -1.864180 -2.230144 0.090139

22 1 0 0.068886 1.365450 -1.890941

23 1 0 0.063787 -1.331050 -1.924253

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2196274 0.8796814 0.6747347

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4305664250 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.503256442656E-01 A.U. after 15 cycles

Convg = 0.2934D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000218471 0.002939397 -0.000430256

2 6 -0.001051760 0.000461249 -0.000682414

3 6 -0.001327353 -0.002039870 0.001827206

4 6 0.003051912 -0.000896289 -0.000751965

5 1 -0.000135480 -0.000007930 -0.000306396

6 1 0.000065984 -0.000261621 0.000087598

7 6 -0.000319788 -0.000065759 0.001391383

8 1 0.000013707 -0.000163071 -0.000180378

9 1 -0.000251516 0.000059619 0.000173192

10 6 -0.000223338 -0.000017530 -0.000178955

11 1 -0.000007133 0.000025740 0.000050365

12 1 0.000081943 0.000008350 -0.000030955

13 1 -0.000071689 -0.000127744 0.000057446

14 1 0.000517338 0.000230702 -0.000294560

15 8 -0.000416791 -0.000244719 0.000069098

16 6 0.001025048 -0.002210302 -0.000860952

17 6 -0.000614403 0.001624647 -0.000428519

18 6 -0.000163481 -0.000433741 0.000271565

19 8 -0.000121631 0.000187837 -0.000167366

20 6 -0.000040151 0.000590741 0.000362278

21 8 -0.000044292 -0.000287928 -0.000014258

22 1 0.000149887 0.000338327 0.000116439

23 1 -0.000335484 0.000289894 -0.000079595

-------------------------------------------------------------------

Cartesian Forces: Max 0.003051912 RMS 0.000806877

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.002918775 RMS 0.000431926

Search for a saddle point.

Step number 46 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 33 34 37

41 43 45 46

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0

Eigenvalues --- -0.07126 -0.00013 0.00329 0.00634 0.00825

Eigenvalues --- 0.00945 0.01134 0.01366 0.01917 0.02282

Eigenvalues --- 0.02554 0.02803 0.03059 0.03090 0.03217

Eigenvalues --- 0.03517 0.03537 0.03645 0.03768 0.03846

Eigenvalues --- 0.04181 0.04190 0.04511 0.04818 0.05999

Eigenvalues --- 0.06340 0.06385 0.06714 0.07343 0.08316

Eigenvalues --- 0.08854 0.09130 0.09934 0.10058 0.10513

Eigenvalues --- 0.12129 0.13872 0.14648 0.17057 0.21855

Eigenvalues --- 0.26009 0.27546 0.28757 0.29847 0.30232

Eigenvalues --- 0.31139 0.31305 0.31792 0.31985 0.32397

Eigenvalues --- 0.32560 0.33231 0.35653 0.37172 0.39044

Eigenvalues --- 0.39702 0.40441 0.43419 0.47662 0.50249

Eigenvalues --- 0.57541 1.08495 1.10874

Eigenvectors required to have negative eigenvalues:

R6 R10 D4 D71 D30

1 -0.58349 -0.50520 -0.15076 -0.14583 0.14141

D86 D73 D1 D85 D35

1 0.13971 0.13967 -0.13183 0.12710 -0.12546

RFO step: Lambda0=9.899871061D-07 Lambda=-8.69716426D-04.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.12911025 RMS(Int)= 0.00592405

Iteration 2 RMS(Cart)= 0.00805152 RMS(Int)= 0.00199850

Iteration 3 RMS(Cart)= 0.00002342 RMS(Int)= 0.00199845

Iteration 4 RMS(Cart)= 0.00000005 RMS(Int)= 0.00199845

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63768 -0.00121 0.00000 -0.01484 -0.01402 2.62367

R2 2.64353 -0.00292 0.00000 -0.01708 -0.01572 2.62782

R3 2.07758 -0.00009 0.00000 0.00139 0.00139 2.07897

R4 2.81791 -0.00151 0.00000 -0.00939 -0.00969 2.80822

R5 2.08306 -0.00007 0.00000 0.00200 0.00200 2.08506

R6 4.08969 -0.00024 0.00000 0.02986 0.02946 4.11914

R7 2.63938 -0.00265 0.00000 -0.02817 -0.02770 2.61168

R8 2.81490 -0.00037 0.00000 0.00201 0.00214 2.81704

R9 2.08299 -0.00011 0.00000 0.00157 0.00157 2.08456

R10 4.11445 -0.00075 0.00000 -0.01232 -0.01264 4.10181

R11 2.07733 -0.00011 0.00000 0.00538 0.00538 2.08271

R12 2.12414 0.00000 0.00000 0.00057 0.00057 2.12471

R13 2.12769 -0.00012 0.00000 0.00097 0.00097 2.12866

R14 2.87652 -0.00058 0.00000 -0.00367 -0.00390 2.87263

R15 2.12429 0.00001 0.00000 -0.00060 -0.00060 2.12369

R16 2.12830 -0.00001 0.00000 0.00023 0.00023 2.12853

R17 2.66403 -0.00026 0.00000 0.00189 0.00224 2.66627

R18 2.66421 -0.00040 0.00000 -0.00110 -0.00054 2.66367

R19 2.66914 -0.00225 0.00000 -0.02529 -0.02693 2.64221

R20 2.81132 -0.00050 0.00000 -0.00159 -0.00193 2.80940

R21 2.06354 0.00008 0.00000 0.00234 0.00234 2.06588

R22 2.81391 -0.00037 0.00000 0.00449 0.00449 2.81840

R23 2.06532 -0.00014 0.00000 -0.00172 -0.00172 2.06360

R24 2.30638 0.00021 0.00000 0.00088 0.00088 2.30726

R25 2.30637 0.00016 0.00000 -0.00028 -0.00028 2.30609

A1 2.06152 0.00022 0.00000 -0.00159 -0.00331 2.05821

A2 2.10705 0.00000 0.00000 0.00718 0.00777 2.11482

A3 2.10113 -0.00021 0.00000 0.00016 0.00049 2.10162

A4 2.08803 -0.00009 0.00000 -0.00163 -0.00119 2.08684

A5 2.09548 0.00040 0.00000 0.03481 0.03521 2.13069

A6 1.62980 -0.00031 0.00000 -0.03379 -0.03538 1.59441

A7 2.02636 -0.00030 0.00000 -0.03088 -0.03126 1.99510

A8 1.73829 0.00029 0.00000 0.02516 0.02256 1.76085

A9 1.70461 0.00001 0.00000 0.00563 0.00952 1.71413

A10 2.09069 0.00000 0.00000 -0.00919 -0.00881 2.08187

A11 2.10337 0.00007 0.00000 0.00687 0.00720 2.11057

A12 1.60882 -0.00004 0.00000 0.03149 0.02875 1.63757

A13 2.02213 -0.00009 0.00000 -0.00215 -0.00257 2.01956

A14 1.74599 0.00019 0.00000 -0.02147 -0.02287 1.72312

A15 1.70279 -0.00008 0.00000 0.00091 0.00399 1.70678

A16 2.05931 0.00052 0.00000 0.01382 0.01224 2.07156

A17 2.10492 -0.00053 0.00000 -0.02297 -0.02245 2.08247

A18 2.10629 0.00001 0.00000 0.00838 0.00918 2.11547

A19 1.92260 0.00009 0.00000 0.00411 0.00460 1.92720

A20 1.87681 -0.00007 0.00000 -0.01300 -0.01237 1.86444

A21 1.97860 -0.00015 0.00000 0.01062 0.00872 1.98732

A22 1.85470 -0.00001 0.00000 0.00045 0.00018 1.85487

A23 1.91875 0.00018 0.00000 0.00297 0.00228 1.92103

A24 1.90776 -0.00005 0.00000 -0.00627 -0.00447 1.90330

A25 1.98427 -0.00050 0.00000 -0.01071 -0.01264 1.97163

A26 1.92321 0.00015 0.00000 0.00388 0.00466 1.92787

A27 1.87154 0.00016 0.00000 0.00604 0.00648 1.87802

A28 1.91930 0.00019 0.00000 0.00639 0.00577 1.92506

A29 1.90473 0.00010 0.00000 -0.00050 0.00134 1.90607

A30 1.85570 -0.00008 0.00000 -0.00489 -0.00521 1.85049

A31 1.88368 -0.00028 0.00000 -0.00011 -0.00026 1.88342

A32 1.87172 0.00002 0.00000 0.02139 0.01182 1.88354

A33 1.72208 -0.00002 0.00000 0.06437 0.06735 1.78942

A34 1.57026 -0.00005 0.00000 -0.07662 -0.07193 1.49833

A35 1.86805 0.00030 0.00000 0.00598 0.00627 1.87431

A36 2.19753 -0.00013 0.00000 0.02087 0.02067 2.21820

A37 2.10813 -0.00016 0.00000 -0.02699 -0.02646 2.08167

A38 1.87715 -0.00013 0.00000 -0.01092 -0.02034 1.85682

A39 1.75514 -0.00009 0.00000 -0.07480 -0.07049 1.68465

A40 1.55893 0.00019 0.00000 0.05809 0.06159 1.62052

A41 1.86502 0.00027 0.00000 0.00352 0.00328 1.86830

A42 2.20050 -0.00029 0.00000 -0.01203 -0.01182 2.18868

A43 2.09578 0.00002 0.00000 0.01800 0.01852 2.11430

A44 1.90356 -0.00015 0.00000 -0.00395 -0.00492 1.89863

A45 2.02568 0.00020 0.00000 0.00341 0.00372 2.02941

A46 2.35394 -0.00006 0.00000 0.00061 0.00099 2.35493

A47 1.90428 -0.00015 0.00000 -0.00468 -0.00519 1.89909

A48 2.02449 0.00033 0.00000 0.01177 0.01198 2.03647

A49 2.35439 -0.00018 0.00000 -0.00701 -0.00678 2.34761

D1 -0.60276 -0.00010 0.00000 -0.02201 -0.02222 -0.62498

D2 2.95629 -0.00006 0.00000 -0.02094 -0.02243 2.93385

D3 1.19574 0.00004 0.00000 -0.01318 -0.01717 1.17857

D4 2.71388 -0.00019 0.00000 -0.05897 -0.05779 2.65609

D5 -0.01027 -0.00015 0.00000 -0.05789 -0.05800 -0.06826

D6 -1.77081 -0.00005 0.00000 -0.05013 -0.05273 -1.82354

D7 -0.00378 0.00001 0.00000 0.06511 0.06508 0.06129

D8 -2.97623 -0.00005 0.00000 0.06931 0.07076 -2.90547

D9 2.96339 0.00012 0.00000 0.10266 0.10112 3.06451

D10 -0.00906 0.00006 0.00000 0.10686 0.10681 0.09775

D11 2.74660 -0.00005 0.00000 -0.05181 -0.05301 2.69359

D12 -1.52254 -0.00006 0.00000 -0.05636 -0.05729 -1.57982

D13 0.58833 -0.00026 0.00000 -0.06659 -0.06605 0.52228

D14 -0.79644 0.00007 0.00000 -0.03787 -0.03788 -0.83432

D15 1.21762 0.00007 0.00000 -0.04241 -0.04216 1.17546

D16 -2.95470 -0.00013 0.00000 -0.05264 -0.05093 -3.00562

D17 1.01005 0.00016 0.00000 -0.02669 -0.02448 0.98557

D18 3.02410 0.00016 0.00000 -0.03124 -0.02876 2.99535

D19 -1.14821 -0.00004 0.00000 -0.04147 -0.03752 -1.18573

D20 -0.99676 0.00030 0.00000 -0.18662 -0.18494 -1.18170

D21 -2.94483 0.00008 0.00000 -0.15595 -0.15583 -3.10065

D22 1.23509 0.00003 0.00000 -0.17932 -0.17824 1.05685

D23 1.11196 0.00019 0.00000 -0.19188 -0.19096 0.92100

D24 -0.83610 -0.00003 0.00000 -0.16121 -0.16185 -0.99795

D25 -2.93937 -0.00008 0.00000 -0.18458 -0.18426 -3.12363

D26 -3.10774 -0.00005 0.00000 -0.21648 -0.21538 2.96006

D27 1.22738 -0.00027 0.00000 -0.18581 -0.18627 1.04111

D28 -0.87588 -0.00032 0.00000 -0.20918 -0.20869 -1.08457

D29 0.59847 0.00009 0.00000 -0.02093 -0.02034 0.57813

D30 -2.71241 0.00009 0.00000 -0.02831 -0.02932 -2.74173

D31 -2.94398 0.00000 0.00000 -0.03425 -0.03273 -2.97671

D32 0.02833 0.00000 0.00000 -0.04163 -0.04171 -0.01339

D33 -1.19697 -0.00011 0.00000 -0.01313 -0.00916 -1.20613

D34 1.77533 -0.00011 0.00000 -0.02051 -0.01815 1.75719

D35 -0.56198 0.00000 0.00000 -0.06339 -0.06375 -0.62572

D36 -2.72559 0.00000 0.00000 -0.06692 -0.06559 -2.79118

D37 1.54496 -0.00007 0.00000 -0.06648 -0.06546 1.47951

D38 2.96247 0.00005 0.00000 -0.05279 -0.05426 2.90820

D39 0.79886 0.00005 0.00000 -0.05632 -0.05611 0.74275

D40 -1.21378 -0.00002 0.00000 -0.05587 -0.05597 -1.26975

D41 1.15515 0.00007 0.00000 -0.04157 -0.04586 1.10929

D42 -1.00846 0.00007 0.00000 -0.04510 -0.04770 -1.05617

D43 -3.02110 0.00000 0.00000 -0.04466 -0.04757 -3.06867

D44 1.07715 -0.00033 0.00000 -0.19638 -0.19772 0.87943

D45 3.01356 -0.00001 0.00000 -0.15872 -0.15877 2.85479

D46 -1.15468 -0.00018 0.00000 -0.19386 -0.19535 -1.35003

D47 -1.03070 -0.00035 0.00000 -0.19094 -0.19146 -1.22216

D48 0.90572 -0.00003 0.00000 -0.15327 -0.15251 0.75320

D49 3.02065 -0.00020 0.00000 -0.18841 -0.18909 2.83156

D50 -3.09116 -0.00028 0.00000 -0.18368 -0.18432 3.00770

D51 -1.15475 0.00005 0.00000 -0.14601 -0.14538 -1.30013

D52 0.96019 -0.00013 0.00000 -0.18115 -0.18196 0.77823

D53 -0.01765 0.00007 0.00000 0.10056 0.10037 0.08272

D54 2.14808 0.00005 0.00000 0.10276 0.10164 2.24972

D55 -2.10584 0.00011 0.00000 0.10019 0.09941 -2.00644

D56 -2.17801 -0.00009 0.00000 0.08522 0.08612 -2.09189

D57 -0.01228 -0.00010 0.00000 0.08741 0.08739 0.07511

D58 2.01698 -0.00004 0.00000 0.08484 0.08515 2.10213

D59 2.07568 -0.00015 0.00000 0.08660 0.08719 2.16287

D60 -2.04178 -0.00017 0.00000 0.08879 0.08846 -1.95332

D61 -0.01252 -0.00010 0.00000 0.08622 0.08623 0.07371

D62 -0.01891 -0.00003 0.00000 0.03327 0.03480 0.01589

D63 3.11971 -0.00001 0.00000 0.05435 0.05672 -3.10676

D64 0.01421 0.00007 0.00000 -0.00167 -0.00362 0.01060

D65 -3.12111 -0.00003 0.00000 -0.01155 -0.01435 -3.13546

D66 -0.04565 0.00022 0.00000 0.22092 0.21983 0.17418

D67 1.82642 0.00018 0.00000 0.13349 0.13425 1.96067

D68 -1.83323 0.00021 0.00000 0.15847 0.16055 -1.67268

D69 -1.87958 0.00011 0.00000 0.13776 0.13589 -1.74368

D70 -0.00751 0.00006 0.00000 0.05033 0.05032 0.04281

D71 2.61603 0.00010 0.00000 0.07531 0.07661 2.69264

D72 1.75111 0.00011 0.00000 0.14683 0.14353 1.89463

D73 -2.66001 0.00006 0.00000 0.05940 0.05795 -2.60206

D74 -0.03647 0.00010 0.00000 0.08438 0.08424 0.04777

D75 -1.92283 -0.00012 0.00000 -0.10312 -0.09713 -2.01996

D76 1.22253 -0.00015 0.00000 -0.12984 -0.12490 1.09764

D77 0.01654 -0.00002 0.00000 -0.05334 -0.05434 -0.03780

D78 -3.12129 -0.00005 0.00000 -0.08005 -0.08210 3.07979

D79 2.69924 -0.00002 0.00000 -0.04634 -0.04633 2.65291

D80 -0.43859 -0.00004 0.00000 -0.07306 -0.07409 -0.51268

D81 1.95358 -0.00018 0.00000 -0.07278 -0.07868 1.87489

D82 -1.19597 -0.00004 0.00000 -0.06014 -0.06513 -1.26110

D83 -0.00384 -0.00009 0.00000 -0.03182 -0.03057 -0.03442

D84 3.12979 0.00005 0.00000 -0.01918 -0.01702 3.11277

D85 -2.66462 0.00000 0.00000 -0.04467 -0.04498 -2.70961

D86 0.46901 0.00013 0.00000 -0.03203 -0.03143 0.43758

Item Value Threshold Converged?

Maximum Force 0.002919 0.000450 NO

RMS Force 0.000432 0.000300 NO

Maximum Displacement 0.518343 0.001800 NO

RMS Displacement 0.130182 0.001200 NO

Predicted change in Energy=-8.852734D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.093209 1.529219 0.416437

2 6 0 0.236780 1.315155 0.080408

3 6 0 -0.811031 3.773845 -0.339279

4 6 0 -1.613947 2.805530 0.233195

5 1 0 -1.681014 0.756973 0.934545

6 1 0 -2.581854 3.064489 0.692296

7 6 0 0.819690 2.019691 -1.090993

8 1 0 1.932186 2.128321 -0.969719

9 1 0 0.663235 1.351566 -1.984298

10 6 0 0.190491 3.375277 -1.368998

11 1 0 0.986983 4.161947 -1.467479

12 1 0 -0.337989 3.341697 -2.363128

13 1 0 -1.125958 4.830793 -0.361859

14 1 0 0.774246 0.396611 0.371653

15 8 0 2.806422 3.720880 0.868996

16 6 0 0.512372 3.897719 1.376733

17 6 0 0.908590 2.598679 1.709083

18 6 0 1.700362 4.595379 0.818040

19 8 0 1.903952 5.696615 0.331674

20 6 0 2.367036 2.497475 1.414026

21 8 0 3.205853 1.619734 1.537154

22 1 0 -0.280989 4.485473 1.846035

23 1 0 0.441392 1.969937 2.469936

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.388384 0.000000

3 C 2.385179 2.705403 0.000000

4 C 1.390581 2.381125 1.382041 0.000000

5 H 1.100143 2.172338 3.388365 2.166328 0.000000

6 H 2.156204 3.373318 2.168675 1.102124 2.488941

7 C 2.484369 1.486047 2.510255 2.879862 3.456990

8 H 3.381326 2.153696 3.260436 3.805348 4.308368

9 H 2.979964 2.108601 3.278259 3.495261 3.790605

10 C 2.871166 2.519330 1.490713 2.479442 3.957823

11 H 3.848064 3.326106 2.157849 3.390723 4.947906

12 H 3.403148 3.226159 2.122849 2.942183 4.399905

13 H 3.392227 3.796362 1.103099 2.166544 4.311004

14 H 2.184535 1.103366 3.797925 3.394927 2.544604

15 O 4.496143 3.607276 3.814276 4.558703 5.378301

16 C 3.018253 2.902766 2.170585 2.649866 3.856263

17 C 2.611872 2.179758 2.921284 2.929886 3.270755

18 C 4.167332 3.666884 2.884684 3.811856 5.116702

19 O 5.133941 4.694655 3.393870 4.554524 6.133148

20 C 3.729074 2.777482 3.847507 4.163831 4.432377

21 O 4.443662 3.321185 4.929154 5.131949 4.998897

22 H 3.382734 3.665575 2.358593 2.683327 4.085658

23 H 2.601170 2.486050 3.565717 3.150499 2.886748

6 7 8 9 10

6 H 0.000000

7 C 3.980229 0.000000

8 H 4.900537 1.124347 0.000000

9 H 4.541901 1.126439 1.800820 0.000000

10 C 3.468634 1.520129 2.178950 2.167369 0.000000

11 H 4.313426 2.181511 2.297131 2.875788 1.123809

12 H 3.800973 2.169389 2.927040 2.259775 1.126372

13 H 2.520060 3.495637 4.126148 4.235392 2.205877

14 H 4.299278 2.185357 2.477685 2.544556 3.499012

15 O 5.430984 3.268440 2.584842 4.283478 3.459935

16 C 3.276731 3.116265 3.263814 4.219264 2.813467

17 C 3.665247 2.860691 2.906022 3.905964 3.254744

18 C 4.549375 3.324779 3.055520 4.410335 2.924294

19 O 5.213501 4.088933 3.798308 5.077653 3.349156

20 C 5.033281 2.982897 2.451043 3.970472 3.640482

21 O 6.024837 3.572240 2.857500 4.351718 4.540932

22 H 2.940118 3.989700 4.287515 5.038292 3.433842

23 H 3.673972 3.581312 3.752170 4.502421 4.095772

11 12 13 14 15

11 H 0.000000

12 H 1.797373 0.000000

13 H 2.476746 2.615986 0.000000

14 H 4.195881 4.170087 4.879629 0.000000

15 O 2.993996 4.525232 4.267379 3.927830 0.000000

16 C 2.895620 3.875415 2.564655 3.651920 2.356212

17 C 3.541257 4.323071 3.662038 2.579897 2.359416

18 C 2.433181 3.980757 3.071753 4.322800 1.410927

19 O 2.536334 4.223020 3.226607 5.419214 2.237565

20 C 3.602511 4.721945 4.560608 2.834987 1.409552

21 O 4.518192 5.544022 5.716795 2.960935 2.240713

22 H 3.562555 4.362171 2.389145 4.472820 3.327358

23 H 4.539363 5.084060 4.319739 2.643659 3.349952

16 17 18 19 20

16 C 0.000000

17 C 1.398196 0.000000

18 C 1.486670 2.325440 0.000000

19 O 2.502932 3.533442 1.220951 0.000000

20 C 2.324189 1.491431 2.280538 3.408875 0.000000

21 O 3.531260 2.503060 3.411465 4.446245 1.220330

22 H 1.093216 2.234692 2.234861 2.921322 3.339282

23 H 2.217313 1.092011 3.347643 4.538654 2.258616

21 22 23

21 O 0.000000

22 H 4.523930 0.000000

23 H 2.938532 2.690541 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.203980 -0.987866 -0.521217

2 6 0 1.193050 -1.391339 0.340664

3 6 0 1.537038 1.259078 -0.079055

4 6 0 2.350185 0.374005 -0.761312

5 1 0 2.784836 -1.721011 -1.100373

6 1 0 2.982897 0.709398 -1.599085

7 6 0 0.856700 -0.552289 1.520154

8 1 0 -0.210159 -0.722773 1.831446

9 1 0 1.496417 -0.916803 2.372654

10 6 0 1.108041 0.932210 1.310673

11 1 0 0.195220 1.525351 1.589758

12 1 0 1.924762 1.271841 2.008047

13 1 0 1.510744 2.328304 -0.349040

14 1 0 0.888860 -2.447898 0.433224

15 8 0 -2.084919 0.112276 0.260021

16 6 0 -0.259635 0.645633 -1.131239

17 6 0 -0.338045 -0.749089 -1.071642

18 6 0 -1.340646 1.188769 -0.267175

19 8 0 -1.687125 2.306835 0.080105

20 6 0 -1.511157 -1.084765 -0.214032

21 8 0 -2.040070 -2.124933 0.143050

22 1 0 0.115699 1.250049 -1.961254

23 1 0 0.010572 -1.435953 -1.845704

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2229793 0.8855634 0.6777994

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.0630772087 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.487554849075E-01 A.U. after 16 cycles

Convg = 0.6766D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000322339 -0.011294894 0.002454984

2 6 0.003298318 -0.005699891 -0.001701085

3 6 0.004109078 0.008166911 -0.009729004

4 6 -0.013434502 0.002979892 0.004297028

5 1 0.001211113 0.000561329 0.002110650

6 1 0.000160636 0.000637495 -0.001664104

7 6 0.002990277 0.001452156 -0.003095175

8 1 -0.000030993 0.000194150 0.000303723

9 1 0.000327750 0.000026333 -0.000478647

10 6 0.000090400 0.001188376 -0.000471644

11 1 0.000032135 -0.000090009 0.000281226

12 1 -0.000390356 0.000038443 0.000337631

13 1 0.000262517 -0.000405568 0.000380170

14 1 -0.002168163 -0.000209886 0.002107243

15 8 0.001128601 -0.000058976 -0.000103504

16 6 -0.004564630 0.010288877 0.002158679

17 6 0.006456573 -0.004184107 0.003692342

18 6 0.001826503 -0.000149676 -0.002680120

19 8 0.000847082 -0.000791154 0.001951780

20 6 -0.002185097 -0.000989874 -0.000325058

21 8 0.000246353 0.001320870 -0.000346623

22 1 -0.000351412 -0.000844170 0.001669905

23 1 0.000460156 -0.002136625 -0.001150397

-------------------------------------------------------------------

Cartesian Forces: Max 0.013434502 RMS 0.003503228

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011717889 RMS 0.001824762

Search for a saddle point.

Step number 47 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 36 46 47

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0

Eigenvalues --- -0.07125 -0.00061 0.00391 0.00616 0.00833

Eigenvalues --- 0.01059 0.01123 0.01337 0.01915 0.02295

Eigenvalues --- 0.02544 0.02809 0.03064 0.03095 0.03211

Eigenvalues --- 0.03531 0.03563 0.03649 0.03817 0.03854

Eigenvalues --- 0.04180 0.04201 0.04496 0.04829 0.06004

Eigenvalues --- 0.06334 0.06412 0.06789 0.07353 0.08331

Eigenvalues --- 0.08888 0.09126 0.09940 0.10084 0.10560

Eigenvalues --- 0.12109 0.13885 0.14588 0.17105 0.21897

Eigenvalues --- 0.26047 0.27563 0.28742 0.29854 0.30259

Eigenvalues --- 0.31155 0.31313 0.31801 0.31985 0.32407

Eigenvalues --- 0.32601 0.33231 0.35633 0.37148 0.39043

Eigenvalues --- 0.39699 0.40446 0.43377 0.47700 0.50236

Eigenvalues --- 0.57980 1.08498 1.10878

Eigenvectors required to have negative eigenvalues:

R6 R10 D4 D71 D86

1 0.58338 0.50374 0.14952 0.14761 -0.14614

D30 D73 D85 D1 R19

1 -0.14422 -0.13908 -0.13339 0.13195 -0.12367

RFO step: Lambda0=1.136860103D-04 Lambda=-3.16461332D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.06481451 RMS(Int)= 0.00261857

Iteration 2 RMS(Cart)= 0.00310749 RMS(Int)= 0.00066064

Iteration 3 RMS(Cart)= 0.00000484 RMS(Int)= 0.00066063

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00066063

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62367 0.00499 0.00000 0.02133 0.02157 2.64524

R2 2.62782 0.01172 0.00000 0.02033 0.02060 2.64842

R3 2.07897 -0.00005 0.00000 -0.00334 -0.00334 2.07563

R4 2.80822 0.00574 0.00000 0.03507 0.03523 2.84345

R5 2.08506 -0.00033 0.00000 -0.00642 -0.00642 2.07864

R6 4.11914 0.00192 0.00000 -0.03980 -0.03987 4.07927

R7 2.61168 0.01105 0.00000 0.05053 0.05054 2.66222

R8 2.81704 0.00092 0.00000 -0.00135 -0.00138 2.81566

R9 2.08456 -0.00047 0.00000 -0.00460 -0.00460 2.07995

R10 4.10181 0.00490 0.00000 -0.04105 -0.04122 4.06059

R11 2.08271 -0.00068 0.00000 -0.00941 -0.00941 2.07330

R12 2.12471 0.00002 0.00000 0.00097 0.00097 2.12567

R13 2.12866 0.00032 0.00000 -0.00225 -0.00225 2.12641

R14 2.87263 0.00320 0.00000 0.00400 0.00411 2.87674

R15 2.12369 -0.00006 0.00000 -0.00034 -0.00034 2.12335

R16 2.12853 -0.00012 0.00000 -0.00024 -0.00024 2.12829

R17 2.66627 0.00016 0.00000 -0.00579 -0.00584 2.66043

R18 2.66367 0.00010 0.00000 0.00587 0.00549 2.66916

R19 2.64221 0.00892 0.00000 0.04551 0.04536 2.68757

R20 2.80940 0.00231 0.00000 0.01558 0.01595 2.82535

R21 2.06588 0.00052 0.00000 -0.00023 -0.00023 2.06565

R22 2.81840 -0.00097 0.00000 -0.02510 -0.02532 2.79307

R23 2.06360 0.00023 0.00000 -0.00133 -0.00133 2.06227

R24 2.30726 -0.00135 0.00000 -0.00179 -0.00179 2.30548

R25 2.30609 -0.00082 0.00000 0.00033 0.00033 2.30642

A1 2.05821 -0.00071 0.00000 0.00466 0.00377 2.06199

A2 2.11482 -0.00017 0.00000 -0.02022 -0.02093 2.09389

A3 2.10162 0.00085 0.00000 0.00662 0.00596 2.10758

A4 2.08684 0.00048 0.00000 0.02339 0.02273 2.10956

A5 2.13069 -0.00179 0.00000 -0.07110 -0.07142 2.05927

A6 1.59441 0.00087 0.00000 -0.01570 -0.01549 1.57893

A7 1.99510 0.00162 0.00000 0.05857 0.05914 2.05423

A8 1.76085 -0.00144 0.00000 -0.01770 -0.01783 1.74303

A9 1.71413 -0.00042 0.00000 0.00120 0.00090 1.71503

A10 2.08187 0.00033 0.00000 -0.01678 -0.01819 2.06368

A11 2.11057 -0.00060 0.00000 -0.00973 -0.00959 2.10098

A12 1.63757 0.00011 0.00000 0.03135 0.03198 1.66955

A13 2.01956 0.00044 0.00000 0.01155 0.01200 2.03156

A14 1.72312 -0.00086 0.00000 0.02066 0.02031 1.74343

A15 1.70678 0.00031 0.00000 -0.01547 -0.01534 1.69144

A16 2.07156 -0.00220 0.00000 -0.02161 -0.02202 2.04954

A17 2.08247 0.00228 0.00000 0.03187 0.03205 2.11452

A18 2.11547 -0.00013 0.00000 -0.01237 -0.01216 2.10331

A19 1.92720 -0.00034 0.00000 -0.01253 -0.01221 1.91499

A20 1.86444 -0.00003 0.00000 0.02995 0.03052 1.89495

A21 1.98732 0.00091 0.00000 -0.01381 -0.01572 1.97160

A22 1.85487 0.00013 0.00000 -0.00923 -0.00934 1.84554

A23 1.92103 -0.00054 0.00000 -0.00585 -0.00609 1.91494

A24 1.90330 -0.00015 0.00000 0.01322 0.01419 1.91749

A25 1.97163 0.00171 0.00000 0.00708 0.00474 1.97637

A26 1.92787 -0.00068 0.00000 -0.00187 -0.00109 1.92678

A27 1.87802 -0.00067 0.00000 -0.01351 -0.01284 1.86517

A28 1.92506 -0.00060 0.00000 -0.00691 -0.00649 1.91858

A29 1.90607 -0.00025 0.00000 0.00215 0.00314 1.90921

A30 1.85049 0.00043 0.00000 0.01343 0.01307 1.86356

A31 1.88342 0.00095 0.00000 0.00010 -0.00171 1.88171

A32 1.88354 -0.00036 0.00000 -0.01409 -0.01464 1.86890

A33 1.78942 0.00080 0.00000 0.02154 0.02165 1.81107

A34 1.49833 0.00075 0.00000 0.07050 0.07070 1.56903

A35 1.87431 -0.00210 0.00000 -0.02587 -0.02634 1.84797

A36 2.21820 0.00043 0.00000 -0.03359 -0.03384 2.18436

A37 2.08167 0.00123 0.00000 0.02123 0.01825 2.09992

A38 1.85682 0.00091 0.00000 0.00584 0.00505 1.86187

A39 1.68465 0.00030 0.00000 -0.02014 -0.01963 1.66502

A40 1.62052 -0.00156 0.00000 -0.04853 -0.04804 1.57248

A41 1.86830 -0.00073 0.00000 0.00942 0.00872 1.87702

A42 2.18868 0.00117 0.00000 0.02134 0.02102 2.20970

A43 2.11430 -0.00021 0.00000 0.00161 0.00021 2.11452

A44 1.89863 0.00062 0.00000 0.01187 0.01093 1.90957

A45 2.02941 -0.00116 0.00000 -0.00556 -0.00568 2.02372

A46 2.35493 0.00055 0.00000 -0.00530 -0.00543 2.34950

A47 1.89909 0.00126 0.00000 0.00369 0.00212 1.90121

A48 2.03647 -0.00191 0.00000 -0.02165 -0.02106 2.01541

A49 2.34761 0.00065 0.00000 0.01810 0.01865 2.36627

D1 -0.62498 0.00146 0.00000 0.05353 0.05436 -0.57062

D2 2.93385 0.00018 0.00000 0.00878 0.01099 2.94484

D3 1.17857 0.00037 0.00000 0.02746 0.02759 1.20616

D4 2.65609 0.00167 0.00000 0.12551 0.12535 2.78144

D5 -0.06826 0.00040 0.00000 0.08076 0.08198 0.01371

D6 -1.82354 0.00059 0.00000 0.09944 0.09858 -1.72497

D7 0.06129 -0.00073 0.00000 -0.04714 -0.04667 0.01462

D8 -2.90547 -0.00045 0.00000 -0.03243 -0.03227 -2.93773

D9 3.06451 -0.00103 0.00000 -0.12079 -0.12048 2.94402

D10 0.09775 -0.00075 0.00000 -0.10608 -0.10608 -0.00833

D11 2.69359 0.00000 0.00000 -0.11667 -0.11716 2.57643

D12 -1.57982 -0.00004 0.00000 -0.11738 -0.11775 -1.69757

D13 0.52228 0.00030 0.00000 -0.08856 -0.08846 0.43382

D14 -0.83432 0.00041 0.00000 -0.10449 -0.10367 -0.93799

D15 1.17546 0.00037 0.00000 -0.10521 -0.10426 1.07120

D16 -3.00562 0.00072 0.00000 -0.07638 -0.07497 -3.08060

D17 0.98557 -0.00030 0.00000 -0.09388 -0.09378 0.89179

D18 2.99535 -0.00034 0.00000 -0.09460 -0.09437 2.90098

D19 -1.18573 0.00000 0.00000 -0.06578 -0.06508 -1.25081

D20 -1.18170 -0.00107 0.00000 -0.04838 -0.04859 -1.23029

D21 -3.10065 -0.00061 0.00000 -0.05262 -0.05205 3.13048

D22 1.05685 -0.00018 0.00000 -0.04362 -0.04377 1.01308

D23 0.92100 -0.00058 0.00000 -0.03054 -0.03105 0.88995

D24 -0.99795 -0.00011 0.00000 -0.03479 -0.03451 -1.03246

D25 -3.12363 0.00032 0.00000 -0.02578 -0.02623 3.13333

D26 2.96006 0.00063 0.00000 0.02676 0.02662 2.98668

D27 1.04111 0.00110 0.00000 0.02251 0.02316 1.06427

D28 -1.08457 0.00153 0.00000 0.03151 0.03144 -1.05313

D29 0.57813 -0.00017 0.00000 0.07392 0.07271 0.65084

D30 -2.74173 -0.00021 0.00000 0.06349 0.06302 -2.67871

D31 -2.97671 0.00038 0.00000 0.03518 0.03458 -2.94213

D32 -0.01339 0.00034 0.00000 0.02474 0.02488 0.01150

D33 -1.20613 0.00071 0.00000 0.03465 0.03438 -1.17176

D34 1.75719 0.00067 0.00000 0.02422 0.02468 1.78187

D35 -0.62572 0.00009 0.00000 -0.11343 -0.11384 -0.73956

D36 -2.79118 0.00015 0.00000 -0.10815 -0.10798 -2.89916

D37 1.47951 0.00038 0.00000 -0.11554 -0.11574 1.36377

D38 2.90820 -0.00019 0.00000 -0.07215 -0.07258 2.83563

D39 0.74275 -0.00014 0.00000 -0.06687 -0.06672 0.67603

D40 -1.26975 0.00009 0.00000 -0.07427 -0.07447 -1.34422

D41 1.10929 -0.00021 0.00000 -0.06855 -0.06929 1.04000

D42 -1.05617 -0.00015 0.00000 -0.06327 -0.06343 -1.11960

D43 -3.06867 0.00008 0.00000 -0.07066 -0.07119 -3.13985

D44 0.87943 0.00176 0.00000 -0.03430 -0.03401 0.84542

D45 2.85479 -0.00037 0.00000 -0.05894 -0.05954 2.79525

D46 -1.35003 0.00109 0.00000 -0.02123 -0.02110 -1.37114

D47 -1.22216 0.00154 0.00000 -0.02736 -0.02674 -1.24889

D48 0.75320 -0.00058 0.00000 -0.05201 -0.05227 0.70093

D49 2.83156 0.00087 0.00000 -0.01429 -0.01383 2.81773

D50 3.00770 0.00121 0.00000 -0.04042 -0.04005 2.96765

D51 -1.30013 -0.00091 0.00000 -0.06507 -0.06559 -1.36572

D52 0.77823 0.00055 0.00000 -0.02736 -0.02715 0.75109

D53 0.08272 -0.00002 0.00000 0.11414 0.11405 0.19678

D54 2.24972 -0.00012 0.00000 0.11161 0.11115 2.36087

D55 -2.00644 -0.00009 0.00000 0.12516 0.12507 -1.88137

D56 -2.09189 0.00018 0.00000 0.14571 0.14603 -1.94586

D57 0.07511 0.00008 0.00000 0.14318 0.14312 0.21823

D58 2.10213 0.00010 0.00000 0.15673 0.15705 2.25918

D59 2.16287 0.00042 0.00000 0.15250 0.15261 2.31548

D60 -1.95332 0.00032 0.00000 0.14998 0.14970 -1.80362

D61 0.07371 0.00034 0.00000 0.16352 0.16362 0.23733

D62 0.01589 0.00008 0.00000 -0.08724 -0.08713 -0.07125

D63 -3.10676 -0.00042 0.00000 -0.13176 -0.13172 3.04471

D64 0.01060 -0.00017 0.00000 0.10173 0.10162 0.11221

D65 -3.13546 0.00015 0.00000 0.12927 0.12838 -3.00708

D66 0.17418 -0.00092 0.00000 0.04555 0.04570 0.21987

D67 1.96067 -0.00052 0.00000 0.02889 0.02904 1.98971

D68 -1.67268 -0.00020 0.00000 0.09436 0.09510 -1.57759

D69 -1.74368 -0.00072 0.00000 0.03909 0.03920 -1.70449

D70 0.04281 -0.00031 0.00000 0.02243 0.02253 0.06534

D71 2.69264 0.00001 0.00000 0.08790 0.08859 2.78123

D72 1.89463 -0.00003 0.00000 0.11296 0.11183 2.00646

D73 -2.60206 0.00038 0.00000 0.09631 0.09517 -2.50689

D74 0.04777 0.00070 0.00000 0.16177 0.16123 0.20900

D75 -2.01996 0.00103 0.00000 0.05553 0.05663 -1.96333

D76 1.09764 0.00163 0.00000 0.11198 0.11301 1.21065

D77 -0.03780 0.00019 0.00000 0.03947 0.03950 0.00170

D78 3.07979 0.00079 0.00000 0.09592 0.09589 -3.10750

D79 2.65291 -0.00060 0.00000 -0.04458 -0.04549 2.60742

D80 -0.51268 0.00000 0.00000 0.01188 0.01090 -0.50178

D81 1.87489 0.00122 0.00000 -0.07656 -0.07741 1.79748

D82 -1.26110 0.00082 0.00000 -0.11090 -0.11177 -1.37287

D83 -0.03442 0.00030 0.00000 -0.07761 -0.07754 -0.11195

D84 3.11277 -0.00010 0.00000 -0.11195 -0.11189 3.00088

D85 -2.70961 -0.00048 0.00000 -0.14629 -0.14616 -2.85577

D86 0.43758 -0.00088 0.00000 -0.18063 -0.18052 0.25706

Item Value Threshold Converged?

Maximum Force 0.011718 0.000450 NO

RMS Force 0.001825 0.000300 NO

Maximum Displacement 0.323302 0.001800 NO

RMS Displacement 0.064807 0.001200 NO

Predicted change in Energy=-2.242626D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.086547 1.517344 0.422985

2 6 0 0.253292 1.325470 0.065978

3 6 0 -0.821445 3.782443 -0.329973

4 6 0 -1.646719 2.787428 0.229976

5 1 0 -1.610018 0.757154 1.018397

6 1 0 -2.621192 3.049386 0.660675

7 6 0 0.858267 2.072086 -1.091890

8 1 0 1.946442 2.271266 -0.888159

9 1 0 0.834319 1.406842 -1.999120

10 6 0 0.143748 3.382308 -1.392207

11 1 0 0.896690 4.198308 -1.564726

12 1 0 -0.445476 3.276738 -2.346195

13 1 0 -1.141762 4.835467 -0.331237

14 1 0 0.745277 0.395875 0.388056

15 8 0 2.796376 3.624171 0.786986

16 6 0 0.513072 3.920106 1.348519

17 6 0 0.887064 2.592377 1.694809

18 6 0 1.739996 4.554738 0.776460

19 8 0 2.011062 5.665318 0.350373

20 6 0 2.333540 2.452249 1.425275

21 8 0 3.182463 1.602741 1.642760

22 1 0 -0.223813 4.525910 1.882237

23 1 0 0.378964 1.937281 2.404479

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.399800 0.000000

3 C 2.401645 2.710821 0.000000

4 C 1.401484 2.402968 1.408785 0.000000

5 H 1.098374 2.168412 3.404750 2.178295 0.000000

6 H 2.181463 3.404145 2.181249 1.097142 2.530763

7 C 2.526833 1.504689 2.515407 2.921300 3.503539

8 H 3.389177 2.161403 3.202566 3.798349 4.309977

9 H 3.093304 2.146821 3.342317 3.609769 3.937294

10 C 2.878653 2.523665 1.489982 2.488198 3.972171

11 H 3.882240 3.365464 2.156280 3.417669 4.979724

12 H 3.342873 3.180299 2.112402 2.884279 4.361759

13 H 3.403210 3.797898 1.100665 2.182751 4.321274

14 H 2.148137 1.099968 3.799871 3.386171 2.464806

15 O 4.432642 3.503021 3.789627 4.555380 5.262096

16 C 3.031280 2.905947 2.148772 2.683056 3.823710

17 C 2.582320 2.158659 2.904307 2.933229 3.171908

18 C 4.164139 3.625361 2.895101 3.858998 5.069790

19 O 5.177465 4.690939 3.468599 4.655760 6.135841

20 C 3.684512 2.728507 3.847628 4.169358 4.311676

21 O 4.440675 3.338137 4.967298 5.169181 4.906396

22 H 3.453287 3.710692 2.409103 2.788717 4.107469

23 H 2.500078 2.420474 3.510389 3.091052 2.696289

6 7 8 9 10

6 H 0.000000

7 C 4.016619 0.000000

8 H 4.885451 1.124857 0.000000

9 H 4.659722 1.125250 1.793956 0.000000

10 C 3.459776 1.522304 2.176737 2.178921 0.000000

11 H 4.318324 2.178502 2.296348 2.825751 1.123628

12 H 3.718426 2.173526 2.976259 2.292346 1.126243

13 H 2.522436 3.494994 4.052443 4.294438 2.211303

14 H 4.295177 2.238903 2.566829 2.593952 3.528449

15 O 5.449438 3.113746 2.314920 4.065539 3.441485

16 C 3.324890 3.080574 3.126652 4.198378 2.817305

17 C 3.685939 2.835000 2.810181 3.879869 3.272029

18 C 4.615132 3.229820 2.833341 4.293407 2.936956

19 O 5.328899 4.039848 3.613547 5.003944 3.425723

20 C 5.048817 2.942291 2.352569 3.881626 3.687601

21 O 6.061326 3.619459 2.894862 4.337677 4.648835

22 H 3.069163 4.004695 4.179536 5.090496 3.487823

23 H 3.643976 3.531643 3.661967 4.458744 4.069184

11 12 13 14 15

11 H 0.000000

12 H 1.805933 0.000000

13 H 2.466324 2.640928 0.000000

14 H 4.277239 4.146491 4.877322 0.000000

15 O 3.077172 4.521852 4.269262 3.845523 0.000000

16 C 2.951534 3.870872 2.529416 3.660138 2.369890

17 C 3.633685 4.309725 3.640391 2.559751 2.352491

18 C 2.513833 4.020018 3.100054 4.293770 1.407837

19 O 2.657357 4.360203 3.330698 5.419470 2.230163

20 C 3.748782 4.756753 4.565390 2.797691 1.412456

21 O 4.716958 5.645881 5.748574 2.995110 2.228809

22 H 3.639286 4.414658 2.416180 4.497654 3.336802

23 H 4.597268 5.004274 4.265704 2.564387 3.362405

16 17 18 19 20

16 C 0.000000

17 C 1.422199 0.000000

18 C 1.495109 2.328458 0.000000

19 O 2.507197 3.537491 1.220006 0.000000

20 C 2.339786 1.478031 2.278972 3.403413 0.000000

21 O 3.547168 2.500188 3.397863 4.421196 1.220505

22 H 1.093093 2.237795 2.253912 2.939307 3.323994

23 H 2.250473 1.091306 3.369560 4.558657 2.245975

21 22 23

21 O 0.000000

22 H 4.494995 0.000000

23 H 2.924336 2.708703 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.172666 -1.071807 -0.471096

2 6 0 1.136894 -1.387788 0.415906

3 6 0 1.575480 1.229990 -0.134940

4 6 0 2.399600 0.278906 -0.768138

5 1 0 2.649212 -1.864849 -1.063053

6 1 0 3.062111 0.575592 -1.590802

7 6 0 0.780345 -0.462413 1.547560

8 1 0 -0.323445 -0.524417 1.755184

9 1 0 1.287928 -0.827952 2.482936

10 6 0 1.171818 0.983794 1.278033

11 1 0 0.330556 1.669031 1.570039

12 1 0 2.053605 1.258775 1.922440

13 1 0 1.580102 2.279415 -0.466826

14 1 0 0.835850 -2.442136 0.503385

15 8 0 -2.020844 0.125807 0.321692

16 6 0 -0.231511 0.648315 -1.141746

17 6 0 -0.326718 -0.767355 -1.044475

18 6 0 -1.316296 1.192287 -0.268425

19 8 0 -1.717106 2.312109 0.003171

20 6 0 -1.502150 -1.078182 -0.204045

21 8 0 -2.111391 -2.090350 0.102509

22 1 0 0.089061 1.197975 -2.030543

23 1 0 0.069001 -1.496453 -1.753539

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2256848 0.8823212 0.6768565

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.9973058097 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.470654387667E-01 A.U. after 15 cycles

Convg = 0.6500D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.003240897 0.013002319 -0.003893659

2 6 0.000058070 0.007606568 -0.004029623

3 6 -0.001069533 -0.007067755 0.006945586

4 6 0.011924518 -0.002042178 0.000079214

5 1 -0.001936519 -0.000708302 -0.001421432

6 1 -0.000887843 -0.000774108 -0.000292927

7 6 -0.005333965 -0.006571136 0.007712916

8 1 -0.000396114 -0.001015991 -0.001425367

9 1 -0.001959698 0.000267178 0.001108835

10 6 0.000290333 -0.000859322 0.000116791

11 1 0.000098907 -0.000217684 0.000449241

12 1 0.000754589 -0.000067781 -0.000480585

13 1 -0.000854974 0.000150183 -0.000696839

14 1 0.004173417 -0.000438994 -0.002340549

15 8 0.000528259 0.001721328 0.003204313

16 6 0.001289626 -0.007885234 -0.003518428

17 6 -0.005111165 0.001217732 -0.005133813

18 6 -0.003613980 0.000097071 0.002902165

19 8 -0.000489936 0.001063676 -0.001821835

20 6 0.005407443 0.002291153 0.000369717

21 8 -0.000767631 -0.002223649 -0.000903235

22 1 -0.000098172 -0.000013945 -0.000925631

23 1 0.001235267 0.002468872 0.003995149

-------------------------------------------------------------------

Cartesian Forces: Max 0.013002319 RMS 0.003658008

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.012207985 RMS 0.001975504

Search for a saddle point.

Step number 48 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 47 48

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07164 0.00002 0.00373 0.00807 0.00865

Eigenvalues --- 0.01060 0.01136 0.01343 0.01940 0.02324

Eigenvalues --- 0.02515 0.02781 0.03070 0.03174 0.03177

Eigenvalues --- 0.03533 0.03583 0.03656 0.03840 0.04000

Eigenvalues --- 0.04178 0.04275 0.04494 0.04875 0.06022

Eigenvalues --- 0.06335 0.06422 0.06883 0.07355 0.08339

Eigenvalues --- 0.08933 0.09103 0.09895 0.10031 0.10463

Eigenvalues --- 0.12093 0.13844 0.14428 0.17122 0.21985

Eigenvalues --- 0.26113 0.27559 0.28772 0.29869 0.30239

Eigenvalues --- 0.31163 0.31312 0.31804 0.31985 0.32412

Eigenvalues --- 0.32636 0.33247 0.35609 0.37136 0.39038

Eigenvalues --- 0.39694 0.40448 0.43330 0.47800 0.50305

Eigenvalues --- 0.58490 1.08508 1.10880

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D71

1 0.58021 0.50758 -0.14638 0.14247 0.14247

D73 D86 D1 D35 D29

1 -0.14229 -0.13478 0.12899 0.12684 -0.12509

RFO step: Lambda0=1.322913344D-04 Lambda=-4.41015637D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.05423081 RMS(Int)= 0.00118910

Iteration 2 RMS(Cart)= 0.00147751 RMS(Int)= 0.00034729

Iteration 3 RMS(Cart)= 0.00000103 RMS(Int)= 0.00034729

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00034729

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64524 -0.00067 0.00000 -0.01023 -0.01044 2.63479

R2 2.64842 -0.01194 0.00000 -0.00912 -0.00938 2.63904

R3 2.07563 0.00064 0.00000 0.00293 0.00293 2.07856

R4 2.84345 -0.01221 0.00000 -0.03641 -0.03611 2.80734

R5 2.07864 0.00155 0.00000 0.00588 0.00588 2.08452

R6 4.07927 0.00112 0.00000 0.08346 0.08343 4.16270

R7 2.66222 -0.00976 0.00000 -0.02404 -0.02408 2.63814

R8 2.81566 -0.00099 0.00000 -0.00066 -0.00064 2.81501

R9 2.07995 0.00039 0.00000 0.00294 0.00294 2.08289

R10 4.06059 -0.00405 0.00000 -0.00085 -0.00088 4.05971

R11 2.07330 0.00049 0.00000 0.00357 0.00357 2.07687

R12 2.12567 -0.00082 0.00000 -0.00019 -0.00019 2.12549

R13 2.12641 -0.00101 0.00000 0.00044 0.00044 2.12685

R14 2.87674 -0.00246 0.00000 -0.00082 -0.00043 2.87631

R15 2.12335 -0.00016 0.00000 -0.00047 -0.00047 2.12288

R16 2.12829 0.00002 0.00000 0.00061 0.00061 2.12890

R17 2.66043 0.00039 0.00000 0.00283 0.00289 2.66331

R18 2.66916 -0.00004 0.00000 -0.00189 -0.00198 2.66717

R19 2.68757 -0.00525 0.00000 -0.01938 -0.01953 2.66804

R20 2.82535 -0.00270 0.00000 -0.00880 -0.00867 2.81667

R21 2.06565 -0.00039 0.00000 0.00159 0.00159 2.06724

R22 2.79307 0.00367 0.00000 0.01790 0.01779 2.81087

R23 2.06227 0.00054 0.00000 0.00061 0.00061 2.06288

R24 2.30548 0.00150 0.00000 0.00091 0.00091 2.30638

R25 2.30642 0.00085 0.00000 -0.00025 -0.00025 2.30617

A1 2.06199 0.00069 0.00000 0.00353 0.00334 2.06532

A2 2.09389 0.00086 0.00000 0.01090 0.01083 2.10471

A3 2.10758 -0.00142 0.00000 -0.00911 -0.00926 2.09832

A4 2.10956 -0.00102 0.00000 -0.00590 -0.00577 2.10379

A5 2.05927 0.00316 0.00000 0.04395 0.04375 2.10301

A6 1.57893 -0.00111 0.00000 0.01150 0.01127 1.59019

A7 2.05423 -0.00263 0.00000 -0.03815 -0.03802 2.01621

A8 1.74303 0.00249 0.00000 -0.01169 -0.01226 1.73077

A9 1.71503 0.00018 0.00000 0.00447 0.00432 1.71935

A10 2.06368 -0.00075 0.00000 0.00789 0.00788 2.07156

A11 2.10098 -0.00030 0.00000 -0.00169 -0.00198 2.09901

A12 1.66955 -0.00007 0.00000 -0.01741 -0.01727 1.65228

A13 2.03156 0.00063 0.00000 -0.00180 -0.00152 2.03004

A14 1.74343 0.00159 0.00000 0.00625 0.00558 1.74901

A15 1.69144 -0.00055 0.00000 0.00148 0.00189 1.69332

A16 2.04954 0.00162 0.00000 0.00544 0.00549 2.05504

A17 2.11452 -0.00150 0.00000 -0.01087 -0.01108 2.10344

A18 2.10331 0.00007 0.00000 0.00926 0.00915 2.11246

A19 1.91499 -0.00012 0.00000 0.00407 0.00409 1.91908

A20 1.89495 -0.00055 0.00000 -0.00987 -0.00977 1.88519

A21 1.97160 0.00067 0.00000 0.01121 0.01095 1.98255

A22 1.84554 0.00022 0.00000 0.00300 0.00298 1.84852

A23 1.91494 0.00008 0.00000 0.00030 0.00014 1.91508

A24 1.91749 -0.00033 0.00000 -0.00937 -0.00912 1.90837

A25 1.97637 -0.00200 0.00000 -0.00251 -0.00319 1.97318

A26 1.92678 0.00113 0.00000 0.00226 0.00248 1.92926

A27 1.86517 0.00057 0.00000 0.00062 0.00076 1.86594

A28 1.91858 0.00068 0.00000 0.00749 0.00757 1.92615

A29 1.90921 0.00001 0.00000 -0.00816 -0.00784 1.90136

A30 1.86356 -0.00032 0.00000 0.00003 -0.00005 1.86351

A31 1.88171 -0.00069 0.00000 0.00224 0.00150 1.88321

A32 1.86890 0.00060 0.00000 0.02327 0.02229 1.89119

A33 1.81107 0.00032 0.00000 -0.02220 -0.02178 1.78930

A34 1.56903 -0.00098 0.00000 -0.02081 -0.02076 1.54827

A35 1.84797 0.00135 0.00000 0.01448 0.01430 1.86227

A36 2.18436 0.00025 0.00000 0.00864 0.00926 2.19362

A37 2.09992 -0.00161 0.00000 -0.01254 -0.01314 2.08678

A38 1.86187 -0.00195 0.00000 -0.01316 -0.01434 1.84753

A39 1.66502 0.00184 0.00000 0.04450 0.04512 1.71014

A40 1.57248 0.00153 0.00000 0.00482 0.00532 1.57780

A41 1.87702 0.00018 0.00000 -0.00585 -0.00618 1.87084

A42 2.20970 -0.00077 0.00000 -0.00436 -0.00408 2.20562

A43 2.11452 -0.00001 0.00000 -0.00392 -0.00445 2.11007

A44 1.90957 0.00059 0.00000 -0.00367 -0.00400 1.90557

A45 2.02372 0.00020 0.00000 0.00237 0.00250 2.02622

A46 2.34950 -0.00080 0.00000 0.00166 0.00179 2.35129

A47 1.90121 -0.00133 0.00000 0.00077 0.00008 1.90128

A48 2.01541 0.00231 0.00000 0.01119 0.01153 2.02694

A49 2.36627 -0.00097 0.00000 -0.01179 -0.01146 2.35481

D1 -0.57062 -0.00176 0.00000 -0.00621 -0.00615 -0.57677

D2 2.94484 0.00027 0.00000 0.00194 0.00196 2.94680

D3 1.20616 0.00035 0.00000 -0.01367 -0.01442 1.19174

D4 2.78144 -0.00228 0.00000 -0.03300 -0.03284 2.74860

D5 0.01371 -0.00026 0.00000 -0.02485 -0.02473 -0.01102

D6 -1.72497 -0.00018 0.00000 -0.04046 -0.04111 -1.76608

D7 0.01462 0.00041 0.00000 0.00786 0.00793 0.02255

D8 -2.93773 -0.00075 0.00000 -0.01594 -0.01550 -2.95324

D9 2.94402 0.00123 0.00000 0.03740 0.03705 2.98107

D10 -0.00833 0.00007 0.00000 0.01361 0.01361 0.00528

D11 2.57643 0.00084 0.00000 0.03330 0.03315 2.60958

D12 -1.69757 0.00072 0.00000 0.03361 0.03347 -1.66410

D13 0.43382 0.00036 0.00000 0.02209 0.02211 0.45594

D14 -0.93799 0.00002 0.00000 0.04214 0.04207 -0.89592

D15 1.07120 -0.00009 0.00000 0.04245 0.04240 1.11359

D16 -3.08060 -0.00046 0.00000 0.03093 0.03104 -3.04956

D17 0.89179 0.00086 0.00000 0.02832 0.02871 0.92050

D18 2.90098 0.00075 0.00000 0.02863 0.02904 2.93001

D19 -1.25081 0.00039 0.00000 0.01711 0.01768 -1.23314

D20 -1.23029 0.00214 0.00000 0.07155 0.07110 -1.15920

D21 3.13048 0.00170 0.00000 0.06481 0.06504 -3.08766

D22 1.01308 0.00143 0.00000 0.06557 0.06535 1.07843

D23 0.88995 0.00115 0.00000 0.06657 0.06606 0.95601

D24 -1.03246 0.00072 0.00000 0.05983 0.06001 -0.97245

D25 3.13333 0.00045 0.00000 0.06058 0.06031 -3.08955

D26 2.98668 -0.00089 0.00000 0.02463 0.02422 3.01091

D27 1.06427 -0.00133 0.00000 0.01789 0.01817 1.08244

D28 -1.05313 -0.00160 0.00000 0.01865 0.01847 -1.03466

D29 0.65084 0.00018 0.00000 -0.02725 -0.02735 0.62349

D30 -2.67871 0.00114 0.00000 -0.00590 -0.00609 -2.68480

D31 -2.94213 -0.00069 0.00000 -0.01691 -0.01680 -2.95893

D32 0.01150 0.00027 0.00000 0.00443 0.00446 0.01596

D33 -1.17176 -0.00145 0.00000 -0.02629 -0.02559 -1.19735

D34 1.78187 -0.00048 0.00000 -0.00495 -0.00433 1.77754

D35 -0.73956 0.00002 0.00000 0.04622 0.04611 -0.69345

D36 -2.89916 -0.00026 0.00000 0.03651 0.03662 -2.86254

D37 1.36377 -0.00079 0.00000 0.03497 0.03497 1.39874

D38 2.83563 0.00108 0.00000 0.03639 0.03622 2.87185

D39 0.67603 0.00079 0.00000 0.02669 0.02672 0.70275

D40 -1.34422 0.00027 0.00000 0.02514 0.02507 -1.31915

D41 1.04000 0.00066 0.00000 0.03178 0.03142 1.07142

D42 -1.11960 0.00037 0.00000 0.02207 0.02193 -1.09767

D43 -3.13985 -0.00015 0.00000 0.02052 0.02028 -3.11958

D44 0.84542 0.00016 0.00000 0.06345 0.06407 0.90950

D45 2.79525 0.00204 0.00000 0.07908 0.07898 2.87423

D46 -1.37114 0.00013 0.00000 0.05684 0.05720 -1.31394

D47 -1.24889 0.00061 0.00000 0.05843 0.05919 -1.18970

D48 0.70093 0.00249 0.00000 0.07405 0.07410 0.77503

D49 2.81773 0.00058 0.00000 0.05181 0.05232 2.87005

D50 2.96765 -0.00027 0.00000 0.05846 0.05896 3.02661

D51 -1.36572 0.00161 0.00000 0.07409 0.07387 -1.29185

D52 0.75109 -0.00030 0.00000 0.05185 0.05208 0.80317

D53 0.19678 -0.00071 0.00000 -0.04141 -0.04143 0.15535

D54 2.36087 -0.00018 0.00000 -0.03457 -0.03472 2.32614

D55 -1.88137 -0.00016 0.00000 -0.03497 -0.03503 -1.91640

D56 -1.94586 -0.00108 0.00000 -0.05472 -0.05462 -2.00047

D57 0.21823 -0.00054 0.00000 -0.04789 -0.04791 0.17032

D58 2.25918 -0.00052 0.00000 -0.04828 -0.04822 2.21096

D59 2.31548 -0.00120 0.00000 -0.05315 -0.05308 2.26240

D60 -1.80362 -0.00066 0.00000 -0.04631 -0.04638 -1.85000

D61 0.23733 -0.00064 0.00000 -0.04671 -0.04669 0.19064

D62 -0.07125 0.00087 0.00000 0.05095 0.05132 -0.01993

D63 3.04471 0.00062 0.00000 0.06297 0.06351 3.10822

D64 0.11221 -0.00108 0.00000 -0.06586 -0.06620 0.04602

D65 -3.00708 -0.00108 0.00000 -0.07172 -0.07228 -3.07936

D66 0.21987 -0.00018 0.00000 -0.07489 -0.07466 0.14522

D67 1.98971 0.00119 0.00000 -0.03261 -0.03235 1.95735

D68 -1.57759 -0.00023 0.00000 -0.06829 -0.06800 -1.64558

D69 -1.70449 -0.00138 0.00000 -0.06585 -0.06588 -1.77037

D70 0.06534 -0.00001 0.00000 -0.02357 -0.02358 0.04177

D71 2.78123 -0.00144 0.00000 -0.05925 -0.05922 2.72201

D72 2.00646 -0.00088 0.00000 -0.07975 -0.07981 1.92666

D73 -2.50689 0.00049 0.00000 -0.03747 -0.03750 -2.54439

D74 0.20900 -0.00093 0.00000 -0.07315 -0.07314 0.13586

D75 -1.96333 -0.00189 0.00000 -0.03879 -0.03766 -2.00099

D76 1.21065 -0.00160 0.00000 -0.05395 -0.05305 1.15760

D77 0.00170 -0.00057 0.00000 -0.01655 -0.01663 -0.01493

D78 -3.10750 -0.00028 0.00000 -0.03171 -0.03202 -3.13952

D79 2.60742 -0.00038 0.00000 0.00432 0.00438 2.61180

D80 -0.50178 -0.00009 0.00000 -0.01085 -0.01101 -0.51279

D81 1.79748 -0.00075 0.00000 0.05722 0.05629 1.85377

D82 -1.37287 -0.00070 0.00000 0.06528 0.06449 -1.30838

D83 -0.11195 0.00062 0.00000 0.05614 0.05631 -0.05564

D84 3.00088 0.00067 0.00000 0.06420 0.06451 3.06539

D85 -2.85577 0.00218 0.00000 0.08957 0.08945 -2.76632

D86 0.25706 0.00223 0.00000 0.09763 0.09766 0.35472

Item Value Threshold Converged?

Maximum Force 0.012208 0.000450 NO

RMS Force 0.001976 0.000300 NO

Maximum Displacement 0.219589 0.001800 NO

RMS Displacement 0.054298 0.001200 NO

Predicted change in Energy=-2.605701D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.114106 1.534735 0.413763

2 6 0 0.213462 1.298924 0.058865

3 6 0 -0.793817 3.781650 -0.336715

4 6 0 -1.632972 2.817401 0.224518

5 1 0 -1.681620 0.786876 0.986888

6 1 0 -2.608376 3.093141 0.649280

7 6 0 0.826628 2.015367 -1.089042

8 1 0 1.928255 2.155064 -0.910194

9 1 0 0.742658 1.354941 -1.996509

10 6 0 0.179227 3.361100 -1.383308

11 1 0 0.965884 4.149585 -1.529728

12 1 0 -0.392060 3.288125 -2.351530

13 1 0 -1.095053 4.841852 -0.347395

14 1 0 0.714950 0.362950 0.357610

15 8 0 2.805736 3.728179 0.843083

16 6 0 0.507120 3.895495 1.369105

17 6 0 0.925283 2.587569 1.697482

18 6 0 1.699498 4.601102 0.819555

19 8 0 1.910619 5.723791 0.389926

20 6 0 2.381767 2.505702 1.406885

21 8 0 3.245013 1.657091 1.561721

22 1 0 -0.266288 4.467770 1.889716

23 1 0 0.461790 1.924595 2.430482

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394273 0.000000

3 C 2.390487 2.708324 0.000000

4 C 1.396520 2.396358 1.396044 0.000000

5 H 1.099927 2.171349 3.392461 2.169472 0.000000

6 H 2.171852 3.395670 2.176891 1.099031 2.508329

7 C 2.501176 1.485582 2.512288 2.901436 3.479941

8 H 3.375445 2.147689 3.222473 3.795866 4.301402

9 H 3.047837 2.123146 3.317316 3.565862 3.885934

10 C 2.870154 2.516666 1.489642 2.482897 3.963233

11 H 3.865353 3.349035 2.157592 3.406779 4.964922

12 H 3.352995 3.183329 2.112926 2.897839 4.366263

13 H 3.393633 3.798631 1.102219 2.171369 4.308968

14 H 2.172943 1.103081 3.800786 3.399233 2.513813

15 O 4.512281 3.638154 3.788346 4.573212 5.367338

16 C 3.018980 2.923208 2.148306 2.655628 3.821020

17 C 2.629734 2.202807 2.918748 2.960931 3.247058

18 C 4.181344 3.700180 2.867940 3.826358 5.099832

19 O 5.166983 4.750725 3.407916 4.586011 6.134630

20 C 3.761675 2.824008 3.840901 4.196818 4.431916

21 O 4.509401 3.402523 4.942667 5.189333 5.035814

22 H 3.391154 3.691038 2.388733 2.713748 4.045646

23 H 2.588937 2.465299 3.561261 3.170395 2.823575

6 7 8 9 10

6 H 0.000000

7 C 3.997826 0.000000

8 H 4.888043 1.124759 0.000000

9 H 4.609878 1.125483 1.796084 0.000000

10 C 3.460339 1.522077 2.176571 2.172130 0.000000

11 H 4.317347 2.183685 2.299586 2.842138 1.123377

12 H 3.735631 2.167715 2.957218 2.269543 1.126564

13 H 2.518233 3.497415 4.083621 4.272623 2.211228

14 H 4.310860 2.199036 2.508208 2.554739 3.508091

15 O 5.454672 3.253260 2.513692 4.236961 3.462675

16 C 3.296701 3.111182 3.200614 4.223418 2.822919

17 C 3.720360 2.846377 2.827187 3.898499 3.262854

18 C 4.567354 3.330266 3.004574 4.402650 2.949820

19 O 5.235351 4.137002 3.798214 5.113322 3.424089

20 C 5.081396 2.981365 2.386939 3.948927 3.656237

21 O 6.095651 3.606036 2.844678 4.360514 4.579945

22 H 2.985576 4.010206 4.243127 5.080397 3.483661

23 H 3.736857 3.539548 3.655647 4.472320 4.085142

11 12 13 14 15

11 H 0.000000

12 H 1.805957 0.000000

13 H 2.474794 2.631506 0.000000

14 H 4.238351 4.137821 4.881978 0.000000

15 O 3.031975 4.541487 4.227725 3.991471 0.000000

16 C 2.945889 3.875636 2.531585 3.680379 2.363965

17 C 3.585586 4.315167 3.653091 2.605461 2.359469

18 C 2.502237 4.019242 3.037968 4.375461 1.409365

19 O 2.656260 4.330170 3.217999 5.492657 2.233619

20 C 3.651133 4.736242 4.541297 2.910437 1.411408

21 O 4.578648 5.585885 5.711708 3.086406 2.235802

22 H 3.648574 4.404038 2.414841 4.489959 3.328629

23 H 4.570334 5.045385 4.318651 2.607609 3.356610

16 17 18 19 20

16 C 0.000000

17 C 1.411865 0.000000

18 C 1.490520 2.329051 0.000000

19 O 2.504250 3.537863 1.220485 0.000000

20 C 2.333935 1.487446 2.280603 3.407680 0.000000

21 O 3.541697 2.503072 3.406850 4.437541 1.220372

22 H 1.093936 2.234268 2.242172 2.926753 3.330921

23 H 2.238978 1.091627 3.360163 4.549380 2.252054

21 22 23

21 O 0.000000

22 H 4.509627 0.000000

23 H 2.927907 2.700049 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.227458 -0.966266 -0.546251

2 6 0 1.236017 -1.399320 0.333241

3 6 0 1.516810 1.264818 -0.064932

4 6 0 2.366040 0.406022 -0.765086

5 1 0 2.765195 -1.685353 -1.181539

6 1 0 3.007963 0.780002 -1.574988

7 6 0 0.861719 -0.577318 1.512718

8 1 0 -0.222660 -0.738312 1.764288

9 1 0 1.443483 -0.955135 2.399011

10 6 0 1.131320 0.909431 1.329389

11 1 0 0.241558 1.511415 1.657893

12 1 0 1.990251 1.209919 1.993537

13 1 0 1.468279 2.334137 -0.327778

14 1 0 0.971020 -2.468283 0.395550

15 8 0 -2.073808 0.110451 0.290688

16 6 0 -0.254365 0.655217 -1.116858

17 6 0 -0.342688 -0.752748 -1.060313

18 6 0 -1.344082 1.187875 -0.250577

19 8 0 -1.726178 2.304722 0.059646

20 6 0 -1.517315 -1.085789 -0.210707

21 8 0 -2.082338 -2.118191 0.112099

22 1 0 0.085461 1.239242 -1.977165

23 1 0 0.022564 -1.455017 -1.812017

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2239151 0.8732222 0.6707904

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.1436066964 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.494476076765E-01 A.U. after 15 cycles

Convg = 0.5110D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001611819 -0.001068883 0.000901034

2 6 -0.002396963 -0.001528917 0.002659663

3 6 -0.001551313 0.000692682 -0.000652162

4 6 0.001140631 0.000834371 0.000244936

5 1 -0.000054774 -0.000227736 -0.000479072

6 1 0.000007661 0.000081631 0.000011850

7 6 0.002124555 0.001740937 -0.001886443

8 1 0.000339798 -0.000277483 -0.000570809

9 1 -0.000842884 -0.000094066 -0.000078974

10 6 -0.000066905 -0.000375962 -0.000098591

11 1 0.000107720 -0.000431733 0.000593552

12 1 0.000556475 0.000618922 -0.000364068

13 1 0.000143029 -0.000002887 -0.000655654

14 1 -0.000293035 0.000662065 0.000881309

15 8 -0.000454649 -0.000288836 0.000861690

16 6 0.000609438 -0.002062008 0.002534439

17 6 0.000579172 0.001478296 -0.002662564

18 6 0.000309663 -0.000044376 0.000234586

19 8 -0.000075907 -0.000240806 -0.000384137

20 6 -0.001334835 0.000914662 0.000058344

21 8 -0.000359330 -0.000093745 -0.000918392

22 1 -0.000545269 -0.000581857 -0.000428409

23 1 0.000445903 0.000295731 0.000197875

-------------------------------------------------------------------

Cartesian Forces: Max 0.002662564 RMS 0.000991269

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.002994334 RMS 0.000453441

Search for a saddle point.

Step number 49 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 47 48 49

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07180 -0.00158 0.00411 0.00808 0.00852

Eigenvalues --- 0.01061 0.01150 0.01349 0.01938 0.02328

Eigenvalues --- 0.02537 0.02797 0.03080 0.03190 0.03265

Eigenvalues --- 0.03538 0.03583 0.03656 0.03842 0.04016

Eigenvalues --- 0.04189 0.04329 0.04579 0.04868 0.06047

Eigenvalues --- 0.06347 0.06476 0.06895 0.07358 0.08360

Eigenvalues --- 0.08952 0.09116 0.09936 0.10060 0.10504

Eigenvalues --- 0.12105 0.13866 0.14477 0.17116 0.21972

Eigenvalues --- 0.26084 0.27614 0.28905 0.29876 0.30269

Eigenvalues --- 0.31168 0.31321 0.31826 0.31985 0.32413

Eigenvalues --- 0.32627 0.33287 0.35718 0.37192 0.39080

Eigenvalues --- 0.39701 0.40449 0.43365 0.47836 0.50469

Eigenvalues --- 0.58549 1.08508 1.10884

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D73

1 0.58118 0.50743 -0.14583 0.14356 -0.14329

D71 D86 D1 D35 D29

1 0.14205 -0.13252 0.13011 0.12809 -0.12520

RFO step: Lambda0=1.723556505D-06 Lambda=-3.28406174D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.10861793 RMS(Int)= 0.00464420

Iteration 2 RMS(Cart)= 0.00604657 RMS(Int)= 0.00126066

Iteration 3 RMS(Cart)= 0.00001253 RMS(Int)= 0.00126063

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00126063

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63479 -0.00156 0.00000 -0.00276 -0.00141 2.63338

R2 2.63904 0.00086 0.00000 0.00483 0.00689 2.64593

R3 2.07856 -0.00007 0.00000 -0.00206 -0.00206 2.07650

R4 2.80734 0.00299 0.00000 0.04098 0.04015 2.84750

R5 2.08452 -0.00046 0.00000 -0.00733 -0.00733 2.07719

R6 4.16270 -0.00104 0.00000 -0.13602 -0.13645 4.02625

R7 2.63814 -0.00044 0.00000 0.00158 0.00218 2.64032

R8 2.81501 0.00057 0.00000 0.00427 0.00402 2.81903

R9 2.08289 -0.00004 0.00000 -0.00178 -0.00178 2.08111

R10 4.05971 0.00030 0.00000 0.05168 0.05167 4.11138

R11 2.07687 0.00002 0.00000 0.00143 0.00143 2.07830

R12 2.12549 0.00021 0.00000 -0.00139 -0.00139 2.12410

R13 2.12685 0.00018 0.00000 0.00088 0.00088 2.12773

R14 2.87631 -0.00011 0.00000 -0.00064 -0.00198 2.87433

R15 2.12288 -0.00030 0.00000 -0.00009 -0.00009 2.12278

R16 2.12890 -0.00001 0.00000 -0.00094 -0.00094 2.12796

R17 2.66331 -0.00073 0.00000 -0.00279 -0.00256 2.66075

R18 2.66717 -0.00093 0.00000 -0.00748 -0.00748 2.65969

R19 2.66804 -0.00202 0.00000 -0.00420 -0.00508 2.66296

R20 2.81667 -0.00016 0.00000 -0.00184 -0.00170 2.81498

R21 2.06724 -0.00012 0.00000 -0.00493 -0.00493 2.06231

R22 2.81087 -0.00153 0.00000 -0.01545 -0.01567 2.79519

R23 2.06288 -0.00024 0.00000 0.00221 0.00221 2.06509

R24 2.30638 -0.00010 0.00000 -0.00030 -0.00030 2.30608

R25 2.30617 -0.00031 0.00000 0.00075 0.00075 2.30692

A1 2.06532 -0.00028 0.00000 -0.00821 -0.00940 2.05592

A2 2.10471 0.00003 0.00000 -0.00496 -0.00447 2.10024

A3 2.09832 0.00028 0.00000 0.01648 0.01688 2.11520

A4 2.10379 0.00023 0.00000 -0.00979 -0.01070 2.09309

A5 2.10301 -0.00028 0.00000 -0.02239 -0.02148 2.08153

A6 1.59019 -0.00009 0.00000 0.02590 0.02448 1.61468

A7 2.01621 0.00017 0.00000 0.02504 0.02507 2.04128

A8 1.73077 -0.00020 0.00000 0.01925 0.01868 1.74945

A9 1.71935 -0.00004 0.00000 -0.02839 -0.02677 1.69258

A10 2.07156 0.00020 0.00000 0.01574 0.01455 2.08610

A11 2.09901 0.00022 0.00000 0.01173 0.01291 2.11192

A12 1.65228 -0.00080 0.00000 -0.05181 -0.05305 1.59923

A13 2.03004 -0.00031 0.00000 -0.01261 -0.01311 2.01693

A14 1.74901 0.00013 0.00000 -0.00037 -0.00063 1.74838

A15 1.69332 0.00043 0.00000 0.01890 0.02055 1.71388

A16 2.05504 0.00046 0.00000 0.01469 0.01275 2.06779

A17 2.10344 -0.00017 0.00000 -0.00079 0.00004 2.10348

A18 2.11246 -0.00029 0.00000 -0.01462 -0.01363 2.09883

A19 1.91908 0.00020 0.00000 -0.00217 -0.00086 1.91822

A20 1.88519 0.00007 0.00000 -0.00920 -0.00821 1.87698

A21 1.98255 -0.00038 0.00000 -0.00515 -0.00894 1.97362

A22 1.84852 -0.00001 0.00000 0.00932 0.00873 1.85725

A23 1.91508 0.00010 0.00000 0.00943 0.01002 1.92510

A24 1.90837 0.00006 0.00000 -0.00151 0.00003 1.90840

A25 1.97318 0.00001 0.00000 0.01794 0.01474 1.98792

A26 1.92926 0.00014 0.00000 -0.00409 -0.00307 1.92619

A27 1.86594 0.00003 0.00000 0.00294 0.00371 1.86964

A28 1.92615 -0.00026 0.00000 -0.01575 -0.01518 1.91097

A29 1.90136 0.00016 0.00000 0.00849 0.00966 1.91102

A30 1.86351 -0.00008 0.00000 -0.01023 -0.01067 1.85284

A31 1.88321 -0.00029 0.00000 -0.00044 -0.00059 1.88261

A32 1.89119 0.00017 0.00000 -0.02009 -0.02559 1.86560

A33 1.78930 -0.00064 0.00000 -0.07690 -0.07587 1.71342

A34 1.54827 0.00010 0.00000 0.02969 0.03286 1.58113

A35 1.86227 0.00007 0.00000 -0.00040 -0.00083 1.86144

A36 2.19362 -0.00005 0.00000 0.00583 0.00475 2.19837

A37 2.08678 0.00015 0.00000 0.02893 0.02862 2.11541

A38 1.84753 0.00056 0.00000 0.05019 0.04512 1.89265

A39 1.71014 -0.00041 0.00000 0.00836 0.01063 1.72077

A40 1.57780 -0.00029 0.00000 -0.02403 -0.02225 1.55556

A41 1.87084 0.00020 0.00000 0.00144 0.00178 1.87262

A42 2.20562 -0.00017 0.00000 -0.01300 -0.01295 2.19267

A43 2.11007 0.00004 0.00000 -0.00304 -0.00361 2.10646

A44 1.90557 -0.00028 0.00000 -0.00248 -0.00261 1.90295

A45 2.02622 0.00009 0.00000 -0.00161 -0.00177 2.02445

A46 2.35129 0.00020 0.00000 0.00452 0.00439 2.35568

A47 1.90128 0.00031 0.00000 0.00449 0.00382 1.90510

A48 2.02694 -0.00023 0.00000 -0.00736 -0.00722 2.01972

A49 2.35481 -0.00008 0.00000 0.00335 0.00351 2.35832

D1 -0.57677 0.00020 0.00000 -0.01655 -0.01657 -0.59334

D2 2.94680 -0.00020 0.00000 -0.00015 -0.00121 2.94560

D3 1.19174 -0.00006 0.00000 0.02029 0.01832 1.21006

D4 2.74860 0.00002 0.00000 -0.03855 -0.03770 2.71090

D5 -0.01102 -0.00037 0.00000 -0.02215 -0.02233 -0.03335

D6 -1.76608 -0.00024 0.00000 -0.00171 -0.00281 -1.76889

D7 0.02255 -0.00002 0.00000 -0.03215 -0.03211 -0.00955

D8 -2.95324 0.00003 0.00000 -0.02594 -0.02520 -2.97844

D9 2.98107 0.00013 0.00000 -0.01256 -0.01315 2.96793

D10 0.00528 0.00018 0.00000 -0.00634 -0.00624 -0.00096

D11 2.60958 0.00004 0.00000 0.12640 0.12534 2.73491

D12 -1.66410 0.00016 0.00000 0.13123 0.13071 -1.53339

D13 0.45594 0.00003 0.00000 0.11943 0.11934 0.57528

D14 -0.89592 0.00032 0.00000 0.10128 0.10081 -0.79511

D15 1.11359 0.00044 0.00000 0.10611 0.10618 1.21977

D16 -3.04956 0.00031 0.00000 0.09431 0.09481 -2.95475

D17 0.92050 0.00021 0.00000 0.08620 0.08760 1.00811

D18 2.93001 0.00033 0.00000 0.09104 0.09297 3.02299

D19 -1.23314 0.00021 0.00000 0.07923 0.08161 -1.15153

D20 -1.15920 0.00012 0.00000 0.12893 0.13036 -1.02883

D21 -3.08766 -0.00008 0.00000 0.11158 0.11193 -2.97573

D22 1.07843 -0.00003 0.00000 0.11793 0.11843 1.19686

D23 0.95601 0.00031 0.00000 0.12646 0.12738 1.08339

D24 -0.97245 0.00011 0.00000 0.10910 0.10894 -0.86351

D25 -3.08955 0.00016 0.00000 0.11545 0.11545 -2.97410

D26 3.01091 0.00043 0.00000 0.15009 0.15100 -3.12128

D27 1.08244 0.00022 0.00000 0.13273 0.13256 1.21501

D28 -1.03466 0.00027 0.00000 0.13908 0.13907 -0.89559

D29 0.62349 -0.00007 0.00000 -0.01855 -0.01853 0.60497

D30 -2.68480 -0.00010 0.00000 -0.02340 -0.02406 -2.70886

D31 -2.95893 0.00015 0.00000 0.01582 0.01674 -2.94220

D32 0.01596 0.00011 0.00000 0.01097 0.01120 0.02716

D33 -1.19735 0.00021 0.00000 0.00870 0.01052 -1.18683

D34 1.77754 0.00017 0.00000 0.00385 0.00499 1.78253

D35 -0.69345 0.00042 0.00000 0.12247 0.12261 -0.57084

D36 -2.86254 0.00064 0.00000 0.13302 0.13406 -2.72848

D37 1.39874 0.00064 0.00000 0.14563 0.14624 1.54498

D38 2.87185 0.00008 0.00000 0.08372 0.08316 2.95500

D39 0.70275 0.00031 0.00000 0.09427 0.09462 0.79737

D40 -1.31915 0.00031 0.00000 0.10688 0.10679 -1.21236

D41 1.07142 -0.00039 0.00000 0.06587 0.06379 1.13521

D42 -1.09767 -0.00016 0.00000 0.07642 0.07525 -1.02242

D43 -3.11958 -0.00016 0.00000 0.08903 0.08742 -3.03216

D44 0.90950 0.00017 0.00000 0.14285 0.14011 1.04961

D45 2.87423 0.00002 0.00000 0.10006 0.09965 2.97388

D46 -1.31394 0.00014 0.00000 0.12920 0.12805 -1.18590

D47 -1.18970 0.00014 0.00000 0.13990 0.13799 -1.05171

D48 0.77503 0.00000 0.00000 0.09712 0.09753 0.87256

D49 2.87005 0.00011 0.00000 0.12626 0.12593 2.99597

D50 3.02661 0.00032 0.00000 0.14802 0.14619 -3.11039

D51 -1.29185 0.00017 0.00000 0.10523 0.10573 -1.18612

D52 0.80317 0.00029 0.00000 0.13437 0.13412 0.93729

D53 0.15535 -0.00016 0.00000 -0.15790 -0.15771 -0.00236

D54 2.32614 -0.00017 0.00000 -0.16211 -0.16265 2.16349

D55 -1.91640 -0.00032 0.00000 -0.17851 -0.17859 -2.09500

D56 -2.00047 -0.00022 0.00000 -0.15854 -0.15774 -2.15821

D57 0.17032 -0.00022 0.00000 -0.16275 -0.16267 0.00765

D58 2.21096 -0.00037 0.00000 -0.17915 -0.17861 2.03234

D59 2.26240 -0.00029 0.00000 -0.17419 -0.17402 2.08838

D60 -1.85000 -0.00030 0.00000 -0.17840 -0.17895 -2.02895

D61 0.19064 -0.00045 0.00000 -0.19480 -0.19490 -0.00426

D62 -0.01993 0.00010 0.00000 0.01323 0.01413 -0.00579

D63 3.10822 0.00032 0.00000 0.03951 0.04072 -3.13425

D64 0.04602 -0.00016 0.00000 -0.03532 -0.03639 0.00962

D65 -3.07936 -0.00029 0.00000 -0.06021 -0.06154 -3.14090

D66 0.14522 -0.00055 0.00000 -0.16162 -0.16281 -0.01759

D67 1.95735 -0.00072 0.00000 -0.13232 -0.13204 1.82532

D68 -1.64558 -0.00054 0.00000 -0.16497 -0.16383 -1.80942

D69 -1.77037 0.00008 0.00000 -0.06489 -0.06645 -1.83682

D70 0.04177 -0.00009 0.00000 -0.03559 -0.03567 0.00609

D71 2.72201 0.00008 0.00000 -0.06824 -0.06747 2.65455

D72 1.92666 -0.00030 0.00000 -0.13555 -0.13767 1.78899

D73 -2.54439 -0.00047 0.00000 -0.10625 -0.10689 -2.65128

D74 0.13586 -0.00030 0.00000 -0.13890 -0.13869 -0.00283

D75 -2.00099 0.00006 0.00000 0.07029 0.07295 -1.92804

D76 1.15760 -0.00021 0.00000 0.03717 0.03926 1.19685

D77 -0.01493 0.00000 0.00000 0.01511 0.01454 -0.00039

D78 -3.13952 -0.00027 0.00000 -0.01802 -0.01916 3.12451

D79 2.61180 0.00028 0.00000 0.07261 0.07319 2.68500

D80 -0.51279 0.00001 0.00000 0.03948 0.03950 -0.47329

D81 1.85377 0.00064 0.00000 0.10260 0.09919 1.95296

D82 -1.30838 0.00080 0.00000 0.13402 0.13115 -1.17723

D83 -0.05564 0.00014 0.00000 0.04497 0.04573 -0.00992

D84 3.06539 0.00030 0.00000 0.07639 0.07769 -3.14010

D85 -2.76632 0.00005 0.00000 0.07874 0.07871 -2.68761

D86 0.35472 0.00021 0.00000 0.11016 0.11068 0.46540

Item Value Threshold Converged?

Maximum Force 0.002994 0.000450 NO

RMS Force 0.000453 0.000300 NO

Maximum Displacement 0.578994 0.001800 NO

RMS Displacement 0.108456 0.001200 NO

Predicted change in Energy=-3.180794D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.126994 1.566543 0.461898

2 6 0 0.197321 1.291402 0.126629

3 6 0 -0.748076 3.787880 -0.374871

4 6 0 -1.613983 2.852287 0.196993

5 1 0 -1.710443 0.847776 1.053849

6 1 0 -2.596190 3.167133 0.578668

7 6 0 0.815213 1.936727 -1.086755

8 1 0 1.933791 1.961756 -0.979092

9 1 0 0.595476 1.275944 -1.971537

10 6 0 0.279625 3.334544 -1.356547

11 1 0 1.134097 4.062873 -1.392325

12 1 0 -0.199502 3.363242 -2.375196

13 1 0 -1.020630 4.853459 -0.430197

14 1 0 0.661084 0.362470 0.487538

15 8 0 2.732666 3.842830 0.805936

16 6 0 0.458004 3.869667 1.434033

17 6 0 0.948606 2.567813 1.658233

18 6 0 1.594694 4.667221 0.894761

19 8 0 1.738263 5.819322 0.518937

20 6 0 2.375824 2.562812 1.269754

21 8 0 3.265492 1.727010 1.255331

22 1 0 -0.362220 4.347005 1.972896

23 1 0 0.571481 1.865290 2.405523

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.393527 0.000000

3 C 2.403768 2.716189 0.000000

4 C 1.400168 2.392099 1.397196 0.000000

5 H 1.098838 2.167050 3.407580 2.182103 0.000000

6 H 2.175790 3.395057 2.170274 1.099788 2.527798

7 C 2.511479 1.506830 2.525356 2.896076 3.485246

8 H 3.406031 2.165022 3.300337 3.842255 4.319055

9 H 2.995490 2.135666 3.265624 3.474060 3.827996

10 C 2.900198 2.526068 1.491769 2.496360 3.994296

11 H 3.844780 3.296335 2.157176 3.397557 4.940852

12 H 3.483887 3.272480 2.117204 2.979595 4.513188

13 H 3.407486 3.805485 1.101274 2.179478 4.327093

14 H 2.155845 1.099202 3.803014 3.385193 2.486034

15 O 4.494087 3.660494 3.675989 4.499483 5.364049

16 C 2.960007 2.902535 2.175650 2.618866 3.738787

17 C 2.596512 2.130602 2.915614 2.963615 3.224028

18 C 4.148392 3.733474 2.806025 3.751863 5.053454

19 O 5.128262 4.799007 3.332796 4.488262 6.074206

20 C 3.730269 2.769312 3.736888 4.141639 4.436839

21 O 4.466455 3.298090 4.797237 5.118165 5.057033

22 H 3.255605 3.613655 2.444078 2.637219 3.860953

23 H 2.598412 2.379643 3.628798 3.260065 2.840693

6 7 8 9 10

6 H 0.000000

7 C 3.990640 0.000000

8 H 4.939663 1.124026 0.000000

9 H 4.501875 1.125948 1.801769 0.000000

10 C 3.470360 1.521031 2.182495 2.171591 0.000000

11 H 4.313027 2.171533 2.285818 2.896994 1.123327

12 H 3.808922 2.173632 2.909332 2.269745 1.126069

13 H 2.518709 3.508378 4.170352 4.217362 2.203609

14 H 4.299333 2.231689 2.515651 2.624079 3.518435

15 O 5.376330 3.300323 2.713478 4.344058 3.309395

16 C 3.248585 3.196597 3.411926 4.283014 2.847019

17 C 3.753695 2.819756 2.879821 3.868961 3.181872

18 C 4.462476 3.462599 3.308451 4.551358 2.928109

19 O 5.081846 4.301722 4.142841 5.305724 3.437904

20 C 5.056058 2.894930 2.369381 3.915563 3.447764

21 O 6.073808 3.396059 2.611739 4.212496 4.280360

22 H 2.885583 4.069061 4.435686 5.089907 3.538678

23 H 3.881537 3.501502 3.649769 4.416624 4.049329

11 12 13 14 15

11 H 0.000000

12 H 1.798334 0.000000

13 H 2.488687 2.584187 0.000000

14 H 4.177392 4.235621 4.882559 0.000000

15 O 2.726938 4.352840 4.078802 4.062725 0.000000

16 C 2.912512 3.898591 2.574793 3.638341 2.359940

17 C 3.402280 4.268420 3.669279 2.513312 2.352646

18 C 2.410010 3.951218 2.937707 4.423611 1.408009

19 O 2.665155 4.261839 3.073310 5.562242 2.231082

20 C 3.298292 4.534165 4.435402 2.897188 1.407448

21 O 4.124219 5.278652 5.566555 3.038819 2.227679

22 H 3.693834 4.460962 2.542609 4.373781 3.345790

23 H 4.423749 5.068881 4.416478 2.438271 3.337673

16 17 18 19 20

16 C 0.000000

17 C 1.409177 0.000000

18 C 1.489621 2.325474 0.000000

19 O 2.505518 3.534665 1.220325 0.000000

20 C 2.326562 1.479152 2.275812 3.402215 0.000000

21 O 3.536228 2.497447 3.400944 4.429642 1.220772

22 H 1.091326 2.232219 2.257084 2.948516 3.342849

23 H 2.230291 1.092797 3.343678 4.533757 2.243248

21 22 23

21 O 0.000000

22 H 4.532061 0.000000

23 H 2.932535 2.686610 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.288087 -0.689947 -0.662719

2 6 0 1.345123 -1.350346 0.122526

3 6 0 1.350145 1.365612 0.157671

4 6 0 2.292765 0.710003 -0.638445

5 1 0 2.894687 -1.248565 -1.388962

6 1 0 2.908628 1.278897 -1.350207

7 6 0 0.926168 -0.764554 1.446105

8 1 0 -0.089225 -1.152617 1.732144

9 1 0 1.643189 -1.143509 2.227151

10 6 0 0.931063 0.756452 1.453306

11 1 0 -0.084196 1.133109 1.752042

12 1 0 1.646572 1.126196 2.240305

13 1 0 1.190078 2.451608 0.069380

14 1 0 1.192823 -2.430221 -0.015021

15 8 0 -2.057931 -0.008501 0.256285

16 6 0 -0.281007 0.706531 -1.122332

17 6 0 -0.270184 -0.702515 -1.106524

18 6 0 -1.415438 1.134439 -0.256922

19 8 0 -1.873540 2.209142 0.095707

20 6 0 -1.391407 -1.141226 -0.247290

21 8 0 -1.836135 -2.220316 0.110570

22 1 0 0.083017 1.341112 -1.932138

23 1 0 0.103387 -1.345307 -1.907442

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2175531 0.8978544 0.6870416

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.8531333222 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.495608279371E-01 A.U. after 16 cycles

Convg = 0.4277D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.005429703 0.007630286 -0.004746277

2 6 0.006505808 0.005768876 -0.008607101

3 6 0.002450268 -0.004676892 0.002015831

4 6 0.000371807 -0.003383470 0.001113539

5 1 -0.001178533 0.000830463 0.000011433

6 1 0.000056767 -0.000634964 0.000085224

7 6 -0.006489157 -0.006311393 0.009059188

8 1 -0.000670291 -0.000140065 -0.000610155

9 1 -0.000213849 0.000136163 0.001037258

10 6 -0.000412377 0.000105296 0.000633328

11 1 0.000112354 0.001054269 0.000017982

12 1 -0.000028813 -0.000561627 -0.000046022

13 1 -0.000675458 0.000131980 0.000572762

14 1 0.002731569 -0.001988371 -0.002187760

15 8 0.001710277 0.001844106 -0.000882652

16 6 -0.000205531 0.004468162 -0.005010365

17 6 -0.004984233 -0.005541337 0.003053607

18 6 -0.002376257 0.001159172 0.000849375

19 8 -0.000093689 0.001360684 0.000358708

20 6 0.007021674 -0.001201727 -0.000086868

21 8 0.000858672 -0.001447514 0.000886460

22 1 0.000114452 0.000776218 0.000050421

23 1 0.000824245 0.000621686 0.002432084

-------------------------------------------------------------------

Cartesian Forces: Max 0.009059188 RMS 0.003141496

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.012305026 RMS 0.001668020

Search for a saddle point.

Step number 50 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 43 45 46 49

50

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07121 0.00186 0.00292 0.00447 0.00716

Eigenvalues --- 0.00937 0.01122 0.01292 0.01717 0.02320

Eigenvalues --- 0.02533 0.02788 0.03082 0.03142 0.03285

Eigenvalues --- 0.03473 0.03592 0.03625 0.03819 0.04047

Eigenvalues --- 0.04183 0.04300 0.04737 0.04855 0.06070

Eigenvalues --- 0.06362 0.06670 0.06889 0.07345 0.08313

Eigenvalues --- 0.08971 0.09154 0.10033 0.10108 0.10671

Eigenvalues --- 0.12126 0.13887 0.14624 0.17051 0.21921

Eigenvalues --- 0.26047 0.27765 0.29319 0.29860 0.30331

Eigenvalues --- 0.31171 0.31332 0.31879 0.31995 0.32413

Eigenvalues --- 0.32616 0.33424 0.36197 0.37354 0.39330

Eigenvalues --- 0.39705 0.40455 0.43614 0.47913 0.51177

Eigenvalues --- 0.58904 1.08534 1.10909

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 -0.57222 -0.50815 -0.15191 0.14523 0.14483

D4 D86 D1 D29 D35

1 -0.13136 0.13102 -0.12989 0.12950 -0.12863

RFO step: Lambda0=3.257996999D-05 Lambda=-1.77068855D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.02015773 RMS(Int)= 0.00014233

Iteration 2 RMS(Cart)= 0.00016812 RMS(Int)= 0.00005706

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00005706

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63338 0.00476 0.00000 0.00267 0.00267 2.63605

R2 2.64593 -0.00697 0.00000 -0.00898 -0.00900 2.63693

R3 2.07650 0.00009 0.00000 0.00103 0.00103 2.07753

R4 2.84750 -0.01231 0.00000 -0.03386 -0.03390 2.81360

R5 2.07719 0.00211 0.00000 0.00634 0.00634 2.08354

R6 4.02625 0.00338 0.00000 0.06337 0.06333 4.08959

R7 2.64032 -0.00159 0.00000 -0.00496 -0.00499 2.63533

R8 2.81903 -0.00196 0.00000 -0.00445 -0.00446 2.81458

R9 2.08111 0.00027 0.00000 0.00184 0.00184 2.08295

R10 4.11138 -0.00101 0.00000 -0.00046 -0.00039 4.11100

R11 2.07830 -0.00020 0.00000 -0.00082 -0.00082 2.07748

R12 2.12410 -0.00073 0.00000 0.00017 0.00017 2.12427

R13 2.12773 -0.00085 0.00000 -0.00004 -0.00004 2.12769

R14 2.87433 -0.00012 0.00000 0.00240 0.00235 2.87669

R15 2.12278 0.00077 0.00000 0.00174 0.00174 2.12452

R16 2.12796 0.00004 0.00000 0.00010 0.00010 2.12806

R17 2.66075 0.00293 0.00000 0.00392 0.00392 2.66468

R18 2.65969 0.00332 0.00000 0.00417 0.00414 2.66383

R19 2.66296 0.00459 0.00000 0.00232 0.00240 2.66535

R20 2.81498 -0.00003 0.00000 -0.00319 -0.00316 2.81182

R21 2.06231 0.00028 0.00000 0.00212 0.00212 2.06443

R22 2.79519 0.00694 0.00000 0.01938 0.01935 2.81454

R23 2.06509 0.00098 0.00000 -0.00001 -0.00001 2.06508

R24 2.30608 0.00116 0.00000 0.00065 0.00065 2.30673

R25 2.30692 0.00161 0.00000 -0.00036 -0.00036 2.30657

A1 2.05592 0.00119 0.00000 0.00711 0.00705 2.06298

A2 2.10024 0.00088 0.00000 0.01004 0.01007 2.11031

A3 2.11520 -0.00207 0.00000 -0.01662 -0.01660 2.09860

A4 2.09309 -0.00139 0.00000 -0.00637 -0.00632 2.08677

A5 2.08153 0.00220 0.00000 0.01857 0.01844 2.09997

A6 1.61468 0.00024 0.00000 0.00650 0.00638 1.62106

A7 2.04128 -0.00134 0.00000 -0.01647 -0.01645 2.02482

A8 1.74945 0.00129 0.00000 -0.00598 -0.00599 1.74346

A9 1.69258 -0.00006 0.00000 0.01183 0.01177 1.70435

A10 2.08610 -0.00062 0.00000 0.00283 0.00285 2.08895

A11 2.11192 -0.00075 0.00000 -0.00897 -0.00896 2.10296

A12 1.59923 0.00202 0.00000 0.01391 0.01390 1.61313

A13 2.01693 0.00100 0.00000 0.00410 0.00405 2.02098

A14 1.74838 0.00000 0.00000 -0.00584 -0.00584 1.74254

A15 1.71388 -0.00122 0.00000 -0.00366 -0.00361 1.71026

A16 2.06779 -0.00059 0.00000 -0.00614 -0.00623 2.06156

A17 2.10348 -0.00025 0.00000 -0.00243 -0.00241 2.10107

A18 2.09883 0.00093 0.00000 0.00996 0.00999 2.10882

A19 1.91822 -0.00040 0.00000 0.00577 0.00581 1.92403

A20 1.87698 -0.00068 0.00000 -0.00576 -0.00576 1.87122

A21 1.97362 0.00148 0.00000 0.00811 0.00808 1.98170

A22 1.85725 0.00019 0.00000 -0.00055 -0.00056 1.85669

A23 1.92510 -0.00032 0.00000 -0.00670 -0.00676 1.91834

A24 1.90840 -0.00035 0.00000 -0.00138 -0.00135 1.90705

A25 1.98792 -0.00084 0.00000 -0.00627 -0.00627 1.98165

A26 1.92619 0.00013 0.00000 -0.00207 -0.00208 1.92411

A27 1.86964 0.00015 0.00000 0.00454 0.00453 1.87418

A28 1.91097 0.00086 0.00000 0.00793 0.00794 1.91891

A29 1.91102 -0.00021 0.00000 -0.00370 -0.00371 1.90731

A30 1.85284 -0.00006 0.00000 -0.00021 -0.00020 1.85264

A31 1.88261 0.00089 0.00000 0.00102 0.00102 1.88364

A32 1.86560 -0.00035 0.00000 0.00843 0.00834 1.87394

A33 1.71342 0.00176 0.00000 0.01743 0.01733 1.73075

A34 1.58113 -0.00075 0.00000 -0.01551 -0.01545 1.56568

A35 1.86144 0.00046 0.00000 0.00691 0.00679 1.86823

A36 2.19837 0.00032 0.00000 0.00002 0.00001 2.19838

A37 2.11541 -0.00105 0.00000 -0.01114 -0.01107 2.10434

A38 1.89265 -0.00207 0.00000 -0.01587 -0.01584 1.87681

A39 1.72077 0.00181 0.00000 0.02077 0.02075 1.74152

A40 1.55556 0.00150 0.00000 0.01249 0.01255 1.56810

A41 1.87262 -0.00052 0.00000 -0.00655 -0.00645 1.86617

A42 2.19267 0.00013 0.00000 0.00478 0.00476 2.19743

A43 2.10646 -0.00022 0.00000 -0.00686 -0.00709 2.09937

A44 1.90295 0.00089 0.00000 0.00020 0.00024 1.90319

A45 2.02445 0.00004 0.00000 0.00155 0.00151 2.02596

A46 2.35568 -0.00093 0.00000 -0.00163 -0.00167 2.35401

A47 1.90510 -0.00172 0.00000 -0.00160 -0.00164 1.90346

A48 2.01972 0.00174 0.00000 0.00741 0.00740 2.02712

A49 2.35832 -0.00002 0.00000 -0.00570 -0.00571 2.35260

D1 -0.59334 -0.00121 0.00000 -0.01194 -0.01198 -0.60532

D2 2.94560 0.00056 0.00000 0.00378 0.00388 2.94947

D3 1.21006 0.00019 0.00000 -0.01617 -0.01630 1.19376

D4 2.71090 -0.00104 0.00000 -0.01397 -0.01401 2.69689

D5 -0.03335 0.00074 0.00000 0.00175 0.00185 -0.03150

D6 -1.76889 0.00037 0.00000 -0.01820 -0.01833 -1.78722

D7 -0.00955 0.00040 0.00000 0.01800 0.01801 0.00845

D8 -2.97844 -0.00029 0.00000 0.00792 0.00799 -2.97045

D9 2.96793 0.00051 0.00000 0.02269 0.02262 2.99054

D10 -0.00096 -0.00017 0.00000 0.01260 0.01260 0.01164

D11 2.73491 0.00065 0.00000 -0.00009 -0.00013 2.73478

D12 -1.53339 0.00029 0.00000 -0.00090 -0.00096 -1.53435

D13 0.57528 0.00031 0.00000 -0.00154 -0.00159 0.57369

D14 -0.79511 -0.00030 0.00000 -0.00773 -0.00767 -0.80278

D15 1.21977 -0.00066 0.00000 -0.00855 -0.00849 1.21127

D16 -2.95475 -0.00064 0.00000 -0.00918 -0.00912 -2.96387

D17 1.00811 -0.00005 0.00000 -0.00239 -0.00233 1.00577

D18 3.02299 -0.00041 0.00000 -0.00321 -0.00316 3.01982

D19 -1.15153 -0.00039 0.00000 -0.00384 -0.00379 -1.15532

D20 -1.02883 0.00100 0.00000 -0.00309 -0.00306 -1.03189

D21 -2.97573 0.00142 0.00000 0.00007 0.00021 -2.97552

D22 1.19686 0.00127 0.00000 0.00343 0.00334 1.20020

D23 1.08339 -0.00017 0.00000 -0.00905 -0.00903 1.07436

D24 -0.86351 0.00025 0.00000 -0.00590 -0.00576 -0.86926

D25 -2.97410 0.00010 0.00000 -0.00254 -0.00263 -2.97673

D26 -3.12128 -0.00127 0.00000 -0.02444 -0.02446 3.13744

D27 1.21501 -0.00085 0.00000 -0.02129 -0.02119 1.19382

D28 -0.89559 -0.00100 0.00000 -0.01793 -0.01807 -0.91365

D29 0.60497 -0.00007 0.00000 -0.01119 -0.01115 0.59382

D30 -2.70886 0.00050 0.00000 -0.00239 -0.00236 -2.71122

D31 -2.94220 -0.00086 0.00000 -0.01603 -0.01598 -2.95817

D32 0.02716 -0.00030 0.00000 -0.00723 -0.00719 0.01997

D33 -1.18683 -0.00116 0.00000 -0.01302 -0.01304 -1.19987

D34 1.78253 -0.00059 0.00000 -0.00423 -0.00425 1.77828

D35 -0.57084 -0.00077 0.00000 -0.00268 -0.00267 -0.57351

D36 -2.72848 -0.00139 0.00000 -0.00689 -0.00689 -2.73536

D37 1.54498 -0.00146 0.00000 -0.00810 -0.00809 1.53688

D38 2.95500 0.00036 0.00000 0.00486 0.00487 2.95988

D39 0.79737 -0.00026 0.00000 0.00064 0.00065 0.79802

D40 -1.21236 -0.00033 0.00000 -0.00056 -0.00055 -1.21292

D41 1.13521 0.00146 0.00000 0.01096 0.01096 1.14617

D42 -1.02242 0.00084 0.00000 0.00674 0.00673 -1.01569

D43 -3.03216 0.00077 0.00000 0.00554 0.00553 -3.02663

D44 1.04961 0.00007 0.00000 -0.00972 -0.00981 1.03980

D45 2.97388 0.00113 0.00000 0.00653 0.00659 2.98047

D46 -1.18590 0.00012 0.00000 -0.00574 -0.00578 -1.19168

D47 -1.05171 0.00025 0.00000 -0.01493 -0.01502 -1.06673

D48 0.87256 0.00131 0.00000 0.00131 0.00138 0.87395

D49 2.99597 0.00029 0.00000 -0.01096 -0.01099 2.98498

D50 -3.11039 -0.00046 0.00000 -0.01670 -0.01678 -3.12717

D51 -1.18612 0.00060 0.00000 -0.00045 -0.00038 -1.18649

D52 0.93729 -0.00042 0.00000 -0.01272 -0.01275 0.92454

D53 -0.00236 -0.00040 0.00000 0.00420 0.00423 0.00186

D54 2.16349 -0.00017 0.00000 0.00306 0.00305 2.16655

D55 -2.09500 0.00012 0.00000 0.00521 0.00520 -2.08980

D56 -2.15821 -0.00071 0.00000 -0.00416 -0.00411 -2.16232

D57 0.00765 -0.00048 0.00000 -0.00530 -0.00528 0.00237

D58 2.03234 -0.00019 0.00000 -0.00315 -0.00314 2.02920

D59 2.08838 -0.00055 0.00000 0.00121 0.00124 2.08961

D60 -2.02895 -0.00032 0.00000 0.00007 0.00006 -2.02889

D61 -0.00426 -0.00002 0.00000 0.00222 0.00221 -0.00205

D62 -0.00579 0.00007 0.00000 0.00010 0.00009 -0.00570

D63 -3.13425 -0.00040 0.00000 -0.00688 -0.00693 -3.14117

D64 0.00962 -0.00004 0.00000 0.00180 0.00178 0.01141

D65 -3.14090 0.00007 0.00000 0.01202 0.01206 -3.12885

D66 -0.01759 0.00111 0.00000 0.01431 0.01429 -0.00331

D67 1.82532 0.00207 0.00000 0.02840 0.02843 1.85375

D68 -1.80942 0.00072 0.00000 0.00815 0.00812 -1.80129

D69 -1.83682 -0.00089 0.00000 -0.01104 -0.01112 -1.84794

D70 0.00609 0.00007 0.00000 0.00305 0.00302 0.00912

D71 2.65455 -0.00128 0.00000 -0.01720 -0.01728 2.63726

D72 1.78899 -0.00003 0.00000 0.00063 0.00059 1.78959

D73 -2.65128 0.00093 0.00000 0.01472 0.01474 -2.63654

D74 -0.00283 -0.00041 0.00000 -0.00553 -0.00557 -0.00840

D75 -1.92804 -0.00049 0.00000 -0.01948 -0.01961 -1.94765

D76 1.19685 0.00013 0.00000 -0.01058 -0.01067 1.18618

D77 -0.00039 -0.00010 0.00000 -0.00207 -0.00206 -0.00245

D78 3.12451 0.00052 0.00000 0.00683 0.00687 3.13138

D79 2.68500 -0.00048 0.00000 -0.00964 -0.00966 2.67534

D80 -0.47329 0.00014 0.00000 -0.00074 -0.00072 -0.47401

D81 1.95296 -0.00169 0.00000 -0.01397 -0.01397 1.93899

D82 -1.17723 -0.00184 0.00000 -0.02711 -0.02707 -1.20430

D83 -0.00992 -0.00001 0.00000 -0.00309 -0.00305 -0.01297

D84 -3.14010 -0.00017 0.00000 -0.01623 -0.01615 3.12693

D85 -2.68761 0.00113 0.00000 0.01202 0.01188 -2.67573

D86 0.46540 0.00098 0.00000 -0.00113 -0.00123 0.46417

Item Value Threshold Converged?

Maximum Force 0.012305 0.000450 NO

RMS Force 0.001668 0.000300 NO

Maximum Displacement 0.112699 0.001800 NO

RMS Displacement 0.020157 0.001200 NO

Predicted change in Energy=-8.856061D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.138851 1.563220 0.440450

2 6 0 0.186909 1.283356 0.108959

3 6 0 -0.753529 3.781301 -0.370639

4 6 0 -1.621477 2.849986 0.198669

5 1 0 -1.741234 0.844714 1.014491

6 1 0 -2.601748 3.158628 0.589044

7 6 0 0.797528 1.929289 -1.085494

8 1 0 1.916752 1.955267 -0.984011

9 1 0 0.574198 1.270816 -1.971068

10 6 0 0.268758 3.330961 -1.355759

11 1 0 1.121924 4.062173 -1.392800

12 1 0 -0.210899 3.357469 -2.374276

13 1 0 -1.031050 4.846872 -0.420598

14 1 0 0.658803 0.345552 0.445823

15 8 0 2.757061 3.856248 0.825694

16 6 0 0.473607 3.872178 1.423363

17 6 0 0.962411 2.571482 1.665469

18 6 0 1.609787 4.673300 0.892990

19 8 0 1.749253 5.826210 0.516985

20 6 0 2.405185 2.574723 1.295762

21 8 0 3.299735 1.744524 1.314968

22 1 0 -0.348480 4.357667 1.954319

23 1 0 0.588956 1.877070 2.422118

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394937 0.000000

3 C 2.392953 2.711857 0.000000

4 C 1.395404 2.394293 1.394558 0.000000

5 H 1.099381 2.174886 3.393772 2.168184 0.000000

6 H 2.169672 3.394663 2.173620 1.099356 2.505132

7 C 2.492404 1.488893 2.519275 2.889350 3.468653

8 H 3.394038 2.153695 3.292572 3.836446 4.313722

9 H 2.972449 2.115812 3.259873 3.467351 3.802150

10 C 2.886631 2.518886 1.489409 2.494107 3.979897

11 H 3.836232 3.294140 2.154305 3.395353 4.934042

12 H 3.464550 3.259855 2.118641 2.977803 4.487717

13 H 3.396380 3.802960 1.102250 2.172476 4.310582

14 H 2.171244 1.102559 3.803376 3.396020 2.516490

15 O 4.537016 3.706637 3.709592 4.536222 5.416607

16 C 2.982855 2.917508 2.175445 2.633273 3.773359

17 C 2.632976 2.164115 2.924696 2.984215 3.273407

18 C 4.175213 3.759123 2.824479 3.774602 5.089418

19 O 5.149766 4.821299 3.351634 4.507888 6.102976

20 C 3.783502 2.827875 3.769642 4.182510 4.501648

21 O 4.527549 3.369988 4.839286 5.165897 5.129455

22 H 3.274969 3.625381 2.429340 2.641199 3.894083

23 H 2.647796 2.421744 3.637012 3.282728 2.911522

6 7 8 9 10

6 H 0.000000

7 C 3.983771 0.000000

8 H 4.933500 1.124115 0.000000

9 H 4.494957 1.125924 1.801445 0.000000

10 C 3.471565 1.522276 2.178673 2.171657 0.000000

11 H 4.313912 2.179189 2.288649 2.902770 1.124249

12 H 3.812737 2.171999 2.902741 2.265629 1.126121

13 H 2.517268 3.506861 4.167536 4.215324 2.204997

14 H 4.308724 2.207352 2.493600 2.589331 3.508632

15 O 5.409206 3.347473 2.755881 4.389900 3.350569

16 C 3.265432 3.189687 3.398922 4.277776 2.838732

17 C 3.769172 2.829734 2.882748 3.881603 3.191517

18 C 4.485938 3.479045 3.317389 4.566418 2.942296

19 O 5.104155 4.319688 4.155147 5.321915 3.453303

20 C 5.090164 2.944746 2.412397 3.965460 3.488092

21 O 6.111805 3.472376 2.691164 4.295462 4.340092

22 H 2.894631 4.055961 4.420021 5.078253 3.520189

23 H 3.896555 3.514196 3.656621 4.434845 4.060626

11 12 13 14 15

11 H 0.000000

12 H 1.798977 0.000000

13 H 2.489222 2.589947 0.000000

14 H 4.172324 4.216750 4.885506 0.000000

15 O 2.763655 4.392877 4.109059 4.107551 0.000000

16 C 2.896064 3.893010 2.571811 3.664284 2.360429

17 C 3.405967 4.279482 3.674638 2.556263 2.361486

18 C 2.415848 3.965013 2.954600 4.453508 1.410086

19 O 2.674443 4.277413 3.093259 5.588538 2.234218

20 C 3.329810 4.574469 4.462764 2.956594 1.409641

21 O 4.176885 5.341972 5.602897 3.112404 2.234561

22 H 3.667780 4.444779 2.519019 4.403096 3.342095

23 H 4.428581 5.082985 4.418731 2.501234 3.341616

16 17 18 19 20

16 C 0.000000

17 C 1.410445 0.000000

18 C 1.487951 2.330978 0.000000

19 O 2.503405 3.539970 1.220668 0.000000

20 C 2.330379 1.489393 2.280112 3.407185 0.000000

21 O 3.539162 2.503956 3.407598 4.438573 1.220582

22 H 1.092447 2.234351 2.249634 2.936500 3.345932

23 H 2.234116 1.092792 3.346525 4.535584 2.248129

21 22 23

21 O 0.000000

22 H 4.532854 0.000000

23 H 2.931156 2.692765 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.300851 -0.713470 -0.658120

2 6 0 1.357637 -1.363078 0.138251

3 6 0 1.378706 1.348689 0.131419

4 6 0 2.308461 0.681892 -0.665907

5 1 0 2.917273 -1.274534 -1.374967

6 1 0 2.921616 1.230514 -1.395043

7 6 0 0.956598 -0.762194 1.440137

8 1 0 -0.059059 -1.135702 1.744387

9 1 0 1.679181 -1.138331 2.217376

10 6 0 0.969705 0.760023 1.436996

11 1 0 -0.038547 1.152854 1.742031

12 1 0 1.697158 1.127224 2.214249

13 1 0 1.231495 2.436204 0.028488

14 1 0 1.197044 -2.449173 0.037038

15 8 0 -2.080531 0.015892 0.267104

16 6 0 -0.287469 0.699371 -1.107456

17 6 0 -0.295271 -0.711014 -1.097106

18 6 0 -1.413457 1.148021 -0.244402

19 8 0 -1.854177 2.232453 0.101726

20 6 0 -1.435736 -1.131968 -0.236625

21 8 0 -1.905100 -2.205827 0.104469

22 1 0 0.076737 1.332899 -1.919513

23 1 0 0.055406 -1.359734 -1.903569

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2196771 0.8823672 0.6762596

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6346516516 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.503850579308E-01 A.U. after 14 cycles

Convg = 0.9581D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000612280 -0.000983641 0.000129896

2 6 -0.000320408 -0.000174189 0.001011152

3 6 0.000013024 0.000062231 0.000533977

4 6 -0.000276723 0.000652035 -0.000720875

5 1 0.000375023 -0.000168332 0.000445579

6 1 -0.000068297 0.000158923 0.000010482

7 6 0.000458746 0.000397027 -0.000390100

8 1 0.000005929 -0.000163529 -0.000174013

9 1 0.000064473 0.000124423 -0.000272193

10 6 0.000457757 -0.000022292 -0.000133230

11 1 -0.000040244 0.000042924 0.000066690

12 1 -0.000126551 -0.000233184 0.000060386

13 1 0.000214582 0.000042507 0.000411548

14 1 0.000132241 0.000185672 -0.000210555

15 8 -0.000348643 -0.000177197 -0.000026465

16 6 -0.000296865 0.000201368 -0.001108450

17 6 0.000780751 -0.000086735 0.000068270

18 6 0.000002792 -0.000215977 -0.000109580

19 8 0.000138283 -0.000077431 0.000481650

20 6 -0.000494686 0.000072607 0.000048204

21 8 -0.000103470 0.000240649 0.000024866

22 1 0.000060760 0.000087285 -0.000110963

23 1 -0.000016192 0.000034856 -0.000036274

-------------------------------------------------------------------

Cartesian Forces: Max 0.001108450 RMS 0.000347113

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000931141 RMS 0.000180716

Search for a saddle point.

Step number 51 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06996 0.00085 0.00399 0.00695 0.00783

Eigenvalues --- 0.01049 0.01163 0.01401 0.01855 0.02326

Eigenvalues --- 0.02555 0.02824 0.03087 0.03124 0.03272

Eigenvalues --- 0.03504 0.03591 0.03611 0.03822 0.04101

Eigenvalues --- 0.04227 0.04308 0.04689 0.04841 0.06032

Eigenvalues --- 0.06361 0.06623 0.06878 0.07339 0.08297

Eigenvalues --- 0.09003 0.09261 0.10026 0.10138 0.10746

Eigenvalues --- 0.12145 0.13889 0.14643 0.17113 0.21965

Eigenvalues --- 0.26057 0.27769 0.29417 0.29877 0.30366

Eigenvalues --- 0.31187 0.31344 0.31889 0.32000 0.32422

Eigenvalues --- 0.32637 0.33476 0.36351 0.37422 0.39403

Eigenvalues --- 0.39720 0.40460 0.43748 0.47980 0.51460

Eigenvalues --- 0.59374 1.08557 1.10937

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 0.57136 0.50227 0.15022 -0.14920 -0.14689

D4 D86 D1 D35 R19

1 0.14140 -0.13383 0.13332 0.13030 -0.12933

RFO step: Lambda0=2.574360993D-06 Lambda=-8.45012947D-05.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.01083518 RMS(Int)= 0.00005263

Iteration 2 RMS(Cart)= 0.00007200 RMS(Int)= 0.00001868

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001868

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63605 0.00031 0.00000 -0.00022 -0.00022 2.63583

R2 2.63693 0.00093 0.00000 0.00303 0.00304 2.63998

R3 2.07753 0.00014 0.00000 0.00024 0.00024 2.07777

R4 2.81360 0.00090 0.00000 0.00431 0.00431 2.81791

R5 2.08354 -0.00017 0.00000 -0.00058 -0.00058 2.08296

R6 4.08959 -0.00014 0.00000 0.00997 0.00997 4.09955

R7 2.63533 0.00009 0.00000 0.00012 0.00013 2.63546

R8 2.81458 0.00031 0.00000 0.00166 0.00165 2.81623

R9 2.08295 -0.00003 0.00000 -0.00001 -0.00001 2.08294

R10 4.11100 -0.00061 0.00000 -0.01101 -0.01101 4.09999

R11 2.07748 0.00011 0.00000 0.00045 0.00045 2.07794

R12 2.12427 -0.00001 0.00000 -0.00015 -0.00015 2.12412

R13 2.12769 0.00013 0.00000 0.00049 0.00049 2.12818

R14 2.87669 -0.00013 0.00000 -0.00117 -0.00118 2.87550

R15 2.12452 0.00000 0.00000 -0.00037 -0.00037 2.12415

R16 2.12806 -0.00001 0.00000 0.00000 0.00000 2.12806

R17 2.66468 -0.00036 0.00000 -0.00086 -0.00087 2.66381

R18 2.66383 -0.00035 0.00000 0.00060 0.00059 2.66443

R19 2.66535 0.00021 0.00000 -0.00009 -0.00007 2.66528

R20 2.81182 -0.00030 0.00000 0.00053 0.00054 2.81236

R21 2.06443 -0.00006 0.00000 0.00035 0.00035 2.06478

R22 2.81454 -0.00064 0.00000 -0.00261 -0.00261 2.81193

R23 2.06508 -0.00004 0.00000 -0.00041 -0.00041 2.06467

R24 2.30673 -0.00021 0.00000 -0.00028 -0.00028 2.30645

R25 2.30657 -0.00024 0.00000 -0.00023 -0.00023 2.30633

A1 2.06298 -0.00032 0.00000 -0.00283 -0.00286 2.06012

A2 2.11031 -0.00024 0.00000 -0.00229 -0.00231 2.10800

A3 2.09860 0.00054 0.00000 0.00352 0.00350 2.10209

A4 2.08677 0.00019 0.00000 0.00243 0.00244 2.08921

A5 2.09997 -0.00005 0.00000 0.00412 0.00412 2.10409

A6 1.62106 0.00004 0.00000 -0.00394 -0.00397 1.61709

A7 2.02482 -0.00013 0.00000 -0.00507 -0.00508 2.01974

A8 1.74346 -0.00013 0.00000 0.00060 0.00059 1.74406

A9 1.70435 0.00007 0.00000 0.00001 0.00005 1.70440

A10 2.08895 0.00008 0.00000 -0.00204 -0.00203 2.08692

A11 2.10296 -0.00009 0.00000 0.00121 0.00123 2.10419

A12 1.61313 0.00011 0.00000 0.00831 0.00829 1.62142

A13 2.02098 0.00005 0.00000 0.00105 0.00103 2.02201

A14 1.74254 -0.00008 0.00000 -0.00248 -0.00249 1.74005

A15 1.71026 -0.00014 0.00000 -0.00665 -0.00663 1.70363

A16 2.06156 0.00001 0.00000 0.00153 0.00152 2.06308

A17 2.10107 0.00013 0.00000 -0.00094 -0.00095 2.10012

A18 2.10882 -0.00017 0.00000 -0.00194 -0.00195 2.10687

A19 1.92403 0.00007 0.00000 -0.00046 -0.00046 1.92357

A20 1.87122 0.00023 0.00000 0.00293 0.00293 1.87415

A21 1.98170 -0.00018 0.00000 -0.00051 -0.00051 1.98119

A22 1.85669 -0.00011 0.00000 -0.00192 -0.00192 1.85477

A23 1.91834 0.00006 0.00000 0.00171 0.00171 1.92005

A24 1.90705 -0.00005 0.00000 -0.00188 -0.00187 1.90518

A25 1.98165 0.00020 0.00000 -0.00001 -0.00002 1.98163

A26 1.92411 -0.00012 0.00000 -0.00038 -0.00037 1.92374

A27 1.87418 -0.00005 0.00000 -0.00104 -0.00104 1.87313

A28 1.91891 -0.00004 0.00000 0.00085 0.00085 1.91975

A29 1.90731 -0.00012 0.00000 -0.00184 -0.00183 1.90548

A30 1.85264 0.00012 0.00000 0.00253 0.00253 1.85516

A31 1.88364 0.00006 0.00000 0.00030 0.00029 1.88392

A32 1.87394 0.00011 0.00000 0.00292 0.00283 1.87677

A33 1.73075 0.00019 0.00000 0.01509 0.01511 1.74586

A34 1.56568 -0.00008 0.00000 -0.00605 -0.00600 1.55968

A35 1.86823 -0.00011 0.00000 -0.00104 -0.00108 1.86715

A36 2.19838 0.00005 0.00000 0.00027 0.00025 2.19863

A37 2.10434 -0.00005 0.00000 -0.00451 -0.00451 2.09982

A38 1.87681 -0.00001 0.00000 -0.00279 -0.00285 1.87396

A39 1.74152 0.00008 0.00000 -0.00618 -0.00616 1.73536

A40 1.56810 -0.00007 0.00000 -0.00193 -0.00189 1.56621

A41 1.86617 -0.00005 0.00000 0.00143 0.00144 1.86761

A42 2.19743 0.00007 0.00000 0.00124 0.00122 2.19864

A43 2.09937 -0.00001 0.00000 0.00286 0.00282 2.10219

A44 1.90319 -0.00001 0.00000 -0.00008 -0.00009 1.90311

A45 2.02596 -0.00006 0.00000 0.00059 0.00057 2.02653

A46 2.35401 0.00006 0.00000 -0.00045 -0.00047 2.35354

A47 1.90346 0.00010 0.00000 -0.00062 -0.00063 1.90283

A48 2.02712 -0.00015 0.00000 -0.00105 -0.00104 2.02608

A49 2.35260 0.00005 0.00000 0.00166 0.00166 2.35427

D1 -0.60532 0.00006 0.00000 0.00447 0.00447 -0.60086

D2 2.94947 0.00006 0.00000 0.00157 0.00154 2.95102

D3 1.19376 -0.00004 0.00000 0.00327 0.00324 1.19700

D4 2.69689 0.00017 0.00000 0.01545 0.01545 2.71233

D5 -0.03150 0.00017 0.00000 0.01255 0.01252 -0.01898

D6 -1.78722 0.00007 0.00000 0.01425 0.01422 -1.77300

D7 0.00845 -0.00013 0.00000 -0.00639 -0.00639 0.00207

D8 -2.97045 0.00006 0.00000 0.00300 0.00303 -2.96743

D9 2.99054 -0.00031 0.00000 -0.01784 -0.01788 2.97267

D10 0.01164 -0.00012 0.00000 -0.00845 -0.00847 0.00317

D11 2.73478 0.00009 0.00000 -0.00177 -0.00177 2.73301

D12 -1.53435 0.00011 0.00000 -0.00265 -0.00266 -1.53701

D13 0.57369 0.00009 0.00000 -0.00329 -0.00329 0.57040

D14 -0.80278 0.00010 0.00000 0.00304 0.00304 -0.79974

D15 1.21127 0.00012 0.00000 0.00216 0.00215 1.21343

D16 -2.96387 0.00010 0.00000 0.00152 0.00152 -2.96235

D17 1.00577 0.00006 0.00000 0.00188 0.00190 1.00767

D18 3.01982 0.00009 0.00000 0.00100 0.00102 3.02084

D19 -1.15532 0.00007 0.00000 0.00035 0.00038 -1.15494

D20 -1.03189 -0.00016 0.00000 -0.01790 -0.01788 -1.04977

D21 -2.97552 -0.00014 0.00000 -0.01609 -0.01609 -2.99161

D22 1.20020 -0.00012 0.00000 -0.01800 -0.01800 1.18220

D23 1.07436 0.00002 0.00000 -0.01622 -0.01619 1.05817

D24 -0.86926 0.00005 0.00000 -0.01441 -0.01441 -0.88367

D25 -2.97673 0.00006 0.00000 -0.01632 -0.01632 -2.99305

D26 3.13744 -0.00013 0.00000 -0.02136 -0.02134 3.11610

D27 1.19382 -0.00011 0.00000 -0.01955 -0.01956 1.17426

D28 -0.91365 -0.00009 0.00000 -0.02146 -0.02147 -0.93512

D29 0.59382 0.00008 0.00000 0.00724 0.00725 0.60106

D30 -2.71122 -0.00008 0.00000 -0.00209 -0.00210 -2.71332

D31 -2.95817 0.00021 0.00000 0.00809 0.00811 -2.95007

D32 0.01997 0.00005 0.00000 -0.00124 -0.00124 0.01873

D33 -1.19987 0.00010 0.00000 0.00554 0.00558 -1.19429

D34 1.77828 -0.00006 0.00000 -0.00379 -0.00377 1.77451

D35 -0.57351 -0.00005 0.00000 -0.00626 -0.00626 -0.57976

D36 -2.73536 -0.00005 0.00000 -0.00708 -0.00707 -2.74243

D37 1.53688 -0.00010 0.00000 -0.00930 -0.00929 1.52759

D38 2.95988 -0.00014 0.00000 -0.00715 -0.00717 2.95271

D39 0.79802 -0.00014 0.00000 -0.00798 -0.00798 0.79004

D40 -1.21292 -0.00019 0.00000 -0.01020 -0.01020 -1.22312

D41 1.14617 0.00006 0.00000 0.00153 0.00150 1.14766

D42 -1.01569 0.00005 0.00000 0.00070 0.00069 -1.01500

D43 -3.02663 0.00000 0.00000 -0.00152 -0.00154 -3.02817

D44 1.03980 0.00009 0.00000 -0.01815 -0.01817 1.02162

D45 2.98047 0.00007 0.00000 -0.01242 -0.01239 2.96809

D46 -1.19168 0.00003 0.00000 -0.01675 -0.01675 -1.20843

D47 -1.06673 -0.00001 0.00000 -0.01756 -0.01759 -1.08432

D48 0.87395 -0.00002 0.00000 -0.01183 -0.01180 0.86215

D49 2.98498 -0.00007 0.00000 -0.01617 -0.01617 2.96882

D50 -3.12717 0.00000 0.00000 -0.01623 -0.01627 3.13975

D51 -1.18649 -0.00001 0.00000 -0.01050 -0.01048 -1.19698

D52 0.92454 -0.00006 0.00000 -0.01484 -0.01485 0.90969

D53 0.00186 -0.00002 0.00000 0.00518 0.00518 0.00705

D54 2.16655 -0.00006 0.00000 0.00534 0.00533 2.17188

D55 -2.08980 -0.00001 0.00000 0.00781 0.00780 -2.08199

D56 -2.16232 -0.00002 0.00000 0.00484 0.00484 -2.15748

D57 0.00237 -0.00006 0.00000 0.00500 0.00499 0.00736

D58 2.02920 -0.00001 0.00000 0.00747 0.00747 2.03667

D59 2.08961 0.00011 0.00000 0.00726 0.00727 2.09688

D60 -2.02889 0.00007 0.00000 0.00742 0.00742 -2.02147

D61 -0.00205 0.00012 0.00000 0.00989 0.00989 0.00784

D62 -0.00570 -0.00012 0.00000 -0.00982 -0.00981 -0.01551

D63 -3.14117 -0.00022 0.00000 -0.01841 -0.01840 3.12361

D64 0.01141 0.00002 0.00000 0.00570 0.00569 0.01710

D65 -3.12885 0.00009 0.00000 0.00851 0.00849 -3.12036

D66 -0.00331 -0.00002 0.00000 0.01865 0.01865 0.01534

D67 1.85375 0.00005 0.00000 0.01114 0.01115 1.86489

D68 -1.80129 0.00005 0.00000 0.02287 0.02289 -1.77840

D69 -1.84794 -0.00023 0.00000 0.00094 0.00093 -1.84701

D70 0.00912 -0.00016 0.00000 -0.00657 -0.00657 0.00254

D71 2.63726 -0.00016 0.00000 0.00516 0.00517 2.64243

D72 1.78959 -0.00001 0.00000 0.01312 0.01311 1.80270

D73 -2.63654 0.00006 0.00000 0.00562 0.00561 -2.63093

D74 -0.00840 0.00007 0.00000 0.01735 0.01735 0.00896

D75 -1.94765 0.00001 0.00000 0.00155 0.00158 -1.94608

D76 1.18618 0.00014 0.00000 0.01245 0.01247 1.19865

D77 -0.00245 0.00018 0.00000 0.01034 0.01033 0.00788

D78 3.13138 0.00031 0.00000 0.02124 0.02122 -3.13058

D79 2.67534 0.00001 0.00000 0.00050 0.00052 2.67586

D80 -0.47401 0.00013 0.00000 0.01140 0.01141 -0.46260

D81 1.93899 0.00011 0.00000 -0.00427 -0.00431 1.93468

D82 -1.20430 0.00001 0.00000 -0.00783 -0.00787 -1.21216

D83 -0.01297 0.00010 0.00000 0.00078 0.00079 -0.01217

D84 3.12693 0.00000 0.00000 -0.00278 -0.00276 3.12417

D85 -2.67573 0.00006 0.00000 -0.00962 -0.00964 -2.68537

D86 0.46417 -0.00004 0.00000 -0.01318 -0.01319 0.45098

Item Value Threshold Converged?

Maximum Force 0.000931 0.000450 NO

RMS Force 0.000181 0.000300 YES

Maximum Displacement 0.048753 0.001800 NO

RMS Displacement 0.010832 0.001200 NO

Predicted change in Energy=-4.144060D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.136381 1.555814 0.440626

2 6 0 0.189724 1.283319 0.104887

3 6 0 -0.759936 3.778895 -0.368409

4 6 0 -1.624260 2.842112 0.197597

5 1 0 -1.727574 0.837224 1.026316

6 1 0 -2.603558 3.148394 0.592918

7 6 0 0.798332 1.935363 -1.090115

8 1 0 1.917293 1.966210 -0.988004

9 1 0 0.580583 1.278984 -1.978956

10 6 0 0.261195 3.333565 -1.358317

11 1 0 1.109538 4.069853 -1.399389

12 1 0 -0.224838 3.354594 -2.373934

13 1 0 -1.038906 4.844366 -0.411903

14 1 0 0.671439 0.349387 0.437586

15 8 0 2.762107 3.843172 0.826677

16 6 0 0.475900 3.877874 1.412088

17 6 0 0.956949 2.577014 1.668208

18 6 0 1.621970 4.669806 0.888436

19 8 0 1.775052 5.824270 0.523132

20 6 0 2.400175 2.567551 1.306016

21 8 0 3.291030 1.733997 1.338950

22 1 0 -0.342993 4.374460 1.938074

23 1 0 0.570761 1.886780 2.421971

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394822 0.000000

3 C 2.395483 2.711782 0.000000

4 C 1.397015 2.393526 1.394626 0.000000

5 H 1.099506 2.173491 3.396324 2.171871 0.000000

6 H 2.170740 3.393981 2.172700 1.099597 2.509321

7 C 2.496065 1.491173 2.519458 2.889524 3.473528

8 H 3.396224 2.155284 3.292003 3.836073 4.314761

9 H 2.979762 2.120186 3.261964 3.470171 3.815023

10 C 2.889605 2.519838 1.490284 2.493459 3.984144

11 H 3.840599 3.297526 2.154648 3.395786 4.937929

12 H 3.462408 3.256777 2.118605 2.972169 4.489662

13 H 3.398659 3.802323 1.102245 2.173282 4.312764

14 H 2.173405 1.102255 3.802629 3.397279 2.517906

15 O 4.536436 3.700132 3.719832 4.542915 5.406738

16 C 2.989172 2.919313 2.169621 2.637890 3.774874

17 C 2.632838 2.169390 2.922332 2.982552 3.262754

18 C 4.184015 3.759465 2.836699 3.788897 5.091871

19 O 5.167492 4.827881 3.377066 4.533715 6.114918

20 C 3.778855 2.824546 3.775892 4.183307 4.484482

21 O 4.521140 3.368103 4.848403 5.166303 5.107674

22 H 3.288857 3.633114 2.418348 2.649340 3.906458

23 H 2.636210 2.424507 3.624511 3.267815 2.886480

6 7 8 9 10

6 H 0.000000

7 C 3.984583 0.000000

8 H 4.933049 1.124034 0.000000

9 H 4.499776 1.126182 1.800294 0.000000

10 C 3.471083 1.521650 2.179324 2.169909 0.000000

11 H 4.313404 2.179116 2.290637 2.899076 1.124052

12 H 3.808285 2.170089 2.904675 2.261166 1.126120

13 H 2.516769 3.506810 4.165908 4.217861 2.206463

14 H 4.310936 2.205741 2.489695 2.590768 3.506977

15 O 5.415507 3.342190 2.744041 4.382428 3.359831

16 C 3.268982 3.184074 3.390061 4.273683 2.831522

17 C 3.762969 2.836409 2.889776 3.889516 3.196295

18 C 4.500791 3.474222 3.304190 4.561151 2.947058

19 O 5.131999 4.322053 4.145889 5.324174 3.469183

20 C 5.087557 2.950763 2.420189 3.970184 3.501527

21 O 6.107639 3.486323 2.712156 4.308371 4.360478

22 H 2.902213 4.052375 4.412539 5.077213 3.509231

23 H 3.874713 3.519787 3.667069 4.442710 4.059507

11 12 13 14 15

11 H 0.000000

12 H 1.800526 0.000000

13 H 2.488134 2.594550 0.000000

14 H 4.172322 4.211796 4.883825 0.000000

15 O 2.781679 4.405049 4.121185 4.090087 0.000000

16 C 2.888382 3.885719 2.560407 3.665802 2.360223

17 C 3.414967 4.282542 3.667586 2.560911 2.360069

18 C 2.420056 3.972850 2.966751 4.446661 1.409628

19 O 2.686443 4.300215 3.122957 5.585662 2.234093

20 C 3.352890 4.588264 4.467932 2.943289 1.409954

21 O 4.208756 5.364063 5.611437 3.097073 2.234010

22 H 3.652573 4.432550 2.495496 4.413813 3.340526

23 H 4.433833 5.078204 4.401043 2.512269 3.342818

16 17 18 19 20

16 C 0.000000

17 C 1.410406 0.000000

18 C 1.488236 2.330253 0.000000

19 O 2.503297 3.539092 1.220520 0.000000

20 C 2.330458 1.488010 2.280231 3.407332 0.000000

21 O 3.539281 2.503401 3.407007 4.437802 1.220458

22 H 1.092632 2.234612 2.247232 2.930892 3.345055

23 H 2.234573 1.092576 3.346940 4.534285 2.248458

21 22 23

21 O 0.000000

22 H 4.531789 0.000000

23 H 2.931918 2.694003 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.300018 -0.725577 -0.655740

2 6 0 1.356134 -1.360756 0.151205

3 6 0 1.386916 1.350610 0.114994

4 6 0 2.314196 0.671237 -0.674682

5 1 0 2.900898 -1.298597 -1.376507

6 1 0 2.924800 1.210339 -1.413360

7 6 0 0.958179 -0.743323 1.448897

8 1 0 -0.059009 -1.109008 1.757208

9 1 0 1.677462 -1.113743 2.232292

10 6 0 0.980794 0.778036 1.429592

11 1 0 -0.022832 1.181242 1.735621

12 1 0 1.717030 1.146813 2.197775

13 1 0 1.239858 2.436688 -0.002274

14 1 0 1.185506 -2.446361 0.065685

15 8 0 -2.078918 0.009027 0.274060

16 6 0 -0.289001 0.700853 -1.100068

17 6 0 -0.295868 -0.709527 -1.095005

18 6 0 -1.419879 1.144077 -0.240119

19 8 0 -1.874534 2.226432 0.093746

20 6 0 -1.432842 -1.136112 -0.235068

21 8 0 -1.902429 -2.211276 0.101128

22 1 0 0.068673 1.338009 -1.912439

23 1 0 0.062774 -1.355957 -1.899510

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2199967 0.8796568 0.6746213

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4578519688 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504081314818E-01 A.U. after 14 cycles

Convg = 0.4067D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000432666 0.000707173 -0.000254814

2 6 0.000246524 0.000323055 -0.000815539

3 6 0.000572198 -0.000632221 -0.000229787

4 6 -0.000070345 -0.000124298 0.000515663

5 1 -0.000011290 0.000040783 -0.000107383

6 1 -0.000055372 -0.000046904 -0.000163719

7 6 -0.000360936 -0.000458042 0.000807277

8 1 -0.000015822 -0.000023907 0.000094706

9 1 -0.000061836 -0.000030450 0.000157398

10 6 -0.000122790 0.000411928 0.000149831

11 1 -0.000033878 0.000040340 0.000010246

12 1 -0.000024845 0.000004499 -0.000001408

13 1 -0.000036101 -0.000104789 0.000068289

14 1 -0.000091539 0.000042611 0.000164354

15 8 0.000002398 -0.000098422 -0.000022867

16 6 -0.000348763 0.000052759 0.000045067

17 6 -0.000110037 -0.000194738 -0.000428861

18 6 0.000025103 -0.000270212 -0.000062854

19 8 0.000031518 0.000000039 -0.000000103

20 6 -0.000001925 0.000461196 -0.000002274

21 8 -0.000023478 -0.000101631 -0.000101077

22 1 -0.000024573 -0.000050784 0.000097599

23 1 0.000083123 0.000052016 0.000080253

-------------------------------------------------------------------

Cartesian Forces: Max 0.000815539 RMS 0.000261041

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.001090323 RMS 0.000131169

Search for a saddle point.

Step number 52 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06905 -0.00008 0.00440 0.00684 0.00802

Eigenvalues --- 0.01093 0.01143 0.01398 0.01846 0.02375

Eigenvalues --- 0.02569 0.02821 0.03099 0.03138 0.03313

Eigenvalues --- 0.03533 0.03589 0.03626 0.03821 0.04124

Eigenvalues --- 0.04251 0.04324 0.04730 0.04840 0.06067

Eigenvalues --- 0.06366 0.06596 0.06878 0.07349 0.08294

Eigenvalues --- 0.08983 0.09251 0.10025 0.10126 0.10757

Eigenvalues --- 0.12206 0.13877 0.14643 0.17114 0.21977

Eigenvalues --- 0.26067 0.27777 0.29461 0.29896 0.30395

Eigenvalues --- 0.31198 0.31346 0.31888 0.32007 0.32424

Eigenvalues --- 0.32654 0.33495 0.36530 0.37498 0.39469

Eigenvalues --- 0.39734 0.40462 0.43839 0.48004 0.51564

Eigenvalues --- 0.59794 1.08562 1.10941

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D4

1 -0.56944 -0.50324 0.15463 -0.15293 -0.14311

D30 D1 D79 R19 D86

1 0.14050 -0.13297 -0.13230 0.13134 0.13093

RFO step: Lambda0=1.059993198D-06 Lambda=-1.23181223D-04.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.983

Iteration 1 RMS(Cart)= 0.16365323 RMS(Int)= 0.02794437

Iteration 2 RMS(Cart)= 0.04350696 RMS(Int)= 0.00455056

Iteration 3 RMS(Cart)= 0.00102252 RMS(Int)= 0.00450269

Iteration 4 RMS(Cart)= 0.00000320 RMS(Int)= 0.00450269

Iteration 5 RMS(Cart)= 0.00000002 RMS(Int)= 0.00450269

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63583 -0.00032 0.00000 0.00786 0.00955 2.64538

R2 2.63998 -0.00048 0.00000 0.01155 0.01462 2.65459

R3 2.07777 -0.00008 0.00000 -0.00086 -0.00086 2.07691

R4 2.81791 -0.00109 0.00000 0.02496 0.02432 2.84223

R5 2.08296 -0.00003 0.00000 -0.00033 -0.00033 2.08263

R6 4.09955 -0.00034 0.00000 -0.08675 -0.08780 4.01176

R7 2.63546 -0.00014 0.00000 -0.00630 -0.00509 2.63037

R8 2.81623 -0.00043 0.00000 0.01556 0.01636 2.83259

R9 2.08294 -0.00009 0.00000 -0.00100 -0.00100 2.08194

R10 4.09999 -0.00028 0.00000 0.07220 0.07139 4.17138

R11 2.07794 -0.00002 0.00000 -0.00028 -0.00028 2.07766

R12 2.12412 -0.00001 0.00000 -0.00369 -0.00369 2.12043

R13 2.12818 -0.00009 0.00000 0.00176 0.00176 2.12993

R14 2.87550 0.00012 0.00000 -0.00458 -0.00441 2.87109

R15 2.12415 0.00000 0.00000 0.00180 0.00180 2.12595

R16 2.12806 0.00001 0.00000 -0.00072 -0.00072 2.12734

R17 2.66381 -0.00005 0.00000 0.00294 0.00400 2.66781

R18 2.66443 -0.00019 0.00000 0.00444 0.00533 2.66976

R19 2.66528 -0.00025 0.00000 0.00011 -0.00455 2.66073

R20 2.81236 0.00000 0.00000 -0.01455 -0.01477 2.79759

R21 2.06478 0.00004 0.00000 -0.00111 -0.00111 2.06367

R22 2.81193 -0.00001 0.00000 -0.00120 -0.00168 2.81026

R23 2.06467 -0.00001 0.00000 0.00555 0.00555 2.07022

R24 2.30645 0.00000 0.00000 -0.00023 -0.00023 2.30621

R25 2.30633 0.00005 0.00000 -0.00062 -0.00062 2.30571

A1 2.06012 0.00025 0.00000 -0.02092 -0.02291 2.03721

A2 2.10800 -0.00008 0.00000 0.00536 0.00634 2.11435

A3 2.10209 -0.00016 0.00000 0.01386 0.01414 2.11623

A4 2.08921 -0.00001 0.00000 -0.01827 -0.01898 2.07023

A5 2.10409 0.00001 0.00000 0.01173 0.01150 2.11559

A6 1.61709 -0.00001 0.00000 0.08763 0.08307 1.70016

A7 2.01974 0.00003 0.00000 -0.01431 -0.01406 2.00568

A8 1.74406 -0.00003 0.00000 -0.01126 -0.01535 1.72871

A9 1.70440 -0.00003 0.00000 -0.02520 -0.01908 1.68532

A10 2.08692 0.00011 0.00000 -0.00416 -0.00568 2.08124

A11 2.10419 -0.00009 0.00000 0.03654 0.03731 2.14150

A12 1.62142 0.00005 0.00000 -0.06558 -0.06889 1.55253

A13 2.02201 -0.00001 0.00000 -0.00884 -0.00933 2.01268

A14 1.74005 -0.00005 0.00000 0.00189 -0.00432 1.73573

A15 1.70363 -0.00002 0.00000 0.00689 0.01467 1.71831

A16 2.06308 -0.00023 0.00000 0.02670 0.02320 2.08628

A17 2.10012 0.00012 0.00000 -0.01173 -0.01131 2.08880

A18 2.10687 0.00012 0.00000 -0.02215 -0.02068 2.08618

A19 1.92357 -0.00011 0.00000 0.00613 0.00923 1.93279

A20 1.87415 -0.00011 0.00000 0.00963 0.01170 1.88585

A21 1.98119 0.00013 0.00000 -0.01609 -0.02479 1.95640

A22 1.85477 0.00006 0.00000 0.00123 -0.00014 1.85463

A23 1.92005 0.00003 0.00000 0.01089 0.01165 1.93171

A24 1.90518 0.00000 0.00000 -0.01103 -0.00648 1.89870

A25 1.98163 -0.00019 0.00000 0.02224 0.01737 1.99900

A26 1.92374 0.00004 0.00000 -0.01112 -0.00968 1.91406

A27 1.87313 0.00003 0.00000 -0.00632 -0.00473 1.86840

A28 1.91975 0.00011 0.00000 -0.00383 -0.00438 1.91537

A29 1.90548 0.00004 0.00000 -0.00712 -0.00356 1.90192

A30 1.85516 -0.00003 0.00000 0.00506 0.00427 1.85944

A31 1.88392 -0.00010 0.00000 0.00542 0.00474 1.88866

A32 1.87677 -0.00006 0.00000 -0.00127 -0.02117 1.85560

A33 1.74586 -0.00007 0.00000 -0.08038 -0.06977 1.67609

A34 1.55968 0.00010 0.00000 0.03179 0.03908 1.59876

A35 1.86715 -0.00006 0.00000 0.01863 0.01905 1.88621

A36 2.19863 -0.00002 0.00000 -0.01382 -0.01302 2.18561

A37 2.09982 0.00009 0.00000 0.01636 0.01539 2.11521

A38 1.87396 0.00001 0.00000 0.01267 -0.00871 1.86525

A39 1.73536 -0.00008 0.00000 0.14002 0.14854 1.88389

A40 1.56621 0.00007 0.00000 -0.04597 -0.03590 1.53031

A41 1.86761 0.00002 0.00000 -0.01146 -0.01199 1.85562

A42 2.19864 -0.00007 0.00000 -0.00207 -0.00190 2.19674

A43 2.10219 0.00005 0.00000 -0.03386 -0.03677 2.06542

A44 1.90311 0.00008 0.00000 -0.01244 -0.01418 1.88893

A45 2.02653 -0.00007 0.00000 0.00595 0.00685 2.03338

A46 2.35354 0.00000 0.00000 0.00648 0.00731 2.36085

A47 1.90283 0.00007 0.00000 0.00034 -0.00124 1.90159

A48 2.02608 0.00002 0.00000 -0.00598 -0.00515 2.02093

A49 2.35427 -0.00009 0.00000 0.00562 0.00637 2.36064

D1 -0.60086 0.00003 0.00000 -0.03512 -0.03643 -0.63729

D2 2.95102 -0.00005 0.00000 0.02641 0.02287 2.97389

D3 1.19700 -0.00001 0.00000 0.00074 -0.00913 1.18787

D4 2.71233 0.00000 0.00000 -0.02523 -0.02266 2.68968

D5 -0.01898 -0.00008 0.00000 0.03630 0.03665 0.01767

D6 -1.77300 -0.00005 0.00000 0.01063 0.00464 -1.76836

D7 0.00207 0.00002 0.00000 -0.04629 -0.04571 -0.04364

D8 -2.96743 -0.00008 0.00000 0.00256 0.00658 -2.96084

D9 2.97267 0.00006 0.00000 -0.05700 -0.06030 2.91237

D10 0.00317 -0.00004 0.00000 -0.00814 -0.00801 -0.00484

D11 2.73301 -0.00003 0.00000 0.17638 0.17271 2.90572

D12 -1.53701 -0.00008 0.00000 0.18638 0.18411 -1.35290

D13 0.57040 -0.00008 0.00000 0.16917 0.16864 0.73904

D14 -0.79974 0.00005 0.00000 0.12374 0.12300 -0.67675

D15 1.21343 0.00000 0.00000 0.13374 0.13439 1.34782

D16 -2.96235 -0.00001 0.00000 0.11653 0.11893 -2.84343

D17 1.00767 0.00000 0.00000 0.08450 0.08933 1.09700

D18 3.02084 -0.00005 0.00000 0.09449 0.10072 3.12157

D19 -1.15494 -0.00005 0.00000 0.07729 0.08526 -1.06968

D20 -1.04977 0.00012 0.00000 0.28160 0.28187 -0.76790

D21 -2.99161 0.00013 0.00000 0.23424 0.23395 -2.75766

D22 1.18220 0.00007 0.00000 0.26433 0.26473 1.44693

D23 1.05817 0.00010 0.00000 0.28132 0.27963 1.33780

D24 -0.88367 0.00011 0.00000 0.23396 0.23172 -0.65195

D25 -2.99305 0.00006 0.00000 0.26405 0.26250 -2.73055

D26 3.11610 0.00011 0.00000 0.25683 0.25674 -2.91035

D27 1.17426 0.00012 0.00000 0.20947 0.20882 1.38308

D28 -0.93512 0.00007 0.00000 0.23956 0.23960 -0.69552

D29 0.60106 -0.00004 0.00000 -0.01585 -0.01508 0.58598

D30 -2.71332 0.00006 0.00000 -0.06381 -0.06634 -2.77966

D31 -2.95007 -0.00004 0.00000 0.04765 0.05185 -2.89822

D32 0.01873 0.00006 0.00000 -0.00030 0.00059 0.01932

D33 -1.19429 -0.00004 0.00000 0.02164 0.03055 -1.16374

D34 1.77451 0.00006 0.00000 -0.02632 -0.02071 1.75380

D35 -0.57976 0.00002 0.00000 0.15144 0.15079 -0.42897

D36 -2.74243 -0.00003 0.00000 0.14869 0.15134 -2.59110

D37 1.52759 -0.00003 0.00000 0.15197 0.15385 1.68144

D38 2.95271 0.00003 0.00000 0.08050 0.07799 3.03071

D39 0.79004 -0.00001 0.00000 0.07775 0.07854 0.86858

D40 -1.22312 -0.00002 0.00000 0.08103 0.08105 -1.14207

D41 1.14766 0.00008 0.00000 0.07415 0.06620 1.21386

D42 -1.01500 0.00003 0.00000 0.07139 0.06674 -0.94826

D43 -3.02817 0.00003 0.00000 0.07467 0.06925 -2.95891

D44 1.02162 0.00009 0.00000 0.26627 0.26366 1.28528

D45 2.96809 -0.00002 0.00000 0.25337 0.25195 -3.06315

D46 -1.20843 0.00009 0.00000 0.26898 0.26756 -0.94086

D47 -1.08432 -0.00002 0.00000 0.28524 0.28404 -0.80027

D48 0.86215 -0.00013 0.00000 0.27234 0.27233 1.13447

D49 2.96882 -0.00002 0.00000 0.28795 0.28795 -3.02642

D50 3.13975 0.00001 0.00000 0.29218 0.29097 -2.85247

D51 -1.19698 -0.00010 0.00000 0.27928 0.27925 -0.91772

D52 0.90969 0.00000 0.00000 0.29489 0.29487 1.20457

D53 0.00705 -0.00002 0.00000 -0.20529 -0.20477 -0.19772

D54 2.17188 -0.00002 0.00000 -0.20655 -0.20818 1.96370

D55 -2.08199 0.00004 0.00000 -0.20673 -0.20755 -2.28954

D56 -2.15748 0.00000 0.00000 -0.20995 -0.20753 -2.36501

D57 0.00736 0.00000 0.00000 -0.21120 -0.21094 -0.20358

D58 2.03667 0.00006 0.00000 -0.21138 -0.21032 1.82635

D59 2.09688 -0.00008 0.00000 -0.21123 -0.21018 1.88669

D60 -2.02147 -0.00008 0.00000 -0.21249 -0.21359 -2.23507

D61 0.00784 -0.00002 0.00000 -0.21266 -0.21297 -0.20513

D62 -0.01551 0.00000 0.00000 -0.01324 -0.00830 -0.02381

D63 3.12361 0.00001 0.00000 -0.01875 -0.01183 3.11179

D64 0.01710 0.00002 0.00000 -0.03955 -0.04434 -0.02724

D65 -3.12036 -0.00005 0.00000 -0.03434 -0.04157 3.12126

D66 0.01534 -0.00002 0.00000 -0.32570 -0.32338 -0.30805

D67 1.86489 -0.00010 0.00000 -0.16784 -0.16411 1.70079

D68 -1.77840 -0.00009 0.00000 -0.27400 -0.26827 -2.04668

D69 -1.84701 0.00010 0.00000 -0.24242 -0.24415 -2.09116

D70 0.00254 0.00002 0.00000 -0.08456 -0.08487 -0.08232

D71 2.64243 0.00004 0.00000 -0.19071 -0.18903 2.45340

D72 1.80270 0.00005 0.00000 -0.29124 -0.29513 1.50757

D73 -2.63093 -0.00003 0.00000 -0.13338 -0.13585 -2.76678

D74 0.00896 -0.00001 0.00000 -0.23953 -0.24002 -0.23106

D75 -1.94608 0.00010 0.00000 0.09104 0.10571 -1.84037

D76 1.19865 0.00008 0.00000 0.09803 0.11020 1.30885

D77 0.00788 -0.00002 0.00000 0.06331 0.06063 0.06851

D78 -3.13058 -0.00003 0.00000 0.07030 0.06513 -3.06546

D79 2.67586 0.00000 0.00000 0.09820 0.09916 2.77502

D80 -0.46260 -0.00002 0.00000 0.10519 0.10365 -0.35895

D81 1.93468 -0.00004 0.00000 0.14516 0.13105 2.06572

D82 -1.21216 0.00004 0.00000 0.13851 0.12746 -1.08471

D83 -0.01217 -0.00003 0.00000 0.07959 0.08175 0.06957

D84 3.12417 0.00005 0.00000 0.07294 0.07816 -3.08086

D85 -2.68537 0.00000 0.00000 0.16819 0.16531 -2.52006

D86 0.45098 0.00008 0.00000 0.16155 0.16172 0.61270

Item Value Threshold Converged?

Maximum Force 0.001090 0.000450 NO

RMS Force 0.000131 0.000300 YES

Maximum Displacement 0.767082 0.001800 NO

RMS Displacement 0.199737 0.001200 NO

Predicted change in Energy=-2.623294D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.218082 1.626396 0.477110

2 6 0 0.098959 1.254466 0.182614

3 6 0 -0.663527 3.790572 -0.443431

4 6 0 -1.600690 2.930497 0.121790

5 1 0 -1.857903 0.997461 1.111920

6 1 0 -2.559414 3.332969 0.479072

7 6 0 0.724827 1.764371 -1.086413

8 1 0 1.834593 1.598875 -1.076558

9 1 0 0.322280 1.153942 -1.944149

10 6 0 0.402885 3.228362 -1.334224

11 1 0 1.339241 3.844710 -1.239394

12 1 0 0.045203 3.350018 -2.394672

13 1 0 -0.831071 4.875536 -0.535966

14 1 0 0.525738 0.313134 0.565160

15 8 0 2.663741 4.113890 0.840729

16 6 0 0.430235 3.793562 1.473931

17 6 0 1.063244 2.539576 1.570231

18 6 0 1.446963 4.791539 1.071504

19 8 0 1.458904 6.001545 0.913049

20 6 0 2.463130 2.741780 1.110921

21 8 0 3.429780 2.018828 0.933028

22 1 0 -0.467491 4.089642 2.020730

23 1 0 0.872053 1.781337 2.337476

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.399877 0.000000

3 C 2.416316 2.721241 0.000000

4 C 1.404749 2.387799 1.391934 0.000000

5 H 1.099052 2.181507 3.412788 2.187040 0.000000

6 H 2.170614 3.387478 2.157499 1.099448 2.519368

7 C 2.497706 1.504043 2.538985 2.868385 3.477257

8 H 3.425415 2.171764 3.383045 3.874329 4.334243

9 H 2.908337 2.140818 3.189952 3.334976 3.757292

10 C 2.911143 2.507874 1.498942 2.494597 4.008953

11 H 3.795681 3.204648 2.155821 3.366274 4.884387

12 H 3.579650 3.322143 2.122199 3.036041 4.631688

13 H 3.425348 3.807028 1.101717 2.192746 4.336979

14 H 2.184792 1.102083 3.811060 3.401302 2.539487

15 O 4.624759 3.897118 3.581105 4.483599 5.498268

16 C 2.899519 2.867796 2.207397 2.588015 3.631090

17 C 2.689471 2.122930 2.932842 3.057342 3.334856

18 C 4.180178 3.888203 2.784085 3.695080 5.031779

19 O 5.147642 4.991768 3.351589 4.406647 6.006798

20 C 3.898348 2.943325 3.645814 4.186720 4.659826

21 O 4.686628 3.498820 4.667856 5.176376 5.388394

22 H 3.002287 3.426041 2.489972 2.496743 3.510095

23 H 2.802433 2.349191 3.758786 3.513443 3.093398

6 7 8 9 10

6 H 0.000000

7 C 3.962005 0.000000

8 H 4.973366 1.122081 0.000000

9 H 4.350209 1.127111 1.799381 0.000000

10 C 3.474795 1.519318 2.184355 2.163729 0.000000

11 H 4.291213 2.174561 2.305573 2.961608 1.125006

12 H 3.878495 2.165111 2.829460 2.258870 1.125739

13 H 2.529227 3.521812 4.258464 4.142881 2.207498

14 H 4.317983 2.207582 2.462005 2.654239 3.481566

15 O 5.293580 3.604651 3.269370 4.690340 3.259762

16 C 3.184320 3.280208 3.646076 4.320014 2.864600

17 C 3.865715 2.788050 2.912970 3.849659 3.057181

18 C 4.304585 3.787061 3.867497 4.857076 3.053055

19 O 4.843192 4.742401 4.845946 5.740623 3.722359

20 C 5.096537 2.967373 2.546833 4.054371 3.234208

21 O 6.148454 3.385212 2.599889 4.322353 3.970579

22 H 2.706548 4.059907 4.593115 4.996233 3.571424

23 H 4.199546 3.427095 3.551817 4.362131 3.974340

11 12 13 14 15

11 H 0.000000

12 H 1.803862 0.000000

13 H 2.503530 2.559267 0.000000

14 H 4.048484 4.267808 4.885583 0.000000

15 O 2.480660 4.231792 3.832637 4.369524 0.000000

16 C 2.861999 3.912936 2.607920 3.598383 2.343524

17 C 3.110231 4.172970 3.671676 2.501224 2.360557

18 C 2.499668 4.007155 2.789346 4.600124 1.411742

19 O 3.049470 4.468799 2.934540 5.774932 2.240559

20 C 2.829057 4.301803 4.256397 3.154308 1.412776

21 O 3.524715 4.929606 5.336064 3.387945 2.232626

22 H 3.735328 4.506182 2.699355 4.167397 3.346282

23 H 4.155691 5.053480 4.553171 2.327371 3.300182

16 17 18 19 20

16 C 0.000000

17 C 1.407997 0.000000

18 C 1.480418 2.338227 0.000000

19 O 2.499588 3.545937 1.220396 0.000000

20 C 2.317474 1.487123 2.288157 3.416679 0.000000

21 O 3.526971 2.505534 3.411549 4.443736 1.220130

22 H 1.092046 2.224591 2.249182 2.931438 3.351571

23 H 2.233822 1.095511 3.315798 4.492610 2.226750

21 22 23

21 O 0.000000

22 H 4.545337 0.000000

23 H 2.927600 2.687560 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.390308 -0.169814 -0.839728

2 6 0 1.618054 -1.180254 -0.254671

3 6 0 1.126656 1.384104 0.511977

4 6 0 2.140465 1.144434 -0.411186

5 1 0 3.026118 -0.373731 -1.712699

6 1 0 2.590635 1.988565 -0.953013

7 6 0 1.252244 -1.056939 1.198987

8 1 0 0.445350 -1.788381 1.469134

9 1 0 2.154467 -1.341792 1.811549

10 6 0 0.838493 0.358115 1.566081

11 1 0 -0.256010 0.378828 1.825453

12 1 0 1.393599 0.672780 2.493513

13 1 0 0.734706 2.393130 0.716971

14 1 0 1.638477 -2.211663 -0.642440

15 8 0 -2.103310 -0.140618 0.253407

16 6 0 -0.348959 0.765629 -1.008763

17 6 0 -0.244376 -0.634448 -1.115070

18 6 0 -1.547813 1.076328 -0.197682

19 8 0 -2.126843 2.096840 0.137945

20 6 0 -1.325189 -1.199994 -0.264460

21 8 0 -1.673766 -2.323068 0.060987

22 1 0 0.047647 1.483466 -1.729859

23 1 0 0.057069 -1.189414 -2.010217

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2244357 0.8703459 0.6670939

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 469.8500913575 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.464919187497E-01 A.U. after 16 cycles

Convg = 0.5779D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.006601862 0.010038338 -0.004739040

2 6 0.004736370 -0.000738326 -0.010273352

3 6 0.010194773 -0.010409995 -0.001523292

4 6 -0.002841465 -0.004494779 0.007063740

5 1 -0.000315764 0.000938801 -0.001484107

6 1 -0.002035040 -0.000811035 -0.000846592

7 6 -0.007090839 -0.001069262 0.007605087

8 1 0.000027620 0.000820153 0.001634558

9 1 -0.000078572 -0.000641338 0.001972504

10 6 -0.002580675 0.005907270 0.000269006

11 1 -0.000429251 0.000187532 0.000036996

12 1 0.000253262 0.000241289 -0.000127643

13 1 -0.002224150 -0.001204854 0.000861823

14 1 -0.001836036 -0.000627356 0.000095260

15 8 0.001322911 0.000452972 -0.000812123

16 6 -0.006148080 0.004545512 0.001464892

17 6 -0.003208202 -0.003916319 0.003149716

18 6 0.003136971 -0.003085281 -0.002060124

19 8 0.000349268 -0.000715955 -0.000550380

20 6 0.003532732 0.003181304 -0.002573043

21 8 -0.000096658 -0.000204798 0.000379055

22 1 0.000412725 0.001437897 0.000606435

23 1 -0.001683765 0.000168229 -0.000149376

-------------------------------------------------------------------

Cartesian Forces: Max 0.010409995 RMS 0.003661123

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.011301221 RMS 0.001686376

Search for a saddle point.

Step number 53 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 30 52 53

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06430 0.00017 0.00220 0.00689 0.00819

Eigenvalues --- 0.01078 0.01106 0.01374 0.01810 0.02440

Eigenvalues --- 0.02599 0.02806 0.03113 0.03153 0.03320

Eigenvalues --- 0.03552 0.03598 0.03663 0.03820 0.04102

Eigenvalues --- 0.04261 0.04407 0.04711 0.04973 0.06103

Eigenvalues --- 0.06331 0.06516 0.06767 0.07337 0.08266

Eigenvalues --- 0.08914 0.09261 0.10003 0.10033 0.10949

Eigenvalues --- 0.12200 0.13871 0.14721 0.16961 0.21880

Eigenvalues --- 0.26004 0.27753 0.29453 0.29829 0.30404

Eigenvalues --- 0.31143 0.31340 0.31873 0.32008 0.32421

Eigenvalues --- 0.32584 0.33454 0.36636 0.37514 0.39573

Eigenvalues --- 0.39741 0.40454 0.43864 0.47848 0.51561

Eigenvalues --- 0.59628 1.08556 1.10940

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D71 D4

1 -0.57988 -0.49524 0.16235 -0.14958 -0.14400

D73 R19 D29 D13 D1

1 0.13872 0.13006 0.12910 0.12841 -0.12772

RFO step: Lambda0=3.579210631D-05 Lambda=-4.49341756D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.06588881 RMS(Int)= 0.00168294

Iteration 2 RMS(Cart)= 0.00229755 RMS(Int)= 0.00045473

Iteration 3 RMS(Cart)= 0.00000194 RMS(Int)= 0.00045473

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00045473

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64538 -0.00360 0.00000 -0.00969 -0.00949 2.63589

R2 2.65459 -0.00780 0.00000 -0.01747 -0.01700 2.63760

R3 2.07691 -0.00121 0.00000 0.00037 0.00037 2.07728

R4 2.84223 -0.01130 0.00000 -0.02713 -0.02741 2.81482

R5 2.08263 -0.00014 0.00000 -0.00027 -0.00027 2.08236

R6 4.01176 -0.00034 0.00000 0.05504 0.05471 4.06647

R7 2.63037 0.00121 0.00000 0.00553 0.00578 2.63615

R8 2.83259 -0.00591 0.00000 -0.01916 -0.01887 2.81372

R9 2.08194 -0.00092 0.00000 0.00117 0.00117 2.08312

R10 4.17138 -0.00218 0.00000 -0.03285 -0.03280 4.13858

R11 2.07766 0.00120 0.00000 0.00083 0.00083 2.07849

R12 2.12043 -0.00008 0.00000 0.00206 0.00206 2.12249

R13 2.12993 -0.00113 0.00000 -0.00156 -0.00156 2.12837

R14 2.87109 -0.00014 0.00000 0.00403 0.00406 2.87515

R15 2.12595 -0.00025 0.00000 -0.00124 -0.00124 2.12472

R16 2.12734 0.00007 0.00000 0.00017 0.00017 2.12751

R17 2.66781 0.00023 0.00000 -0.00433 -0.00420 2.66360

R18 2.66976 -0.00091 0.00000 -0.00842 -0.00834 2.66142

R19 2.66073 0.00064 0.00000 0.00650 0.00583 2.66656

R20 2.79759 0.00238 0.00000 0.01216 0.01216 2.80975

R21 2.06367 0.00035 0.00000 -0.00120 -0.00120 2.06247

R22 2.81026 0.00457 0.00000 0.00982 0.00975 2.82000

R23 2.07022 0.00007 0.00000 -0.00299 -0.00299 2.06723

R24 2.30621 -0.00063 0.00000 0.00003 0.00003 2.30625

R25 2.30571 -0.00001 0.00000 0.00032 0.00032 2.30603

A1 2.03721 0.00434 0.00000 0.02840 0.02833 2.06554

A2 2.11435 -0.00113 0.00000 -0.00564 -0.00569 2.10866

A3 2.11623 -0.00305 0.00000 -0.01954 -0.01968 2.09655

A4 2.07023 -0.00124 0.00000 0.00081 0.00045 2.07067

A5 2.11559 0.00022 0.00000 -0.01538 -0.01535 2.10024

A6 1.70016 -0.00072 0.00000 -0.03692 -0.03738 1.66278

A7 2.00568 0.00110 0.00000 0.02428 0.02442 2.03009

A8 1.72871 0.00032 0.00000 0.00212 0.00162 1.73033

A9 1.68532 0.00028 0.00000 0.01460 0.01482 1.70014

A10 2.08124 0.00156 0.00000 0.02186 0.02119 2.10243

A11 2.14150 -0.00109 0.00000 -0.03258 -0.03239 2.10911

A12 1.55253 0.00098 0.00000 0.02600 0.02524 1.57777

A13 2.01268 -0.00070 0.00000 0.00024 0.00025 2.01293

A14 1.73573 0.00070 0.00000 0.02050 0.01971 1.75544

A15 1.71831 -0.00094 0.00000 -0.01517 -0.01444 1.70386

A16 2.08628 -0.00385 0.00000 -0.03154 -0.03178 2.05451

A17 2.08880 0.00118 0.00000 0.01486 0.01449 2.10329

A18 2.08618 0.00296 0.00000 0.02508 0.02487 2.11105

A19 1.93279 -0.00127 0.00000 -0.00205 -0.00164 1.93116

A20 1.88585 -0.00151 0.00000 -0.01810 -0.01793 1.86792

A21 1.95640 0.00208 0.00000 0.01867 0.01764 1.97405

A22 1.85463 0.00089 0.00000 0.00455 0.00435 1.85897

A23 1.93171 -0.00020 0.00000 -0.00938 -0.00907 1.92263

A24 1.89870 -0.00007 0.00000 0.00543 0.00585 1.90455

A25 1.99900 -0.00234 0.00000 -0.01634 -0.01677 1.98223

A26 1.91406 0.00048 0.00000 0.00440 0.00445 1.91851

A27 1.86840 0.00073 0.00000 0.01031 0.01051 1.87891

A28 1.91537 0.00116 0.00000 0.00512 0.00534 1.92071

A29 1.90192 0.00052 0.00000 0.00188 0.00197 1.90389

A30 1.85944 -0.00046 0.00000 -0.00463 -0.00473 1.85471

A31 1.88866 -0.00101 0.00000 -0.00625 -0.00642 1.88224

A32 1.85560 -0.00142 0.00000 -0.00345 -0.00528 1.85032

A33 1.67609 0.00045 0.00000 -0.00068 0.00022 1.67630

A34 1.59876 0.00048 0.00000 -0.00225 -0.00153 1.59723

A35 1.88621 -0.00166 0.00000 -0.01469 -0.01478 1.87143

A36 2.18561 0.00056 0.00000 0.01145 0.01173 2.19734

A37 2.11521 0.00139 0.00000 0.00647 0.00633 2.12154

A38 1.86525 -0.00021 0.00000 0.01753 0.01539 1.88064

A39 1.88389 -0.00103 0.00000 -0.06791 -0.06685 1.81705

A40 1.53031 0.00094 0.00000 0.01204 0.01305 1.54336

A41 1.85562 -0.00012 0.00000 0.00419 0.00413 1.85975

A42 2.19674 -0.00061 0.00000 -0.00287 -0.00296 2.19378

A43 2.06542 0.00084 0.00000 0.01846 0.01820 2.08363

A44 1.88893 0.00223 0.00000 0.01479 0.01458 1.90351

A45 2.03338 -0.00170 0.00000 -0.00799 -0.00789 2.02550

A46 2.36085 -0.00053 0.00000 -0.00678 -0.00668 2.35418

A47 1.90159 0.00062 0.00000 0.00549 0.00520 1.90679

A48 2.02093 0.00007 0.00000 0.00425 0.00439 2.02532

A49 2.36064 -0.00068 0.00000 -0.00971 -0.00957 2.35107

D1 -0.63729 0.00058 0.00000 0.01432 0.01397 -0.62332

D2 2.97389 0.00011 0.00000 -0.01556 -0.01583 2.95806

D3 1.18787 0.00018 0.00000 -0.00503 -0.00611 1.18176

D4 2.68968 -0.00005 0.00000 -0.00285 -0.00278 2.68689

D5 0.01767 -0.00052 0.00000 -0.03273 -0.03258 -0.01492

D6 -1.76836 -0.00045 0.00000 -0.02219 -0.02286 -1.79121

D7 -0.04364 0.00056 0.00000 0.02454 0.02464 -0.01901

D8 -2.96084 -0.00126 0.00000 -0.02103 -0.02036 -2.98121

D9 2.91237 0.00140 0.00000 0.04331 0.04281 2.95517

D10 -0.00484 -0.00041 0.00000 -0.00225 -0.00219 -0.00703

D11 2.90572 -0.00089 0.00000 -0.06530 -0.06579 2.83993

D12 -1.35290 -0.00140 0.00000 -0.07146 -0.07173 -1.42463

D13 0.73904 -0.00121 0.00000 -0.06522 -0.06568 0.67335

D14 -0.67675 -0.00064 0.00000 -0.04723 -0.04730 -0.72405

D15 1.34782 -0.00114 0.00000 -0.05340 -0.05325 1.29457

D16 -2.84343 -0.00095 0.00000 -0.04715 -0.04720 -2.89062

D17 1.09700 0.00013 0.00000 -0.02336 -0.02298 1.07402

D18 3.12157 -0.00038 0.00000 -0.02952 -0.02892 3.09264

D19 -1.06968 -0.00019 0.00000 -0.02328 -0.02287 -1.09255

D20 -0.76790 0.00052 0.00000 -0.07916 -0.07954 -0.84744

D21 -2.75766 0.00125 0.00000 -0.06024 -0.06009 -2.81775

D22 1.44693 0.00017 0.00000 -0.07490 -0.07497 1.37196

D23 1.33780 -0.00088 0.00000 -0.08748 -0.08809 1.24971

D24 -0.65195 -0.00015 0.00000 -0.06856 -0.06865 -0.72060

D25 -2.73055 -0.00123 0.00000 -0.08322 -0.08352 -2.81407

D26 -2.91035 0.00039 0.00000 -0.05849 -0.05881 -2.96916

D27 1.38308 0.00112 0.00000 -0.03957 -0.03936 1.34372

D28 -0.69552 0.00004 0.00000 -0.05423 -0.05424 -0.74975

D29 0.58598 -0.00037 0.00000 0.00185 0.00229 0.58827

D30 -2.77966 0.00121 0.00000 0.04604 0.04611 -2.73356

D31 -2.89822 -0.00128 0.00000 -0.03414 -0.03331 -2.93153

D32 0.01932 0.00030 0.00000 0.01004 0.01051 0.02983

D33 -1.16374 -0.00186 0.00000 -0.03822 -0.03763 -1.20137

D34 1.75380 -0.00028 0.00000 0.00596 0.00619 1.75999

D35 -0.42897 -0.00063 0.00000 -0.05754 -0.05740 -0.48637

D36 -2.59110 -0.00082 0.00000 -0.05575 -0.05562 -2.64672

D37 1.68144 -0.00091 0.00000 -0.05809 -0.05806 1.62338

D38 3.03071 0.00033 0.00000 -0.01739 -0.01710 3.01361

D39 0.86858 0.00014 0.00000 -0.01560 -0.01532 0.85326

D40 -1.14207 0.00005 0.00000 -0.01794 -0.01776 -1.15983

D41 1.21386 0.00124 0.00000 -0.01097 -0.01109 1.20277

D42 -0.94826 0.00104 0.00000 -0.00918 -0.00931 -0.95758

D43 -2.95891 0.00095 0.00000 -0.01152 -0.01176 -2.97067

D44 1.28528 0.00026 0.00000 -0.06509 -0.06493 1.22036

D45 -3.06315 -0.00167 0.00000 -0.08175 -0.08175 3.13828

D46 -0.94086 -0.00016 0.00000 -0.07561 -0.07555 -1.01641

D47 -0.80027 -0.00155 0.00000 -0.09350 -0.09354 -0.89381

D48 1.13447 -0.00348 0.00000 -0.11017 -0.11035 1.02412

D49 -3.02642 -0.00197 0.00000 -0.10402 -0.10416 -3.13058

D50 -2.85247 -0.00075 0.00000 -0.09495 -0.09481 -2.94728

D51 -0.91772 -0.00268 0.00000 -0.11162 -0.11163 -1.02935

D52 1.20457 -0.00117 0.00000 -0.10547 -0.10543 1.09913

D53 -0.19772 0.00002 0.00000 0.07172 0.07183 -0.12589

D54 1.96370 -0.00015 0.00000 0.06953 0.06956 2.03326

D55 -2.28954 0.00024 0.00000 0.06791 0.06800 -2.22154

D56 -2.36501 0.00030 0.00000 0.06773 0.06789 -2.29712

D57 -0.20358 0.00013 0.00000 0.06554 0.06562 -0.13797

D58 1.82635 0.00053 0.00000 0.06393 0.06406 1.89042

D59 1.88669 -0.00062 0.00000 0.06434 0.06436 1.95106

D60 -2.23507 -0.00079 0.00000 0.06215 0.06209 -2.17298

D61 -0.20513 -0.00039 0.00000 0.06054 0.06054 -0.14459

D62 -0.02381 0.00035 0.00000 0.00907 0.00964 -0.01417

D63 3.11179 0.00063 0.00000 0.01160 0.01227 3.12405

D64 -0.02724 -0.00001 0.00000 0.01453 0.01411 -0.01313

D65 3.12126 -0.00025 0.00000 0.01068 0.00987 3.13113

D66 -0.30805 0.00131 0.00000 0.09905 0.09906 -0.20899

D67 1.70079 -0.00002 0.00000 0.03150 0.03164 1.73243

D68 -2.04668 0.00051 0.00000 0.07079 0.07110 -1.97557

D69 -2.09116 0.00199 0.00000 0.10660 0.10623 -1.98492

D70 -0.08232 0.00066 0.00000 0.03905 0.03882 -0.04350

D71 2.45340 0.00119 0.00000 0.07835 0.07828 2.53168

D72 1.50757 0.00107 0.00000 0.09880 0.09836 1.60594

D73 -2.76678 -0.00026 0.00000 0.03125 0.03095 -2.73583

D74 -0.23106 0.00027 0.00000 0.07055 0.07041 -0.16065

D75 -1.84037 0.00118 0.00000 -0.02364 -0.02236 -1.86273

D76 1.30885 0.00082 0.00000 -0.02687 -0.02571 1.28314

D77 0.06851 -0.00056 0.00000 -0.03094 -0.03122 0.03729

D78 -3.06546 -0.00092 0.00000 -0.03417 -0.03458 -3.10003

D79 2.77502 0.00010 0.00000 -0.02163 -0.02173 2.75329

D80 -0.35895 -0.00026 0.00000 -0.02486 -0.02508 -0.38403

D81 2.06572 -0.00108 0.00000 -0.04274 -0.04404 2.02169

D82 -1.08471 -0.00077 0.00000 -0.03771 -0.03857 -1.12327

D83 0.06957 -0.00030 0.00000 -0.03318 -0.03316 0.03642

D84 -3.08086 0.00001 0.00000 -0.02814 -0.02769 -3.10854

D85 -2.52006 -0.00022 0.00000 -0.06069 -0.06136 -2.58142

D86 0.61270 0.00009 0.00000 -0.05566 -0.05589 0.55681

Item Value Threshold Converged?

Maximum Force 0.011301 0.000450 NO

RMS Force 0.001686 0.000300 NO

Maximum Displacement 0.298866 0.001800 NO

RMS Displacement 0.065825 0.001200 NO

Predicted change in Energy=-2.889212D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.185138 1.607468 0.454889

2 6 0 0.129730 1.255490 0.150178

3 6 0 -0.681289 3.777083 -0.407707

4 6 0 -1.610200 2.903253 0.157575

5 1 0 -1.821068 0.942677 1.056553

6 1 0 -2.584389 3.267311 0.515589

7 6 0 0.752815 1.818709 -1.079971

8 1 0 1.870664 1.717152 -1.039819

9 1 0 0.404842 1.186713 -1.944852

10 6 0 0.366824 3.268173 -1.334777

11 1 0 1.277843 3.924892 -1.280639

12 1 0 -0.029506 3.364559 -2.384123

13 1 0 -0.893066 4.856329 -0.482058

14 1 0 0.552974 0.308679 0.522578

15 8 0 2.692721 4.029175 0.810280

16 6 0 0.437564 3.829504 1.474234

17 6 0 1.026126 2.554542 1.612892

18 6 0 1.499570 4.755406 0.999278

19 8 0 1.554672 5.949831 0.754895

20 6 0 2.442127 2.688484 1.161334

21 8 0 3.381461 1.918775 1.041650

22 1 0 -0.436445 4.193365 2.017280

23 1 0 0.774765 1.815434 2.379196

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394854 0.000000

3 C 2.388549 2.706922 0.000000

4 C 1.395755 2.396359 1.394991 0.000000

5 H 1.099251 2.173702 3.387774 2.167137 0.000000

6 H 2.171789 3.398146 2.175807 1.099890 2.505838

7 C 2.481146 1.489537 2.518694 2.879513 3.457895

8 H 3.403544 2.158721 3.339962 3.867428 4.315492

9 H 2.909266 2.114135 3.201954 3.380400 3.744684

10 C 2.892997 2.512409 1.488955 2.503778 3.989142

11 H 3.801156 3.238998 2.149897 3.384228 4.894826

12 H 3.533108 3.300942 2.121607 3.028469 4.573123

13 H 3.393859 3.796298 1.102338 2.176676 4.306412

14 H 2.170822 1.101938 3.797192 3.397700 2.514589

15 O 4.585712 3.833795 3.595968 4.495425 5.473701

16 C 2.934224 2.910917 2.190042 2.604777 3.689125

17 C 2.669758 2.151881 2.914222 3.031461 3.318754

18 C 4.172953 3.853161 2.773602 3.716127 5.056364

19 O 5.143217 4.942973 3.327461 4.433378 6.046338

20 C 3.850287 2.902255 3.660965 4.180312 4.607998

21 O 4.614654 3.436338 4.696795 5.164055 5.293325

22 H 3.112631 3.526717 2.472611 2.549626 3.661577

23 H 2.754528 2.387075 3.706075 3.436132 3.041288

6 7 8 9 10

6 H 0.000000

7 C 3.972555 0.000000

8 H 4.966869 1.123171 0.000000

9 H 4.395243 1.126287 1.802521 0.000000

10 C 3.483319 1.521466 2.180414 2.169357 0.000000

11 H 4.309952 2.179892 2.298597 2.949734 1.124352

12 H 3.865904 2.168522 2.851623 2.263765 1.125831

13 H 2.526035 3.506217 4.219447 4.158174 2.199248

14 H 4.312378 2.210948 2.482174 2.623184 3.499003

15 O 5.339960 3.496061 3.073124 4.572169 3.254257

16 C 3.219823 3.265983 3.582775 4.321523 2.865421

17 C 3.840303 2.804935 2.907119 3.861928 3.103658

18 C 4.373455 3.674930 3.677855 4.754145 2.990450

19 O 4.938118 4.590847 4.608299 5.594465 3.601250

20 C 5.100774 2.938322 2.472879 4.006774 3.297498

21 O 6.138946 3.379508 2.579859 4.279646 4.068946

22 H 2.779626 4.079987 4.560728 5.044423 3.568964

23 H 4.106689 3.459239 3.591702 4.385148 4.008798

11 12 13 14 15

11 H 0.000000

12 H 1.800225 0.000000

13 H 2.493623 2.566898 0.000000

14 H 4.105365 4.257534 4.876623 0.000000

15 O 2.526796 4.249287 3.900280 4.301556 0.000000

16 C 2.881752 3.914237 2.579151 3.648997 2.359330

17 C 3.211501 4.212673 3.656546 2.540976 2.365643

18 C 2.436583 3.964837 2.815892 4.571288 1.409518

19 O 2.884513 4.364251 2.952494 5.734106 2.233191

20 C 2.974474 4.374507 4.303928 3.104897 1.408364

21 O 3.720584 5.045880 5.405783 3.295783 2.231968

22 H 3.726544 4.497207 2.625779 4.278302 3.357899

23 H 4.254092 5.073051 4.496162 2.401361 3.322755

16 17 18 19 20

16 C 0.000000

17 C 1.411084 0.000000

18 C 1.486855 2.333340 0.000000

19 O 2.502232 3.541681 1.220414 0.000000

20 C 2.327683 1.492282 2.277464 3.404284 0.000000

21 O 3.536177 2.505618 3.404377 4.434952 1.220297

22 H 1.091414 2.233468 2.258401 2.939955 3.359090

23 H 2.233638 1.093931 3.327605 4.509972 2.241763

21 22 23

21 O 0.000000

22 H 4.549947 0.000000

23 H 2.931651 2.693059 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.374965 -0.331336 -0.770972

2 6 0 1.552519 -1.249963 -0.118803

3 6 0 1.182494 1.383191 0.388159

4 6 0 2.194878 1.026532 -0.502837

5 1 0 3.034837 -0.649010 -1.590730

6 1 0 2.714690 1.787909 -1.102719

7 6 0 1.142386 -0.969890 1.285501

8 1 0 0.257820 -1.599575 1.572824

9 1 0 1.993876 -1.292646 1.948308

10 6 0 0.843639 0.500383 1.538296

11 1 0 -0.237823 0.631688 1.816444

12 1 0 1.442136 0.850411 2.425301

13 1 0 0.862769 2.433277 0.489369

14 1 0 1.544250 -2.307462 -0.428471

15 8 0 -2.087353 -0.107817 0.261752

16 6 0 -0.334952 0.755820 -1.060995

17 6 0 -0.251451 -0.651213 -1.127656

18 6 0 -1.509311 1.087441 -0.211498

19 8 0 -2.052528 2.121841 0.141122

20 6 0 -1.345370 -1.183521 -0.263425

21 8 0 -1.714482 -2.299540 0.064267

22 1 0 0.046321 1.455568 -1.806762

23 1 0 0.077240 -1.230703 -1.995319

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2243598 0.8788486 0.6740931

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5581966719 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.491752881841E-01 A.U. after 15 cycles

Convg = 0.8030D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001730707 -0.001351331 0.002257775

2 6 0.001262403 0.000011528 -0.001015942

3 6 -0.001474949 0.001222360 0.001502460

4 6 0.001756329 0.000757509 -0.001055616

5 1 -0.000011285 -0.000414881 0.000101989

6 1 0.000271582 -0.000013948 -0.000489304

7 6 0.000469071 -0.000181650 -0.000519732

8 1 0.000060550 0.000082169 0.000432480

9 1 0.000426487 -0.000072404 -0.000320171

10 6 -0.000028844 -0.000042064 -0.000098825

11 1 0.000197480 -0.000032470 -0.000149855

12 1 -0.000249940 0.000103728 0.000075231

13 1 -0.000828270 0.000088281 0.000452330

14 1 0.000178886 -0.000072338 -0.000438342

15 8 -0.000365570 -0.000167463 -0.000299547

16 6 0.002116610 -0.000491932 -0.002998004

17 6 -0.000168880 0.000764203 0.001776560

18 6 -0.001082521 0.000156374 0.000600746

19 8 -0.000277647 0.000419405 -0.000327916

20 6 -0.000992218 -0.001366018 0.000508902

21 8 0.000556719 -0.000344541 0.000320466

22 1 0.000746461 0.001173235 0.000361583

23 1 -0.000831748 -0.000227752 -0.000677268

-------------------------------------------------------------------

Cartesian Forces: Max 0.002998004 RMS 0.000873010

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.001322428 RMS 0.000398177

Search for a saddle point.

Step number 54 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 32 39 40 53 54

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06314 0.00046 0.00393 0.00561 0.00791

Eigenvalues --- 0.01096 0.01110 0.01395 0.01797 0.02444

Eigenvalues --- 0.02591 0.02813 0.03106 0.03148 0.03327

Eigenvalues --- 0.03559 0.03586 0.03664 0.03819 0.04116

Eigenvalues --- 0.04310 0.04439 0.04703 0.04970 0.06108

Eigenvalues --- 0.06345 0.06536 0.06799 0.07344 0.08252

Eigenvalues --- 0.08910 0.09278 0.10040 0.10091 0.11069

Eigenvalues --- 0.12332 0.13891 0.14701 0.17054 0.21956

Eigenvalues --- 0.26055 0.27828 0.29508 0.29874 0.30498

Eigenvalues --- 0.31166 0.31345 0.31884 0.32013 0.32428

Eigenvalues --- 0.32621 0.33476 0.36664 0.37552 0.39623

Eigenvalues --- 0.39758 0.40457 0.43879 0.48009 0.51572

Eigenvalues --- 0.59837 1.08562 1.10946

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D4 D71

1 -0.59425 -0.48688 0.15158 -0.14840 -0.14696

D73 D1 R19 D13 D86

1 0.14015 -0.13159 0.12962 0.12562 0.12527

RFO step: Lambda0=1.787470189D-07 Lambda=-2.25011735D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.09750738 RMS(Int)= 0.00347593

Iteration 2 RMS(Cart)= 0.00459576 RMS(Int)= 0.00119899

Iteration 3 RMS(Cart)= 0.00000630 RMS(Int)= 0.00119899

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00119899

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63589 0.00132 0.00000 0.00567 0.00579 2.64168

R2 2.63760 0.00124 0.00000 0.00321 0.00414 2.64173

R3 2.07728 0.00031 0.00000 0.00067 0.00067 2.07795

R4 2.81482 0.00058 0.00000 -0.00020 -0.00018 2.81464

R5 2.08236 -0.00002 0.00000 0.00012 0.00012 2.08248

R6 4.06647 -0.00006 0.00000 0.05291 0.05267 4.11914

R7 2.63615 -0.00088 0.00000 -0.00517 -0.00441 2.63174

R8 2.81372 0.00070 0.00000 0.01033 0.00993 2.82365

R9 2.08312 0.00022 0.00000 -0.00028 -0.00028 2.08284

R10 4.13858 -0.00067 0.00000 -0.06393 -0.06399 4.07459

R11 2.07849 -0.00040 0.00000 -0.00169 -0.00169 2.07680

R12 2.12249 0.00007 0.00000 0.00154 0.00154 2.12403

R13 2.12837 0.00015 0.00000 0.00003 0.00003 2.12841

R14 2.87515 0.00069 0.00000 0.00434 0.00387 2.87903

R15 2.12472 0.00013 0.00000 0.00026 0.00026 2.12498

R16 2.12751 0.00003 0.00000 0.00057 0.00057 2.12808

R17 2.66360 0.00047 0.00000 0.00397 0.00417 2.66777

R18 2.66142 0.00064 0.00000 0.00778 0.00767 2.66909

R19 2.66656 0.00016 0.00000 -0.00389 -0.00436 2.66220

R20 2.80975 -0.00119 0.00000 -0.00347 -0.00325 2.80650

R21 2.06247 -0.00003 0.00000 0.00410 0.00410 2.06658

R22 2.82000 -0.00106 0.00000 -0.01282 -0.01308 2.80692

R23 2.06723 -0.00013 0.00000 -0.00345 -0.00345 2.06378

R24 2.30625 0.00046 0.00000 0.00069 0.00069 2.30694

R25 2.30603 0.00061 0.00000 0.00124 0.00124 2.30726

A1 2.06554 -0.00095 0.00000 -0.01502 -0.01606 2.04948

A2 2.10866 0.00022 0.00000 0.00634 0.00680 2.11546

A3 2.09655 0.00074 0.00000 0.01088 0.01126 2.10781

A4 2.07067 0.00039 0.00000 0.02327 0.02299 2.09366

A5 2.10024 -0.00027 0.00000 0.00072 0.00073 2.10097

A6 1.66278 -0.00011 0.00000 -0.03424 -0.03529 1.62749

A7 2.03009 -0.00006 0.00000 -0.00664 -0.00714 2.02296

A8 1.73033 -0.00027 0.00000 -0.00375 -0.00472 1.72561

A9 1.70014 0.00024 0.00000 -0.00194 -0.00001 1.70013

A10 2.10243 -0.00033 0.00000 -0.02814 -0.02800 2.07443

A11 2.10911 0.00000 0.00000 0.00340 0.00286 2.11197

A12 1.57777 0.00035 0.00000 0.03897 0.03757 1.61534

A13 2.01293 0.00036 0.00000 0.01138 0.01119 2.02412

A14 1.75544 -0.00056 0.00000 -0.01566 -0.01641 1.73903

A15 1.70386 0.00011 0.00000 0.01169 0.01351 1.71737

A16 2.05451 0.00095 0.00000 0.02662 0.02618 2.08069

A17 2.10329 -0.00024 0.00000 -0.01085 -0.01080 2.09249

A18 2.11105 -0.00070 0.00000 -0.01512 -0.01486 2.09619

A19 1.93116 0.00002 0.00000 -0.01189 -0.01120 1.91996

A20 1.86792 0.00020 0.00000 0.01134 0.01166 1.87958

A21 1.97405 -0.00035 0.00000 0.00271 0.00110 1.97515

A22 1.85897 -0.00008 0.00000 -0.00195 -0.00216 1.85681

A23 1.92263 0.00020 0.00000 0.00297 0.00251 1.92515

A24 1.90455 0.00003 0.00000 -0.00315 -0.00178 1.90277

A25 1.98223 0.00046 0.00000 0.01260 0.01063 1.99286

A26 1.91851 -0.00019 0.00000 0.00455 0.00508 1.92359

A27 1.87891 -0.00013 0.00000 -0.01291 -0.01222 1.86669

A28 1.92071 -0.00016 0.00000 -0.00671 -0.00681 1.91390

A29 1.90389 -0.00008 0.00000 0.00189 0.00316 1.90705

A30 1.85471 0.00008 0.00000 -0.00037 -0.00066 1.85404

A31 1.88224 0.00046 0.00000 0.00524 0.00514 1.88738

A32 1.85032 0.00023 0.00000 0.03462 0.02921 1.87953

A33 1.67630 -0.00017 0.00000 0.04365 0.04599 1.72230

A34 1.59723 -0.00008 0.00000 -0.01117 -0.00913 1.58810

A35 1.87143 0.00064 0.00000 0.00305 0.00234 1.87377

A36 2.19734 -0.00016 0.00000 -0.00739 -0.00769 2.18965

A37 2.12154 -0.00049 0.00000 -0.02487 -0.02573 2.09580

A38 1.88064 0.00027 0.00000 0.00081 -0.00424 1.87640

A39 1.81705 -0.00063 0.00000 -0.06214 -0.06051 1.75653

A40 1.54336 0.00004 0.00000 -0.00478 -0.00209 1.54127

A41 1.85975 0.00015 0.00000 0.00752 0.00814 1.86789

A42 2.19378 0.00007 0.00000 0.01766 0.01692 2.21070

A43 2.08363 -0.00007 0.00000 0.01010 0.00828 2.09191

A44 1.90351 -0.00072 0.00000 -0.00745 -0.00731 1.89620

A45 2.02550 0.00062 0.00000 0.00555 0.00539 2.03088

A46 2.35418 0.00010 0.00000 0.00196 0.00183 2.35601

A47 1.90679 -0.00052 0.00000 -0.00692 -0.00745 1.89934

A48 2.02532 0.00031 0.00000 0.00118 0.00144 2.02676

A49 2.35107 0.00021 0.00000 0.00571 0.00594 2.35701

D1 -0.62332 0.00014 0.00000 0.02548 0.02568 -0.59764

D2 2.95806 0.00001 0.00000 -0.01687 -0.01750 2.94056

D3 1.18176 -0.00015 0.00000 0.00638 0.00396 1.18572

D4 2.68689 0.00003 0.00000 0.00970 0.01070 2.69759

D5 -0.01492 -0.00010 0.00000 -0.03265 -0.03248 -0.04739

D6 -1.79121 -0.00026 0.00000 -0.00939 -0.01102 -1.80223

D7 -0.01901 -0.00020 0.00000 0.00578 0.00588 -0.01312

D8 -2.98121 -0.00018 0.00000 0.00323 0.00411 -2.97709

D9 2.95517 -0.00014 0.00000 0.02101 0.02036 2.97553

D10 -0.00703 -0.00012 0.00000 0.01846 0.01859 0.01157

D11 2.83993 -0.00018 0.00000 -0.08797 -0.08871 2.75122

D12 -1.42463 -0.00016 0.00000 -0.09007 -0.09061 -1.51524

D13 0.67335 -0.00020 0.00000 -0.08474 -0.08424 0.58911

D14 -0.72405 -0.00012 0.00000 -0.04586 -0.04586 -0.76991

D15 1.29457 -0.00009 0.00000 -0.04796 -0.04776 1.24681

D16 -2.89062 -0.00014 0.00000 -0.04262 -0.04140 -2.93202

D17 1.07402 -0.00001 0.00000 -0.05199 -0.05038 1.02364

D18 3.09264 0.00002 0.00000 -0.05409 -0.05228 3.04036

D19 -1.09255 -0.00003 0.00000 -0.04875 -0.04591 -1.13847

D20 -0.84744 -0.00069 0.00000 -0.14790 -0.14659 -0.99404

D21 -2.81775 -0.00068 0.00000 -0.12851 -0.12783 -2.94558

D22 1.37196 -0.00054 0.00000 -0.13065 -0.13017 1.24179

D23 1.24971 -0.00037 0.00000 -0.13283 -0.13185 1.11786

D24 -0.72060 -0.00036 0.00000 -0.11344 -0.11308 -0.83368

D25 -2.81407 -0.00022 0.00000 -0.11558 -0.11543 -2.92950

D26 -2.96916 -0.00043 0.00000 -0.14110 -0.14036 -3.10951

D27 1.34372 -0.00042 0.00000 -0.12172 -0.12159 1.22213

D28 -0.74975 -0.00028 0.00000 -0.12385 -0.12393 -0.87369

D29 0.58827 -0.00012 0.00000 0.00664 0.00665 0.59492

D30 -2.73356 -0.00010 0.00000 0.00969 0.00887 -2.72468

D31 -2.93153 0.00003 0.00000 -0.03235 -0.03145 -2.96299

D32 0.02983 0.00006 0.00000 -0.02930 -0.02923 0.00060

D33 -1.20137 0.00037 0.00000 0.00528 0.00784 -1.19353

D34 1.75999 0.00039 0.00000 0.00833 0.01007 1.77006

D35 -0.48637 0.00007 0.00000 -0.06436 -0.06462 -0.55099

D36 -2.64672 0.00009 0.00000 -0.06821 -0.06742 -2.71414

D37 1.62338 0.00017 0.00000 -0.06304 -0.06253 1.56084

D38 3.01361 -0.00001 0.00000 -0.02634 -0.02720 2.98641

D39 0.85326 0.00001 0.00000 -0.03020 -0.03001 0.82325

D40 -1.15983 0.00009 0.00000 -0.02502 -0.02512 -1.18495

D41 1.20277 0.00005 0.00000 -0.03492 -0.03729 1.16548

D42 -0.95758 0.00007 0.00000 -0.03878 -0.04009 -0.99767

D43 -2.97067 0.00015 0.00000 -0.03361 -0.03520 -3.00587

D44 1.22036 -0.00084 0.00000 -0.15251 -0.15369 1.06666

D45 3.13828 -0.00017 0.00000 -0.12678 -0.12667 3.01161

D46 -1.01641 -0.00070 0.00000 -0.14925 -0.14948 -1.16589

D47 -0.89381 -0.00051 0.00000 -0.13046 -0.13113 -1.02494

D48 1.02412 0.00016 0.00000 -0.10473 -0.10411 0.92001

D49 -3.13058 -0.00037 0.00000 -0.12719 -0.12691 3.02570

D50 -2.94728 -0.00078 0.00000 -0.14176 -0.14241 -3.08969

D51 -1.02935 -0.00011 0.00000 -0.11603 -0.11539 -1.14474

D52 1.09913 -0.00064 0.00000 -0.13849 -0.13819 0.96094

D53 -0.12589 0.00022 0.00000 0.10545 0.10567 -0.02022

D54 2.03326 0.00018 0.00000 0.11547 0.11486 2.14812

D55 -2.22154 0.00014 0.00000 0.11232 0.11203 -2.10951

D56 -2.29712 0.00030 0.00000 0.11679 0.11763 -2.17948

D57 -0.13797 0.00026 0.00000 0.12680 0.12683 -0.01114

D58 1.89042 0.00022 0.00000 0.12365 0.12400 2.01441

D59 1.95106 0.00026 0.00000 0.11929 0.11985 2.07091

D60 -2.17298 0.00023 0.00000 0.12930 0.12905 -2.04393

D61 -0.14459 0.00018 0.00000 0.12615 0.12622 -0.01838

D62 -0.01417 -0.00014 0.00000 -0.00417 -0.00310 -0.01727

D63 3.12405 -0.00004 0.00000 0.01093 0.01265 3.13670

D64 -0.01313 0.00016 0.00000 0.02294 0.02179 0.00867

D65 3.13113 0.00015 0.00000 0.03234 0.03080 -3.12125

D66 -0.20899 0.00067 0.00000 0.15887 0.16025 -0.04874

D67 1.73243 0.00014 0.00000 0.09186 0.09337 1.82581

D68 -1.97557 0.00037 0.00000 0.15624 0.15850 -1.81707

D69 -1.98492 0.00054 0.00000 0.09646 0.09649 -1.88843

D70 -0.04350 0.00001 0.00000 0.02945 0.02961 -0.01389

D71 2.53168 0.00024 0.00000 0.09383 0.09474 2.62642

D72 1.60594 0.00067 0.00000 0.16887 0.16822 1.77415

D73 -2.73583 0.00014 0.00000 0.10187 0.10134 -2.63448

D74 -0.16065 0.00037 0.00000 0.16625 0.16647 0.00582

D75 -1.86273 -0.00026 0.00000 -0.07061 -0.06718 -1.92991

D76 1.28314 -0.00038 0.00000 -0.08975 -0.08713 1.19600

D77 0.03729 0.00006 0.00000 -0.01704 -0.01764 0.01965

D78 -3.10003 -0.00006 0.00000 -0.03619 -0.03759 -3.13762

D79 2.75329 0.00002 0.00000 -0.08063 -0.07968 2.67361

D80 -0.38403 -0.00009 0.00000 -0.09977 -0.09963 -0.48366

D81 2.02169 -0.00004 0.00000 -0.05656 -0.05991 1.96178

D82 -1.12327 -0.00003 0.00000 -0.06847 -0.07137 -1.19465

D83 0.03642 -0.00013 0.00000 -0.03346 -0.03273 0.00369

D84 -3.10854 -0.00012 0.00000 -0.04537 -0.04420 3.13045

D85 -2.58142 -0.00040 0.00000 -0.09598 -0.09590 -2.67732

D86 0.55681 -0.00038 0.00000 -0.10789 -0.10737 0.44944

Item Value Threshold Converged?

Maximum Force 0.001322 0.000450 NO

RMS Force 0.000398 0.000300 NO

Maximum Displacement 0.403109 0.001800 NO

RMS Displacement 0.097356 0.001200 NO

Predicted change in Energy=-1.948025D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.160059 1.562759 0.446435

2 6 0 0.163934 1.264465 0.111425

3 6 0 -0.735487 3.788598 -0.365714

4 6 0 -1.612739 2.860106 0.189108

5 1 0 -1.774966 0.856347 1.022633

6 1 0 -2.589107 3.185963 0.574224

7 6 0 0.789433 1.896879 -1.083248

8 1 0 1.908818 1.886280 -0.982180

9 1 0 0.544987 1.256505 -1.976963

10 6 0 0.295109 3.315175 -1.338546

11 1 0 1.168628 4.023123 -1.354440

12 1 0 -0.171111 3.367541 -2.362299

13 1 0 -1.002740 4.856141 -0.426938

14 1 0 0.629695 0.328585 0.460141

15 8 0 2.737342 3.899443 0.808908

16 6 0 0.465634 3.866756 1.423231

17 6 0 0.979086 2.574783 1.650878

18 6 0 1.580360 4.702220 0.908435

19 8 0 1.696722 5.866373 0.559856

20 6 0 2.411488 2.600797 1.258659

21 8 0 3.321253 1.786526 1.254967

22 1 0 -0.355727 4.329704 1.977283

23 1 0 0.633046 1.857941 2.398601

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.397916 0.000000

3 C 2.407116 2.721740 0.000000

4 C 1.397944 2.389283 1.392658 0.000000

5 H 1.099606 2.180870 3.406776 2.176266 0.000000

6 H 2.166403 3.389038 2.163922 1.098996 2.508189

7 C 2.500417 1.489443 2.533543 2.883943 3.477583

8 H 3.400531 2.151103 3.315297 3.836876 4.318599

9 H 2.978898 2.122883 3.263010 3.452417 3.813120

10 C 2.893895 2.514962 1.494209 2.486101 3.988259

11 H 3.836577 3.281519 2.158294 3.386909 4.933932

12 H 3.481989 3.264123 2.117112 2.974132 4.509569

13 H 3.410850 3.814591 1.102189 2.176182 4.323881

14 H 2.174073 1.102001 3.810177 3.392723 2.525336

15 O 4.558641 3.748602 3.667773 4.515260 5.446745

16 C 2.984193 2.929808 2.156182 2.618403 3.774033

17 C 2.655337 2.179752 2.912001 2.989271 3.306436

18 C 4.192798 3.802584 2.796660 3.755889 5.105095

19 O 5.166735 4.871148 3.330085 4.486383 6.112867

20 C 3.806991 2.855420 3.735360 4.172000 4.541499

21 O 4.559161 3.398366 4.805417 5.160708 5.185620

22 H 3.262886 3.625901 2.434470 2.633888 3.871667

23 H 2.667079 2.409035 3.638923 3.306017 2.948729

6 7 8 9 10

6 H 0.000000

7 C 3.977875 0.000000

8 H 4.933853 1.123988 0.000000

9 H 4.478159 1.126304 1.801734 0.000000

10 C 3.463248 1.523515 2.184673 2.169824 0.000000

11 H 4.305944 2.176752 2.291846 2.903556 1.124491

12 H 3.808260 2.172893 2.902579 2.262245 1.126132

13 H 2.511649 3.521344 4.195896 4.213718 2.211339

14 H 4.305615 2.206153 2.478479 2.609155 3.502420

15 O 5.379144 3.374146 2.819091 4.421834 3.304154

16 C 3.242797 3.204325 3.433812 4.287310 2.821477

17 C 3.776868 2.823290 2.876010 3.884267 3.154784

18 C 4.449179 3.530199 3.407614 4.611993 2.936783

19 O 5.055011 4.390882 4.273640 5.386356 3.475207

20 C 5.081027 2.934466 2.405114 3.969912 3.425620

21 O 6.111808 3.448120 2.647593 4.293477 4.268562

22 H 2.874840 4.073927 4.456109 5.088408 3.528113

23 H 3.933735 3.485577 3.613596 4.417583 4.025419

11 12 13 14 15

11 H 0.000000

12 H 1.800130 0.000000

13 H 2.503801 2.579372 0.000000

14 H 4.151236 4.224064 4.893927 0.000000

15 O 2.675114 4.335732 4.053492 4.161110 0.000000

16 C 2.869513 3.871032 2.560884 3.670574 2.353533

17 C 3.341490 4.249354 3.667363 2.566191 2.356926

18 C 2.398187 3.942933 2.911927 4.498157 1.411723

19 O 2.709425 4.274570 3.046543 5.640531 2.239136

20 C 3.224283 4.513209 4.425468 2.995891 1.412423

21 O 4.055263 5.270752 5.563116 3.162566 2.237038

22 H 3.676687 4.448798 2.544806 4.391097 3.334261

23 H 4.365796 5.058827 4.432683 2.469123 3.335103

16 17 18 19 20

16 C 0.000000

17 C 1.408777 0.000000

18 C 1.485137 2.332111 0.000000

19 O 2.501892 3.541172 1.220778 0.000000

20 C 2.327249 1.485358 2.286790 3.415144 0.000000

21 O 3.536980 2.502767 3.413512 4.446058 1.220951

22 H 1.093585 2.228904 2.242686 2.929676 3.341111

23 H 2.239355 1.092106 3.347823 4.536510 2.239232

21 22 23

21 O 0.000000

22 H 4.528761 0.000000

23 H 2.922234 2.695328 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.343099 -0.607330 -0.688783

2 6 0 1.433248 -1.335098 0.083677

3 6 0 1.306014 1.381810 0.184134

4 6 0 2.273159 0.787289 -0.622508

5 1 0 2.986829 -1.103722 -1.429282

6 1 0 2.858159 1.398932 -1.323550

7 6 0 0.999884 -0.814155 1.410046

8 1 0 0.013347 -1.269175 1.698230

9 1 0 1.747357 -1.164542 2.176254

10 6 0 0.915001 0.706229 1.458246

11 1 0 -0.122242 1.017801 1.760781

12 1 0 1.605774 1.091725 2.259744

13 1 0 1.112241 2.465639 0.133258

14 1 0 1.314515 -2.419891 -0.069728

15 8 0 -2.077032 -0.032653 0.266935

16 6 0 -0.302695 0.714285 -1.086923

17 6 0 -0.278040 -0.694165 -1.104607

18 6 0 -1.447248 1.126758 -0.235162

19 8 0 -1.922270 2.195863 0.113647

20 6 0 -1.397580 -1.159466 -0.246461

21 8 0 -1.839839 -2.249313 0.081201

22 1 0 0.041060 1.364998 -1.895831

23 1 0 0.087035 -1.329876 -1.914105

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2191279 0.8834643 0.6750641

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6378209185 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.500380784271E-01 A.U. after 16 cycles

Convg = 0.4424D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.005231703 0.002911328 -0.003955484

2 6 -0.002598467 0.000038438 0.001828899

3 6 0.005448320 -0.004629828 -0.002361196

4 6 -0.004510935 -0.001811324 0.003375083

5 1 0.000733508 0.000708367 -0.000004052

6 1 -0.001277947 -0.000012030 0.000164016

7 6 -0.002559048 0.001610048 0.000960360

8 1 -0.000107674 0.000368540 -0.000585562

9 1 0.000022119 -0.000155601 0.000475845

10 6 -0.000016991 0.002011897 -0.000601065

11 1 -0.000392771 0.000093963 -0.000155809

12 1 0.000224670 -0.000440499 -0.000066322

13 1 0.000222276 -0.000413081 0.000442567

14 1 -0.000155494 -0.000221017 -0.000203178

15 8 0.000485279 0.000431098 -0.000145269

16 6 -0.003953669 0.001790572 0.002763076

17 6 -0.000688813 -0.003462835 -0.000424474

18 6 0.003340870 -0.001894557 -0.002082224

19 8 0.000600839 -0.001162093 0.000921646

20 6 0.002112166 0.002770011 -0.000079544

21 8 -0.000825624 0.001042227 -0.000429550

22 1 -0.000416952 -0.000139172 -0.000536723

23 1 -0.000917366 0.000565547 0.000698962

-------------------------------------------------------------------

Cartesian Forces: Max 0.005448320 RMS 0.001902015

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.004111287 RMS 0.000896891

Search for a saddle point.

Step number 55 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 33 34 36

37 41 43 45 46

50 51 52 54 55

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06365 0.00195 0.00374 0.00545 0.00781

Eigenvalues --- 0.00905 0.01155 0.01361 0.01831 0.02442

Eigenvalues --- 0.02603 0.02820 0.03098 0.03120 0.03336

Eigenvalues --- 0.03565 0.03605 0.03737 0.03824 0.04119

Eigenvalues --- 0.04292 0.04519 0.04708 0.05047 0.06140

Eigenvalues --- 0.06410 0.06632 0.06880 0.07349 0.08492

Eigenvalues --- 0.09188 0.09383 0.10007 0.10145 0.11070

Eigenvalues --- 0.12651 0.13895 0.14713 0.17247 0.22134

Eigenvalues --- 0.26114 0.27964 0.29529 0.29913 0.30680

Eigenvalues --- 0.31214 0.31346 0.31925 0.32022 0.32438

Eigenvalues --- 0.32671 0.33542 0.36674 0.37596 0.39626

Eigenvalues --- 0.39785 0.40462 0.43931 0.48399 0.51607

Eigenvalues --- 0.60530 1.08570 1.10972

Eigenvectors required to have negative eigenvalues:

R6 R10 D4 D73 D71

1 -0.57929 -0.50660 -0.15499 0.15311 -0.14396

D30 D79 R19 D1 D13

1 0.13960 -0.13066 0.13056 -0.13009 0.11869

RFO step: Lambda0=8.944097623D-06 Lambda=-7.50544202D-04.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.02633359 RMS(Int)= 0.00024845

Iteration 2 RMS(Cart)= 0.00031925 RMS(Int)= 0.00008227

Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00008227

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64168 -0.00411 0.00000 -0.00857 -0.00855 2.63313

R2 2.64173 -0.00223 0.00000 -0.00138 -0.00131 2.64042

R3 2.07795 -0.00087 0.00000 -0.00029 -0.00029 2.07766

R4 2.81464 -0.00070 0.00000 -0.00086 -0.00091 2.81373

R5 2.08248 0.00006 0.00000 0.00037 0.00037 2.08285

R6 4.11914 -0.00041 0.00000 -0.01138 -0.01138 4.10776

R7 2.63174 0.00249 0.00000 0.00284 0.00287 2.63462

R8 2.82365 -0.00179 0.00000 -0.00875 -0.00872 2.81492

R9 2.08284 -0.00048 0.00000 -0.00011 -0.00011 2.08273

R10 4.07459 0.00019 0.00000 0.02783 0.02781 4.10240

R11 2.07680 0.00119 0.00000 0.00084 0.00084 2.07764

R12 2.12403 -0.00016 0.00000 -0.00005 -0.00005 2.12398

R13 2.12841 -0.00029 0.00000 -0.00019 -0.00019 2.12822

R14 2.87903 -0.00170 0.00000 -0.00244 -0.00247 2.87656

R15 2.12498 -0.00024 0.00000 -0.00079 -0.00079 2.12419

R16 2.12808 -0.00005 0.00000 0.00005 0.00005 2.12814

R17 2.66777 -0.00168 0.00000 -0.00510 -0.00509 2.66268

R18 2.66909 -0.00155 0.00000 -0.00596 -0.00593 2.66316

R19 2.66220 0.00005 0.00000 0.00117 0.00111 2.66331

R20 2.80650 0.00269 0.00000 0.00645 0.00644 2.81294

R21 2.06658 -0.00002 0.00000 -0.00187 -0.00187 2.06471

R22 2.80692 0.00229 0.00000 0.00434 0.00434 2.81126

R23 2.06378 0.00040 0.00000 0.00092 0.00092 2.06470

R24 2.30694 -0.00131 0.00000 -0.00053 -0.00053 2.30641

R25 2.30726 -0.00131 0.00000 -0.00075 -0.00075 2.30651

A1 2.04948 0.00267 0.00000 0.01319 0.01315 2.06263

A2 2.11546 -0.00147 0.00000 -0.00846 -0.00846 2.10700

A3 2.10781 -0.00120 0.00000 -0.00584 -0.00585 2.10196

A4 2.09366 -0.00072 0.00000 -0.00451 -0.00447 2.08919

A5 2.10097 0.00028 0.00000 0.00201 0.00202 2.10299

A6 1.62749 -0.00034 0.00000 -0.00799 -0.00809 1.61940

A7 2.02296 0.00035 0.00000 -0.00051 -0.00057 2.02239

A8 1.72561 0.00093 0.00000 0.01465 0.01463 1.74024

A9 1.70013 -0.00036 0.00000 0.00156 0.00167 1.70180

A10 2.07443 0.00133 0.00000 0.01730 0.01732 2.09175

A11 2.11197 -0.00051 0.00000 -0.01079 -0.01083 2.10114

A12 1.61534 -0.00057 0.00000 -0.00054 -0.00067 1.61467

A13 2.02412 -0.00093 0.00000 -0.00261 -0.00265 2.02147

A14 1.73903 0.00139 0.00000 0.00272 0.00261 1.74165

A15 1.71737 -0.00048 0.00000 -0.01167 -0.01157 1.70580

A16 2.08069 -0.00305 0.00000 -0.02026 -0.02027 2.06042

A17 2.09249 0.00123 0.00000 0.00874 0.00873 2.10122

A18 2.09619 0.00187 0.00000 0.01227 0.01228 2.10846

A19 1.91996 0.00010 0.00000 0.00495 0.00496 1.92492

A20 1.87958 -0.00043 0.00000 -0.00700 -0.00695 1.87263

A21 1.97515 0.00083 0.00000 0.00610 0.00601 1.98116

A22 1.85681 0.00007 0.00000 -0.00160 -0.00161 1.85521

A23 1.92515 -0.00058 0.00000 -0.00489 -0.00488 1.92027

A24 1.90277 -0.00003 0.00000 0.00190 0.00193 1.90470

A25 1.99286 -0.00125 0.00000 -0.01137 -0.01138 1.98149

A26 1.92359 0.00047 0.00000 0.00044 0.00046 1.92405

A27 1.86669 0.00044 0.00000 0.00656 0.00652 1.87322

A28 1.91390 0.00044 0.00000 0.00608 0.00604 1.91995

A29 1.90705 0.00018 0.00000 -0.00142 -0.00138 1.90568

A30 1.85404 -0.00022 0.00000 0.00045 0.00044 1.85448

A31 1.88738 -0.00111 0.00000 -0.00459 -0.00459 1.88279

A32 1.87953 -0.00032 0.00000 -0.00319 -0.00347 1.87607

A33 1.72230 0.00086 0.00000 0.01161 0.01172 1.73401

A34 1.58810 -0.00029 0.00000 -0.02159 -0.02139 1.56671

A35 1.87377 -0.00143 0.00000 -0.00619 -0.00615 1.86761

A36 2.18965 0.00056 0.00000 0.00906 0.00893 2.19858

A37 2.09580 0.00084 0.00000 0.00572 0.00570 2.10150

A38 1.87640 -0.00065 0.00000 -0.00208 -0.00240 1.87400

A39 1.75653 0.00107 0.00000 -0.01212 -0.01195 1.74458

A40 1.54127 0.00015 0.00000 0.01879 0.01893 1.56019

A41 1.86789 -0.00077 0.00000 -0.00134 -0.00138 1.86651

A42 2.21070 -0.00008 0.00000 -0.01169 -0.01167 2.19902

A43 2.09191 0.00065 0.00000 0.00997 0.01000 2.10191

A44 1.89620 0.00179 0.00000 0.00710 0.00703 1.90323

A45 2.03088 -0.00155 0.00000 -0.00462 -0.00463 2.02626

A46 2.35601 -0.00023 0.00000 -0.00231 -0.00232 2.35370

A47 1.89934 0.00152 0.00000 0.00523 0.00519 1.90453

A48 2.02676 -0.00118 0.00000 -0.00165 -0.00165 2.02510

A49 2.35701 -0.00033 0.00000 -0.00345 -0.00346 2.35355

D1 -0.59764 -0.00003 0.00000 -0.00294 -0.00305 -0.60069

D2 2.94056 0.00014 0.00000 0.00587 0.00573 2.94628

D3 1.18572 0.00072 0.00000 0.00855 0.00836 1.19408

D4 2.69759 0.00004 0.00000 0.00564 0.00564 2.70323

D5 -0.04739 0.00022 0.00000 0.01445 0.01442 -0.03297

D6 -1.80223 0.00080 0.00000 0.01713 0.01705 -1.78518

D7 -0.01312 0.00048 0.00000 0.01566 0.01568 0.00256

D8 -2.97709 0.00002 0.00000 0.00965 0.00977 -2.96732

D9 2.97553 0.00038 0.00000 0.00687 0.00677 2.98230

D10 0.01157 -0.00008 0.00000 0.00086 0.00086 0.01242

D11 2.75122 -0.00006 0.00000 -0.01008 -0.01016 2.74106

D12 -1.51524 -0.00016 0.00000 -0.01326 -0.01334 -1.52858

D13 0.58911 0.00003 0.00000 -0.01187 -0.01197 0.57714

D14 -0.76991 -0.00022 0.00000 -0.01790 -0.01793 -0.78784

D15 1.24681 -0.00033 0.00000 -0.02108 -0.02110 1.22571

D16 -2.93202 -0.00014 0.00000 -0.01970 -0.01973 -2.95175

D17 1.02364 -0.00004 0.00000 -0.00843 -0.00833 1.01531

D18 3.04036 -0.00015 0.00000 -0.01162 -0.01151 3.02886

D19 -1.13847 0.00004 0.00000 -0.01023 -0.01014 -1.14861

D20 -0.99404 -0.00001 0.00000 -0.03318 -0.03319 -1.02722

D21 -2.94558 0.00060 0.00000 -0.02599 -0.02601 -2.97159

D22 1.24179 -0.00017 0.00000 -0.03902 -0.03898 1.20281

D23 1.11786 -0.00067 0.00000 -0.03718 -0.03725 1.08062

D24 -0.83368 -0.00006 0.00000 -0.03000 -0.03007 -0.86375

D25 -2.92950 -0.00083 0.00000 -0.04302 -0.04303 -2.97253

D26 -3.10951 -0.00018 0.00000 -0.03397 -0.03398 3.13969

D27 1.22213 0.00043 0.00000 -0.02678 -0.02680 1.19533

D28 -0.87369 -0.00034 0.00000 -0.03981 -0.03977 -0.91345

D29 0.59492 0.00041 0.00000 -0.00171 -0.00161 0.59331

D30 -2.72468 0.00081 0.00000 0.00393 0.00394 -2.72074

D31 -2.96299 -0.00009 0.00000 0.00844 0.00851 -2.95448

D32 0.00060 0.00030 0.00000 0.01409 0.01406 0.01466

D33 -1.19353 -0.00109 0.00000 -0.00744 -0.00722 -1.20074

D34 1.77006 -0.00069 0.00000 -0.00180 -0.00167 1.76839

D35 -0.55099 -0.00046 0.00000 -0.01456 -0.01454 -0.56552

D36 -2.71414 -0.00048 0.00000 -0.01448 -0.01445 -2.72858

D37 1.56084 -0.00071 0.00000 -0.01883 -0.01880 1.54204

D38 2.98641 -0.00005 0.00000 -0.02198 -0.02200 2.96440

D39 0.82325 -0.00007 0.00000 -0.02190 -0.02191 0.80134

D40 -1.18495 -0.00029 0.00000 -0.02625 -0.02627 -1.21122

D41 1.16548 0.00002 0.00000 -0.00924 -0.00932 1.15616

D42 -0.99767 0.00000 0.00000 -0.00916 -0.00923 -1.00690

D43 -3.00587 -0.00023 0.00000 -0.01351 -0.01359 -3.01946

D44 1.06666 0.00102 0.00000 -0.02037 -0.02037 1.04630

D45 3.01161 -0.00029 0.00000 -0.02336 -0.02338 2.98824

D46 -1.16589 0.00061 0.00000 -0.02030 -0.02042 -1.18631

D47 -1.02494 -0.00042 0.00000 -0.03839 -0.03838 -1.06332

D48 0.92001 -0.00173 0.00000 -0.04138 -0.04139 0.87862

D49 3.02570 -0.00083 0.00000 -0.03832 -0.03843 2.98727

D50 -3.08969 0.00032 0.00000 -0.03318 -0.03314 -3.12284

D51 -1.14474 -0.00098 0.00000 -0.03617 -0.03615 -1.18090

D52 0.96094 -0.00009 0.00000 -0.03312 -0.03319 0.92775

D53 -0.02022 -0.00016 0.00000 0.01341 0.01339 -0.00683

D54 2.14812 -0.00011 0.00000 0.01038 0.01034 2.15846

D55 -2.10951 -0.00003 0.00000 0.01354 0.01349 -2.09602

D56 -2.17948 -0.00046 0.00000 0.00620 0.00621 -2.17327

D57 -0.01114 -0.00041 0.00000 0.00317 0.00316 -0.00798

D58 2.01441 -0.00032 0.00000 0.00632 0.00632 2.02073

D59 2.07091 -0.00019 0.00000 0.00980 0.00980 2.08071

D60 -2.04393 -0.00014 0.00000 0.00677 0.00675 -2.03718

D61 -0.01838 -0.00005 0.00000 0.00992 0.00990 -0.00847

D62 -0.01727 0.00016 0.00000 0.00375 0.00383 -0.01344

D63 3.13670 -0.00017 0.00000 -0.00788 -0.00778 3.12892

D64 0.00867 -0.00005 0.00000 0.00508 0.00503 0.01370

D65 -3.12125 -0.00024 0.00000 -0.00351 -0.00363 -3.12488

D66 -0.04874 -0.00015 0.00000 0.03867 0.03856 -0.01018

D67 1.82581 0.00046 0.00000 0.02353 0.02350 1.84931

D68 -1.81707 0.00022 0.00000 0.02083 0.02091 -1.79616

D69 -1.88843 -0.00039 0.00000 0.02947 0.02934 -1.85909

D70 -0.01389 0.00022 0.00000 0.01433 0.01429 0.00040

D71 2.62642 -0.00002 0.00000 0.01163 0.01169 2.63812

D72 1.77415 -0.00051 0.00000 0.01197 0.01176 1.78591

D73 -2.63448 0.00009 0.00000 -0.00317 -0.00330 -2.63778

D74 0.00582 -0.00014 0.00000 -0.00586 -0.00589 -0.00006

D75 -1.92991 0.00020 0.00000 -0.01093 -0.01070 -1.94061

D76 1.19600 0.00061 0.00000 0.00380 0.00402 1.20003

D77 0.01965 -0.00022 0.00000 -0.01157 -0.01164 0.00801

D78 -3.13762 0.00019 0.00000 0.00316 0.00308 -3.13454

D79 2.67361 -0.00015 0.00000 0.00626 0.00620 2.67981

D80 -0.48366 0.00025 0.00000 0.02099 0.02092 -0.46275

D81 1.96178 -0.00062 0.00000 -0.02001 -0.02025 1.94153

D82 -1.19465 -0.00038 0.00000 -0.00906 -0.00924 -1.20388

D83 0.00369 -0.00010 0.00000 -0.01236 -0.01237 -0.00869

D84 3.13045 0.00015 0.00000 -0.00141 -0.00136 3.12909

D85 -2.67732 0.00034 0.00000 -0.00276 -0.00278 -2.68010

D86 0.44944 0.00058 0.00000 0.00820 0.00824 0.45767

Item Value Threshold Converged?

Maximum Force 0.004111 0.000450 NO

RMS Force 0.000897 0.000300 NO

Maximum Displacement 0.099211 0.001800 NO

RMS Displacement 0.026348 0.001200 NO

Predicted change in Energy=-3.848174D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.141729 1.562067 0.442321

2 6 0 0.180402 1.277955 0.106482

3 6 0 -0.750712 3.778794 -0.371023

4 6 0 -1.622148 2.851196 0.198095

5 1 0 -1.740299 0.845323 1.022655

6 1 0 -2.598619 3.165146 0.593959

7 6 0 0.792652 1.921446 -1.088539

8 1 0 1.912408 1.936162 -0.992542

9 1 0 0.560148 1.268651 -1.976311

10 6 0 0.273746 3.327678 -1.353807

11 1 0 1.130683 4.054532 -1.383589

12 1 0 -0.202689 3.360124 -2.373707

13 1 0 -1.025183 4.845124 -0.418986

14 1 0 0.654831 0.342505 0.445141

15 8 0 2.755026 3.864212 0.821596

16 6 0 0.472130 3.872119 1.420272

17 6 0 0.966030 2.574836 1.664044

18 6 0 1.607872 4.678991 0.896050

19 8 0 1.747227 5.836590 0.535273

20 6 0 2.406072 2.581951 1.290758

21 8 0 3.303723 1.755091 1.307467

22 1 0 -0.351012 4.355755 1.951591

23 1 0 0.593038 1.876760 2.417256

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.393391 0.000000

3 C 2.393387 2.710937 0.000000

4 C 1.397248 2.394299 1.394178 0.000000

5 H 1.099453 2.171552 3.395125 2.171955 0.000000

6 H 2.171494 3.394419 2.173135 1.099441 2.510393

7 C 2.492894 1.488961 2.519235 2.889831 3.468577

8 H 3.395075 2.154283 3.297542 3.840311 4.311986

9 H 2.971912 2.117149 3.255168 3.463366 3.803296

10 C 2.889123 2.518437 1.489592 2.495967 3.983220

11 H 3.835386 3.291311 2.154291 3.395264 4.932705

12 H 3.470565 3.260908 2.118102 2.981281 4.497082

13 H 3.396159 3.801874 1.102132 2.170923 4.311396

14 H 2.171398 1.102197 3.801283 3.396939 2.514557

15 O 4.541853 3.718710 3.704030 4.535924 5.418678

16 C 2.982829 2.922471 2.170896 2.630969 3.770204

17 C 2.638362 2.173732 2.922022 2.987313 3.275181

18 C 4.181075 3.772020 2.824668 3.776374 5.091492

19 O 5.160064 4.839417 3.360892 4.514305 6.108448

20 C 3.787731 2.838402 3.762876 4.182459 4.503349

21 O 4.532966 3.380112 4.832302 5.166852 5.133318

22 H 3.272280 3.627627 2.426351 2.637088 3.887952

23 H 2.647417 2.422501 3.632891 3.283481 2.907445

6 7 8 9 10

6 H 0.000000

7 C 3.984760 0.000000

8 H 4.937282 1.123959 0.000000

9 H 4.492304 1.126205 1.800550 0.000000

10 C 3.474291 1.522209 2.179918 2.170053 0.000000

11 H 4.313861 2.179765 2.291616 2.904817 1.124075

12 H 3.819102 2.170750 2.899813 2.261438 1.126161

13 H 2.514774 3.507238 4.173783 4.210664 2.205391

14 H 4.309801 2.205498 2.487604 2.594252 3.506094

15 O 5.403891 3.357658 2.778215 4.402580 3.343201

16 C 3.257622 3.194056 3.412331 4.280487 2.833953

17 C 3.768324 2.834377 2.891537 3.888836 3.186448

18 C 4.480798 3.493884 3.344044 4.580240 2.944112

19 O 5.101611 4.344690 4.192236 5.346333 3.469064

20 C 5.086510 2.949652 2.423677 3.975668 3.478023

21 O 6.110237 3.474765 2.694176 4.306626 4.328530

22 H 2.883133 4.059091 4.432315 5.078271 3.517516

23 H 3.895000 3.511757 3.656636 4.435573 4.053150

11 12 13 14 15

11 H 0.000000

12 H 1.800115 0.000000

13 H 2.490632 2.588948 0.000000

14 H 4.165313 4.217495 4.882903 0.000000

15 O 2.745461 4.383165 4.097708 4.117640 0.000000

16 C 2.885933 3.887389 2.563505 3.666392 2.360104

17 C 3.391855 4.276214 3.668535 2.562396 2.360661

18 C 2.411309 3.963439 2.947863 4.462814 1.409032

19 O 2.690333 4.289197 3.095136 5.602359 2.233365

20 C 3.308663 4.565029 4.451819 2.965979 1.409282

21 O 4.153471 5.331238 5.591813 3.123401 2.232830

22 H 3.661910 4.440887 2.512693 4.403099 3.341553

23 H 4.413409 5.078078 4.412946 2.499398 3.342198

16 17 18 19 20

16 C 0.000000

17 C 1.409363 0.000000

18 C 1.488544 2.330073 0.000000

19 O 2.503646 3.538846 1.220499 0.000000

20 C 2.328399 1.487655 2.278265 3.405512 0.000000

21 O 3.537295 2.502787 3.405050 4.435944 1.220555

22 H 1.092596 2.233596 2.248527 2.932821 3.344337

23 H 2.233842 1.092594 3.346110 4.533682 2.247973

21 22 23

21 O 0.000000

22 H 4.531604 0.000000

23 H 2.931595 2.693230 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.310362 -0.687142 -0.667757

2 6 0 1.380628 -1.354360 0.127199

3 6 0 1.364106 1.356483 0.142487

4 6 0 2.301633 0.710066 -0.661826

5 1 0 2.925958 -1.237143 -1.393936

6 1 0 2.901492 1.273130 -1.391139

7 6 0 0.974214 -0.770369 1.435170

8 1 0 -0.031692 -1.166180 1.743019

9 1 0 1.707649 -1.136240 2.207536

10 6 0 0.959870 0.751755 1.442403

11 1 0 -0.055948 1.125306 1.745912

12 1 0 1.679479 1.124962 2.224144

13 1 0 1.202140 2.442480 0.047231

14 1 0 1.227393 -2.440263 0.016870

15 8 0 -2.079921 -0.000654 0.271699

16 6 0 -0.292709 0.703934 -1.099259

17 6 0 -0.292347 -0.705428 -1.099647

18 6 0 -1.426325 1.138771 -0.238099

19 8 0 -1.884331 2.217667 0.102241

20 6 0 -1.425785 -1.139494 -0.239403

21 8 0 -1.887078 -2.218274 0.097046

22 1 0 0.065878 1.345987 -1.907311

23 1 0 0.066405 -1.347243 -1.907813

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2204848 0.8803256 0.6752576

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5432971911 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504067765031E-01 A.U. after 15 cycles

Convg = 0.6585D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000631924 -0.000349173 0.000008655

2 6 0.000120845 -0.000467465 -0.000116610

3 6 -0.000772807 -0.000079400 -0.000067419

4 6 0.000627812 0.000029364 -0.000239007

5 1 0.000015830 0.000190823 0.000356159

6 1 -0.000079879 -0.000044581 -0.000203707

7 6 0.000246454 0.000414949 -0.000384838

8 1 0.000028906 0.000020368 0.000076854

9 1 0.000034574 -0.000036497 -0.000020583

10 6 -0.000017342 -0.000110088 -0.000047176

11 1 -0.000026424 0.000018326 -0.000040770

12 1 -0.000007074 -0.000069837 0.000010990

13 1 0.000154291 0.000198835 0.000126251

14 1 -0.000000363 -0.000063135 -0.000012724

15 8 0.000151212 0.000089208 -0.000116319

16 6 0.000279149 0.000546876 0.000525830

17 6 -0.000215294 0.000317072 0.000530168

18 6 -0.000415381 0.000248553 -0.000199663

19 8 -0.000034200 0.000226917 0.000141200

20 6 0.000587015 -0.000845426 -0.000108624

21 8 0.000038158 -0.000188775 0.000037535

22 1 -0.000084188 0.000024560 -0.000160991

23 1 0.000000630 -0.000071473 -0.000095209

-------------------------------------------------------------------

Cartesian Forces: Max 0.000845426 RMS 0.000273692

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000570051 RMS 0.000137027

Search for a saddle point.

Step number 56 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 43 45 46 50

51 52 55 56

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06813 0.00129 0.00366 0.00761 0.00769

Eigenvalues --- 0.01072 0.01145 0.01376 0.01859 0.02441

Eigenvalues --- 0.02608 0.02830 0.03109 0.03134 0.03324

Eigenvalues --- 0.03564 0.03602 0.03751 0.03816 0.04129

Eigenvalues --- 0.04298 0.04521 0.04670 0.05016 0.06163

Eigenvalues --- 0.06463 0.06659 0.06955 0.07363 0.08510

Eigenvalues --- 0.09205 0.09602 0.10026 0.10191 0.11085

Eigenvalues --- 0.12677 0.13896 0.14749 0.17206 0.22261

Eigenvalues --- 0.26139 0.27999 0.29571 0.29916 0.30793

Eigenvalues --- 0.31263 0.31354 0.31924 0.32025 0.32442

Eigenvalues --- 0.32688 0.33569 0.36726 0.37713 0.39647

Eigenvalues --- 0.39814 0.40466 0.43974 0.48498 0.51783

Eigenvalues --- 0.60956 1.08587 1.10995

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D4

1 -0.57555 -0.51499 0.15048 -0.14443 -0.14275

D30 D1 R19 D79 D29

1 0.13318 -0.12945 0.12773 -0.12717 0.12450

RFO step: Lambda0=4.349354955D-06 Lambda=-4.35324500D-05.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.01308651 RMS(Int)= 0.00006300

Iteration 2 RMS(Cart)= 0.00007993 RMS(Int)= 0.00002040

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002040

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63313 0.00043 0.00000 0.00225 0.00225 2.63538

R2 2.64042 0.00006 0.00000 -0.00125 -0.00124 2.63917

R3 2.07766 0.00005 0.00000 0.00009 0.00009 2.07775

R4 2.81373 0.00047 0.00000 0.00202 0.00203 2.81576

R5 2.08285 0.00005 0.00000 0.00014 0.00014 2.08299

R6 4.10776 0.00030 0.00000 -0.00634 -0.00634 4.10141

R7 2.63462 -0.00024 0.00000 0.00003 0.00003 2.63465

R8 2.81492 0.00016 0.00000 0.00051 0.00050 2.81542

R9 2.08273 0.00015 0.00000 0.00045 0.00045 2.08318

R10 4.10240 0.00042 0.00000 -0.00388 -0.00389 4.09851

R11 2.07764 -0.00002 0.00000 0.00010 0.00010 2.07774

R12 2.12398 0.00004 0.00000 0.00022 0.00022 2.12420

R13 2.12822 0.00003 0.00000 -0.00014 -0.00014 2.12808

R14 2.87656 0.00000 0.00000 -0.00031 -0.00030 2.87626

R15 2.12419 -0.00001 0.00000 -0.00029 -0.00029 2.12390

R16 2.12814 -0.00001 0.00000 0.00010 0.00010 2.12824

R17 2.66268 0.00057 0.00000 0.00217 0.00217 2.66485

R18 2.66316 0.00051 0.00000 0.00132 0.00132 2.66448

R19 2.66331 0.00043 0.00000 0.00226 0.00225 2.66556

R20 2.81294 -0.00006 0.00000 -0.00103 -0.00103 2.81191

R21 2.06471 0.00000 0.00000 0.00006 0.00006 2.06476

R22 2.81126 0.00045 0.00000 0.00101 0.00101 2.81227

R23 2.06470 -0.00002 0.00000 -0.00010 -0.00010 2.06460

R24 2.30641 0.00017 0.00000 0.00012 0.00012 2.30653

R25 2.30651 0.00016 0.00000 0.00001 0.00001 2.30652

A1 2.06263 -0.00022 0.00000 -0.00238 -0.00240 2.06023

A2 2.10700 0.00023 0.00000 0.00161 0.00161 2.10861

A3 2.10196 -0.00002 0.00000 -0.00031 -0.00032 2.10164

A4 2.08919 -0.00004 0.00000 0.00023 0.00023 2.08942

A5 2.10299 -0.00001 0.00000 -0.00043 -0.00043 2.10256

A6 1.61940 0.00004 0.00000 -0.00249 -0.00251 1.61689

A7 2.02239 0.00007 0.00000 -0.00022 -0.00022 2.02217

A8 1.74024 -0.00006 0.00000 0.00297 0.00295 1.74318

A9 1.70180 -0.00003 0.00000 0.00067 0.00070 1.70249

A10 2.09175 -0.00011 0.00000 -0.00442 -0.00443 2.08732

A11 2.10114 0.00011 0.00000 0.00148 0.00148 2.10261

A12 1.61467 0.00008 0.00000 0.00672 0.00671 1.62138

A13 2.02147 0.00001 0.00000 0.00147 0.00147 2.02294

A14 1.74165 -0.00002 0.00000 0.00052 0.00050 1.74215

A15 1.70580 -0.00008 0.00000 -0.00369 -0.00366 1.70214

A16 2.06042 0.00033 0.00000 0.00236 0.00234 2.06276

A17 2.10122 -0.00014 0.00000 -0.00009 -0.00010 2.10112

A18 2.10846 -0.00018 0.00000 -0.00126 -0.00126 2.10720

A19 1.92492 0.00000 0.00000 -0.00164 -0.00162 1.92329

A20 1.87263 0.00001 0.00000 0.00042 0.00042 1.87305

A21 1.98116 -0.00006 0.00000 0.00038 0.00035 1.98150

A22 1.85521 0.00000 0.00000 -0.00025 -0.00025 1.85496

A23 1.92027 0.00005 0.00000 0.00021 0.00020 1.92047

A24 1.90470 0.00001 0.00000 0.00088 0.00090 1.90560

A25 1.98149 0.00011 0.00000 -0.00069 -0.00073 1.98075

A26 1.92405 -0.00006 0.00000 0.00086 0.00087 1.92492

A27 1.87322 0.00001 0.00000 -0.00077 -0.00075 1.87246

A28 1.91995 -0.00001 0.00000 0.00069 0.00070 1.92065

A29 1.90568 -0.00007 0.00000 -0.00083 -0.00081 1.90487

A30 1.85448 0.00002 0.00000 0.00077 0.00076 1.85524

A31 1.88279 0.00023 0.00000 0.00140 0.00140 1.88419

A32 1.87607 -0.00012 0.00000 -0.00068 -0.00078 1.87529

A33 1.73401 -0.00001 0.00000 0.00804 0.00808 1.74210

A34 1.56671 0.00005 0.00000 -0.00529 -0.00526 1.56146

A35 1.86761 0.00008 0.00000 -0.00069 -0.00069 1.86692

A36 2.19858 -0.00001 0.00000 0.00026 0.00026 2.19884

A37 2.10150 -0.00003 0.00000 -0.00004 -0.00004 2.10145

A38 1.87400 0.00005 0.00000 0.00099 0.00090 1.87490

A39 1.74458 -0.00018 0.00000 -0.01134 -0.01130 1.73328

A40 1.56019 -0.00003 0.00000 0.00695 0.00699 1.56719

A41 1.86651 0.00018 0.00000 0.00172 0.00172 1.86823

A42 2.19902 -0.00002 0.00000 -0.00125 -0.00126 2.19777

A43 2.10191 -0.00010 0.00000 0.00048 0.00049 2.10240

A44 1.90323 -0.00011 0.00000 -0.00015 -0.00016 1.90307

A45 2.02626 0.00017 0.00000 0.00034 0.00033 2.02659

A46 2.35370 -0.00007 0.00000 -0.00018 -0.00018 2.35351

A47 1.90453 -0.00038 0.00000 -0.00233 -0.00234 1.90219

A48 2.02510 0.00033 0.00000 0.00235 0.00235 2.02745

A49 2.35355 0.00005 0.00000 -0.00001 -0.00001 2.35354

D1 -0.60069 0.00007 0.00000 0.00064 0.00063 -0.60006

D2 2.94628 0.00000 0.00000 0.00185 0.00184 2.94812

D3 1.19408 0.00001 0.00000 0.00265 0.00261 1.19669

D4 2.70323 0.00017 0.00000 0.00818 0.00819 2.71143

D5 -0.03297 0.00011 0.00000 0.00940 0.00940 -0.02358

D6 -1.78518 0.00012 0.00000 0.01020 0.01017 -1.77500

D7 0.00256 -0.00006 0.00000 -0.00185 -0.00185 0.00070

D8 -2.96732 -0.00008 0.00000 -0.00827 -0.00826 -2.97558

D9 2.98230 -0.00014 0.00000 -0.00919 -0.00920 2.97310

D10 0.01242 -0.00016 0.00000 -0.01561 -0.01561 -0.00318

D11 2.74106 -0.00004 0.00000 -0.00744 -0.00745 2.73361

D12 -1.52858 -0.00004 0.00000 -0.00835 -0.00836 -1.53694

D13 0.57714 -0.00006 0.00000 -0.00672 -0.00672 0.57043

D14 -0.78784 0.00000 0.00000 -0.00865 -0.00865 -0.79649

D15 1.22571 0.00001 0.00000 -0.00957 -0.00956 1.21615

D16 -2.95175 -0.00001 0.00000 -0.00793 -0.00792 -2.95967

D17 1.01531 -0.00004 0.00000 -0.00635 -0.00633 1.00898

D18 3.02886 -0.00004 0.00000 -0.00726 -0.00724 3.02162

D19 -1.14861 -0.00006 0.00000 -0.00563 -0.00560 -1.15420

D20 -1.02722 0.00003 0.00000 -0.01890 -0.01890 -1.04613

D21 -2.97159 -0.00011 0.00000 -0.01650 -0.01650 -2.98810

D22 1.20281 0.00001 0.00000 -0.01732 -0.01730 1.18551

D23 1.08062 -0.00002 0.00000 -0.01876 -0.01877 1.06184

D24 -0.86375 -0.00016 0.00000 -0.01636 -0.01637 -0.88012

D25 -2.97253 -0.00004 0.00000 -0.01718 -0.01718 -2.98971

D26 3.13969 0.00004 0.00000 -0.01810 -0.01810 3.12159

D27 1.19533 -0.00011 0.00000 -0.01570 -0.01571 1.17962

D28 -0.91345 0.00002 0.00000 -0.01652 -0.01651 -0.92996

D29 0.59331 0.00004 0.00000 0.00904 0.00904 0.60235

D30 -2.72074 0.00006 0.00000 0.01561 0.01559 -2.70515

D31 -2.95448 0.00006 0.00000 0.00521 0.00523 -2.94925

D32 0.01466 0.00008 0.00000 0.01178 0.01178 0.02644

D33 -1.20074 0.00004 0.00000 0.00518 0.00524 -1.19550

D34 1.76839 0.00005 0.00000 0.01176 0.01180 1.78019

D35 -0.56552 -0.00001 0.00000 -0.01459 -0.01458 -0.58010

D36 -2.72858 -0.00003 0.00000 -0.01566 -0.01564 -2.74422

D37 1.54204 -0.00002 0.00000 -0.01659 -0.01657 1.52547

D38 2.96440 -0.00005 0.00000 -0.01101 -0.01102 2.95338

D39 0.80134 -0.00007 0.00000 -0.01208 -0.01207 0.78927

D40 -1.21122 -0.00007 0.00000 -0.01301 -0.01301 -1.22423

D41 1.15616 0.00004 0.00000 -0.00748 -0.00752 1.14864

D42 -1.00690 0.00003 0.00000 -0.00855 -0.00857 -1.01547

D43 -3.01946 0.00003 0.00000 -0.00949 -0.00951 -3.02897

D44 1.04630 -0.00012 0.00000 -0.02055 -0.02054 1.02576

D45 2.98824 -0.00007 0.00000 -0.01828 -0.01827 2.96997

D46 -1.18631 -0.00010 0.00000 -0.01857 -0.01857 -1.20488

D47 -1.06332 -0.00002 0.00000 -0.01763 -0.01761 -1.08093

D48 0.87862 0.00002 0.00000 -0.01535 -0.01534 0.86329

D49 2.98727 0.00000 0.00000 -0.01564 -0.01564 2.97162

D50 -3.12284 0.00000 0.00000 -0.01830 -0.01829 -3.14113

D51 -1.18090 0.00004 0.00000 -0.01602 -0.01602 -1.19692

D52 0.92775 0.00002 0.00000 -0.01632 -0.01633 0.91142

D53 -0.00683 0.00004 0.00000 0.01351 0.01352 0.00669

D54 2.15846 0.00004 0.00000 0.01467 0.01467 2.17313

D55 -2.09602 0.00001 0.00000 0.01552 0.01552 -2.08050

D56 -2.17327 0.00005 0.00000 0.01523 0.01524 -2.15803

D57 -0.00798 0.00004 0.00000 0.01639 0.01639 0.00841

D58 2.02073 0.00002 0.00000 0.01723 0.01724 2.03797

D59 2.08071 0.00002 0.00000 0.01490 0.01491 2.09562

D60 -2.03718 0.00001 0.00000 0.01606 0.01606 -2.02112

D61 -0.00847 -0.00001 0.00000 0.01691 0.01691 0.00843

D62 -0.01344 0.00000 0.00000 -0.00319 -0.00317 -0.01661

D63 3.12892 0.00000 0.00000 -0.00843 -0.00841 3.12051

D64 0.01370 -0.00004 0.00000 0.00386 0.00384 0.01754

D65 -3.12488 -0.00001 0.00000 0.00277 0.00274 -3.12215

D66 -0.01018 0.00002 0.00000 0.02123 0.02123 0.01105

D67 1.84931 -0.00009 0.00000 0.00959 0.00960 1.85891

D68 -1.79616 0.00002 0.00000 0.01180 0.01183 -1.78433

D69 -1.85909 0.00005 0.00000 0.01274 0.01274 -1.84635

D70 0.00040 -0.00005 0.00000 0.00111 0.00111 0.00151

D71 2.63812 0.00005 0.00000 0.00332 0.00334 2.64145

D72 1.78591 -0.00002 0.00000 0.01377 0.01375 1.79967

D73 -2.63778 -0.00012 0.00000 0.00213 0.00212 -2.63566

D74 -0.00006 -0.00002 0.00000 0.00435 0.00435 0.00429

D75 -1.94061 0.00014 0.00000 -0.00100 -0.00093 -1.94154

D76 1.20003 0.00015 0.00000 0.00565 0.00570 1.20573

D77 0.00801 0.00003 0.00000 0.00123 0.00122 0.00923

D78 -3.13454 0.00004 0.00000 0.00787 0.00785 -3.12669

D79 2.67981 0.00010 0.00000 0.00039 0.00040 2.68020

D80 -0.46275 0.00011 0.00000 0.00704 0.00703 -0.45572

D81 1.94153 0.00010 0.00000 -0.00600 -0.00606 1.93547

D82 -1.20388 0.00007 0.00000 -0.00460 -0.00465 -1.20854

D83 -0.00869 0.00006 0.00000 -0.00310 -0.00309 -0.01177

D84 3.12909 0.00003 0.00000 -0.00170 -0.00168 3.12741

D85 -2.68010 -0.00006 0.00000 -0.00453 -0.00453 -2.68463

D86 0.45767 -0.00009 0.00000 -0.00313 -0.00313 0.45455

Item Value Threshold Converged?

Maximum Force 0.000570 0.000450 NO

RMS Force 0.000137 0.000300 YES

Maximum Displacement 0.048352 0.001800 NO

RMS Displacement 0.013085 0.001200 NO

Predicted change in Energy=-1.988015D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.136500 1.557322 0.441880

2 6 0 0.188754 1.282815 0.105410

3 6 0 -0.756965 3.779051 -0.366570

4 6 0 -1.622684 2.843781 0.198746

5 1 0 -1.729335 0.839556 1.026909

6 1 0 -2.604447 3.150002 0.587657

7 6 0 0.797597 1.933590 -1.088744

8 1 0 1.916710 1.961749 -0.987049

9 1 0 0.577712 1.277089 -1.976903

10 6 0 0.262984 3.333216 -1.356827

11 1 0 1.112113 4.068300 -1.399560

12 1 0 -0.224548 3.354155 -2.371832

13 1 0 -1.035633 4.844783 -0.408803

14 1 0 0.668778 0.349122 0.441269

15 8 0 2.759857 3.844354 0.819994

16 6 0 0.475896 3.878207 1.415025

17 6 0 0.958864 2.577289 1.668035

18 6 0 1.619534 4.671157 0.888280

19 8 0 1.771544 5.827006 0.526777

20 6 0 2.400678 2.567997 1.299530

21 8 0 3.290477 1.732935 1.325836

22 1 0 -0.343580 4.372588 1.942164

23 1 0 0.575792 1.886942 2.423231

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394584 0.000000

3 C 2.394518 2.710783 0.000000

4 C 1.396591 2.393039 1.394195 0.000000

5 H 1.099500 2.173639 3.395279 2.171209 0.000000

6 H 2.170887 3.394249 2.172427 1.099492 2.509367

7 C 2.495019 1.490034 2.518715 2.888570 3.472504

8 H 3.395216 2.154124 3.291827 3.835544 4.313814

9 H 2.977846 2.118337 3.261036 3.468388 3.812714

10 C 2.889239 2.519482 1.489857 2.493009 3.983700

11 H 3.840856 3.297947 2.155038 3.396048 4.938256

12 H 3.460815 3.255456 2.117801 2.970376 4.487653

13 H 3.397239 3.801468 1.102372 2.172039 4.310955

14 H 2.172275 1.102273 3.801284 3.396018 2.516833

15 O 4.533771 3.699011 3.712174 4.538035 5.405966

16 C 2.988869 2.921233 2.168838 2.636932 3.774530

17 C 2.633313 2.170375 2.920260 2.982317 3.264532

18 C 4.182220 3.760436 2.831652 3.785068 5.090708

19 O 5.166635 4.830367 3.374247 4.530785 6.113995

20 C 3.777387 2.823158 3.770047 4.180338 4.485403

21 O 4.517780 3.363440 4.840725 5.161730 5.107445

22 H 3.287141 3.633696 2.419385 2.648181 3.903886

23 H 2.639383 2.426327 3.624819 3.270653 2.891426

6 7 8 9 10

6 H 0.000000

7 C 3.982949 0.000000

8 H 4.932799 1.124077 0.000000

9 H 4.495654 1.126131 1.800413 0.000000

10 C 3.469401 1.522049 2.180016 2.170532 0.000000

11 H 4.313366 2.180026 2.292401 2.899961 1.123920

12 H 3.803179 2.170046 2.905409 2.261370 1.126215

13 H 2.515232 3.506864 4.166844 4.217850 2.206806

14 H 4.310495 2.206371 2.489577 2.591713 3.507511

15 O 5.414043 3.338377 2.742354 4.378955 3.351744

16 C 3.271595 3.186516 3.393923 4.275671 2.832933

17 C 3.767281 2.835522 2.888915 3.888621 3.194599

18 C 4.499589 3.475410 3.308484 4.562277 2.944626

19 O 5.130239 4.326334 4.153668 5.328733 3.470260

20 C 5.088887 2.945537 2.414582 3.965434 3.494499

21 O 6.107628 3.476335 2.699820 4.298253 4.350091

22 H 2.905327 4.054306 4.416033 5.078384 3.511631

23 H 3.883114 3.519281 3.665197 4.442197 4.059359

11 12 13 14 15

11 H 0.000000

12 H 1.800549 0.000000

13 H 2.489446 2.594862 0.000000

14 H 4.173426 4.212101 4.882480 0.000000

15 O 2.773379 4.397126 4.112973 4.090561 0.000000

16 C 2.891850 3.886584 2.558386 3.666039 2.360442

17 C 3.414196 4.280713 3.665079 2.560045 2.359704

18 C 2.419737 3.970323 2.960150 4.447892 1.410178

19 O 2.690477 4.301314 3.117742 5.588436 2.234647

20 C 3.346101 4.581348 4.462106 2.942702 1.409983

21 O 4.198450 5.353177 5.604267 3.093655 2.235067

22 H 3.657698 4.434178 2.495787 4.412010 3.342098

23 H 4.433926 5.077981 4.400674 2.510321 3.342450

16 17 18 19 20

16 C 0.000000

17 C 1.410553 0.000000

18 C 1.487998 2.329975 0.000000

19 O 2.503099 3.538866 1.220564 0.000000

20 C 2.331260 1.488190 2.280920 3.407946 0.000000

21 O 3.540058 2.503289 3.408322 4.439265 1.220559

22 H 1.092625 2.234862 2.248029 2.931279 3.346712

23 H 2.234188 1.092541 3.346241 4.533262 2.248722

21 22 23

21 O 0.000000

22 H 4.533653 0.000000

23 H 2.932151 2.693531 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.302223 -0.714302 -0.657499

2 6 0 1.360975 -1.357689 0.145603

3 6 0 1.378585 1.352932 0.121701

4 6 0 2.310221 0.682214 -0.669483

5 1 0 2.907465 -1.280632 -1.379893

6 1 0 2.924329 1.228601 -1.399699

7 6 0 0.958949 -0.748808 1.444772

8 1 0 -0.056452 -1.121744 1.750433

9 1 0 1.679952 -1.119815 2.226232

10 6 0 0.973690 0.773123 1.433019

11 1 0 -0.031462 1.170502 1.741169

12 1 0 1.708635 1.141253 2.202888

13 1 0 1.227291 2.438934 0.007975

14 1 0 1.194523 -2.443242 0.051406

15 8 0 -2.076124 0.003264 0.275378

16 6 0 -0.291078 0.703958 -1.100966

17 6 0 -0.293868 -0.706590 -1.098621

18 6 0 -1.422075 1.141852 -0.238857

19 8 0 -1.881682 2.222126 0.095131

20 6 0 -1.427579 -1.139060 -0.237007

21 8 0 -1.890482 -2.217128 0.099525

22 1 0 0.066689 1.343895 -1.911098

23 1 0 0.065079 -1.349631 -1.905654

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2196434 0.8810628 0.6753921

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5500027277 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504135570420E-01 A.U. after 14 cycles

Convg = 0.6129D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000132944 0.000283340 -0.000105228

2 6 0.000090027 0.000037993 0.000168199

3 6 0.000463331 0.000237237 -0.000171550

4 6 -0.000712052 -0.000275832 0.000171459

5 1 0.000040238 -0.000005291 -0.000060210

6 1 0.000010411 0.000022418 0.000141769

7 6 0.000016139 -0.000150448 0.000226760

8 1 -0.000009486 0.000028273 -0.000051181

9 1 -0.000025057 0.000034609 -0.000005943

10 6 -0.000012656 -0.000009868 -0.000027649

11 1 0.000013453 0.000009844 0.000067781

12 1 0.000030779 0.000028107 -0.000008058

13 1 0.000048013 -0.000091961 -0.000061315

14 1 0.000020356 0.000007027 -0.000029143

15 8 -0.000114593 -0.000006898 0.000030521

16 6 -0.000132560 -0.000401119 -0.000189186

17 6 -0.000073342 -0.000053769 -0.000235181

18 6 0.000419117 -0.000242542 0.000179235

19 8 0.000057159 -0.000226984 -0.000065412

20 6 -0.000316069 0.000572061 -0.000041543

21 8 -0.000073733 0.000244150 -0.000066336

22 1 0.000070035 -0.000018076 0.000115840

23 1 0.000057545 -0.000022271 0.000016372

-------------------------------------------------------------------

Cartesian Forces: Max 0.000712052 RMS 0.000183668

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000524866 RMS 0.000106354

Search for a saddle point.

Step number 57 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06975 0.00179 0.00427 0.00736 0.00769

Eigenvalues --- 0.01076 0.01171 0.01366 0.01904 0.02410

Eigenvalues --- 0.02617 0.02833 0.03105 0.03152 0.03331

Eigenvalues --- 0.03567 0.03603 0.03766 0.03814 0.04140

Eigenvalues --- 0.04327 0.04564 0.04719 0.05007 0.06172

Eigenvalues --- 0.06416 0.06634 0.07011 0.07368 0.08508

Eigenvalues --- 0.09226 0.09652 0.10060 0.10237 0.10994

Eigenvalues --- 0.12682 0.13872 0.14747 0.17170 0.22277

Eigenvalues --- 0.26159 0.28023 0.29573 0.29945 0.30854

Eigenvalues --- 0.31286 0.31370 0.31930 0.32031 0.32449

Eigenvalues --- 0.32705 0.33586 0.36752 0.37751 0.39679

Eigenvalues --- 0.39856 0.40476 0.44061 0.48530 0.52255

Eigenvalues --- 0.61291 1.08612 1.11025

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D4

1 0.57266 0.51403 -0.15475 0.14769 0.14010

D1 D79 R19 D30 D35

1 0.13155 0.13131 -0.13036 -0.12631 0.12617

RFO step: Lambda0=7.435588735D-07 Lambda=-1.38242469D-05.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00687025 RMS(Int)= 0.00001684

Iteration 2 RMS(Cart)= 0.00002211 RMS(Int)= 0.00000567

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000567

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63538 0.00004 0.00000 -0.00009 -0.00009 2.63529

R2 2.63917 -0.00004 0.00000 0.00024 0.00025 2.63942

R3 2.07775 -0.00005 0.00000 -0.00002 -0.00002 2.07774

R4 2.81576 -0.00016 0.00000 -0.00028 -0.00028 2.81548

R5 2.08299 -0.00001 0.00000 -0.00004 -0.00004 2.08296

R6 4.10141 -0.00020 0.00000 -0.00078 -0.00078 4.10064

R7 2.63465 0.00050 0.00000 0.00063 0.00063 2.63527

R8 2.81542 -0.00006 0.00000 -0.00012 -0.00012 2.81530

R9 2.08318 -0.00010 0.00000 -0.00022 -0.00022 2.08296

R10 4.09851 -0.00009 0.00000 0.00281 0.00281 4.10132

R11 2.07774 0.00005 0.00000 -0.00002 -0.00002 2.07772

R12 2.12420 -0.00001 0.00000 -0.00015 -0.00015 2.12405

R13 2.12808 -0.00001 0.00000 0.00007 0.00007 2.12815

R14 2.87626 -0.00004 0.00000 -0.00001 -0.00001 2.87624

R15 2.12390 0.00001 0.00000 0.00017 0.00017 2.12407

R16 2.12824 -0.00001 0.00000 -0.00007 -0.00007 2.12816

R17 2.66485 -0.00052 0.00000 -0.00113 -0.00113 2.66372

R18 2.66448 -0.00042 0.00000 -0.00064 -0.00064 2.66384

R19 2.66556 -0.00038 0.00000 -0.00074 -0.00075 2.66481

R20 2.81191 0.00011 0.00000 0.00045 0.00045 2.81236

R21 2.06476 0.00000 0.00000 -0.00009 -0.00009 2.06468

R22 2.81227 -0.00019 0.00000 0.00021 0.00021 2.81248

R23 2.06460 0.00001 0.00000 0.00007 0.00007 2.06467

R24 2.30653 -0.00019 0.00000 -0.00006 -0.00006 2.30648

R25 2.30652 -0.00022 0.00000 -0.00006 -0.00006 2.30646

A1 2.06023 0.00017 0.00000 0.00129 0.00129 2.06152

A2 2.10861 -0.00012 0.00000 -0.00079 -0.00079 2.10782

A3 2.10164 -0.00004 0.00000 -0.00042 -0.00042 2.10122

A4 2.08942 0.00002 0.00000 -0.00036 -0.00036 2.08906

A5 2.10256 0.00004 0.00000 0.00030 0.00030 2.10286

A6 1.61689 -0.00001 0.00000 0.00193 0.00192 1.61882

A7 2.02217 -0.00006 0.00000 -0.00016 -0.00016 2.02201

A8 1.74318 -0.00004 0.00000 -0.00139 -0.00139 1.74179

A9 1.70249 0.00004 0.00000 -0.00001 0.00000 1.70249

A10 2.08732 0.00009 0.00000 0.00161 0.00161 2.08893

A11 2.10261 -0.00003 0.00000 0.00048 0.00048 2.10309

A12 1.62138 0.00000 0.00000 -0.00282 -0.00282 1.61856

A13 2.02294 -0.00004 0.00000 -0.00101 -0.00102 2.02192

A14 1.74215 -0.00007 0.00000 -0.00016 -0.00016 1.74199

A15 1.70214 0.00005 0.00000 0.00037 0.00038 1.70252

A16 2.06276 -0.00029 0.00000 -0.00134 -0.00135 2.06141

A17 2.10112 0.00011 0.00000 0.00026 0.00026 2.10138

A18 2.10720 0.00017 0.00000 0.00065 0.00065 2.10785

A19 1.92329 0.00001 0.00000 0.00098 0.00099 1.92428

A20 1.87305 0.00002 0.00000 0.00001 0.00001 1.87306

A21 1.98150 0.00003 0.00000 -0.00037 -0.00038 1.98112

A22 1.85496 0.00001 0.00000 0.00013 0.00013 1.85509

A23 1.92047 -0.00004 0.00000 -0.00016 -0.00016 1.92031

A24 1.90560 -0.00003 0.00000 -0.00057 -0.00057 1.90503

A25 1.98075 -0.00001 0.00000 0.00061 0.00060 1.98135

A26 1.92492 -0.00001 0.00000 -0.00077 -0.00076 1.92416

A27 1.87246 0.00000 0.00000 0.00043 0.00043 1.87289

A28 1.92065 -0.00002 0.00000 -0.00026 -0.00026 1.92039

A29 1.90487 0.00003 0.00000 0.00013 0.00014 1.90500

A30 1.85524 0.00000 0.00000 -0.00017 -0.00017 1.85507

A31 1.88419 -0.00022 0.00000 -0.00074 -0.00074 1.88344

A32 1.87529 0.00005 0.00000 -0.00007 -0.00009 1.87520

A33 1.74210 0.00002 0.00000 -0.00423 -0.00422 1.73787

A34 1.56146 0.00000 0.00000 0.00279 0.00280 1.56426

A35 1.86692 -0.00008 0.00000 0.00031 0.00031 1.86723

A36 2.19884 0.00002 0.00000 -0.00009 -0.00009 2.19875

A37 2.10145 0.00003 0.00000 0.00026 0.00026 2.10172

A38 1.87490 0.00005 0.00000 0.00029 0.00027 1.87517

A39 1.73328 0.00006 0.00000 0.00500 0.00501 1.73829

A40 1.56719 -0.00004 0.00000 -0.00300 -0.00299 1.56420

A41 1.86823 -0.00018 0.00000 -0.00107 -0.00107 1.86716

A42 2.19777 0.00007 0.00000 0.00140 0.00140 2.19916

A43 2.10240 0.00008 0.00000 -0.00119 -0.00119 2.10121

A44 1.90307 0.00016 0.00000 0.00034 0.00034 1.90341

A45 2.02659 -0.00021 0.00000 -0.00037 -0.00037 2.02622

A46 2.35351 0.00005 0.00000 0.00004 0.00004 2.35355

A47 1.90219 0.00032 0.00000 0.00118 0.00118 1.90337

A48 2.02745 -0.00032 0.00000 -0.00132 -0.00132 2.02613

A49 2.35354 0.00000 0.00000 0.00014 0.00014 2.35368

D1 -0.60006 0.00001 0.00000 0.00027 0.00026 -0.59980

D2 2.94812 0.00001 0.00000 0.00094 0.00093 2.94905

D3 1.19669 -0.00003 0.00000 -0.00026 -0.00028 1.19641

D4 2.71143 0.00001 0.00000 -0.00023 -0.00023 2.71120

D5 -0.02358 0.00001 0.00000 0.00044 0.00044 -0.02314

D6 -1.77500 -0.00004 0.00000 -0.00076 -0.00077 -1.77577

D7 0.00070 0.00001 0.00000 -0.00076 -0.00076 -0.00006

D8 -2.97558 0.00006 0.00000 0.00208 0.00209 -2.97350

D9 2.97310 0.00000 0.00000 -0.00031 -0.00031 2.97279

D10 -0.00318 0.00006 0.00000 0.00254 0.00254 -0.00064

D11 2.73361 -0.00003 0.00000 0.00361 0.00361 2.73722

D12 -1.53694 0.00000 0.00000 0.00429 0.00428 -1.53265

D13 0.57043 0.00000 0.00000 0.00334 0.00334 0.57377

D14 -0.79649 0.00000 0.00000 0.00308 0.00308 -0.79341

D15 1.21615 0.00002 0.00000 0.00375 0.00375 1.21990

D16 -2.95967 0.00002 0.00000 0.00281 0.00281 -2.95686

D17 1.00898 0.00000 0.00000 0.00227 0.00228 1.01126

D18 3.02162 0.00003 0.00000 0.00294 0.00295 3.02457

D19 -1.15420 0.00003 0.00000 0.00200 0.00201 -1.15220

D20 -1.04613 -0.00002 0.00000 0.01035 0.01036 -1.03577

D21 -2.98810 0.00014 0.00000 0.00943 0.00943 -2.97867

D22 1.18551 0.00005 0.00000 0.01074 0.01074 1.19625

D23 1.06184 0.00000 0.00000 0.01021 0.01021 1.07205

D24 -0.88012 0.00015 0.00000 0.00928 0.00928 -0.87085

D25 -2.98971 0.00007 0.00000 0.01060 0.01060 -2.97911

D26 3.12159 -0.00006 0.00000 0.00970 0.00970 3.13129

D27 1.17962 0.00009 0.00000 0.00877 0.00877 1.18839

D28 -0.92996 0.00001 0.00000 0.01008 0.01009 -0.91988

D29 0.60235 -0.00002 0.00000 -0.00228 -0.00228 0.60006

D30 -2.70515 -0.00008 0.00000 -0.00518 -0.00519 -2.71034

D31 -2.94925 0.00000 0.00000 0.00049 0.00049 -2.94876

D32 0.02644 -0.00006 0.00000 -0.00241 -0.00241 0.02403

D33 -1.19550 0.00005 0.00000 -0.00072 -0.00071 -1.19621

D34 1.78019 -0.00001 0.00000 -0.00362 -0.00361 1.77658

D35 -0.58010 -0.00002 0.00000 0.00567 0.00567 -0.57443

D36 -2.74422 0.00002 0.00000 0.00615 0.00616 -2.73807

D37 1.52547 0.00002 0.00000 0.00651 0.00651 1.53198

D38 2.95338 -0.00004 0.00000 0.00272 0.00272 2.95610

D39 0.78927 0.00000 0.00000 0.00320 0.00320 0.79247

D40 -1.22423 0.00000 0.00000 0.00356 0.00356 -1.22067

D41 1.14864 -0.00004 0.00000 0.00268 0.00267 1.15131

D42 -1.01547 0.00000 0.00000 0.00316 0.00315 -1.01232

D43 -3.02897 -0.00001 0.00000 0.00352 0.00351 -3.02546

D44 1.02576 0.00009 0.00000 0.01075 0.01075 1.03651

D45 2.96997 0.00002 0.00000 0.00935 0.00935 2.97932

D46 -1.20488 0.00006 0.00000 0.00978 0.00978 -1.19510

D47 -1.08093 0.00002 0.00000 0.00977 0.00977 -1.07116

D48 0.86329 -0.00005 0.00000 0.00837 0.00837 0.87166

D49 2.97162 -0.00002 0.00000 0.00880 0.00880 2.98042

D50 -3.14113 0.00006 0.00000 0.01077 0.01077 -3.13036

D51 -1.19692 0.00000 0.00000 0.00937 0.00937 -1.18754

D52 0.91142 0.00003 0.00000 0.00980 0.00979 0.92122

D53 0.00669 -0.00002 0.00000 -0.00630 -0.00630 0.00039

D54 2.17313 -0.00005 0.00000 -0.00705 -0.00706 2.16607

D55 -2.08050 -0.00003 0.00000 -0.00732 -0.00733 -2.08783

D56 -2.15803 -0.00002 0.00000 -0.00719 -0.00719 -2.16522

D57 0.00841 -0.00005 0.00000 -0.00795 -0.00795 0.00046

D58 2.03797 -0.00004 0.00000 -0.00822 -0.00822 2.02975

D59 2.09562 0.00001 0.00000 -0.00693 -0.00693 2.08869

D60 -2.02112 -0.00002 0.00000 -0.00769 -0.00769 -2.02881

D61 0.00843 0.00000 0.00000 -0.00796 -0.00796 0.00047

D62 -0.01661 -0.00002 0.00000 0.00014 0.00014 -0.01647

D63 3.12051 0.00001 0.00000 0.00233 0.00234 3.12285

D64 0.01754 0.00003 0.00000 -0.00105 -0.00106 0.01648

D65 -3.12215 0.00002 0.00000 -0.00074 -0.00075 -3.12290

D66 0.01105 0.00000 0.00000 -0.01145 -0.01145 -0.00040

D67 1.85891 0.00002 0.00000 -0.00615 -0.00614 1.85277

D68 -1.78433 -0.00003 0.00000 -0.00838 -0.00837 -1.79270

D69 -1.84635 -0.00001 0.00000 -0.00678 -0.00678 -1.85313

D70 0.00151 0.00001 0.00000 -0.00148 -0.00148 0.00003

D71 2.64145 -0.00004 0.00000 -0.00371 -0.00371 2.63774

D72 1.79967 0.00005 0.00000 -0.00784 -0.00785 1.79182

D73 -2.63566 0.00006 0.00000 -0.00254 -0.00254 -2.63820

D74 0.00429 0.00002 0.00000 -0.00477 -0.00477 -0.00049

D75 -1.94154 -0.00003 0.00000 0.00255 0.00257 -1.93897

D76 1.20573 -0.00006 0.00000 -0.00023 -0.00022 1.20551

D77 0.00923 0.00001 0.00000 0.00089 0.00088 0.01011

D78 -3.12669 -0.00002 0.00000 -0.00189 -0.00190 -3.12859

D79 2.68020 -0.00004 0.00000 0.00175 0.00175 2.68195

D80 -0.45572 -0.00008 0.00000 -0.00103 -0.00103 -0.45675

D81 1.93547 0.00001 0.00000 0.00358 0.00356 1.93903

D82 -1.20854 0.00002 0.00000 0.00319 0.00318 -1.20536

D83 -0.01177 -0.00002 0.00000 0.00161 0.00161 -0.01016

D84 3.12741 -0.00001 0.00000 0.00122 0.00123 3.12864

D85 -2.68463 0.00002 0.00000 0.00280 0.00280 -2.68183

D86 0.45455 0.00003 0.00000 0.00242 0.00242 0.45696

Item Value Threshold Converged?

Maximum Force 0.000525 0.000450 NO

RMS Force 0.000106 0.000300 YES

Maximum Displacement 0.024604 0.001800 NO

RMS Displacement 0.006871 0.001200 NO

Predicted change in Energy=-6.560870D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.139643 1.560243 0.442462

2 6 0 0.184829 1.280838 0.107145

3 6 0 -0.753851 3.779116 -0.369178

4 6 0 -1.623299 2.847360 0.197033

5 1 0 -1.734446 0.844861 1.028396

6 1 0 -2.603564 3.157109 0.586897

7 6 0 0.795807 1.927601 -1.087911

8 1 0 1.915206 1.949666 -0.988756

9 1 0 0.570198 1.272517 -1.975728

10 6 0 0.268507 3.330102 -1.355411

11 1 0 1.121205 4.061513 -1.392048

12 1 0 -0.213520 3.355703 -2.372892

13 1 0 -1.028493 4.845685 -0.413537

14 1 0 0.661754 0.346042 0.444288

15 8 0 2.756654 3.854148 0.818981

16 6 0 0.473611 3.874932 1.418130

17 6 0 0.962140 2.575439 1.665521

18 6 0 1.613260 4.675170 0.893092

19 8 0 1.759320 5.832639 0.534430

20 6 0 2.403070 2.574553 1.293014

21 8 0 3.296848 1.743620 1.312816

22 1 0 -0.347925 4.363401 1.947476

23 1 0 0.585930 1.880748 2.420238

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394536 0.000000

3 C 2.393949 2.710978 0.000000

4 C 1.396721 2.394034 1.394527 0.000000

5 H 1.099491 2.173107 3.394795 2.171064 0.000000

6 H 2.171154 3.394951 2.173111 1.099481 2.509338

7 C 2.494587 1.489885 2.519152 2.889483 3.471781

8 H 3.395900 2.154655 3.294637 3.838356 4.313868

9 H 2.975565 2.118240 3.258397 3.465899 3.810385

10 C 2.889227 2.519039 1.489793 2.494404 3.983814

11 H 3.838387 3.294926 2.154494 3.395828 4.935599

12 H 3.465198 3.257965 2.118043 2.974963 4.492917

13 H 3.396942 3.801499 1.102254 2.172531 4.310932

14 H 2.172399 1.102255 3.801534 3.396939 2.516302

15 O 4.537058 3.707144 3.706885 4.537007 5.410142

16 C 2.985348 2.920857 2.170326 2.635150 3.769448

17 C 2.635145 2.169963 2.921210 2.985782 3.266864

18 C 4.181425 3.765584 2.828331 3.781627 5.088881

19 O 5.163896 4.835338 3.368901 4.524140 6.109692

20 C 3.781941 2.828529 3.765635 4.181776 4.492315

21 O 4.524776 3.369343 4.835340 5.164404 5.118846

22 H 3.278655 3.629440 2.423438 2.643673 3.891949

23 H 2.644225 2.423051 3.630380 3.279890 2.897315

6 7 8 9 10

6 H 0.000000

7 C 3.984018 0.000000

8 H 4.935574 1.123998 0.000000

9 H 4.493496 1.126168 1.800469 0.000000

10 C 3.471495 1.522042 2.179830 2.170131 0.000000

11 H 4.313708 2.179900 2.291939 2.902204 1.124010

12 H 3.809475 2.170113 2.902456 2.260889 1.126176

13 H 2.516546 3.506860 4.169313 4.214710 2.205975

14 H 4.311002 2.206113 2.489250 2.592917 3.506875

15 O 5.410330 3.345555 2.757354 4.388144 3.345666

16 C 3.267296 3.190008 3.402639 4.277870 2.833979

17 C 3.770413 2.833505 2.888791 3.887148 3.190090

18 C 4.492201 3.484500 3.325793 4.571231 2.945053

19 O 5.118200 4.337012 4.173953 5.339440 3.472279

20 C 5.089632 2.944596 2.415568 3.967290 3.484447

21 O 6.110628 3.471678 2.692327 4.297800 4.336729

22 H 2.897278 4.056454 4.423725 5.078193 3.515218

23 H 3.893984 3.514734 3.659641 4.437873 4.056712

11 12 13 14 15

11 H 0.000000

12 H 1.800476 0.000000

13 H 2.488696 2.592932 0.000000

14 H 4.169886 4.214341 4.882580 0.000000

15 O 2.757960 4.388443 4.102388 4.103146 0.000000

16 C 2.889860 3.887621 2.560016 3.665628 2.360445

17 C 3.403300 4.277823 3.665940 2.559658 2.360510

18 C 2.416725 3.967968 2.952154 4.455125 1.409582

19 O 2.693585 4.298818 3.105580 5.596028 2.233847

20 C 3.326227 4.571171 4.454883 2.952757 1.409642

21 O 4.174009 5.339096 5.595684 3.106652 2.233833

22 H 3.660861 4.438367 2.504027 4.406608 3.342343

23 H 4.424453 5.078259 4.407663 2.503088 3.342211

16 17 18 19 20

16 C 0.000000

17 C 1.410158 0.000000

18 C 1.488236 2.330124 0.000000

19 O 2.503316 3.538957 1.220535 0.000000

20 C 2.330119 1.488302 2.279546 3.406610 0.000000

21 O 3.538962 2.503435 3.406556 4.437337 1.220525

22 H 1.092579 2.234407 2.248372 2.931867 3.346083

23 H 2.234638 1.092578 3.346099 4.533273 2.248110

21 22 23

21 O 0.000000

22 H 4.533257 0.000000

23 H 2.931597 2.694282 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306789 -0.698250 -0.663511

2 6 0 1.370382 -1.355629 0.133812

3 6 0 1.370515 1.355348 0.134687

4 6 0 2.306906 0.698471 -0.663052

5 1 0 2.915215 -1.254297 -1.391184

6 1 0 2.915832 1.255041 -1.389894

7 6 0 0.965311 -0.761589 1.438723

8 1 0 -0.045617 -1.146320 1.744301

9 1 0 1.692050 -1.131454 2.215450

10 6 0 0.965710 0.760452 1.439185

11 1 0 -0.044855 1.145618 1.745459

12 1 0 1.693024 1.129434 2.215806

13 1 0 1.211315 2.441166 0.031632

14 1 0 1.211453 -2.441413 0.029986

15 8 0 -2.077023 0.000338 0.274075

16 6 0 -0.291768 0.705083 -1.099933

17 6 0 -0.291955 -0.705075 -1.099945

18 6 0 -1.424795 1.139958 -0.238551

19 8 0 -1.885601 2.218972 0.097743

20 6 0 -1.425195 -1.139588 -0.238548

21 8 0 -1.886437 -2.218365 0.097872

22 1 0 0.066765 1.346921 -1.908158

23 1 0 0.065907 -1.347360 -1.908111

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2201347 0.8808815 0.6754472

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5639786115 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504197335157E-01 A.U. after 13 cycles

Convg = 0.7519D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000075110 0.000033879 -0.000022849

2 6 0.000003564 0.000090384 0.000007933

3 6 0.000027384 -0.000059958 0.000082262

4 6 0.000077674 0.000016030 -0.000049433

5 1 0.000006685 -0.000011430 -0.000019279

6 1 0.000010796 0.000007095 0.000008933

7 6 -0.000079596 -0.000047822 0.000058144

8 1 0.000001788 -0.000013260 0.000004287

9 1 0.000006366 -0.000008870 0.000009921

10 6 -0.000035135 0.000023133 -0.000008090

11 1 0.000004518 -0.000001492 0.000008322

12 1 0.000002874 0.000012492 -0.000003260

13 1 -0.000027985 -0.000018820 0.000007538

14 1 -0.000018607 -0.000001216 -0.000008246

15 8 -0.000024726 -0.000030469 0.000032191

16 6 -0.000017431 0.000016569 -0.000089813

17 6 0.000084930 -0.000068044 -0.000078637

18 6 -0.000046319 0.000014701 0.000019541

19 8 -0.000016297 0.000023843 -0.000008048

20 6 -0.000038182 0.000018806 0.000001057

21 8 -0.000000454 -0.000036513 0.000013980

22 1 0.000020874 0.000007943 0.000011639

23 1 -0.000017832 0.000033018 0.000021910

-------------------------------------------------------------------

Cartesian Forces: Max 0.000090384 RMS 0.000036332

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000104603 RMS 0.000020634

Search for a saddle point.

Step number 58 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06956 0.00155 0.00454 0.00745 0.00796

Eigenvalues --- 0.01077 0.01208 0.01330 0.01892 0.02402

Eigenvalues --- 0.02620 0.02830 0.03103 0.03159 0.03335

Eigenvalues --- 0.03563 0.03593 0.03762 0.03815 0.04135

Eigenvalues --- 0.04334 0.04559 0.04734 0.04970 0.06161

Eigenvalues --- 0.06421 0.06622 0.07038 0.07375 0.08497

Eigenvalues --- 0.09232 0.09675 0.10052 0.10260 0.10950

Eigenvalues --- 0.12699 0.13862 0.14763 0.17103 0.22317

Eigenvalues --- 0.26168 0.28055 0.29593 0.29949 0.30906

Eigenvalues --- 0.31303 0.31384 0.31929 0.32034 0.32451

Eigenvalues --- 0.32720 0.33600 0.36785 0.37811 0.39703

Eigenvalues --- 0.39893 0.40480 0.44204 0.48554 0.52465

Eigenvalues --- 0.61506 1.08623 1.11041

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D4

1 0.57049 0.51124 0.15337 -0.15044 0.13746

D1 R19 D30 D29 D35

1 0.13380 -0.13030 -0.12785 -0.12680 0.12638

RFO step: Lambda0=6.545300228D-08 Lambda=-3.94806009D-07.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00045194 RMS(Int)= 0.00000014

Iteration 2 RMS(Cart)= 0.00000016 RMS(Int)= 0.00000004

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63529 -0.00010 0.00000 -0.00039 -0.00039 2.63491

R2 2.63942 -0.00004 0.00000 0.00008 0.00008 2.63950

R3 2.07774 -0.00001 0.00000 -0.00002 -0.00002 2.07771

R4 2.81548 -0.00010 0.00000 -0.00023 -0.00023 2.81525

R5 2.08296 -0.00001 0.00000 -0.00002 -0.00002 2.08294

R6 4.10064 -0.00004 0.00000 0.00066 0.00066 4.10130

R7 2.63527 -0.00010 0.00000 -0.00034 -0.00034 2.63493

R8 2.81530 -0.00003 0.00000 -0.00011 -0.00011 2.81519

R9 2.08296 -0.00001 0.00000 -0.00002 -0.00002 2.08294

R10 4.10132 -0.00007 0.00000 0.00028 0.00028 4.10161

R11 2.07772 0.00000 0.00000 0.00001 0.00001 2.07772

R12 2.12405 0.00000 0.00000 0.00004 0.00004 2.12409

R13 2.12815 0.00000 0.00000 0.00000 0.00000 2.12815

R14 2.87624 0.00002 0.00000 0.00009 0.00009 2.87633

R15 2.12407 0.00000 0.00000 0.00002 0.00002 2.12409

R16 2.12816 0.00000 0.00000 -0.00002 -0.00002 2.12814

R17 2.66372 0.00003 0.00000 0.00020 0.00020 2.66392

R18 2.66384 0.00000 0.00000 -0.00003 -0.00003 2.66381

R19 2.66481 0.00001 0.00000 -0.00006 -0.00006 2.66476

R20 2.81236 -0.00006 0.00000 -0.00018 -0.00018 2.81218

R21 2.06468 -0.00001 0.00000 0.00000 0.00000 2.06467

R22 2.81248 -0.00007 0.00000 -0.00028 -0.00028 2.81220

R23 2.06467 0.00000 0.00000 0.00002 0.00002 2.06469

R24 2.30648 0.00002 0.00000 0.00000 0.00000 2.30648

R25 2.30646 0.00002 0.00000 0.00002 0.00002 2.30648

A1 2.06152 0.00001 0.00000 -0.00003 -0.00003 2.06149

A2 2.10782 -0.00002 0.00000 0.00002 0.00002 2.10784

A3 2.10122 0.00001 0.00000 0.00006 0.00006 2.10129

A4 2.08906 -0.00001 0.00000 -0.00005 -0.00005 2.08901

A5 2.10286 0.00000 0.00000 -0.00004 -0.00004 2.10282

A6 1.61882 0.00000 0.00000 -0.00015 -0.00015 1.61867

A7 2.02201 0.00000 0.00000 0.00010 0.00010 2.02211

A8 1.74179 0.00002 0.00000 -0.00001 -0.00001 1.74178

A9 1.70249 0.00000 0.00000 0.00015 0.00015 1.70263

A10 2.08893 -0.00001 0.00000 0.00025 0.00025 2.08919

A11 2.10309 -0.00001 0.00000 -0.00039 -0.00039 2.10270

A12 1.61856 0.00000 0.00000 -0.00017 -0.00017 1.61839

A13 2.02192 0.00001 0.00000 0.00025 0.00025 2.02218

A14 1.74199 0.00002 0.00000 -0.00022 -0.00022 1.74177

A15 1.70252 -0.00001 0.00000 0.00007 0.00007 1.70259

A16 2.06141 0.00001 0.00000 0.00015 0.00015 2.06157

A17 2.10138 0.00000 0.00000 -0.00008 -0.00008 2.10131

A18 2.10785 -0.00001 0.00000 -0.00013 -0.00013 2.10772

A19 1.92428 -0.00001 0.00000 -0.00017 -0.00017 1.92411

A20 1.87306 -0.00001 0.00000 -0.00015 -0.00015 1.87291

A21 1.98112 0.00001 0.00000 0.00017 0.00017 1.98129

A22 1.85509 0.00000 0.00000 -0.00006 -0.00006 1.85503

A23 1.92031 0.00001 0.00000 0.00003 0.00003 1.92034

A24 1.90503 0.00001 0.00000 0.00016 0.00016 1.90520

A25 1.98135 -0.00003 0.00000 -0.00014 -0.00014 1.98121

A26 1.92416 0.00001 0.00000 0.00000 0.00000 1.92416

A27 1.87289 0.00001 0.00000 0.00015 0.00015 1.87304

A28 1.92039 0.00001 0.00000 -0.00010 -0.00010 1.92029

A29 1.90500 0.00001 0.00000 0.00016 0.00016 1.90516

A30 1.85507 0.00000 0.00000 -0.00005 -0.00005 1.85502

A31 1.88344 0.00003 0.00000 0.00014 0.00014 1.88358

A32 1.87520 0.00000 0.00000 -0.00012 -0.00012 1.87507

A33 1.73787 0.00000 0.00000 0.00024 0.00024 1.73811

A34 1.56426 0.00001 0.00000 0.00007 0.00007 1.56433

A35 1.86723 0.00002 0.00000 0.00007 0.00007 1.86730

A36 2.19875 -0.00001 0.00000 0.00004 0.00004 2.19878

A37 2.10172 -0.00001 0.00000 -0.00021 -0.00021 2.10151

A38 1.87517 -0.00001 0.00000 0.00007 0.00007 1.87524

A39 1.73829 0.00000 0.00000 0.00013 0.00013 1.73841

A40 1.56420 0.00001 0.00000 -0.00011 -0.00011 1.56409

A41 1.86716 0.00002 0.00000 0.00013 0.00013 1.86729

A42 2.19916 -0.00003 0.00000 -0.00066 -0.00066 2.19850

A43 2.10121 0.00000 0.00000 0.00052 0.00052 2.10172

A44 1.90341 -0.00004 0.00000 -0.00020 -0.00020 1.90321

A45 2.02622 0.00004 0.00000 0.00014 0.00014 2.02636

A46 2.35355 0.00000 0.00000 0.00006 0.00006 2.35361

A47 1.90337 -0.00002 0.00000 -0.00013 -0.00013 1.90324

A48 2.02613 0.00005 0.00000 0.00033 0.00033 2.02647

A49 2.35368 -0.00002 0.00000 -0.00020 -0.00020 2.35348

D1 -0.59980 -0.00001 0.00000 0.00005 0.00005 -0.59975

D2 2.94905 0.00000 0.00000 0.00002 0.00002 2.94907

D3 1.19641 0.00000 0.00000 -0.00006 -0.00006 1.19636

D4 2.71120 -0.00002 0.00000 -0.00035 -0.00035 2.71085

D5 -0.02314 0.00000 0.00000 -0.00038 -0.00038 -0.02352

D6 -1.77577 0.00000 0.00000 -0.00046 -0.00046 -1.77623

D7 -0.00006 0.00000 0.00000 0.00006 0.00006 0.00000

D8 -2.97350 0.00001 0.00000 0.00044 0.00044 -2.97305

D9 2.97279 0.00000 0.00000 0.00046 0.00046 2.97325

D10 -0.00064 0.00001 0.00000 0.00084 0.00084 0.00019

D11 2.73722 0.00001 0.00000 0.00051 0.00051 2.73773

D12 -1.53265 0.00000 0.00000 0.00027 0.00027 -1.53238

D13 0.57377 0.00000 0.00000 0.00047 0.00047 0.57424

D14 -0.79341 0.00000 0.00000 0.00051 0.00051 -0.79290

D15 1.21990 -0.00002 0.00000 0.00027 0.00027 1.22017

D16 -2.95686 -0.00001 0.00000 0.00048 0.00048 -2.95639

D17 1.01126 0.00001 0.00000 0.00071 0.00071 1.01196

D18 3.02457 0.00000 0.00000 0.00046 0.00046 3.02503

D19 -1.15220 0.00000 0.00000 0.00067 0.00067 -1.15153

D20 -1.03577 0.00001 0.00000 0.00012 0.00012 -1.03566

D21 -2.97867 0.00000 0.00000 -0.00010 -0.00010 -2.97877

D22 1.19625 -0.00001 0.00000 -0.00062 -0.00062 1.19563

D23 1.07205 0.00001 0.00000 0.00003 0.00003 1.07208

D24 -0.87085 -0.00001 0.00000 -0.00019 -0.00019 -0.87104

D25 -2.97911 -0.00002 0.00000 -0.00071 -0.00071 -2.97982

D26 3.13129 0.00002 0.00000 0.00016 0.00016 3.13145

D27 1.18839 0.00000 0.00000 -0.00005 -0.00005 1.18834

D28 -0.91988 -0.00001 0.00000 -0.00057 -0.00057 -0.92045

D29 0.60006 0.00001 0.00000 -0.00058 -0.00058 0.59948

D30 -2.71034 0.00000 0.00000 -0.00096 -0.00096 -2.71130

D31 -2.94876 0.00000 0.00000 -0.00019 -0.00019 -2.94895

D32 0.02403 0.00000 0.00000 -0.00057 -0.00057 0.02345

D33 -1.19621 -0.00001 0.00000 -0.00027 -0.00027 -1.19648

D34 1.77658 -0.00001 0.00000 -0.00065 -0.00065 1.77593

D35 -0.57443 0.00000 0.00000 0.00111 0.00111 -0.57332

D36 -2.73807 0.00000 0.00000 0.00135 0.00135 -2.73672

D37 1.53198 0.00000 0.00000 0.00132 0.00132 1.53331

D38 2.95610 0.00001 0.00000 0.00089 0.00089 2.95699

D39 0.79247 0.00001 0.00000 0.00112 0.00112 0.79359

D40 -1.22067 0.00001 0.00000 0.00110 0.00110 -1.21957

D41 1.15131 0.00001 0.00000 0.00085 0.00085 1.15216

D42 -1.01232 0.00001 0.00000 0.00108 0.00108 -1.01124

D43 -3.02546 0.00001 0.00000 0.00106 0.00106 -3.02440

D44 1.03651 -0.00001 0.00000 0.00012 0.00012 1.03663

D45 2.97932 0.00001 0.00000 0.00026 0.00026 2.97958

D46 -1.19510 0.00000 0.00000 0.00008 0.00008 -1.19502

D47 -1.07116 0.00000 0.00000 -0.00007 -0.00007 -1.07122

D48 0.87166 0.00001 0.00000 0.00007 0.00007 0.87173

D49 2.98042 0.00000 0.00000 -0.00011 -0.00011 2.98031

D50 -3.13036 -0.00002 0.00000 -0.00030 -0.00030 -3.13066

D51 -1.18754 0.00000 0.00000 -0.00016 -0.00016 -1.18771

D52 0.92122 -0.00001 0.00000 -0.00034 -0.00034 0.92088

D53 0.00039 0.00000 0.00000 -0.00097 -0.00097 -0.00058

D54 2.16607 -0.00001 0.00000 -0.00115 -0.00115 2.16492

D55 -2.08783 0.00000 0.00000 -0.00118 -0.00118 -2.08900

D56 -2.16522 0.00000 0.00000 -0.00090 -0.00090 -2.16612

D57 0.00046 0.00000 0.00000 -0.00108 -0.00108 -0.00062

D58 2.02975 0.00000 0.00000 -0.00111 -0.00111 2.02864

D59 2.08869 0.00000 0.00000 -0.00094 -0.00094 2.08776

D60 -2.02881 -0.00001 0.00000 -0.00112 -0.00112 -2.02993

D61 0.00047 0.00000 0.00000 -0.00114 -0.00114 -0.00067

D62 -0.01647 0.00000 0.00000 0.00026 0.00026 -0.01621

D63 3.12285 0.00000 0.00000 0.00014 0.00014 3.12299

D64 0.01648 0.00000 0.00000 -0.00038 -0.00038 0.01610

D65 -3.12290 0.00000 0.00000 -0.00017 -0.00017 -3.12307

D66 -0.00040 0.00000 0.00000 -0.00018 -0.00018 -0.00057

D67 1.85277 0.00001 0.00000 0.00005 0.00005 1.85282

D68 -1.79270 0.00000 0.00000 0.00022 0.00022 -1.79248

D69 -1.85313 -0.00001 0.00000 -0.00043 -0.00043 -1.85356

D70 0.00003 0.00000 0.00000 -0.00020 -0.00020 -0.00017

D71 2.63774 -0.00001 0.00000 -0.00002 -0.00002 2.63772

D72 1.79182 0.00000 0.00000 -0.00017 -0.00017 1.79165

D73 -2.63820 0.00001 0.00000 0.00006 0.00006 -2.63815

D74 -0.00049 0.00000 0.00000 0.00023 0.00023 -0.00025

D75 -1.93897 0.00000 0.00000 -0.00001 -0.00001 -1.93898

D76 1.20551 0.00000 0.00000 0.00014 0.00014 1.20565

D77 0.01011 0.00000 0.00000 -0.00003 -0.00003 0.01008

D78 -3.12859 0.00000 0.00000 0.00012 0.00012 -3.12847

D79 2.68195 -0.00001 0.00000 -0.00019 -0.00019 2.68176

D80 -0.45675 -0.00001 0.00000 -0.00004 -0.00004 -0.45679

D81 1.93903 0.00000 0.00000 0.00054 0.00054 1.93957

D82 -1.20536 -0.00001 0.00000 0.00026 0.00026 -1.20510

D83 -0.01016 0.00000 0.00000 0.00037 0.00037 -0.00979

D84 3.12864 0.00000 0.00000 0.00009 0.00009 3.12873

D85 -2.68183 0.00002 0.00000 0.00060 0.00060 -2.68123

D86 0.45696 0.00001 0.00000 0.00033 0.00033 0.45729

Item Value Threshold Converged?

Maximum Force 0.000105 0.000450 YES

RMS Force 0.000021 0.000300 YES

Maximum Displacement 0.001859 0.001800 NO

RMS Displacement 0.000452 0.001200 YES

Predicted change in Energy=-1.646785D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.139426 1.560089 0.442536

2 6 0 0.184756 1.280602 0.106993

3 6 0 -0.753903 3.778887 -0.369415

4 6 0 -1.623027 2.847268 0.197074

5 1 0 -1.734275 0.844663 1.028345

6 1 0 -2.603005 3.157213 0.587511

7 6 0 0.795412 1.927250 -1.088142

8 1 0 1.914876 1.948696 -0.989351

9 1 0 0.569215 1.272195 -1.975829

10 6 0 0.268728 3.330086 -1.355376

11 1 0 1.121768 4.061158 -1.391103

12 1 0 -0.212625 3.356479 -2.373142

13 1 0 -1.029047 4.845316 -0.413740

14 1 0 0.661646 0.345791 0.444117

15 8 0 2.756675 3.854560 0.819380

16 6 0 0.473660 3.875086 1.417986

17 6 0 0.962336 2.575671 1.665332

18 6 0 1.613144 4.675590 0.893265

19 8 0 1.759099 5.833147 0.534846

20 6 0 2.403133 2.574783 1.292913

21 8 0 3.296743 1.743652 1.312765

22 1 0 -0.347898 4.363488 1.947356

23 1 0 0.585614 1.881337 2.420138

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394332 0.000000

3 C 2.393941 2.710991 0.000000

4 C 1.396764 2.393875 1.394346 0.000000

5 H 1.099478 2.172928 3.394780 2.171132 0.000000

6 H 2.171148 3.394728 2.172870 1.099483 2.509365

7 C 2.494270 1.489766 2.519028 2.889128 3.471431

8 H 3.395596 2.154444 3.294890 3.838201 4.313501

9 H 2.975034 2.118024 3.258022 3.465297 3.809713

10 C 2.889339 2.519119 1.489737 2.494384 3.983903

11 H 3.838044 3.294507 2.154453 3.395547 4.935237

12 H 3.466125 3.258565 2.118097 2.975658 4.493858

13 H 3.396779 3.801535 1.102243 2.172120 4.310706

14 H 2.172183 1.102246 3.801547 3.396784 2.516075

15 O 4.537203 3.707765 3.707171 4.536925 5.410340

16 C 2.985425 2.921219 2.170476 2.634982 3.769650

17 C 2.635155 2.170312 2.921198 2.985573 3.267086

18 C 4.181643 3.766226 2.828665 3.781566 5.089151

19 O 5.164203 4.836040 3.369400 4.524195 6.110007

20 C 3.781861 2.828871 3.765644 4.181516 4.492378

21 O 4.524443 3.369386 4.835250 5.163997 5.118615

22 H 3.278726 3.629717 2.423639 2.643551 3.892140

23 H 2.643836 2.423264 3.629959 3.279196 2.897182

6 7 8 9 10

6 H 0.000000

7 C 3.983699 0.000000

8 H 4.935408 1.124019 0.000000

9 H 4.492992 1.126166 1.800443 0.000000

10 C 3.471534 1.522091 2.179912 2.170292 0.000000

11 H 4.313463 2.179876 2.291926 2.902677 1.124020

12 H 3.810392 2.170267 2.902239 2.261276 1.126163

13 H 2.515858 3.506933 4.169942 4.214469 2.206087

14 H 4.310754 2.206065 2.488919 2.592857 3.506933

15 O 5.409826 3.346597 2.759067 4.389394 3.345820

16 C 3.266634 3.190340 3.403432 4.278101 2.833824

17 C 3.769820 2.833714 2.889251 3.887370 3.189814

18 C 4.491644 3.485402 3.327347 4.572153 2.945203

19 O 5.117749 4.338066 4.175692 5.340561 3.472673

20 C 5.089031 2.945079 2.416425 3.967955 3.484194

21 O 6.109924 3.471991 2.692831 4.298434 4.336430

22 H 2.896513 4.056682 4.424434 5.078245 3.515137

23 H 3.892771 3.514847 3.660066 4.438000 4.056328

11 12 13 14 15

11 H 0.000000

12 H 1.800438 0.000000

13 H 2.489206 2.592766 0.000000

14 H 4.169377 4.214919 4.882631 0.000000

15 O 2.757143 4.388282 4.102910 4.103831 0.000000

16 C 2.888884 3.887492 2.560214 3.666017 2.360277

17 C 3.402041 4.277787 3.665983 2.560107 2.360263

18 C 2.416053 3.967732 2.952666 4.455810 1.409685

19 O 2.693588 4.298601 3.106346 5.596759 2.234037

20 C 3.324929 4.570908 4.455092 2.953243 1.409629

21 O 4.172799 5.338800 5.595855 3.106815 2.234063

22 H 3.660141 4.438364 2.504176 4.406903 3.342112

23 H 4.423193 5.078263 4.407172 2.503665 3.342086

16 17 18 19 20

16 C 0.000000

17 C 1.410129 0.000000

18 C 1.488140 2.330085 0.000000

19 O 2.503257 3.538924 1.220535 0.000000

20 C 2.330085 1.488151 2.279735 3.406814 0.000000

21 O 3.538910 2.503201 3.406867 4.437733 1.220537

22 H 1.092578 2.234399 2.248155 2.931642 3.346033

23 H 2.234251 1.092589 3.345894 4.533012 2.248306

21 22 23

21 O 0.000000

22 H 4.533173 0.000000

23 H 2.931800 2.693704 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306911 -0.697260 -0.663971

2 6 0 1.371311 -1.355197 0.133482

3 6 0 1.370097 1.355793 0.134969

4 6 0 2.306270 0.699503 -0.663193

5 1 0 2.915598 -1.252866 -1.391745

6 1 0 2.914301 1.256499 -1.390461

7 6 0 0.966497 -0.761594 1.438535

8 1 0 -0.043895 -1.147417 1.744585

9 1 0 1.693999 -1.131039 2.214744

10 6 0 0.965388 0.760496 1.439250

11 1 0 -0.045773 1.144507 1.745043

12 1 0 1.691838 1.130236 2.216301

13 1 0 1.210818 2.441591 0.031947

14 1 0 1.212951 -2.441039 0.029476

15 8 0 -2.077252 -0.000510 0.274036

16 6 0 -0.292318 0.705240 -1.099585

17 6 0 -0.291945 -0.704889 -1.099780

18 6 0 -1.425486 1.139629 -0.238308

19 8 0 -1.886797 2.218423 0.098000

20 6 0 -1.424746 -1.140105 -0.238420

21 8 0 -1.885190 -2.219310 0.097764

22 1 0 0.065805 1.347356 -1.907769

23 1 0 0.066390 -1.346347 -1.908407

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200595 0.8808482 0.6753885

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5584147721 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504198093112E-01 A.U. after 11 cycles

Convg = 0.5223D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000043305 0.000008426 0.000005649

2 6 0.000039618 -0.000008706 -0.000018869

3 6 0.000001781 0.000023520 0.000014539

4 6 -0.000018060 -0.000009154 0.000004993

5 1 -0.000001172 -0.000001660 0.000008870

6 1 -0.000007844 -0.000005225 0.000000487

7 6 0.000012155 -0.000005646 -0.000003141

8 1 -0.000000807 0.000006641 -0.000001787

9 1 -0.000000281 0.000006342 -0.000006500

10 6 0.000008318 -0.000016704 -0.000005269

11 1 -0.000000388 0.000000660 -0.000002672

12 1 -0.000000280 -0.000002981 -0.000000122

13 1 0.000005335 0.000007830 -0.000009265

14 1 0.000002703 -0.000002168 -0.000001241

15 8 0.000017019 0.000018103 -0.000013223

16 6 -0.000010206 -0.000015711 0.000012955

17 6 -0.000069368 0.000019529 0.000027228

18 6 0.000039710 -0.000023633 -0.000003219

19 8 0.000008014 -0.000020099 -0.000001898

20 6 -0.000001467 0.000011704 0.000010052

21 8 0.000005336 0.000022427 -0.000013540

22 1 -0.000003580 -0.000004148 -0.000001042

23 1 0.000016771 -0.000009346 -0.000002985

-------------------------------------------------------------------

Cartesian Forces: Max 0.000069368 RMS 0.000015918

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000048569 RMS 0.000009685

Search for a saddle point.

Step number 59 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58 59

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.06976 -0.00023 0.00351 0.00736 0.00790

Eigenvalues --- 0.01063 0.01202 0.01312 0.01908 0.02396

Eigenvalues --- 0.02668 0.02832 0.03107 0.03292 0.03340

Eigenvalues --- 0.03566 0.03580 0.03782 0.03844 0.04125

Eigenvalues --- 0.04371 0.04577 0.04741 0.04975 0.06166

Eigenvalues --- 0.06416 0.06592 0.07033 0.07375 0.08484

Eigenvalues --- 0.09219 0.09710 0.10087 0.10270 0.10904

Eigenvalues --- 0.12713 0.13859 0.14770 0.17051 0.22378

Eigenvalues --- 0.26175 0.28127 0.29607 0.29956 0.30985

Eigenvalues --- 0.31335 0.31420 0.31935 0.32041 0.32454

Eigenvalues --- 0.32765 0.33627 0.36811 0.37884 0.39721

Eigenvalues --- 0.39953 0.40489 0.44401 0.48578 0.52678

Eigenvalues --- 0.61761 1.08633 1.11058

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D4

1 -0.56708 -0.51000 -0.15311 0.14921 -0.13598

D30 D1 D35 R19 D29

1 0.13431 -0.13315 -0.13144 0.13036 0.12978

RFO step: Lambda0=9.637125820D-10 Lambda=-2.33529599D-04.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.06202938 RMS(Int)= 0.00241301

Iteration 2 RMS(Cart)= 0.00286283 RMS(Int)= 0.00050207

Iteration 3 RMS(Cart)= 0.00000402 RMS(Int)= 0.00050206

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00050206

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63491 0.00005 0.00000 0.00903 0.00915 2.64406

R2 2.63950 0.00000 0.00000 -0.00304 -0.00282 2.63668

R3 2.07771 0.00001 0.00000 -0.00080 -0.00080 2.07692

R4 2.81525 0.00001 0.00000 -0.00079 -0.00091 2.81434

R5 2.08294 0.00000 0.00000 0.00042 0.00042 2.08336

R6 4.10130 0.00001 0.00000 -0.04054 -0.04057 4.06073

R7 2.63493 0.00003 0.00000 0.00478 0.00486 2.63979

R8 2.81519 0.00002 0.00000 0.00370 0.00374 2.81893

R9 2.08294 0.00001 0.00000 0.00137 0.00137 2.08431

R10 4.10161 0.00001 0.00000 0.01532 0.01528 4.11689

R11 2.07772 0.00001 0.00000 0.00187 0.00187 2.07960

R12 2.12409 0.00000 0.00000 -0.00065 -0.00065 2.12344

R13 2.12815 0.00000 0.00000 0.00133 0.00133 2.12948

R14 2.87633 -0.00001 0.00000 -0.00167 -0.00177 2.87456

R15 2.12409 0.00000 0.00000 0.00203 0.00203 2.12612

R16 2.12814 0.00000 0.00000 -0.00245 -0.00245 2.12569

R17 2.66392 -0.00003 0.00000 -0.00959 -0.00960 2.65432

R18 2.66381 -0.00001 0.00000 -0.00188 -0.00190 2.66191

R19 2.66476 -0.00002 0.00000 -0.00319 -0.00329 2.66147

R20 2.81218 0.00003 0.00000 0.01048 0.01049 2.82267

R21 2.06467 0.00000 0.00000 0.00052 0.00052 2.06519

R22 2.81220 0.00003 0.00000 0.01242 0.01242 2.82462

R23 2.06469 0.00000 0.00000 0.00004 0.00004 2.06473

R24 2.30648 -0.00002 0.00000 -0.00032 -0.00032 2.30616

R25 2.30648 -0.00001 0.00000 -0.00036 -0.00036 2.30612

A1 2.06149 0.00000 0.00000 -0.00907 -0.00972 2.05178

A2 2.10784 0.00000 0.00000 0.01083 0.01110 2.11894

A3 2.10129 0.00000 0.00000 0.00044 0.00075 2.10204

A4 2.08901 0.00000 0.00000 -0.01524 -0.01623 2.07278

A5 2.10282 0.00000 0.00000 0.00885 0.00894 2.11176

A6 1.61867 -0.00001 0.00000 0.00551 0.00606 1.62473

A7 2.02211 0.00000 0.00000 -0.00133 -0.00060 2.02151

A8 1.74178 0.00000 0.00000 0.02834 0.02790 1.76968

A9 1.70263 0.00000 0.00000 -0.01392 -0.01389 1.68875

A10 2.08919 0.00000 0.00000 0.01154 0.01047 2.09965

A11 2.10270 0.00000 0.00000 0.00138 0.00156 2.10426

A12 1.61839 0.00000 0.00000 -0.00976 -0.00931 1.60908

A13 2.02218 -0.00001 0.00000 -0.01079 -0.00989 2.01229

A14 1.74177 0.00000 0.00000 -0.02776 -0.02818 1.71358

A15 1.70259 0.00000 0.00000 0.03267 0.03269 1.73528

A16 2.06157 -0.00001 0.00000 0.00994 0.00930 2.07087

A17 2.10131 0.00000 0.00000 -0.00465 -0.00431 2.09699

A18 2.10772 0.00001 0.00000 -0.00622 -0.00591 2.10181

A19 1.92411 0.00001 0.00000 0.00904 0.01007 1.93419

A20 1.87291 0.00001 0.00000 -0.00933 -0.00844 1.86447

A21 1.98129 0.00000 0.00000 0.00112 -0.00208 1.97921

A22 1.85503 0.00000 0.00000 0.00591 0.00545 1.86048

A23 1.92034 0.00000 0.00000 -0.00309 -0.00210 1.91824

A24 1.90520 0.00000 0.00000 -0.00359 -0.00274 1.90246

A25 1.98121 0.00001 0.00000 0.00116 -0.00191 1.97930

A26 1.92416 0.00000 0.00000 -0.00878 -0.00789 1.91627

A27 1.87304 0.00000 0.00000 0.01735 0.01818 1.89122

A28 1.92029 -0.00001 0.00000 -0.00828 -0.00749 1.91280

A29 1.90516 0.00000 0.00000 0.00867 0.00948 1.91465

A30 1.85502 0.00000 0.00000 -0.00999 -0.01036 1.84466

A31 1.88358 -0.00002 0.00000 -0.00948 -0.00962 1.87396

A32 1.87507 0.00001 0.00000 -0.00932 -0.00978 1.86529

A33 1.73811 0.00000 0.00000 0.00858 0.00864 1.74675

A34 1.56433 -0.00001 0.00000 0.00989 0.01015 1.57448

A35 1.86730 -0.00001 0.00000 -0.00554 -0.00570 1.86160

A36 2.19878 0.00000 0.00000 0.00069 0.00097 2.19976

A37 2.10151 0.00001 0.00000 0.00028 0.00017 2.10168

A38 1.87524 0.00000 0.00000 0.01345 0.01274 1.88798

A39 1.73841 0.00000 0.00000 0.00122 0.00172 1.74014

A40 1.56409 0.00000 0.00000 0.00159 0.00155 1.56564

A41 1.86729 -0.00001 0.00000 -0.00474 -0.00506 1.86224

A42 2.19850 0.00001 0.00000 0.01855 0.01877 2.21727

A43 2.10172 0.00000 0.00000 -0.02313 -0.02318 2.07855

A44 1.90321 0.00003 0.00000 0.01155 0.01144 1.91465

A45 2.02636 -0.00003 0.00000 -0.00736 -0.00736 2.01901

A46 2.35361 0.00000 0.00000 -0.00423 -0.00423 2.34938

A47 1.90324 0.00002 0.00000 0.00832 0.00818 1.91142

A48 2.02647 -0.00004 0.00000 -0.01578 -0.01579 2.01068

A49 2.35348 0.00002 0.00000 0.00750 0.00749 2.36097

D1 -0.59975 0.00000 0.00000 -0.02155 -0.02096 -0.62070

D2 2.94907 0.00000 0.00000 0.00045 0.00075 2.94982

D3 1.19636 0.00000 0.00000 0.01201 0.01193 1.20829

D4 2.71085 0.00000 0.00000 -0.03625 -0.03584 2.67501

D5 -0.02352 0.00000 0.00000 -0.01425 -0.01414 -0.03765

D6 -1.77623 0.00000 0.00000 -0.00269 -0.00295 -1.77918

D7 0.00000 0.00000 0.00000 -0.02238 -0.02228 -0.02228

D8 -2.97305 0.00000 0.00000 -0.01562 -0.01571 -2.98876

D9 2.97325 0.00000 0.00000 -0.00669 -0.00649 2.96676

D10 0.00019 0.00000 0.00000 0.00007 0.00008 0.00028

D11 2.73773 0.00000 0.00000 0.11658 0.11613 2.85386

D12 -1.53238 0.00000 0.00000 0.12309 0.12309 -1.40929

D13 0.57424 0.00000 0.00000 0.11283 0.11263 0.68688

D14 -0.79290 0.00000 0.00000 0.09807 0.09794 -0.69496

D15 1.22017 0.00000 0.00000 0.10459 0.10490 1.32507

D16 -2.95639 0.00000 0.00000 0.09433 0.09444 -2.86195

D17 1.01196 0.00000 0.00000 0.09697 0.09687 1.10883

D18 3.02503 0.00001 0.00000 0.10348 0.10384 3.12887

D19 -1.15153 0.00000 0.00000 0.09322 0.09337 -1.05815

D20 -1.03566 -0.00001 0.00000 0.02969 0.02947 -1.00618

D21 -2.97877 0.00000 0.00000 0.03028 0.03038 -2.94840

D22 1.19563 0.00001 0.00000 0.05341 0.05352 1.24915

D23 1.07208 -0.00001 0.00000 0.01979 0.01894 1.09102

D24 -0.87104 0.00001 0.00000 0.02039 0.01985 -0.85119

D25 -2.97982 0.00001 0.00000 0.04352 0.04299 -2.93683

D26 3.13145 -0.00001 0.00000 0.02156 0.02120 -3.13054

D27 1.18834 0.00000 0.00000 0.02215 0.02210 1.21044

D28 -0.92045 0.00001 0.00000 0.04529 0.04525 -0.87520

D29 0.59948 0.00000 0.00000 -0.02153 -0.02208 0.57740

D30 -2.71130 0.00000 0.00000 -0.02815 -0.02851 -2.73980

D31 -2.94895 0.00000 0.00000 -0.01798 -0.01824 -2.96719

D32 0.02345 0.00000 0.00000 -0.02461 -0.02466 -0.00121

D33 -1.19648 0.00000 0.00000 0.01456 0.01464 -1.18183

D34 1.77593 0.00000 0.00000 0.00794 0.00822 1.78415

D35 -0.57332 -0.00001 0.00000 0.11245 0.11239 -0.46093

D36 -2.73672 0.00000 0.00000 0.12928 0.12957 -2.60715

D37 1.53331 0.00000 0.00000 0.13604 0.13596 1.66927

D38 2.95699 0.00000 0.00000 0.10660 0.10645 3.06344

D39 0.79359 0.00000 0.00000 0.12343 0.12364 0.91722

D40 -1.21957 0.00000 0.00000 0.13020 0.13003 -1.08955

D41 1.15216 -0.00001 0.00000 0.08719 0.08686 1.23902

D42 -1.01124 0.00000 0.00000 0.10402 0.10404 -0.90720

D43 -3.02440 0.00000 0.00000 0.11078 0.11043 -2.91397

D44 1.03663 0.00000 0.00000 0.02940 0.02952 1.06615

D45 2.97958 -0.00001 0.00000 0.02399 0.02375 3.00333

D46 -1.19502 0.00000 0.00000 0.02698 0.02685 -1.16817

D47 -1.07122 0.00000 0.00000 0.02418 0.02485 -1.04637

D48 0.87173 -0.00001 0.00000 0.01876 0.01909 0.89081

D49 2.98031 0.00000 0.00000 0.02175 0.02218 3.00250

D50 -3.13066 0.00001 0.00000 0.03346 0.03386 -3.09680

D51 -1.18771 0.00000 0.00000 0.02804 0.02809 -1.15962

D52 0.92088 0.00001 0.00000 0.03103 0.03119 0.95207

D53 -0.00058 0.00000 0.00000 -0.14590 -0.14582 -0.14640

D54 2.16492 0.00000 0.00000 -0.16298 -0.16320 2.00172

D55 -2.08900 0.00000 0.00000 -0.17472 -0.17450 -2.26351

D56 -2.16612 0.00000 0.00000 -0.15622 -0.15592 -2.32203

D57 -0.00062 0.00000 0.00000 -0.17330 -0.17329 -0.17391

D58 2.02864 0.00000 0.00000 -0.18504 -0.18460 1.84405

D59 2.08776 0.00000 0.00000 -0.15953 -0.15972 1.92804

D60 -2.02993 0.00000 0.00000 -0.17661 -0.17709 -2.20702

D61 -0.00067 0.00000 0.00000 -0.18834 -0.18840 -0.18907

D62 -0.01621 0.00000 0.00000 -0.00596 -0.00578 -0.02199

D63 3.12299 0.00000 0.00000 -0.01959 -0.01927 3.10371

D64 0.01610 0.00000 0.00000 -0.01831 -0.01857 -0.00247

D65 -3.12307 0.00000 0.00000 -0.03506 -0.03512 3.12500

D66 -0.00057 0.00001 0.00000 -0.04011 -0.04015 -0.04072

D67 1.85282 0.00000 0.00000 -0.03520 -0.03513 1.81769

D68 -1.79248 0.00000 0.00000 -0.06218 -0.06237 -1.85484

D69 -1.85356 0.00001 0.00000 -0.04364 -0.04354 -1.89710

D70 -0.00017 0.00000 0.00000 -0.03873 -0.03852 -0.03869

D71 2.63772 0.00000 0.00000 -0.06571 -0.06576 2.57196

D72 1.79165 0.00001 0.00000 -0.03423 -0.03419 1.75746

D73 -2.63815 0.00000 0.00000 -0.02932 -0.02917 -2.66731

D74 -0.00025 0.00000 0.00000 -0.05630 -0.05640 -0.05666

D75 -1.93898 0.00000 0.00000 0.03744 0.03803 -1.90095

D76 1.20565 0.00000 0.00000 0.05471 0.05511 1.26076

D77 0.01008 0.00000 0.00000 0.02901 0.02903 0.03912

D78 -3.12847 0.00000 0.00000 0.04628 0.04611 -3.08236

D79 2.68176 0.00000 0.00000 0.02051 0.02073 2.70249

D80 -0.45679 0.00000 0.00000 0.03778 0.03781 -0.41898

D81 1.93957 0.00000 0.00000 0.05020 0.04983 1.98940

D82 -1.20510 0.00000 0.00000 0.07137 0.07106 -1.13404

D83 -0.00979 0.00000 0.00000 0.03651 0.03682 0.02703

D84 3.12873 0.00000 0.00000 0.05768 0.05805 -3.09641

D85 -2.68123 -0.00001 0.00000 0.04764 0.04750 -2.63373

D86 0.45729 0.00000 0.00000 0.06882 0.06873 0.52602

Item Value Threshold Converged?

Maximum Force 0.000049 0.000450 YES

RMS Force 0.000010 0.000300 YES

Maximum Displacement 0.290552 0.001800 NO

RMS Displacement 0.062077 0.001200 NO

Predicted change in Energy=-6.617932D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.143879 1.558897 0.466104

2 6 0 0.185801 1.276585 0.134527

3 6 0 -0.750883 3.767373 -0.391494

4 6 0 -1.622980 2.837709 0.179950

5 1 0 -1.746831 0.858653 1.061111

6 1 0 -2.610165 3.153643 0.549675

7 6 0 0.760675 1.881501 -1.098992

8 1 0 1.882804 1.823915 -1.086490

9 1 0 0.415461 1.247783 -1.964480

10 6 0 0.318336 3.318496 -1.329841

11 1 0 1.206906 4.004113 -1.251019

12 1 0 -0.062412 3.433680 -2.382023

13 1 0 -1.040976 4.827815 -0.480103

14 1 0 0.677100 0.356743 0.492225

15 8 0 2.745177 3.910159 0.817375

16 6 0 0.453149 3.877156 1.420793

17 6 0 0.963704 2.584962 1.651282

18 6 0 1.593316 4.706418 0.927373

19 8 0 1.732599 5.881842 0.630257

20 6 0 2.402225 2.612976 1.246225

21 8 0 3.303715 1.792260 1.191558

22 1 0 -0.380881 4.343033 1.951523

23 1 0 0.641638 1.877293 2.418923

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.399176 0.000000

3 C 2.401518 2.712582 0.000000

4 C 1.395271 2.389741 1.396917 0.000000

5 H 1.099058 2.183642 3.400387 2.169896 0.000000

6 H 2.167993 3.393099 2.172417 1.100475 2.504774

7 C 2.486147 1.489286 2.518308 2.869118 3.464081

8 H 3.411978 2.161081 3.346096 3.862923 4.326451

9 H 2.904492 2.111730 3.191078 3.358823 3.739136

10 C 2.908553 2.516216 1.491715 2.505860 4.004048

11 H 3.801813 3.225182 2.151224 3.378820 4.895348

12 H 3.577179 3.323807 2.132498 3.058474 4.617706

13 H 3.404662 3.807097 1.102970 2.175987 4.315997

14 H 2.182160 1.102466 3.801643 3.397510 2.539880

15 O 4.558134 3.735292 3.701917 4.542825 5.435922

16 C 2.972583 2.913576 2.178562 2.632575 3.752419

17 C 2.626663 2.148844 2.917335 2.986575 3.267330

18 C 4.196652 3.791234 2.848945 3.794110 5.097035

19 O 5.195086 4.883310 3.417987 4.552958 6.125724

20 C 3.780809 2.816798 3.735887 4.170098 4.508501

21 O 4.512409 3.332360 4.779843 5.136988 5.137768

22 H 3.246544 3.609114 2.440905 2.635769 3.847020

23 H 2.665136 2.405640 3.661962 3.326244 2.930200

6 7 8 9 10

6 H 0.000000

7 C 3.962198 0.000000

8 H 4.963062 1.123675 0.000000

9 H 4.371235 1.126872 1.804408 0.000000

10 C 3.483658 1.521154 2.177281 2.167960 0.000000

11 H 4.305326 2.174331 2.288486 2.955125 1.125095

12 H 3.894139 2.175522 2.837888 2.276148 1.124865

13 H 2.515085 3.508524 4.235518 4.140195 2.201778

14 H 4.316488 2.205412 2.469546 2.626368 3.495800

15 O 5.415134 3.424349 2.953101 4.500504 3.293959

16 C 3.265917 3.229013 3.542058 4.286618 2.810029

17 C 3.782787 2.846065 2.986526 3.893887 3.137144

18 C 4.497002 3.574856 3.528210 4.659647 2.940564

19 O 5.129246 4.465161 4.408690 5.471929 3.523189

20 C 5.089357 2.954621 2.516740 4.014924 3.387694

21 O 6.102407 3.423688 2.685051 4.312661 4.195158

22 H 2.889556 4.082638 4.549698 5.054682 3.507981

23 H 3.961993 3.519931 3.719041 4.434148 4.029247

11 12 13 14 15

11 H 0.000000

12 H 1.793246 0.000000

13 H 2.515108 2.553135 0.000000

14 H 4.077119 4.275011 4.887504 0.000000

15 O 2.579411 4.283192 4.106154 4.124249 0.000000

16 C 2.779001 3.863144 2.597994 3.647698 2.370357

17 C 3.239829 4.247445 3.686725 2.527947 2.371750

18 C 2.321193 3.913233 2.989184 4.466372 1.404603

19 O 2.709505 4.276609 3.168058 5.626708 2.224378

20 C 3.098432 4.462306 4.443125 2.938564 1.408622

21 O 3.905777 5.176442 5.557463 3.073903 2.222044

22 H 3.590572 4.439366 2.565842 4.374858 3.353493

23 H 4.279178 5.095794 4.465549 2.454689 3.335023

16 17 18 19 20

16 C 0.000000

17 C 1.408388 0.000000

18 C 1.493693 2.328311 0.000000

19 O 2.506133 3.535973 1.220368 0.000000

20 C 2.329703 1.494723 2.266826 3.393125 0.000000

21 O 3.539077 2.513041 3.389333 4.416803 1.220348

22 H 1.092851 2.233577 2.253528 2.929245 3.352047

23 H 2.243044 1.092609 3.336819 4.519506 2.239668

21 22 23

21 O 0.000000

22 H 4.545354 0.000000

23 H 2.932629 2.709960 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.341749 -0.543919 -0.715186

2 6 0 1.439901 -1.300121 0.041464

3 6 0 1.301005 1.402210 0.231768

4 6 0 2.273770 0.845069 -0.601719

5 1 0 2.979044 -1.009555 -1.480017

6 1 0 2.859396 1.484316 -1.279547

7 6 0 1.061163 -0.816726 1.398247

8 1 0 0.132585 -1.334529 1.761933

9 1 0 1.892640 -1.119115 2.096135

10 6 0 0.876058 0.691301 1.472430

11 1 0 -0.200348 0.928703 1.697883

12 1 0 1.466048 1.103708 2.336810

13 1 0 1.108930 2.488280 0.221644

14 1 0 1.318700 -2.381741 -0.134152

15 8 0 -2.086839 -0.089666 0.263508

16 6 0 -0.314321 0.742109 -1.072502

17 6 0 -0.250281 -0.663914 -1.123032

18 6 0 -1.493653 1.086866 -0.223127

19 8 0 -2.036574 2.128654 0.107346

20 6 0 -1.357982 -1.175601 -0.259683

21 8 0 -1.745214 -2.278498 0.090917

22 1 0 0.027293 1.429631 -1.850280

23 1 0 0.100270 -1.277262 -1.956527

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2275931 0.8771387 0.6750219

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6113348266 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.494436446738E-01 A.U. after 16 cycles

Convg = 0.2901D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001777858 0.001124203 -0.001925651

2 6 -0.000804258 0.000396379 0.002804710

3 6 0.001845258 -0.002114606 0.000814647

4 6 -0.000396685 0.001482464 -0.000065414

5 1 0.000819179 -0.000154296 0.000221407

6 1 0.000207539 -0.000025860 -0.000543854

7 6 -0.000267569 0.000416435 -0.001470660

8 1 -0.000240095 -0.000019166 0.001124922

9 1 0.000678169 -0.000112146 -0.000122059

10 6 -0.000018393 0.001014843 0.001081162

11 1 -0.000225892 0.000215330 -0.001449162

12 1 -0.001166250 -0.000981518 0.000247528

13 1 0.000258055 -0.000536110 0.001560269

14 1 -0.001065551 -0.000414396 -0.000347004

15 8 -0.002086559 -0.002292456 0.001072244

16 6 0.001124314 0.004511077 -0.002232486

17 6 0.006970560 -0.004717874 -0.003048364

18 6 -0.004832508 0.003747397 0.002171188

19 8 -0.001372967 0.002102318 -0.000854781

20 6 0.000088349 -0.002144137 -0.000835664

21 8 -0.000364666 -0.002465530 0.001661438

22 1 0.000589875 0.000181867 -0.000311931

23 1 -0.001517763 0.000785783 0.000447515

-------------------------------------------------------------------

Cartesian Forces: Max 0.006970560 RMS 0.001819855

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.004727428 RMS 0.001107130

Search for a saddle point.

Step number 60 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 33 38 40 41 44

59 60

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07057 -0.00176 0.00198 0.00752 0.00848

Eigenvalues --- 0.01086 0.01213 0.01359 0.01818 0.02432

Eigenvalues --- 0.02677 0.02819 0.03089 0.03311 0.03336

Eigenvalues --- 0.03574 0.03605 0.03808 0.03851 0.04146

Eigenvalues --- 0.04393 0.04652 0.04770 0.04989 0.06176

Eigenvalues --- 0.06441 0.06619 0.06970 0.07371 0.08502

Eigenvalues --- 0.09244 0.09821 0.10124 0.10308 0.10937

Eigenvalues --- 0.12743 0.13875 0.14885 0.17021 0.22428

Eigenvalues --- 0.26150 0.28237 0.29593 0.29975 0.31078

Eigenvalues --- 0.31365 0.31583 0.31954 0.32042 0.32463

Eigenvalues --- 0.32863 0.33633 0.36845 0.37891 0.39746

Eigenvalues --- 0.40151 0.40510 0.44428 0.48599 0.52802

Eigenvalues --- 0.61853 1.08635 1.11080

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D79

1 -0.56479 -0.51492 0.16037 -0.15206 -0.13697

R19 D1 D4 D29 D30

1 0.13244 -0.13014 -0.12853 0.12702 0.12618

RFO step: Lambda0=7.212844320D-05 Lambda=-1.80805118D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.10572968 RMS(Int)= 0.00441566

Iteration 2 RMS(Cart)= 0.00574710 RMS(Int)= 0.00144721

Iteration 3 RMS(Cart)= 0.00001373 RMS(Int)= 0.00144716

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00144716

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64406 -0.00250 0.00000 -0.02872 -0.02875 2.61531

R2 2.63668 -0.00064 0.00000 0.01265 0.01215 2.64883

R3 2.07692 -0.00023 0.00000 0.00028 0.00028 2.07720

R4 2.81434 0.00050 0.00000 0.00546 0.00566 2.82000

R5 2.08336 -0.00024 0.00000 -0.00165 -0.00165 2.08171

R6 4.06073 -0.00128 0.00000 0.04433 0.04401 4.10474

R7 2.63979 -0.00187 0.00000 -0.01708 -0.01753 2.62226

R8 2.81893 -0.00045 0.00000 -0.00924 -0.00862 2.81032

R9 2.08431 -0.00071 0.00000 -0.00355 -0.00355 2.08077

R10 4.11689 -0.00156 0.00000 0.04239 0.04236 4.15925

R11 2.07960 -0.00038 0.00000 -0.00373 -0.00373 2.07586

R12 2.12344 -0.00023 0.00000 -0.00247 -0.00247 2.12097

R13 2.12948 -0.00005 0.00000 0.00065 0.00065 2.13013

R14 2.87456 0.00057 0.00000 0.00522 0.00619 2.88076

R15 2.12612 -0.00015 0.00000 -0.00276 -0.00276 2.12336

R16 2.12569 0.00006 0.00000 0.00172 0.00172 2.12741

R17 2.65432 0.00394 0.00000 0.02794 0.02795 2.68226

R18 2.66191 0.00194 0.00000 0.00368 0.00380 2.66571

R19 2.66147 0.00473 0.00000 0.00378 0.00328 2.66474

R20 2.82267 -0.00427 0.00000 -0.02565 -0.02577 2.79690

R21 2.06519 -0.00052 0.00000 -0.00065 -0.00065 2.06454

R22 2.82462 -0.00373 0.00000 -0.02765 -0.02757 2.79705

R23 2.06473 0.00025 0.00000 0.00051 0.00051 2.06524

R24 2.30616 0.00208 0.00000 0.00030 0.00030 2.30647

R25 2.30612 0.00131 0.00000 0.00108 0.00108 2.30720

A1 2.05178 0.00111 0.00000 0.01354 0.01332 2.06510

A2 2.11894 -0.00130 0.00000 -0.01977 -0.01988 2.09906

A3 2.10204 0.00018 0.00000 0.00055 -0.00010 2.10194

A4 2.07278 -0.00060 0.00000 0.00144 0.00220 2.07497

A5 2.11176 -0.00016 0.00000 0.01468 0.01363 2.12539

A6 1.62473 0.00004 0.00000 -0.04681 -0.04755 1.57718

A7 2.02151 0.00061 0.00000 -0.00471 -0.00456 2.01695

A8 1.76968 0.00036 0.00000 0.02724 0.02474 1.79443

A9 1.68875 -0.00003 0.00000 -0.00584 -0.00312 1.68563

A10 2.09965 -0.00001 0.00000 0.01290 0.01356 2.11321

A11 2.10426 -0.00063 0.00000 -0.03112 -0.03134 2.07292

A12 1.60908 0.00025 0.00000 0.03705 0.03622 1.64530

A13 2.01229 0.00057 0.00000 0.02607 0.02564 2.03793

A14 1.71358 0.00081 0.00000 -0.02245 -0.02474 1.68885

A15 1.73528 -0.00091 0.00000 -0.03746 -0.03456 1.70072

A16 2.07087 -0.00021 0.00000 -0.01192 -0.01240 2.05847

A17 2.09699 0.00033 0.00000 0.00282 0.00279 2.09978

A18 2.10181 -0.00009 0.00000 0.00628 0.00639 2.10820

A19 1.93419 -0.00026 0.00000 -0.00668 -0.00636 1.92782

A20 1.86447 0.00000 0.00000 -0.00729 -0.00688 1.85758

A21 1.97921 -0.00031 0.00000 0.00605 0.00467 1.98389

A22 1.86048 0.00000 0.00000 0.00976 0.00960 1.87008

A23 1.91824 0.00059 0.00000 0.01339 0.01318 1.93142

A24 1.90246 -0.00001 0.00000 -0.01591 -0.01485 1.88761

A25 1.97930 -0.00014 0.00000 -0.00684 -0.00726 1.97204

A26 1.91627 0.00026 0.00000 0.01034 0.01058 1.92685

A27 1.89122 -0.00014 0.00000 -0.00237 -0.00243 1.88878

A28 1.91280 0.00031 0.00000 0.00631 0.00551 1.91832

A29 1.91465 -0.00029 0.00000 -0.00704 -0.00603 1.90862

A30 1.84466 0.00000 0.00000 -0.00008 -0.00012 1.84454

A31 1.87396 0.00347 0.00000 0.02428 0.02382 1.89779

A32 1.86529 -0.00085 0.00000 -0.01753 -0.02441 1.84088

A33 1.74675 -0.00019 0.00000 0.08576 0.08793 1.83468

A34 1.57448 0.00044 0.00000 -0.02397 -0.02025 1.55423

A35 1.86160 0.00161 0.00000 0.01439 0.01487 1.87647

A36 2.19976 -0.00020 0.00000 0.00065 0.00052 2.20028

A37 2.10168 -0.00121 0.00000 -0.03491 -0.03561 2.06608

A38 1.88798 -0.00030 0.00000 0.01436 0.00810 1.89608

A39 1.74014 -0.00011 0.00000 -0.07201 -0.06796 1.67218

A40 1.56564 0.00037 0.00000 0.02330 0.02635 1.59199

A41 1.86224 0.00127 0.00000 0.01392 0.01358 1.87582

A42 2.21727 -0.00133 0.00000 -0.04716 -0.04652 2.17075

A43 2.07855 0.00005 0.00000 0.04914 0.04907 2.12761

A44 1.91465 -0.00344 0.00000 -0.02932 -0.02991 1.88474

A45 2.01901 0.00344 0.00000 0.01655 0.01665 2.03565

A46 2.34938 0.00001 0.00000 0.01324 0.01336 2.36274

A47 1.91142 -0.00290 0.00000 -0.02194 -0.02209 1.88932

A48 2.01068 0.00438 0.00000 0.04113 0.04111 2.05178

A49 2.36097 -0.00147 0.00000 -0.01939 -0.01930 2.34167

D1 -0.62070 -0.00016 0.00000 0.01028 0.00979 -0.61091

D2 2.94982 0.00012 0.00000 -0.01864 -0.02023 2.92959

D3 1.20829 0.00016 0.00000 0.01488 0.01132 1.21961

D4 2.67501 -0.00009 0.00000 0.05174 0.05237 2.72738

D5 -0.03765 0.00019 0.00000 0.02283 0.02235 -0.01531

D6 -1.77918 0.00023 0.00000 0.05635 0.05390 -1.72529

D7 -0.02228 0.00012 0.00000 0.01611 0.01587 -0.00641

D8 -2.98876 -0.00004 0.00000 0.03366 0.03474 -2.95402

D9 2.96676 -0.00009 0.00000 -0.02683 -0.02862 2.93815

D10 0.00028 -0.00025 0.00000 -0.00929 -0.00974 -0.00946

D11 2.85386 0.00006 0.00000 -0.02094 -0.02171 2.83215

D12 -1.40929 -0.00009 0.00000 -0.01694 -0.01748 -1.42677

D13 0.68688 -0.00028 0.00000 -0.03803 -0.03774 0.64913

D14 -0.69496 -0.00038 0.00000 0.01111 0.01079 -0.68417

D15 1.32507 -0.00052 0.00000 0.01512 0.01502 1.34009

D16 -2.86195 -0.00072 0.00000 -0.00597 -0.00524 -2.86719

D17 1.10883 -0.00003 0.00000 0.01770 0.01917 1.12800

D18 3.12887 -0.00017 0.00000 0.02171 0.02340 -3.13092

D19 -1.05815 -0.00036 0.00000 0.00062 0.00314 -1.05501

D20 -1.00618 0.00081 0.00000 -0.15979 -0.16051 -1.16670

D21 -2.94840 -0.00044 0.00000 -0.14938 -0.14974 -3.09814

D22 1.24915 -0.00055 0.00000 -0.19741 -0.19763 1.05153

D23 1.09102 0.00027 0.00000 -0.16578 -0.16692 0.92411

D24 -0.85119 -0.00099 0.00000 -0.15537 -0.15615 -1.00734

D25 -2.93683 -0.00110 0.00000 -0.20340 -0.20403 -3.14086

D26 -3.13054 0.00098 0.00000 -0.16583 -0.16654 2.98611

D27 1.21044 -0.00027 0.00000 -0.15542 -0.15577 1.05466

D28 -0.87520 -0.00039 0.00000 -0.20345 -0.20366 -1.07886

D29 0.57740 0.00033 0.00000 -0.00636 -0.00571 0.57169

D30 -2.73980 0.00053 0.00000 -0.02433 -0.02507 -2.76487

D31 -2.96719 0.00025 0.00000 0.02208 0.02303 -2.94417

D32 -0.00121 0.00045 0.00000 0.00412 0.00367 0.00246

D33 -1.18183 -0.00078 0.00000 -0.00440 -0.00120 -1.18303

D34 1.78415 -0.00057 0.00000 -0.02236 -0.02055 1.76360

D35 -0.46093 -0.00029 0.00000 -0.02126 -0.02158 -0.48252

D36 -2.60715 -0.00078 0.00000 -0.03235 -0.03152 -2.63866

D37 1.66927 -0.00085 0.00000 -0.03647 -0.03569 1.63358

D38 3.06344 0.00005 0.00000 -0.03576 -0.03726 3.02617

D39 0.91722 -0.00045 0.00000 -0.04685 -0.04719 0.87003

D40 -1.08955 -0.00052 0.00000 -0.05097 -0.05137 -1.14091

D41 1.23902 0.00050 0.00000 0.01164 0.00894 1.24795

D42 -0.90720 0.00001 0.00000 0.00054 -0.00100 -0.90819

D43 -2.91397 -0.00006 0.00000 -0.00357 -0.00517 -2.91913

D44 1.06615 0.00000 0.00000 -0.15265 -0.15171 0.91443

D45 3.00333 0.00141 0.00000 -0.10865 -0.10849 2.89484

D46 -1.16817 0.00025 0.00000 -0.13981 -0.13969 -1.30785

D47 -1.04637 -0.00014 0.00000 -0.16992 -0.16874 -1.21511

D48 0.89081 0.00127 0.00000 -0.12591 -0.12552 0.76530

D49 3.00250 0.00010 0.00000 -0.15707 -0.15671 2.84579

D50 -3.09680 -0.00072 0.00000 -0.18194 -0.18161 3.00477

D51 -1.15962 0.00069 0.00000 -0.13794 -0.13839 -1.29801

D52 0.95207 -0.00047 0.00000 -0.16910 -0.16958 0.78248

D53 -0.14640 0.00016 0.00000 0.03650 0.03647 -0.10994

D54 2.00172 0.00063 0.00000 0.04981 0.04919 2.05091

D55 -2.26351 0.00065 0.00000 0.04931 0.04874 -2.21477

D56 -2.32203 0.00028 0.00000 0.03042 0.03100 -2.29103

D57 -0.17391 0.00076 0.00000 0.04374 0.04372 -0.13018

D58 1.84405 0.00077 0.00000 0.04324 0.04327 1.88732

D59 1.92804 -0.00004 0.00000 0.02026 0.02067 1.94871

D60 -2.20702 0.00043 0.00000 0.03357 0.03339 -2.17363

D61 -0.18907 0.00044 0.00000 0.03307 0.03294 -0.15613

D62 -0.02199 0.00007 0.00000 0.04277 0.04410 0.02211

D63 3.10371 0.00037 0.00000 0.06760 0.06954 -3.10993

D64 -0.00247 -0.00001 0.00000 -0.02940 -0.03112 -0.03359

D65 3.12500 0.00029 0.00000 -0.04071 -0.04352 3.08148

D66 -0.04072 -0.00020 0.00000 0.18421 0.18247 0.14174

D67 1.81769 0.00010 0.00000 0.11477 0.11479 1.93247

D68 -1.85484 0.00026 0.00000 0.16501 0.16503 -1.68981

D69 -1.89710 -0.00029 0.00000 0.08943 0.08779 -1.80931

D70 -0.03869 0.00000 0.00000 0.01999 0.02011 -0.01858

D71 2.57196 0.00016 0.00000 0.07023 0.07035 2.64232

D72 1.75746 -0.00041 0.00000 0.13841 0.13645 1.89391

D73 -2.66731 -0.00011 0.00000 0.06897 0.06877 -2.59854

D74 -0.05666 0.00005 0.00000 0.11921 0.11902 0.06236

D75 -1.90095 0.00034 0.00000 -0.05927 -0.05583 -1.95678

D76 1.26076 -0.00007 0.00000 -0.09060 -0.08810 1.17266

D77 0.03912 -0.00017 0.00000 -0.04050 -0.04062 -0.00151

D78 -3.08236 -0.00058 0.00000 -0.07183 -0.07289 3.12794

D79 2.70249 0.00023 0.00000 -0.07471 -0.07368 2.62881

D80 -0.41898 -0.00018 0.00000 -0.10603 -0.10595 -0.52493

D81 1.98940 -0.00008 0.00000 -0.00416 -0.00835 1.98105

D82 -1.13404 -0.00052 0.00000 0.00967 0.00628 -1.12776

D83 0.02703 -0.00010 0.00000 0.00435 0.00550 0.03253

D84 -3.09641 -0.00054 0.00000 0.01818 0.02013 -3.07628

D85 -2.63373 0.00030 0.00000 -0.00745 -0.00907 -2.64280

D86 0.52602 -0.00014 0.00000 0.00638 0.00556 0.53158

Item Value Threshold Converged?

Maximum Force 0.004727 0.000450 NO

RMS Force 0.001107 0.000300 NO

Maximum Displacement 0.381174 0.001800 NO

RMS Displacement 0.105823 0.001200 NO

Predicted change in Energy=-1.463448D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.072179 1.515547 0.448646

2 6 0 0.247203 1.295484 0.093456

3 6 0 -0.814300 3.741124 -0.384061

4 6 0 -1.626130 2.778778 0.199355

5 1 0 -1.606019 0.787362 1.075558

6 1 0 -2.603649 3.048592 0.621678

7 6 0 0.782860 1.954127 -1.133803

8 1 0 1.905153 1.954492 -1.120728

9 1 0 0.460850 1.315299 -2.004907

10 6 0 0.247039 3.364021 -1.355133

11 1 0 1.091556 4.104338 -1.319436

12 1 0 -0.181922 3.441485 -2.393092

13 1 0 -1.166560 4.783903 -0.414628

14 1 0 0.798974 0.405091 0.434420

15 8 0 2.794070 3.785401 0.914859

16 6 0 0.498144 3.934861 1.372147

17 6 0 0.910253 2.622035 1.680524

18 6 0 1.686146 4.672190 0.886805

19 8 0 1.901125 5.803782 0.483103

20 6 0 2.353042 2.523427 1.365200

21 8 0 3.169062 1.615601 1.389733

22 1 0 -0.291050 4.496638 1.877277

23 1 0 0.439930 1.989426 2.437484

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.383964 0.000000

3 C 2.390208 2.708499 0.000000

4 C 1.401699 2.391809 1.387643 0.000000

5 H 1.099207 2.158041 3.388512 2.175747 0.000000

6 H 2.173837 3.388180 2.166306 1.098499 2.512854

7 C 2.477431 1.492281 2.511253 2.874125 3.456784

8 H 3.394129 2.158085 3.336190 3.859019 4.302812

9 H 2.900035 2.109304 3.183988 3.369871 3.746989

10 C 2.900140 2.525323 1.487155 2.503539 3.997656

11 H 3.809161 3.255589 2.153866 3.383734 4.900534

12 H 3.546445 3.312459 2.127415 3.040674 4.593904

13 H 3.381760 3.798149 1.101094 2.146789 4.287903

14 H 2.175897 1.101594 3.794955 3.401585 2.518170

15 O 4.507491 3.655260 3.835295 4.589489 5.326805

16 C 3.028506 2.943524 2.200979 2.687845 3.797660

17 C 2.582997 2.172133 2.913581 2.941372 3.172323

18 C 4.214823 3.755277 2.955371 3.876696 5.095672

19 O 5.218303 4.817887 3.518532 4.655394 6.149434

20 C 3.686194 2.749498 3.817690 4.154300 4.332664

21 O 4.345547 3.212487 4.850914 5.075810 4.856550

22 H 3.396771 3.703933 2.440951 2.747527 4.016295

23 H 2.542933 2.452176 3.550022 3.146570 2.736002

6 7 8 9 10

6 H 0.000000

7 C 3.968377 0.000000

8 H 4.956040 1.122369 0.000000

9 H 4.392540 1.127215 1.810069 0.000000

10 C 3.483346 1.524432 2.188849 2.159903 0.000000

11 H 4.305470 2.180175 2.307220 2.940476 1.123634

12 H 3.886897 2.174591 2.861109 2.254885 1.125774

13 H 2.480012 3.510709 4.235513 4.148332 2.213340

14 H 4.312889 2.204336 2.458203 2.625476 3.501772

15 O 5.455659 3.405224 2.878545 4.479995 3.437702

16 C 3.312069 3.206892 3.480799 4.274106 2.797672

17 C 3.694674 2.895301 3.046712 3.935978 3.194622

18 C 4.594422 3.505232 3.385859 4.596962 2.967932

19 O 5.282355 4.322586 4.170052 5.330203 3.473838

20 C 5.039584 3.005760 2.589234 4.049393 3.541477

21 O 5.997296 3.489526 2.831030 4.352950 4.373726

22 H 3.003578 4.084635 4.502649 5.075196 3.467107

23 H 3.698967 3.587888 3.848243 4.493297 4.038646

11 12 13 14 15

11 H 0.000000

12 H 1.792725 0.000000

13 H 2.525782 2.585714 0.000000

14 H 4.104394 4.263411 4.874239 0.000000

15 O 2.827074 4.462886 4.295478 3.954457 0.000000

16 C 2.761427 3.857841 2.585474 3.664575 2.345789

17 C 3.351098 4.296359 3.657388 2.545585 2.342740

18 C 2.354462 3.970144 3.137537 4.381765 1.419393

19 O 2.606273 4.265213 3.355111 5.510261 2.248916

20 C 3.361234 4.625325 4.545892 2.787262 1.410635

21 O 4.224860 5.373334 5.664933 2.827591 2.252589

22 H 3.504921 4.400149 2.470196 4.473337 3.309089

23 H 4.360266 5.082287 4.304004 2.579011 3.329548

16 17 18 19 20

16 C 0.000000

17 C 1.410122 0.000000

18 C 1.480054 2.331339 0.000000

19 O 2.500324 3.541068 1.220529 0.000000

20 C 2.330845 1.480133 2.300173 3.426814 0.000000

21 O 3.537383 2.489917 3.434343 4.468837 1.220917

22 H 1.092509 2.235168 2.218368 2.908260 3.338713

23 H 2.218795 1.092880 3.339893 4.528135 2.257199

21 22 23

21 O 0.000000

22 H 4.528846 0.000000

23 H 2.947149 2.671006 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.260370 -0.755947 -0.636231

2 6 0 1.330785 -1.318528 0.220933

3 6 0 1.430463 1.381912 0.037494

4 6 0 2.317578 0.641390 -0.730755

5 1 0 2.802016 -1.385354 -1.356456

6 1 0 2.912096 1.119690 -1.520994

7 6 0 1.011098 -0.616981 1.498640

8 1 0 0.043267 -0.995603 1.922505

9 1 0 1.824643 -0.895438 2.227488

10 6 0 0.985594 0.902046 1.372952

11 1 0 -0.043885 1.287984 1.604854

12 1 0 1.662073 1.352314 2.152056

13 1 0 1.330327 2.460418 -0.160512

14 1 0 1.098029 -2.395020 0.198594

15 8 0 -2.108699 -0.081448 0.243404

16 6 0 -0.346216 0.720542 -1.080679

17 6 0 -0.281333 -0.688047 -1.091214

18 6 0 -1.499258 1.107004 -0.237054

19 8 0 -1.999641 2.161431 0.120008

20 6 0 -1.377918 -1.189962 -0.233090

21 8 0 -1.727306 -2.299060 0.139025

22 1 0 -0.055896 1.383924 -1.898733

23 1 0 0.125520 -1.280869 -1.914268

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2119880 0.8782691 0.6718819

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 469.9795635122 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.479616822146E-01 A.U. after 16 cycles

Convg = 0.2174D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.007086771 -0.000359978 0.004446271

2 6 0.005113533 -0.001606297 -0.007436835

3 6 -0.002919050 0.003714255 -0.002651353

4 6 0.001999707 -0.001454295 0.000967947

5 1 -0.001665171 -0.000142366 0.000013897

6 1 -0.000936681 -0.000437684 -0.000445007

7 6 -0.001527562 0.000564873 -0.000103082

8 1 -0.000175751 0.001023244 0.000782665

9 1 0.001827847 -0.000709422 0.000032941

10 6 0.001693887 -0.001614959 0.000807218

11 1 -0.000065443 0.000516494 -0.000487783

12 1 -0.000868368 -0.000703132 0.000446259

13 1 0.001877306 0.001890878 -0.001259088

14 1 -0.000642259 -0.001048653 0.000379425

15 8 0.003523939 0.002316081 -0.002539834

16 6 -0.003841173 -0.003705773 0.009787091

17 6 -0.005365137 0.007813026 0.004568853

18 6 0.006768611 -0.006977911 -0.003696291

19 8 0.001716942 -0.003236560 0.001953888

20 6 0.000870918 0.003801756 -0.003556253

21 8 0.001756862 0.003987685 0.000210028

22 1 -0.003276311 -0.001715292 -0.001510732

23 1 0.001220127 -0.001915972 -0.000710225

-------------------------------------------------------------------

Cartesian Forces: Max 0.009787091 RMS 0.003126260

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.008022718 RMS 0.001856433

Search for a saddle point.

Step number 61 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 60 61

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0

Eigenvalues --- -0.07103 -0.00102 0.00396 0.00787 0.00853

Eigenvalues --- 0.01085 0.01214 0.01359 0.01842 0.02440

Eigenvalues --- 0.02670 0.02808 0.03074 0.03323 0.03331

Eigenvalues --- 0.03571 0.03606 0.03810 0.03883 0.04142

Eigenvalues --- 0.04399 0.04647 0.04771 0.04950 0.06173

Eigenvalues --- 0.06453 0.06616 0.07070 0.07398 0.08496

Eigenvalues --- 0.09235 0.09912 0.10152 0.10312 0.10885

Eigenvalues --- 0.12765 0.13870 0.14901 0.17058 0.22464

Eigenvalues --- 0.26157 0.28347 0.29604 0.29976 0.31094

Eigenvalues --- 0.31375 0.31721 0.31989 0.32073 0.32464

Eigenvalues --- 0.33051 0.33718 0.36852 0.37892 0.39741

Eigenvalues --- 0.40212 0.40543 0.44446 0.48649 0.52820

Eigenvalues --- 0.61860 1.08636 1.11111

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 R19

1 -0.56709 -0.51393 -0.15437 0.15351 0.13299

D4 D1 D30 D86 D29

1 -0.13187 -0.13063 0.12777 0.12770 0.12704

RFO step: Lambda0=3.174300501D-04 Lambda=-4.33760849D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.09426285 RMS(Int)= 0.01089436

Iteration 2 RMS(Cart)= 0.00993461 RMS(Int)= 0.00111200

Iteration 3 RMS(Cart)= 0.00014438 RMS(Int)= 0.00110216

Iteration 4 RMS(Cart)= 0.00000004 RMS(Int)= 0.00110216

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.61531 0.00802 0.00000 0.03545 0.03592 2.65123

R2 2.64883 0.00066 0.00000 -0.01592 -0.01483 2.63400

R3 2.07720 0.00091 0.00000 0.00180 0.00180 2.07900

R4 2.82000 -0.00062 0.00000 -0.01255 -0.01232 2.80768

R5 2.08171 0.00064 0.00000 0.00318 0.00318 2.08489

R6 4.10474 0.00409 0.00000 -0.00076 -0.00093 4.10380

R7 2.62226 0.00293 0.00000 0.02115 0.02170 2.64396

R8 2.81032 -0.00010 0.00000 0.00712 0.00618 2.81650

R9 2.08077 0.00123 0.00000 0.00407 0.00407 2.08483

R10 4.15925 0.00194 0.00000 -0.11868 -0.11857 4.04068

R11 2.07586 0.00055 0.00000 0.00329 0.00329 2.07915

R12 2.12097 -0.00017 0.00000 0.00549 0.00549 2.12646

R13 2.13013 -0.00015 0.00000 -0.00238 -0.00238 2.12775

R14 2.88076 -0.00133 0.00000 -0.00792 -0.00881 2.87195

R15 2.12336 0.00028 0.00000 -0.00040 -0.00040 2.12296

R16 2.12741 -0.00013 0.00000 0.00114 0.00114 2.12854

R17 2.68226 -0.00550 0.00000 -0.03581 -0.03547 2.64680

R18 2.66571 -0.00367 0.00000 -0.00922 -0.00912 2.65659

R19 2.66474 -0.00574 0.00000 -0.00663 -0.00716 2.65759

R20 2.79690 0.00651 0.00000 0.03637 0.03649 2.83338

R21 2.06454 0.00079 0.00000 0.00346 0.00346 2.06800

R22 2.79705 0.00723 0.00000 0.02331 0.02300 2.82005

R23 2.06524 0.00009 0.00000 -0.00189 -0.00189 2.06335

R24 2.30647 -0.00334 0.00000 -0.00013 -0.00013 2.30633

R25 2.30720 -0.00179 0.00000 -0.00103 -0.00103 2.30617

A1 2.06510 -0.00277 0.00000 -0.01898 -0.02057 2.04452

A2 2.09906 0.00270 0.00000 0.01942 0.02025 2.11931

A3 2.10194 0.00011 0.00000 0.00313 0.00380 2.10575

A4 2.07497 0.00042 0.00000 0.02197 0.02032 2.09529

A5 2.12539 -0.00006 0.00000 -0.01500 -0.01424 2.11115

A6 1.57718 0.00015 0.00000 0.00403 0.00450 1.58168

A7 2.01695 -0.00024 0.00000 -0.00469 -0.00384 2.01311

A8 1.79443 -0.00086 0.00000 -0.02706 -0.02738 1.76704

A9 1.68563 0.00039 0.00000 0.01574 0.01601 1.70163

A10 2.11321 -0.00023 0.00000 -0.04209 -0.04420 2.06902

A11 2.07292 0.00124 0.00000 0.03478 0.03431 2.10723

A12 1.64530 -0.00057 0.00000 0.01187 0.01266 1.65796

A13 2.03793 -0.00088 0.00000 -0.01508 -0.01465 2.02328

A14 1.68885 -0.00062 0.00000 0.03467 0.03440 1.72325

A15 1.70072 0.00088 0.00000 0.01492 0.01492 1.71564

A16 2.05847 0.00124 0.00000 0.01779 0.01594 2.07440

A17 2.09978 -0.00098 0.00000 -0.00351 -0.00293 2.09685

A18 2.10820 -0.00018 0.00000 -0.00635 -0.00604 2.10216

A19 1.92782 -0.00012 0.00000 -0.01227 -0.01019 1.91763

A20 1.85758 -0.00026 0.00000 0.01458 0.01534 1.87292

A21 1.98389 0.00062 0.00000 0.01373 0.00788 1.99177

A22 1.87008 -0.00011 0.00000 -0.02186 -0.02245 1.84763

A23 1.93142 -0.00085 0.00000 -0.01908 -0.01763 1.91379

A24 1.88761 0.00074 0.00000 0.02513 0.02661 1.91422

A25 1.97204 0.00091 0.00000 0.00474 -0.00217 1.96987

A26 1.92685 -0.00042 0.00000 0.00048 0.00236 1.92921

A27 1.88878 -0.00049 0.00000 -0.02126 -0.01902 1.86977

A28 1.91832 -0.00034 0.00000 0.00663 0.00877 1.92709

A29 1.90862 -0.00001 0.00000 -0.00469 -0.00288 1.90574

A30 1.84454 0.00030 0.00000 0.01421 0.01317 1.85771

A31 1.89779 -0.00512 0.00000 -0.03021 -0.03080 1.86699

A32 1.84088 0.00197 0.00000 0.05618 0.05457 1.89545

A33 1.83468 -0.00037 0.00000 -0.02700 -0.02442 1.81026

A34 1.55423 -0.00166 0.00000 -0.02624 -0.02586 1.52838

A35 1.87647 -0.00342 0.00000 -0.03074 -0.03085 1.84562

A36 2.20028 0.00098 0.00000 -0.00166 -0.00084 2.19944

A37 2.06608 0.00273 0.00000 0.03224 0.03146 2.09754

A38 1.89608 -0.00033 0.00000 -0.05172 -0.05216 1.84393

A39 1.67218 0.00092 0.00000 0.00180 0.00111 1.67329

A40 1.59199 -0.00057 0.00000 0.02578 0.02699 1.61898

A41 1.87582 -0.00176 0.00000 -0.00415 -0.00481 1.87101

A42 2.17075 0.00132 0.00000 0.03191 0.03220 2.20295

A43 2.12761 0.00051 0.00000 -0.01907 -0.01876 2.10886

A44 1.88474 0.00605 0.00000 0.04211 0.04158 1.92631

A45 2.03565 -0.00549 0.00000 -0.02451 -0.02446 2.01119

A46 2.36274 -0.00055 0.00000 -0.01729 -0.01724 2.34549

A47 1.88932 0.00426 0.00000 0.02549 0.02429 1.91361

A48 2.05178 -0.00638 0.00000 -0.04577 -0.04539 2.00639

A49 2.34167 0.00212 0.00000 0.02114 0.02152 2.36318

D1 -0.61091 0.00041 0.00000 0.01164 0.01225 -0.59866

D2 2.92959 0.00012 0.00000 0.00583 0.00640 2.93599

D3 1.21961 -0.00043 0.00000 -0.01388 -0.01377 1.20584

D4 2.72738 0.00016 0.00000 -0.00895 -0.00900 2.71838

D5 -0.01531 -0.00013 0.00000 -0.01476 -0.01485 -0.03016

D6 -1.72529 -0.00067 0.00000 -0.03447 -0.03502 -1.76031

D7 -0.00641 -0.00016 0.00000 0.02195 0.02114 0.01473

D8 -2.95402 -0.00058 0.00000 -0.02283 -0.02383 -2.97785

D9 2.93815 0.00039 0.00000 0.04448 0.04416 2.98231

D10 -0.00946 -0.00003 0.00000 -0.00030 -0.00080 -0.01026

D11 2.83215 -0.00062 0.00000 -0.15676 -0.15723 2.67492

D12 -1.42677 -0.00096 0.00000 -0.18073 -0.18050 -1.60727

D13 0.64913 0.00014 0.00000 -0.13203 -0.13174 0.51739

D14 -0.68417 -0.00032 0.00000 -0.15411 -0.15443 -0.83861

D15 1.34009 -0.00066 0.00000 -0.17808 -0.17770 1.16239

D16 -2.86719 0.00044 0.00000 -0.12938 -0.12895 -2.99614

D17 1.12800 -0.00042 0.00000 -0.15230 -0.15207 0.97593

D18 -3.13092 -0.00076 0.00000 -0.17627 -0.17534 2.97693

D19 -1.05501 0.00034 0.00000 -0.12757 -0.12658 -1.18160

D20 -1.16670 -0.00023 0.00000 -0.05621 -0.05522 -1.22191

D21 -3.09814 0.00139 0.00000 -0.04024 -0.03887 -3.13701

D22 1.05153 0.00087 0.00000 -0.02460 -0.02386 1.02767

D23 0.92411 0.00013 0.00000 -0.03612 -0.03681 0.88729

D24 -1.00734 0.00174 0.00000 -0.02015 -0.02047 -1.02780

D25 -3.14086 0.00123 0.00000 -0.00452 -0.00545 3.13688

D26 2.98611 -0.00022 0.00000 -0.04288 -0.04288 2.94323

D27 1.05466 0.00140 0.00000 -0.02691 -0.02653 1.02813

D28 -1.07886 0.00088 0.00000 -0.01128 -0.01152 -1.09037

D29 0.57169 -0.00041 0.00000 0.05481 0.05370 0.62538

D30 -2.76487 -0.00008 0.00000 0.10017 0.09918 -2.66570

D31 -2.94417 -0.00018 0.00000 -0.01608 -0.01731 -2.96148

D32 0.00246 0.00015 0.00000 0.02927 0.02817 0.03063

D33 -1.18303 0.00073 0.00000 0.01429 0.01470 -1.16833

D34 1.76360 0.00106 0.00000 0.05964 0.06018 1.82377

D35 -0.48252 0.00000 0.00000 -0.17333 -0.17232 -0.65484

D36 -2.63866 0.00009 0.00000 -0.18580 -0.18402 -2.82268

D37 1.63358 0.00024 0.00000 -0.19100 -0.19023 1.44335

D38 3.02617 -0.00066 0.00000 -0.11419 -0.11518 2.91099

D39 0.87003 -0.00057 0.00000 -0.12666 -0.12689 0.74314

D40 -1.14091 -0.00042 0.00000 -0.13186 -0.13310 -1.27401

D41 1.24795 -0.00113 0.00000 -0.14655 -0.14710 1.10085

D42 -0.90819 -0.00103 0.00000 -0.15902 -0.15880 -1.06699

D43 -2.91913 -0.00089 0.00000 -0.16422 -0.16502 -3.08415

D44 0.91443 0.00105 0.00000 -0.07110 -0.07109 0.84335

D45 2.89484 -0.00211 0.00000 -0.09346 -0.09423 2.80061

D46 -1.30785 0.00019 0.00000 -0.07124 -0.07154 -1.37940

D47 -1.21511 0.00149 0.00000 -0.03600 -0.03449 -1.24959

D48 0.76530 -0.00167 0.00000 -0.05837 -0.05763 0.70767

D49 2.84579 0.00063 0.00000 -0.03614 -0.03494 2.81085

D50 3.00477 0.00234 0.00000 -0.03088 -0.03062 2.97415

D51 -1.29801 -0.00082 0.00000 -0.05325 -0.05376 -1.35177

D52 0.78248 0.00149 0.00000 -0.03102 -0.03107 0.75141

D53 -0.10994 0.00002 0.00000 0.20511 0.20548 0.09555

D54 2.05091 -0.00013 0.00000 0.21413 0.21365 2.26456

D55 -2.21477 0.00004 0.00000 0.23229 0.23289 -1.98188

D56 -2.29103 0.00038 0.00000 0.22619 0.22698 -2.06405

D57 -0.13018 0.00024 0.00000 0.23521 0.23514 0.10496

D58 1.88732 0.00041 0.00000 0.25337 0.25438 2.14170

D59 1.94871 0.00056 0.00000 0.24843 0.24857 2.19728

D60 -2.17363 0.00042 0.00000 0.25745 0.25674 -1.91689

D61 -0.15613 0.00059 0.00000 0.27561 0.27597 0.11985

D62 0.02211 0.00006 0.00000 -0.01627 -0.01568 0.00643

D63 -3.10993 -0.00061 0.00000 -0.04307 -0.04289 3.13036

D64 -0.03359 0.00021 0.00000 0.05632 0.05608 0.02249

D65 3.08148 0.00048 0.00000 0.08443 0.08235 -3.11936

D66 0.14174 -0.00068 0.00000 0.06723 0.06737 0.20911

D67 1.93247 -0.00050 0.00000 0.04695 0.04670 1.97917

D68 -1.68981 -0.00037 0.00000 0.05742 0.05767 -1.63214

D69 -1.80931 0.00030 0.00000 0.08551 0.08481 -1.72450

D70 -0.01858 0.00048 0.00000 0.06523 0.06414 0.04555

D71 2.64232 0.00062 0.00000 0.07570 0.07511 2.71743

D72 1.89391 -0.00087 0.00000 0.07675 0.07652 1.97043

D73 -2.59854 -0.00070 0.00000 0.05647 0.05585 -2.54269

D74 0.06236 -0.00056 0.00000 0.06695 0.06682 0.12918

D75 -1.95678 -0.00094 0.00000 -0.07047 -0.07043 -2.02722

D76 1.17266 -0.00012 0.00000 -0.03631 -0.03592 1.13674

D77 -0.00151 -0.00032 0.00000 -0.03206 -0.03247 -0.03397

D78 3.12794 0.00051 0.00000 0.00210 0.00205 3.12998

D79 2.62881 0.00030 0.00000 -0.03470 -0.03526 2.59356

D80 -0.52493 0.00113 0.00000 -0.00054 -0.00075 -0.52567

D81 1.98105 -0.00073 0.00000 -0.13160 -0.13344 1.84761

D82 -1.12776 -0.00088 0.00000 -0.16490 -0.16590 -1.29366

D83 0.03253 -0.00031 0.00000 -0.07575 -0.07692 -0.04439

D84 -3.07628 -0.00046 0.00000 -0.10905 -0.10938 3.09753

D85 -2.64280 -0.00074 0.00000 -0.10282 -0.10394 -2.74673

D86 0.53158 -0.00089 0.00000 -0.13612 -0.13640 0.39518

Item Value Threshold Converged?

Maximum Force 0.008023 0.000450 NO

RMS Force 0.001856 0.000300 NO

Maximum Displacement 0.449383 0.001800 NO

RMS Displacement 0.097448 0.001200 NO

Predicted change in Energy=-4.016374D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.091381 1.514559 0.429152

2 6 0 0.252095 1.324208 0.072542

3 6 0 -0.818273 3.780666 -0.327682

4 6 0 -1.628996 2.784648 0.227500

5 1 0 -1.647571 0.753735 0.996732

6 1 0 -2.622855 3.033888 0.628310

7 6 0 0.821033 2.044544 -1.095753

8 1 0 1.930176 2.177406 -0.960148

9 1 0 0.698654 1.376125 -1.993539

10 6 0 0.174478 3.392435 -1.369361

11 1 0 0.959603 4.188100 -1.481514

12 1 0 -0.375582 3.346741 -2.351231

13 1 0 -1.150110 4.832666 -0.345878

14 1 0 0.796889 0.414606 0.377576

15 8 0 2.821500 3.679573 0.857724

16 6 0 0.502030 3.902489 1.349817

17 6 0 0.891993 2.599995 1.709282

18 6 0 1.730140 4.554776 0.789144

19 8 0 1.974258 5.655125 0.321000

20 6 0 2.353490 2.484199 1.430733

21 8 0 3.201063 1.619309 1.582049

22 1 0 -0.262507 4.506064 1.848572

23 1 0 0.413473 1.967148 2.459429

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.402972 0.000000

3 C 2.404709 2.709253 0.000000

4 C 1.393850 2.386503 1.399125 0.000000

5 H 1.100158 2.188217 3.406482 2.171790 0.000000

6 H 2.166435 3.390755 2.174423 1.100239 2.507192

7 C 2.502708 1.485762 2.508262 2.881214 3.484062

8 H 3.391065 2.147173 3.244137 3.800915 4.319316

9 H 3.015430 2.114427 3.295142 3.512108 3.851475

10 C 2.891966 2.522434 1.490426 2.484328 3.985097

11 H 3.873628 3.334297 2.158280 3.404592 4.973321

12 H 3.405847 3.218586 2.116368 2.921789 4.421594

13 H 3.407925 3.801386 1.103246 2.180017 4.322933

14 H 2.185891 1.103278 3.799539 3.394781 2.544356

15 O 4.492393 3.572968 3.829276 4.583120 5.343449

16 C 3.014762 2.888154 2.138234 2.655266 3.828852

17 C 2.598206 2.171640 2.910019 2.930044 3.219594

18 C 4.163351 3.624184 2.888071 3.838306 5.089198

19 O 5.153069 4.667378 3.425290 4.607800 6.131711

20 C 3.716248 2.757920 3.851354 4.171119 4.380793

21 O 4.445808 3.325975 4.947079 5.149979 4.959945

22 H 3.413339 3.680123 2.360331 2.731015 4.089500

23 H 2.567381 2.477225 3.545988 3.133926 2.803526

6 7 8 9 10

6 H 0.000000

7 C 3.976376 0.000000

8 H 4.897637 1.125273 0.000000

9 H 4.544743 1.125957 1.796273 0.000000

10 C 3.456055 1.519772 2.173988 2.174825 0.000000

11 H 4.314808 2.182394 2.292754 2.870098 1.123424

12 H 3.745101 2.168832 2.935809 2.272719 1.126376

13 H 2.520639 3.495904 4.112894 4.252104 2.208238

14 H 4.314877 2.197266 2.486224 2.560539 3.508084

15 O 5.487308 3.239022 2.521036 4.235806 3.471179

16 C 3.322642 3.087805 3.217367 4.195141 2.785924

17 C 3.702826 2.860381 2.895213 3.904628 3.258961

18 C 4.613842 3.268115 2.958365 4.348691 2.903491

19 O 5.300827 4.046407 3.706455 5.029324 3.349073

20 C 5.070508 2.987449 2.447372 3.961307 3.662446

21 O 6.068663 3.607767 2.896444 4.371043 4.584213

22 H 3.037694 3.987755 4.256690 5.047986 3.433106

23 H 3.702731 3.579304 3.746745 4.501062 4.092455

11 12 13 14 15

11 H 0.000000

12 H 1.801946 0.000000

13 H 2.481133 2.613295 0.000000

14 H 4.209744 4.173547 4.881951 0.000000

15 O 3.032704 4.541971 4.307199 3.871641 0.000000

16 C 2.882253 3.844063 2.543654 3.632840 2.381552

17 C 3.564803 4.318812 3.657688 2.560939 2.369312

18 C 2.425709 3.969303 3.108269 4.263960 1.400625

19 O 2.535891 4.241603 3.298915 5.371447 2.215558

20 C 3.650668 4.742896 4.576773 2.795597 1.405807

21 O 4.583475 5.589910 5.742409 2.946542 2.216620

22 H 3.561478 4.358344 2.389585 4.475062 3.343047

23 H 4.556524 5.066393 4.304152 2.625168 3.361019

16 17 18 19 20

16 C 0.000000

17 C 1.406334 0.000000

18 C 1.499362 2.317394 0.000000

19 O 2.509512 3.525967 1.220459 0.000000

20 C 2.333666 1.492304 2.255547 3.380842 0.000000

21 O 3.542827 2.511919 3.377763 4.402625 1.220374

22 H 1.094338 2.232794 2.257299 2.942267 3.332561

23 H 2.232627 1.091878 3.349519 4.539835 2.255930

21 22 23

21 O 0.000000

22 H 4.516714 0.000000

23 H 2.943033 2.697441 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.188575 -1.052745 -0.488032

2 6 0 1.152674 -1.387074 0.397103

3 6 0 1.563318 1.240160 -0.121608

4 6 0 2.384902 0.301187 -0.754760

5 1 0 2.711268 -1.821769 -1.076030

6 1 0 3.074979 0.612597 -1.553098

7 6 0 0.831282 -0.491802 1.538454

8 1 0 -0.249199 -0.614057 1.828028

9 1 0 1.429281 -0.848952 2.423112

10 6 0 1.128005 0.975992 1.279137

11 1 0 0.236876 1.608085 1.540725

12 1 0 1.964931 1.309598 1.955144

13 1 0 1.573941 2.298826 -0.431876

14 1 0 0.814465 -2.431532 0.506397

15 8 0 -2.080584 0.127506 0.262226

16 6 0 -0.221140 0.639454 -1.134972

17 6 0 -0.328494 -0.760896 -1.062371

18 6 0 -1.320325 1.177268 -0.268581

19 8 0 -1.690495 2.297489 0.043827

20 6 0 -1.517592 -1.068996 -0.214969

21 8 0 -2.089149 -2.085916 0.143511

22 1 0 0.130741 1.214044 -1.997295

23 1 0 0.027327 -1.474760 -1.808016

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2343529 0.8808269 0.6773821

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 471.1734289636 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.485358736228E-01 A.U. after 16 cycles

Convg = 0.7510D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.005252106 0.002662463 -0.003062888

2 6 -0.004902038 -0.000726708 0.008158729

3 6 0.003856559 -0.001373594 0.001039835

4 6 -0.004246118 -0.000113247 0.000872901

5 1 0.001151354 0.000198391 -0.001014728

6 1 0.000402018 0.000282690 0.000288946

7 6 0.003591996 -0.000336763 -0.002142533

8 1 0.000212955 -0.000008096 0.000110940

9 1 -0.000771477 0.000498829 -0.000562287

10 6 -0.002005746 -0.000067511 -0.001078758

11 1 0.000027143 -0.000235619 -0.000076830

12 1 0.000387735 0.000133458 -0.000324038

13 1 -0.000250080 -0.001206513 0.000189199

14 1 -0.001470383 -0.000186182 0.000342602

15 8 -0.002591222 -0.001965902 0.000739104

16 6 0.001785379 0.007883883 -0.005021958

17 6 0.006939435 -0.009753081 -0.003719759

18 6 -0.007054912 0.010118108 0.001576930

19 8 -0.001677281 0.003993585 -0.001432354

20 6 -0.000100360 -0.005947793 0.002675530

21 8 -0.000917476 -0.003992228 0.001441798

22 1 0.001482147 0.000195777 0.000592776

23 1 0.000898265 -0.000053947 0.000406840

-------------------------------------------------------------------

Cartesian Forces: Max 0.010118108 RMS 0.003189608

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.010294617 RMS 0.001977389

Search for a saddle point.

Step number 62 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 47 49 61 62

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0

Eigenvalues --- -0.07348 -0.00001 0.00329 0.00792 0.00816

Eigenvalues --- 0.00963 0.01225 0.01356 0.01858 0.02435

Eigenvalues --- 0.02694 0.02818 0.03077 0.03314 0.03330

Eigenvalues --- 0.03568 0.03613 0.03804 0.03935 0.04140

Eigenvalues --- 0.04401 0.04666 0.04786 0.04985 0.06166

Eigenvalues --- 0.06468 0.06619 0.07119 0.07428 0.08491

Eigenvalues --- 0.09225 0.10018 0.10137 0.10377 0.10909

Eigenvalues --- 0.12703 0.13842 0.14816 0.17098 0.22689

Eigenvalues --- 0.26203 0.28425 0.29588 0.30035 0.31081

Eigenvalues --- 0.31380 0.31796 0.32012 0.32203 0.32479

Eigenvalues --- 0.33376 0.34218 0.36803 0.37855 0.39740

Eigenvalues --- 0.40243 0.40613 0.44435 0.48683 0.53042

Eigenvalues --- 0.61800 1.08656 1.11179

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D30

1 0.55984 0.52119 -0.16312 0.14325 -0.13965

R19 D79 D29 D1 D35

1 -0.13824 0.13414 -0.13340 0.12583 0.12540

RFO step: Lambda0=2.578356300D-04 Lambda=-2.86017519D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.06566081 RMS(Int)= 0.00151428

Iteration 2 RMS(Cart)= 0.00207339 RMS(Int)= 0.00056640

Iteration 3 RMS(Cart)= 0.00000129 RMS(Int)= 0.00056640

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00056640

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65123 -0.00513 0.00000 -0.01688 -0.01665 2.63459

R2 2.63400 -0.00075 0.00000 0.00505 0.00556 2.63956

R3 2.07900 -0.00124 0.00000 -0.00142 -0.00142 2.07758

R4 2.80768 0.00350 0.00000 0.00791 0.00785 2.81554

R5 2.08489 -0.00048 0.00000 -0.00178 -0.00178 2.08311

R6 4.10380 -0.00290 0.00000 0.00420 0.00415 4.10796

R7 2.64396 0.00024 0.00000 -0.00833 -0.00808 2.63588

R8 2.81650 0.00097 0.00000 -0.00131 -0.00146 2.81503

R9 2.08483 -0.00108 0.00000 -0.00245 -0.00245 2.08238

R10 4.04068 -0.00084 0.00000 0.05193 0.05182 4.09250

R11 2.07915 -0.00019 0.00000 -0.00172 -0.00172 2.07743

R12 2.12646 0.00022 0.00000 -0.00202 -0.00202 2.12444

R13 2.12775 0.00024 0.00000 0.00008 0.00008 2.12783

R14 2.87195 0.00156 0.00000 0.00429 0.00402 2.87598

R15 2.12296 -0.00014 0.00000 0.00008 0.00008 2.12304

R16 2.12854 0.00009 0.00000 -0.00035 -0.00035 2.12819

R17 2.64680 0.00758 0.00000 0.01501 0.01509 2.66189

R18 2.65659 0.00627 0.00000 0.00550 0.00564 2.66223

R19 2.65759 0.01029 0.00000 0.00706 0.00667 2.66425

R20 2.83338 -0.00518 0.00000 -0.01854 -0.01863 2.81476

R21 2.06800 -0.00066 0.00000 -0.00198 -0.00198 2.06602

R22 2.82005 -0.00528 0.00000 -0.00933 -0.00933 2.81071

R23 2.06335 -0.00008 0.00000 0.00115 0.00115 2.06450

R24 2.30633 0.00381 0.00000 -0.00003 -0.00003 2.30630

R25 2.30617 0.00237 0.00000 0.00006 0.00006 2.30623

A1 2.04452 0.00300 0.00000 0.01503 0.01467 2.05919

A2 2.11931 -0.00236 0.00000 -0.01007 -0.00989 2.10942

A3 2.10575 -0.00059 0.00000 -0.00372 -0.00363 2.10211

A4 2.09529 -0.00073 0.00000 -0.00313 -0.00287 2.09242

A5 2.11115 -0.00007 0.00000 -0.00536 -0.00528 2.10587

A6 1.58168 0.00049 0.00000 0.01963 0.01894 1.60063

A7 2.01311 0.00062 0.00000 0.00501 0.00472 2.01783

A8 1.76704 0.00037 0.00000 -0.01604 -0.01648 1.75056

A9 1.70163 -0.00043 0.00000 0.00448 0.00545 1.70709

A10 2.06902 -0.00013 0.00000 0.01165 0.01192 2.08094

A11 2.10723 -0.00085 0.00000 -0.00585 -0.00607 2.10116

A12 1.65796 0.00088 0.00000 -0.02533 -0.02626 1.63170

A13 2.02328 0.00072 0.00000 0.00359 0.00338 2.02666

A14 1.72325 0.00065 0.00000 0.01581 0.01552 1.73877

A15 1.71564 -0.00096 0.00000 -0.01144 -0.01062 1.70502

A16 2.07440 -0.00134 0.00000 -0.00950 -0.00987 2.06453

A17 2.09685 0.00090 0.00000 0.00243 0.00246 2.09931

A18 2.10216 0.00044 0.00000 0.00451 0.00462 2.10678

A19 1.91763 0.00024 0.00000 0.00442 0.00450 1.92213

A20 1.87292 0.00068 0.00000 0.00086 0.00081 1.87373

A21 1.99177 -0.00098 0.00000 -0.00561 -0.00578 1.98599

A22 1.84763 0.00007 0.00000 0.00543 0.00541 1.85304

A23 1.91379 0.00085 0.00000 0.00421 0.00389 1.91768

A24 1.91422 -0.00081 0.00000 -0.00865 -0.00824 1.90599

A25 1.96987 0.00001 0.00000 0.00690 0.00652 1.97639

A26 1.92921 0.00002 0.00000 -0.00249 -0.00236 1.92686

A27 1.86977 0.00032 0.00000 0.00203 0.00214 1.87191

A28 1.92709 0.00021 0.00000 -0.00525 -0.00547 1.92162

A29 1.90574 -0.00045 0.00000 -0.00156 -0.00112 1.90462

A30 1.85771 -0.00013 0.00000 0.00023 0.00016 1.85788

A31 1.86699 0.00639 0.00000 0.01466 0.01460 1.88160

A32 1.89545 -0.00225 0.00000 -0.01002 -0.01242 1.88303

A33 1.81026 -0.00051 0.00000 -0.03391 -0.03262 1.77764

A34 1.52838 0.00182 0.00000 0.01373 0.01467 1.54304

A35 1.84562 0.00348 0.00000 0.01649 0.01672 1.86234

A36 2.19944 -0.00083 0.00000 -0.00068 -0.00078 2.19866

A37 2.09754 -0.00249 0.00000 -0.00179 -0.00214 2.09540

A38 1.84393 0.00018 0.00000 0.02304 0.02060 1.86453

A39 1.67329 -0.00001 0.00000 0.03770 0.03841 1.71170

A40 1.61898 -0.00013 0.00000 -0.03367 -0.03262 1.58636

A41 1.87101 0.00164 0.00000 -0.00086 -0.00103 1.86998

A42 2.20295 -0.00073 0.00000 -0.00636 -0.00641 2.19653

A43 2.10886 -0.00095 0.00000 -0.00229 -0.00215 2.10670

A44 1.92631 -0.00654 0.00000 -0.01918 -0.01947 1.90685

A45 2.01119 0.00614 0.00000 0.01143 0.01153 2.02272

A46 2.34549 0.00041 0.00000 0.00801 0.00811 2.35360

A47 1.91361 -0.00497 0.00000 -0.00971 -0.00985 1.90376

A48 2.00639 0.00667 0.00000 0.01871 0.01878 2.02517

A49 2.36318 -0.00169 0.00000 -0.00900 -0.00894 2.35425

D1 -0.59866 -0.00022 0.00000 0.00171 0.00153 -0.59713

D2 2.93599 0.00019 0.00000 0.01091 0.01046 2.94644

D3 1.20584 0.00040 0.00000 -0.00572 -0.00681 1.19903

D4 2.71838 -0.00046 0.00000 -0.00593 -0.00566 2.71272

D5 -0.03016 -0.00006 0.00000 0.00327 0.00326 -0.02689

D6 -1.76031 0.00015 0.00000 -0.01336 -0.01400 -1.77431

D7 0.01473 0.00022 0.00000 0.00256 0.00254 0.01726

D8 -2.97785 0.00023 0.00000 0.02155 0.02197 -2.95588

D9 2.98231 0.00026 0.00000 0.00945 0.00903 2.99133

D10 -0.01026 0.00028 0.00000 0.02844 0.02845 0.01819

D11 2.67492 0.00015 0.00000 0.01639 0.01609 2.69102

D12 -1.60727 0.00073 0.00000 0.02550 0.02524 -1.58202

D13 0.51739 -0.00045 0.00000 0.01151 0.01172 0.52910

D14 -0.83861 -0.00036 0.00000 0.00555 0.00553 -0.83307

D15 1.16239 0.00022 0.00000 0.01466 0.01468 1.17707

D16 -2.99614 -0.00096 0.00000 0.00068 0.00115 -2.99498

D17 0.97593 -0.00046 0.00000 0.00370 0.00443 0.98036

D18 2.97693 0.00012 0.00000 0.01282 0.01357 2.99051

D19 -1.18160 -0.00105 0.00000 -0.00117 0.00005 -1.18155

D20 -1.22191 0.00146 0.00000 0.09905 0.10000 -1.12192

D21 -3.13701 -0.00031 0.00000 0.08252 0.08254 -3.05447

D22 1.02767 0.00067 0.00000 0.08539 0.08573 1.11340

D23 0.88729 0.00087 0.00000 0.09839 0.09921 0.98650

D24 -1.02780 -0.00090 0.00000 0.08187 0.08175 -0.94605

D25 3.13688 0.00008 0.00000 0.08474 0.08495 -3.06136

D26 2.94323 0.00149 0.00000 0.10091 0.10156 3.04479

D27 1.02813 -0.00028 0.00000 0.08438 0.08411 1.11224

D28 -1.09037 0.00070 0.00000 0.08725 0.08730 -1.00307

D29 0.62538 0.00039 0.00000 -0.01977 -0.01958 0.60580

D30 -2.66570 0.00041 0.00000 -0.03901 -0.03929 -2.70499

D31 -2.96148 -0.00007 0.00000 0.00488 0.00529 -2.95618

D32 0.03063 -0.00004 0.00000 -0.01436 -0.01442 0.01621

D33 -1.16833 -0.00084 0.00000 -0.02592 -0.02469 -1.19302

D34 1.82377 -0.00082 0.00000 -0.04516 -0.04440 1.77937

D35 -0.65484 -0.00019 0.00000 0.03308 0.03298 -0.62185

D36 -2.82268 -0.00049 0.00000 0.03677 0.03717 -2.78552

D37 1.44335 -0.00053 0.00000 0.03665 0.03700 1.48035

D38 2.91099 0.00063 0.00000 0.01212 0.01165 2.92264

D39 0.74314 0.00033 0.00000 0.01581 0.01584 0.75898

D40 -1.27401 0.00029 0.00000 0.01569 0.01566 -1.25834

D41 1.10085 0.00118 0.00000 0.01572 0.01448 1.11534

D42 -1.06699 0.00088 0.00000 0.01941 0.01867 -1.04833

D43 -3.08415 0.00084 0.00000 0.01929 0.01850 -3.06565

D44 0.84335 -0.00008 0.00000 0.10696 0.10629 0.94963

D45 2.80061 0.00272 0.00000 0.10587 0.10568 2.90629

D46 -1.37940 0.00056 0.00000 0.10436 0.10401 -1.27538

D47 -1.24959 -0.00026 0.00000 0.09774 0.09727 -1.15232

D48 0.70767 0.00253 0.00000 0.09665 0.09667 0.80433

D49 2.81085 0.00038 0.00000 0.09514 0.09500 2.90585

D50 2.97415 -0.00094 0.00000 0.09297 0.09268 3.06684

D51 -1.35177 0.00186 0.00000 0.09188 0.09207 -1.25969

D52 0.75141 -0.00030 0.00000 0.09037 0.09041 0.84182

D53 0.09555 0.00021 0.00000 -0.03142 -0.03141 0.06413

D54 2.26456 0.00040 0.00000 -0.03361 -0.03390 2.23066

D55 -1.98188 0.00010 0.00000 -0.03728 -0.03749 -2.01938

D56 -2.06405 -0.00007 0.00000 -0.03642 -0.03613 -2.10019

D57 0.10496 0.00013 0.00000 -0.03860 -0.03862 0.06634

D58 2.14170 -0.00017 0.00000 -0.04227 -0.04221 2.09949

D59 2.19728 -0.00018 0.00000 -0.04043 -0.04015 2.15713

D60 -1.91689 0.00001 0.00000 -0.04261 -0.04264 -1.95953

D61 0.11985 -0.00028 0.00000 -0.04628 -0.04623 0.07361

D62 0.00643 -0.00014 0.00000 -0.01077 -0.01014 -0.00370

D63 3.13036 0.00046 0.00000 0.00169 0.00244 3.13280

D64 0.02249 0.00008 0.00000 -0.00660 -0.00710 0.01538

D65 -3.11936 0.00023 0.00000 -0.00290 -0.00370 -3.12305

D66 0.20911 -0.00047 0.00000 -0.11181 -0.11184 0.09727

D67 1.97917 0.00015 0.00000 -0.06194 -0.06168 1.91749

D68 -1.63214 -0.00009 0.00000 -0.08304 -0.08234 -1.71448

D69 -1.72450 -0.00055 0.00000 -0.07659 -0.07706 -1.80156

D70 0.04555 0.00007 0.00000 -0.02672 -0.02690 0.01865

D71 2.71743 -0.00017 0.00000 -0.04782 -0.04756 2.66986

D72 1.97043 -0.00027 0.00000 -0.10199 -0.10277 1.86766

D73 -2.54269 0.00035 0.00000 -0.05212 -0.05261 -2.59531

D74 0.12918 0.00011 0.00000 -0.07322 -0.07327 0.05590

D75 -2.02722 0.00159 0.00000 0.04341 0.04516 -1.98206

D76 1.13674 0.00077 0.00000 0.02769 0.02925 1.16599

D77 -0.03397 0.00024 0.00000 0.02458 0.02409 -0.00989

D78 3.12998 -0.00057 0.00000 0.00885 0.00818 3.13816

D79 2.59356 0.00047 0.00000 0.04811 0.04798 2.64154

D80 -0.52567 -0.00035 0.00000 0.03238 0.03208 -0.49360

D81 1.84761 0.00071 0.00000 0.06064 0.05881 1.90642

D82 -1.29366 0.00051 0.00000 0.05585 0.05449 -1.23917

D83 -0.04439 0.00017 0.00000 0.02263 0.02268 -0.02170

D84 3.09753 -0.00003 0.00000 0.01784 0.01836 3.11589

D85 -2.74673 0.00038 0.00000 0.04370 0.04347 -2.70327

D86 0.39518 0.00018 0.00000 0.03892 0.03914 0.43432

Item Value Threshold Converged?

Maximum Force 0.010295 0.000450 NO

RMS Force 0.001977 0.000300 NO

Maximum Displacement 0.252722 0.001800 NO

RMS Displacement 0.065658 0.001200 NO

Predicted change in Energy=-1.676390D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.114504 1.540720 0.432408

2 6 0 0.214419 1.298286 0.087616

3 6 0 -0.786274 3.779372 -0.357530

4 6 0 -1.625353 2.822024 0.212585

5 1 0 -1.692451 0.801295 1.005054

6 1 0 -2.603414 3.107235 0.625595

7 6 0 0.811602 1.982356 -1.093601

8 1 0 1.925734 2.066795 -0.969443

9 1 0 0.645102 1.317144 -1.986709

10 6 0 0.216732 3.354869 -1.373815

11 1 0 1.034863 4.119988 -1.459997

12 1 0 -0.306425 3.333729 -2.370890

13 1 0 -1.088346 4.838699 -0.387055

14 1 0 0.717263 0.370239 0.405458

15 8 0 2.791260 3.776307 0.854742

16 6 0 0.491351 3.890862 1.387554

17 6 0 0.931894 2.585251 1.685904

18 6 0 1.670639 4.629768 0.856588

19 8 0 1.863578 5.763629 0.448405

20 6 0 2.383020 2.528086 1.364622

21 8 0 3.250684 1.673956 1.448314

22 1 0 -0.308206 4.431834 1.900719

23 1 0 0.500432 1.920559 2.437934

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394164 0.000000

3 C 2.396519 2.712072 0.000000

4 C 1.396793 2.392103 1.394847 0.000000

5 H 1.099407 2.173671 3.398049 2.171602 0.000000

6 H 2.169826 3.391446 2.172626 1.099330 2.508227

7 C 2.496724 1.489917 2.514812 2.889622 3.474124

8 H 3.388951 2.153271 3.265325 3.818086 4.311774

9 H 2.999721 2.118648 3.281102 3.500932 3.831566

10 C 2.885441 2.522959 1.489651 2.488748 3.978032

11 H 3.854037 3.321180 2.155921 3.399851 4.952620

12 H 3.424377 3.233970 2.117185 2.945464 4.441992

13 H 3.398363 3.802241 1.101949 2.171387 4.313182

14 H 2.173965 1.102337 3.803283 3.396513 2.520327

15 O 4.520089 3.656388 3.777349 4.563933 5.383025

16 C 3.002372 2.913413 2.165658 2.646394 3.802725

17 C 2.617258 2.173838 2.924662 2.960784 3.245496

18 C 4.180810 3.716270 2.869439 3.813953 5.098002

19 O 5.167416 4.773801 3.407129 4.569605 6.130249

20 C 3.751878 2.801067 3.817846 4.180985 4.440784

21 O 4.483824 3.348362 4.898049 5.159537 5.039107

22 H 3.341346 3.657814 2.398738 2.678835 3.987375

23 H 2.602773 2.448064 3.595194 3.206833 2.848619

6 7 8 9 10

6 H 0.000000

7 C 3.985389 0.000000

8 H 4.913232 1.124204 0.000000

9 H 4.536675 1.125998 1.799118 0.000000

10 C 3.465861 1.521901 2.177921 2.170591 0.000000

11 H 4.314212 2.180267 2.291265 2.878415 1.123464

12 H 3.782378 2.169715 2.924331 2.262656 1.126188

13 H 2.513734 3.502529 4.136098 4.238524 2.208773

14 H 4.308887 2.203406 2.495807 2.573771 3.510607

15 O 5.440834 3.306561 2.645603 4.327508 3.431074

16 C 3.282107 3.146598 3.307583 4.246565 2.826280

17 C 3.727617 2.846682 2.882253 3.895951 3.235065

18 C 4.543016 3.398525 3.157260 4.484367 2.951933

19 O 5.200178 4.216926 3.959891 5.213990 3.440161

20 C 5.074061 2.968170 2.422758 3.964614 3.588232

21 O 6.082896 3.536320 2.784845 4.326171 4.471548

22 H 2.940830 4.027390 4.338402 5.071705 3.486831

23 H 3.785054 3.545755 3.696361 4.467942 4.082543

11 12 13 14 15

11 H 0.000000

12 H 1.801939 0.000000

13 H 2.485109 2.609969 0.000000

14 H 4.200168 4.187877 4.884203 0.000000

15 O 2.925930 4.494022 4.209760 4.013056 0.000000

16 C 2.907998 3.882363 2.557943 3.662012 2.363597

17 C 3.501816 4.307114 3.668318 2.567467 2.359383

18 C 2.455739 4.000640 3.033529 4.388169 1.408613

19 O 2.651476 4.308336 3.204270 5.514031 2.230504

20 C 3.511432 4.672925 4.523017 2.889817 1.408792

21 O 4.399001 5.476695 5.675505 3.034048 2.232326

22 H 3.632561 4.410497 2.451136 4.447915 3.336236

23 H 4.507435 5.076697 4.361229 2.565437 3.346370

16 17 18 19 20

16 C 0.000000

17 C 1.409861 0.000000

18 C 1.489506 2.326705 0.000000

19 O 2.504449 3.535749 1.220442 0.000000

20 C 2.331543 1.487365 2.276544 3.402647 0.000000

21 O 3.540096 2.502737 3.403455 4.432753 1.220403

22 H 1.093290 2.234695 2.246156 2.932497 3.339813

23 H 2.232818 1.092486 3.348112 4.537133 2.250605

21 22 23

21 O 0.000000

22 H 4.525070 0.000000

23 H 2.933265 2.692396 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.252762 -0.867087 -0.599519

2 6 0 1.275387 -1.382212 0.250819

3 6 0 1.468423 1.312633 0.014433

4 6 0 2.343904 0.520743 -0.728563

5 1 0 2.823588 -1.527367 -1.268013

6 1 0 2.974891 0.964389 -1.511864

7 6 0 0.906314 -0.643805 1.491139

8 1 0 -0.145891 -0.898325 1.794321

9 1 0 1.571001 -1.022014 2.317589

10 6 0 1.060697 0.865842 1.375755

11 1 0 0.109388 1.376138 1.686852

12 1 0 1.857160 1.211224 2.093152

13 1 0 1.387622 2.393188 -0.185979

14 1 0 1.040032 -2.459130 0.249483

15 8 0 -2.085320 0.058085 0.270144

16 6 0 -0.270018 0.678431 -1.110595

17 6 0 -0.316757 -0.730277 -1.077950

18 6 0 -1.384898 1.163842 -0.250336

19 8 0 -1.803052 2.262320 0.078256

20 6 0 -1.472111 -1.110855 -0.222044

21 8 0 -1.977259 -2.166780 0.123252

22 1 0 0.084366 1.290088 -1.944604

23 1 0 0.040676 -1.400717 -1.862984

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2219044 0.8778673 0.6739205

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.4020661526 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.501370657628E-01 A.U. after 16 cycles

Convg = 0.3036D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000364550 0.000697691 -0.000506309

2 6 0.000129631 -0.000079711 0.000206198

3 6 0.000350216 -0.000620537 -0.000246155

4 6 -0.000640738 0.000049191 0.000510136

5 1 0.000119477 0.000035766 0.000185816

6 1 -0.000238736 0.000011890 -0.000110856

7 6 0.000819082 -0.000203198 -0.000154766

8 1 0.000147435 -0.000068790 0.000133211

9 1 -0.000222011 0.000028430 -0.000054506

10 6 -0.000092350 -0.000280905 0.000426037

11 1 0.000079864 0.000116538 0.000293833

12 1 0.000127323 0.000199048 -0.000107673

13 1 0.000220420 0.000076427 -0.000100479

14 1 -0.000163994 -0.000011796 0.000362350

15 8 -0.000146168 -0.000245722 -0.000255655

16 6 -0.000165699 0.000939999 0.000485951

17 6 0.000299259 -0.000801705 -0.000698507

18 6 -0.000727282 0.001331169 -0.000344255

19 8 -0.000320681 0.000691079 -0.000130140

20 6 0.000212704 -0.000759893 0.000256811

21 8 0.000118752 -0.000649570 0.000000989

22 1 0.000080480 -0.000248726 -0.000004284

23 1 0.000377566 -0.000206674 -0.000147745

-------------------------------------------------------------------

Cartesian Forces: Max 0.001331169 RMS 0.000394401

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.001125280 RMS 0.000299232

Search for a saddle point.

Step number 63 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

42 47 49 50 51

52 56 57 58 59

62 63

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0

Eigenvalues --- -0.07397 0.00201 0.00260 0.00733 0.00810

Eigenvalues --- 0.00957 0.01193 0.01319 0.01847 0.02431

Eigenvalues --- 0.02697 0.02810 0.03060 0.03329 0.03347

Eigenvalues --- 0.03567 0.03617 0.03807 0.03946 0.04142

Eigenvalues --- 0.04411 0.04689 0.04790 0.04947 0.06161

Eigenvalues --- 0.06476 0.06630 0.07068 0.07404 0.08503

Eigenvalues --- 0.09235 0.10006 0.10147 0.10345 0.10912

Eigenvalues --- 0.12698 0.13844 0.14825 0.17012 0.22678

Eigenvalues --- 0.26199 0.28419 0.29597 0.30035 0.31082

Eigenvalues --- 0.31386 0.31798 0.32013 0.32197 0.32479

Eigenvalues --- 0.33362 0.34196 0.36817 0.37873 0.39740

Eigenvalues --- 0.40232 0.40612 0.44458 0.48705 0.53136

Eigenvalues --- 0.61858 1.08654 1.11177

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D30

1 0.56485 0.51813 -0.15605 0.14597 -0.14046

R19 D79 D29 D1 D4

1 -0.13833 0.13322 -0.13217 0.13040 0.12653

RFO step: Lambda0=1.961777113D-06 Lambda=-4.68974122D-04.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.05111603 RMS(Int)= 0.00088580

Iteration 2 RMS(Cart)= 0.00119868 RMS(Int)= 0.00029887

Iteration 3 RMS(Cart)= 0.00000038 RMS(Int)= 0.00029887

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63459 0.00053 0.00000 0.00136 0.00147 2.63606

R2 2.63956 -0.00010 0.00000 -0.00038 -0.00020 2.63935

R3 2.07758 0.00001 0.00000 0.00033 0.00033 2.07790

R4 2.81554 0.00005 0.00000 -0.00095 -0.00098 2.81455

R5 2.08311 0.00004 0.00000 0.00018 0.00018 2.08330

R6 4.10796 -0.00067 0.00000 -0.01121 -0.01127 4.09669

R7 2.63588 0.00030 0.00000 -0.00117 -0.00111 2.63477

R8 2.81503 -0.00005 0.00000 0.00036 0.00037 2.81540

R9 2.08238 0.00002 0.00000 0.00071 0.00071 2.08310

R10 4.09250 -0.00029 0.00000 0.00337 0.00334 4.09584

R11 2.07743 0.00017 0.00000 0.00043 0.00043 2.07787

R12 2.12444 0.00016 0.00000 -0.00002 -0.00002 2.12442

R13 2.12783 0.00006 0.00000 0.00026 0.00026 2.12809

R14 2.87598 0.00013 0.00000 -0.00026 -0.00027 2.87570

R15 2.12304 0.00011 0.00000 0.00036 0.00036 2.12340

R16 2.12819 0.00003 0.00000 -0.00013 -0.00013 2.12806

R17 2.66189 0.00113 0.00000 0.00058 0.00062 2.66252

R18 2.66223 0.00107 0.00000 0.00052 0.00057 2.66280

R19 2.66425 0.00093 0.00000 -0.00091 -0.00113 2.66312

R20 2.81476 -0.00017 0.00000 -0.00080 -0.00082 2.81393

R21 2.06602 -0.00018 0.00000 -0.00130 -0.00130 2.06472

R22 2.81071 -0.00009 0.00000 0.00225 0.00225 2.81296

R23 2.06450 -0.00013 0.00000 0.00012 0.00012 2.06462

R24 2.30630 0.00063 0.00000 0.00013 0.00013 2.30643

R25 2.30623 0.00054 0.00000 0.00023 0.00023 2.30645

A1 2.05919 0.00028 0.00000 0.00197 0.00180 2.06099

A2 2.10942 -0.00020 0.00000 -0.00028 -0.00019 2.10923

A3 2.10211 -0.00009 0.00000 -0.00154 -0.00149 2.10062

A4 2.09242 0.00008 0.00000 -0.00103 -0.00095 2.09147

A5 2.10587 -0.00001 0.00000 -0.00191 -0.00189 2.10398

A6 1.60063 0.00034 0.00000 0.01532 0.01501 1.61564

A7 2.01783 0.00000 0.00000 0.00130 0.00125 2.01908

A8 1.75056 -0.00048 0.00000 -0.00976 -0.01009 1.74047

A9 1.70709 -0.00005 0.00000 -0.00192 -0.00142 1.70567

A10 2.08094 0.00019 0.00000 0.00514 0.00520 2.08613

A11 2.10116 -0.00016 0.00000 0.00112 0.00118 2.10234

A12 1.63170 0.00054 0.00000 -0.01274 -0.01306 1.61864

A13 2.02666 0.00002 0.00000 -0.00442 -0.00448 2.02218

A14 1.73877 -0.00056 0.00000 0.00624 0.00594 1.74472

A15 1.70502 -0.00010 0.00000 0.00249 0.00299 1.70801

A16 2.06453 -0.00036 0.00000 -0.00228 -0.00250 2.06203

A17 2.09931 0.00021 0.00000 0.00141 0.00147 2.10078

A18 2.10678 0.00016 0.00000 0.00076 0.00087 2.10765

A19 1.92213 -0.00010 0.00000 0.00091 0.00102 1.92316

A20 1.87373 0.00019 0.00000 -0.00042 -0.00035 1.87338

A21 1.98599 -0.00029 0.00000 -0.00332 -0.00364 1.98235

A22 1.85304 0.00003 0.00000 0.00151 0.00146 1.85450

A23 1.91768 0.00029 0.00000 0.00249 0.00241 1.92009

A24 1.90599 -0.00010 0.00000 -0.00093 -0.00066 1.90532

A25 1.97639 0.00028 0.00000 0.00433 0.00403 1.98042

A26 1.92686 -0.00021 0.00000 -0.00156 -0.00146 1.92540

A27 1.87191 -0.00006 0.00000 0.00048 0.00055 1.87246

A28 1.92162 0.00005 0.00000 -0.00313 -0.00321 1.91840

A29 1.90462 -0.00013 0.00000 0.00210 0.00235 1.90697

A30 1.85788 0.00005 0.00000 -0.00247 -0.00252 1.85536

A31 1.88160 0.00074 0.00000 0.00079 0.00076 1.88236

A32 1.88303 -0.00031 0.00000 -0.00275 -0.00416 1.87888

A33 1.77764 -0.00050 0.00000 -0.03609 -0.03555 1.74210

A34 1.54304 0.00039 0.00000 0.01732 0.01791 1.56096

A35 1.86234 0.00052 0.00000 0.00403 0.00402 1.86636

A36 2.19866 -0.00015 0.00000 0.00173 0.00170 2.20036

A37 2.09540 -0.00022 0.00000 0.00348 0.00343 2.09884

A38 1.86453 0.00018 0.00000 0.00949 0.00812 1.87265

A39 1.71170 -0.00037 0.00000 0.02104 0.02163 1.73333

A40 1.58636 0.00002 0.00000 -0.01895 -0.01842 1.56794

A41 1.86998 0.00025 0.00000 -0.00286 -0.00285 1.86713

A42 2.19653 -0.00014 0.00000 0.00115 0.00123 2.19776

A43 2.10670 -0.00004 0.00000 -0.00237 -0.00240 2.10431

A44 1.90685 -0.00083 0.00000 -0.00231 -0.00241 1.90444

A45 2.02272 0.00092 0.00000 0.00314 0.00319 2.02591

A46 2.35360 -0.00009 0.00000 -0.00082 -0.00077 2.35283

A47 1.90376 -0.00068 0.00000 0.00063 0.00055 1.90431

A48 2.02517 0.00073 0.00000 0.00025 0.00028 2.02546

A49 2.35425 -0.00005 0.00000 -0.00087 -0.00083 2.35342

D1 -0.59713 0.00016 0.00000 0.00176 0.00169 -0.59544

D2 2.94644 -0.00004 0.00000 0.00617 0.00593 2.95238

D3 1.19903 -0.00019 0.00000 -0.00063 -0.00126 1.19777

D4 2.71272 0.00021 0.00000 0.00089 0.00106 2.71377

D5 -0.02689 0.00001 0.00000 0.00530 0.00530 -0.02159

D6 -1.77431 -0.00014 0.00000 -0.00150 -0.00190 -1.77621

D7 0.01726 -0.00007 0.00000 -0.01470 -0.01470 0.00256

D8 -2.95588 -0.00010 0.00000 -0.01402 -0.01379 -2.96967

D9 2.99133 -0.00013 0.00000 -0.01371 -0.01394 2.97739

D10 0.01819 -0.00016 0.00000 -0.01303 -0.01303 0.00516

D11 2.69102 -0.00006 0.00000 0.02823 0.02805 2.71906

D12 -1.58202 0.00002 0.00000 0.03026 0.03011 -1.55191

D13 0.52910 -0.00015 0.00000 0.02669 0.02676 0.55587

D14 -0.83307 0.00012 0.00000 0.02336 0.02333 -0.80974

D15 1.17707 0.00020 0.00000 0.02538 0.02540 1.20247

D16 -2.99498 0.00003 0.00000 0.02182 0.02205 -2.97294

D17 0.98036 -0.00020 0.00000 0.01629 0.01666 0.99702

D18 2.99051 -0.00011 0.00000 0.01831 0.01872 3.00923

D19 -1.18155 -0.00028 0.00000 0.01475 0.01537 -1.16618

D20 -1.12192 0.00039 0.00000 0.07369 0.07390 -1.04802

D21 -3.05447 0.00022 0.00000 0.06632 0.06632 -2.98815

D22 1.11340 0.00030 0.00000 0.06986 0.06997 1.18337

D23 0.98650 0.00048 0.00000 0.07476 0.07484 1.06134

D24 -0.94605 0.00031 0.00000 0.06738 0.06726 -0.87878

D25 -3.06136 0.00038 0.00000 0.07092 0.07091 -2.99045

D26 3.04479 0.00035 0.00000 0.07313 0.07326 3.11805

D27 1.11224 0.00017 0.00000 0.06576 0.06569 1.17793

D28 -1.00307 0.00025 0.00000 0.06929 0.06933 -0.93374

D29 0.60580 -0.00014 0.00000 -0.00207 -0.00201 0.60379

D30 -2.70499 -0.00011 0.00000 -0.00269 -0.00287 -2.70786

D31 -2.95618 -0.00003 0.00000 0.00183 0.00207 -2.95411

D32 0.01621 0.00000 0.00000 0.00122 0.00121 0.01742

D33 -1.19302 0.00015 0.00000 -0.00282 -0.00218 -1.19520

D34 1.77937 0.00018 0.00000 -0.00343 -0.00303 1.77634

D35 -0.62185 0.00009 0.00000 0.03008 0.03002 -0.59183

D36 -2.78552 -0.00002 0.00000 0.03220 0.03239 -2.75312

D37 1.48035 0.00007 0.00000 0.03568 0.03583 1.51618

D38 2.92264 0.00003 0.00000 0.02515 0.02492 2.94756

D39 0.75898 -0.00009 0.00000 0.02727 0.02729 0.78627

D40 -1.25834 0.00000 0.00000 0.03075 0.03073 -1.22761

D41 1.11534 0.00045 0.00000 0.02018 0.01957 1.13491

D42 -1.04833 0.00033 0.00000 0.02230 0.02195 -1.02638

D43 -3.06565 0.00042 0.00000 0.02578 0.02539 -3.04026

D44 0.94963 0.00019 0.00000 0.07562 0.07540 1.02503

D45 2.90629 0.00045 0.00000 0.06346 0.06346 2.96974

D46 -1.27538 0.00026 0.00000 0.06767 0.06751 -1.20787

D47 -1.15232 -0.00004 0.00000 0.07223 0.07211 -1.08021

D48 0.80433 0.00022 0.00000 0.06007 0.06017 0.86450

D49 2.90585 0.00004 0.00000 0.06428 0.06422 2.97008

D50 3.06684 0.00011 0.00000 0.07466 0.07452 3.14136

D51 -1.25969 0.00037 0.00000 0.06250 0.06258 -1.19712

D52 0.84182 0.00019 0.00000 0.06671 0.06663 0.90845

D53 0.06413 -0.00010 0.00000 -0.04064 -0.04062 0.02351

D54 2.23066 -0.00013 0.00000 -0.04191 -0.04205 2.18861

D55 -2.01938 -0.00012 0.00000 -0.04546 -0.04556 -2.06494

D56 -2.10019 0.00002 0.00000 -0.04133 -0.04117 -2.14135

D57 0.06634 -0.00001 0.00000 -0.04260 -0.04260 0.02374

D58 2.09949 0.00000 0.00000 -0.04615 -0.04610 2.05339

D59 2.15713 -0.00012 0.00000 -0.04401 -0.04391 2.11322

D60 -1.95953 -0.00014 0.00000 -0.04529 -0.04533 -2.00487

D61 0.07361 -0.00013 0.00000 -0.04884 -0.04884 0.02477

D62 -0.00370 -0.00002 0.00000 -0.01339 -0.01308 -0.01679

D63 3.13280 0.00008 0.00000 -0.01281 -0.01238 3.12042

D64 0.01538 0.00008 0.00000 0.00235 0.00206 0.01745

D65 -3.12305 -0.00006 0.00000 -0.00081 -0.00125 -3.12430

D66 0.09727 -0.00011 0.00000 -0.08405 -0.08414 0.01314

D67 1.91749 -0.00036 0.00000 -0.05791 -0.05780 1.85969

D68 -1.71448 -0.00021 0.00000 -0.06723 -0.06693 -1.78141

D69 -1.80156 0.00035 0.00000 -0.04372 -0.04394 -1.84550

D70 0.01865 0.00010 0.00000 -0.01759 -0.01760 0.00105

D71 2.66986 0.00025 0.00000 -0.02691 -0.02673 2.64314

D72 1.86766 0.00008 0.00000 -0.06251 -0.06292 1.80475

D73 -2.59531 -0.00016 0.00000 -0.03637 -0.03657 -2.63188

D74 0.05590 -0.00002 0.00000 -0.04569 -0.04570 0.01020

D75 -1.98206 0.00031 0.00000 0.03628 0.03720 -1.94485

D76 1.16599 0.00018 0.00000 0.03552 0.03630 1.20229

D77 -0.00989 -0.00005 0.00000 0.01969 0.01953 0.00965

D78 3.13816 -0.00018 0.00000 0.01894 0.01862 -3.12640

D79 2.64154 0.00021 0.00000 0.03650 0.03653 2.67807

D80 -0.49360 0.00008 0.00000 0.03574 0.03563 -0.45797

D81 1.90642 0.00001 0.00000 0.02763 0.02664 1.93306

D82 -1.23917 0.00019 0.00000 0.03165 0.03084 -1.20833

D83 -0.02170 -0.00011 0.00000 0.01011 0.01027 -0.01143

D84 3.11589 0.00007 0.00000 0.01413 0.01447 3.13036

D85 -2.70327 -0.00020 0.00000 0.01765 0.01758 -2.68569

D86 0.43432 -0.00002 0.00000 0.02167 0.02178 0.45610

Item Value Threshold Converged?

Maximum Force 0.001125 0.000450 NO

RMS Force 0.000299 0.000300 YES

Maximum Displacement 0.225136 0.001800 NO

RMS Displacement 0.051133 0.001200 NO

Predicted change in Energy=-2.694223D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.136177 1.559078 0.440332

2 6 0 0.189514 1.284359 0.104278

3 6 0 -0.757060 3.780653 -0.367603

4 6 0 -1.622760 2.845730 0.198473

5 1 0 -1.730820 0.840410 1.022562

6 1 0 -2.602429 3.152655 0.592273

7 6 0 0.803430 1.938838 -1.084448

8 1 0 1.921344 1.977146 -0.972120

9 1 0 0.598409 1.279294 -1.973912

10 6 0 0.259660 3.333083 -1.360381

11 1 0 1.105779 4.070667 -1.411874

12 1 0 -0.233059 3.345989 -2.372908

13 1 0 -1.037316 4.845783 -0.413207

14 1 0 0.669187 0.348645 0.435503

15 8 0 2.760196 3.840855 0.823455

16 6 0 0.473951 3.874010 1.413862

17 6 0 0.955747 2.574461 1.668951

18 6 0 1.620289 4.666343 0.889033

19 8 0 1.773204 5.821924 0.527239

20 6 0 2.398586 2.566160 1.302971

21 8 0 3.288337 1.731096 1.329177

22 1 0 -0.344169 4.371606 1.940035

23 1 0 0.569756 1.884221 2.422768

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394941 0.000000

3 C 2.394135 2.711117 0.000000

4 C 1.396686 2.393969 1.394259 0.000000

5 H 1.099580 2.174401 3.394966 2.170739 0.000000

6 H 2.170822 3.394645 2.172816 1.099560 2.508252

7 C 2.496247 1.489398 2.518189 2.890456 3.473969

8 H 3.393853 2.153560 3.285107 3.832153 4.313841

9 H 2.985908 2.118041 3.267158 3.479450 3.820574

10 C 2.887563 2.519407 1.489848 2.492196 3.981689

11 H 3.842540 3.301783 2.155175 3.396853 4.940378

12 H 3.452969 3.250437 2.117724 2.965389 4.477771

13 H 3.397166 3.802189 1.102328 2.171891 4.311078

14 H 2.173594 1.102433 3.802346 3.397740 2.519228

15 O 4.531557 3.696118 3.713938 4.537750 5.404770

16 C 2.983149 2.915854 2.167423 2.632628 3.770525

17 C 2.629953 2.167873 2.921671 2.980703 3.262268

18 C 4.177862 3.755099 2.831143 3.782707 5.087782

19 O 5.161773 4.824568 3.371909 4.527515 6.110565

20 C 3.775302 2.821325 3.771460 4.179629 4.484288

21 O 4.516188 3.361942 4.842002 5.161373 5.106787

22 H 3.284310 3.631241 2.417623 2.645020 3.903063

23 H 2.635522 2.424832 3.625337 3.267891 2.888385

6 7 8 9 10

6 H 0.000000

7 C 3.985551 0.000000

8 H 4.928861 1.124196 0.000000

9 H 4.510005 1.126135 1.800206 0.000000

10 C 3.469433 1.521756 2.179565 2.170074 0.000000

11 H 4.313949 2.177916 2.289402 2.892244 1.123654

12 H 3.800473 2.171293 2.911596 2.263132 1.126122

13 H 2.515403 3.505601 4.158742 4.222706 2.206252

14 H 4.311673 2.203857 2.490243 2.583873 3.507104

15 O 5.411544 3.329668 2.720509 4.365796 3.358519

16 C 3.264886 3.177262 3.374307 4.269081 2.834598

17 C 3.762202 2.829915 2.874790 3.882731 3.199515

18 C 4.495628 3.464270 3.284251 4.551131 2.947670

19 O 5.125953 4.314667 4.129448 5.317085 3.471060

20 C 5.085196 2.939017 2.398069 3.954064 3.500945

21 O 6.104505 3.470375 2.687969 4.283718 4.355797

22 H 2.898628 4.047572 4.398481 5.076399 3.512248

23 H 3.875873 3.515416 3.655227 4.438192 4.062951

11 12 13 14 15

11 H 0.000000

12 H 1.800341 0.000000

13 H 2.488171 2.595504 0.000000

14 H 4.178141 4.205389 4.884334 0.000000

15 O 2.790449 4.406949 4.118290 4.088808 0.000000

16 C 2.902183 3.888226 2.562510 3.663810 2.361481

17 C 3.428211 4.283123 3.669686 2.560813 2.361070

18 C 2.431815 3.977247 2.964944 4.444412 1.408942

19 O 2.696761 4.308851 3.120306 5.584268 2.233054

20 C 3.362332 4.587567 4.466248 2.942906 1.409093

21 O 4.213136 5.358502 5.607892 3.093504 2.232884

22 H 3.664452 4.434604 2.498609 4.413017 3.341486

23 H 4.446611 5.077380 4.404122 2.513385 3.344286

16 17 18 19 20

16 C 0.000000

17 C 1.409264 0.000000

18 C 1.489070 2.329348 0.000000

19 O 2.503703 3.538044 1.220510 0.000000

20 C 2.329589 1.488554 2.277687 3.404829 0.000000

21 O 3.538364 2.503534 3.404671 4.435494 1.220523

22 H 1.092603 2.234502 2.247348 2.929622 3.344875

23 H 2.233009 1.092547 3.346067 4.532860 2.250245

21 22 23

21 O 0.000000

22 H 4.532167 0.000000

23 H 2.934292 2.693580 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.297552 -0.724751 -0.654851

2 6 0 1.352922 -1.362067 0.149736

3 6 0 1.385019 1.348694 0.119741

4 6 0 2.312530 0.671760 -0.671109

5 1 0 2.902419 -1.295391 -1.374283

6 1 0 2.925495 1.212547 -1.406538

7 6 0 0.946982 -0.747681 1.444358

8 1 0 -0.076326 -1.106933 1.740326

9 1 0 1.655008 -1.128274 2.233046

10 6 0 0.981950 0.773636 1.433700

11 1 0 -0.016600 1.181676 1.748344

12 1 0 1.725824 1.133490 2.198754

13 1 0 1.241887 2.435797 0.006394

14 1 0 1.183438 -2.447869 0.062173

15 8 0 -2.076333 0.011290 0.273793

16 6 0 -0.284568 0.700953 -1.101176

17 6 0 -0.294692 -0.708272 -1.098300

18 6 0 -1.415706 1.144587 -0.240337

19 8 0 -1.870270 2.227387 0.092170

20 6 0 -1.432317 -1.133037 -0.237385

21 8 0 -1.900500 -2.207994 0.101659

22 1 0 0.074051 1.340053 -1.911561

23 1 0 0.063597 -1.353496 -1.903890

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2207606 0.8817589 0.6761367

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6709990991 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.503947139745E-01 A.U. after 15 cycles

Convg = 0.9633D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000065656 0.000144160 -0.000470270

2 6 -0.000176483 -0.000008739 0.000633549

3 6 0.000355476 0.000202350 -0.000371652

4 6 -0.000502234 -0.000692890 0.000568170

5 1 0.000195872 -0.000025559 -0.000050427

6 1 -0.000018509 -0.000020646 -0.000067804

7 6 -0.000084816 -0.000228280 -0.000556165

8 1 -0.000018941 -0.000073418 -0.000247015

9 1 -0.000029357 0.000018329 -0.000055747

10 6 0.000215315 0.000150400 0.000188969

11 1 0.000078745 0.000309066 0.000156245

12 1 0.000020667 -0.000090801 -0.000019768

13 1 0.000175885 -0.000008857 0.000179837

14 1 -0.000187338 0.000038803 0.000198743

15 8 0.000013887 0.000009091 0.000029157

16 6 -0.000091691 0.001853525 -0.000664307

17 6 0.000504340 -0.001222805 -0.000248137

18 6 -0.000639921 0.000561038 0.000108668

19 8 -0.000091430 0.000165908 -0.000147673

20 6 -0.000018393 -0.000733840 0.000357636

21 8 0.000102296 -0.000244411 0.000164057

22 1 -0.000019473 -0.000062820 0.000195367

23 1 0.000281759 -0.000039605 0.000118569

-------------------------------------------------------------------

Cartesian Forces: Max 0.001853525 RMS 0.000386327

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.001498792 RMS 0.000206178

Search for a saddle point.

Step number 64 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58 59 63 64

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0

Eigenvalues --- -0.07286 0.00180 0.00385 0.00768 0.00811

Eigenvalues --- 0.01016 0.01184 0.01346 0.01867 0.02407

Eigenvalues --- 0.02696 0.02809 0.03073 0.03293 0.03326

Eigenvalues --- 0.03553 0.03583 0.03798 0.03959 0.04123

Eigenvalues --- 0.04403 0.04696 0.04800 0.04933 0.06174

Eigenvalues --- 0.06469 0.06609 0.07063 0.07395 0.08495

Eigenvalues --- 0.09211 0.10039 0.10160 0.10380 0.10874

Eigenvalues --- 0.12708 0.13865 0.14866 0.16937 0.22695

Eigenvalues --- 0.26197 0.28426 0.29612 0.30043 0.31082

Eigenvalues --- 0.31395 0.31815 0.32015 0.32211 0.32482

Eigenvalues --- 0.33388 0.34295 0.36849 0.37917 0.39749

Eigenvalues --- 0.40245 0.40631 0.44570 0.48741 0.53203

Eigenvalues --- 0.62052 1.08662 1.11197

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 0.57281 0.50956 0.15232 -0.15135 -0.13809

R19 D1 D4 D29 D79

1 -0.13767 0.13342 0.13057 -0.12802 0.12761

RFO step: Lambda0=3.188676800D-06 Lambda=-5.18908692D-05.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.01067675 RMS(Int)= 0.00005857

Iteration 2 RMS(Cart)= 0.00007404 RMS(Int)= 0.00001404

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001404

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63606 -0.00019 0.00000 -0.00103 -0.00103 2.63503

R2 2.63935 -0.00021 0.00000 -0.00010 -0.00009 2.63926

R3 2.07790 -0.00012 0.00000 -0.00023 -0.00023 2.07768

R4 2.81455 0.00057 0.00000 0.00072 0.00073 2.81528

R5 2.08330 -0.00005 0.00000 -0.00044 -0.00044 2.08285

R6 4.09669 0.00012 0.00000 0.00439 0.00439 4.10107

R7 2.63477 0.00078 0.00000 0.00060 0.00061 2.63538

R8 2.81540 0.00000 0.00000 -0.00018 -0.00019 2.81522

R9 2.08310 -0.00006 0.00000 -0.00029 -0.00029 2.08281

R10 4.09584 -0.00022 0.00000 0.00517 0.00517 4.10101

R11 2.07787 -0.00001 0.00000 -0.00015 -0.00015 2.07772

R12 2.12442 -0.00005 0.00000 -0.00033 -0.00033 2.12409

R13 2.12809 0.00004 0.00000 0.00009 0.00009 2.12818

R14 2.87570 0.00021 0.00000 0.00057 0.00056 2.87627

R15 2.12340 0.00026 0.00000 0.00070 0.00070 2.12410

R16 2.12806 0.00001 0.00000 0.00005 0.00005 2.12811

R17 2.66252 0.00069 0.00000 0.00133 0.00132 2.66384

R18 2.66280 0.00066 0.00000 0.00083 0.00082 2.66362

R19 2.66312 0.00150 0.00000 0.00158 0.00158 2.66470

R20 2.81393 -0.00038 0.00000 -0.00173 -0.00173 2.81220

R21 2.06472 0.00008 0.00000 -0.00003 -0.00003 2.06469

R22 2.81296 -0.00030 0.00000 -0.00085 -0.00085 2.81211

R23 2.06462 0.00001 0.00000 -0.00001 -0.00001 2.06460

R24 2.30643 0.00019 0.00000 0.00002 0.00002 2.30645

R25 2.30645 0.00025 0.00000 0.00001 0.00001 2.30647

A1 2.06099 0.00024 0.00000 0.00049 0.00047 2.06146

A2 2.10923 -0.00029 0.00000 -0.00103 -0.00102 2.10821

A3 2.10062 0.00004 0.00000 0.00025 0.00026 2.10088

A4 2.09147 -0.00006 0.00000 -0.00267 -0.00270 2.08877

A5 2.10398 -0.00011 0.00000 -0.00129 -0.00128 2.10270

A6 1.61564 0.00013 0.00000 0.00270 0.00271 1.61834

A7 2.01908 0.00013 0.00000 0.00331 0.00332 2.02240

A8 1.74047 0.00002 0.00000 0.00183 0.00182 1.74229

A9 1.70567 -0.00007 0.00000 -0.00308 -0.00307 1.70260

A10 2.08613 -0.00007 0.00000 0.00232 0.00229 2.08843

A11 2.10234 0.00006 0.00000 0.00056 0.00055 2.10289

A12 1.61864 0.00013 0.00000 -0.00023 -0.00023 1.61841

A13 2.02218 0.00002 0.00000 0.00005 0.00005 2.02223

A14 1.74472 0.00007 0.00000 -0.00228 -0.00230 1.74242

A15 1.70801 -0.00023 0.00000 -0.00478 -0.00477 1.70324

A16 2.06203 -0.00013 0.00000 -0.00025 -0.00026 2.06177

A17 2.10078 0.00007 0.00000 0.00036 0.00037 2.10115

A18 2.10765 0.00006 0.00000 -0.00015 -0.00014 2.10751

A19 1.92316 0.00008 0.00000 0.00140 0.00143 1.92458

A20 1.87338 0.00011 0.00000 -0.00082 -0.00080 1.87258

A21 1.98235 -0.00013 0.00000 -0.00087 -0.00094 1.98141

A22 1.85450 -0.00008 0.00000 0.00020 0.00019 1.85469

A23 1.92009 0.00000 0.00000 -0.00009 -0.00007 1.92002

A24 1.90532 0.00002 0.00000 0.00023 0.00025 1.90557

A25 1.98042 0.00010 0.00000 0.00093 0.00085 1.98127

A26 1.92540 -0.00015 0.00000 -0.00150 -0.00147 1.92393

A27 1.87246 -0.00002 0.00000 0.00070 0.00072 1.87319

A28 1.91840 0.00018 0.00000 0.00169 0.00172 1.92012

A29 1.90697 -0.00017 0.00000 -0.00163 -0.00160 1.90537

A30 1.85536 0.00006 0.00000 -0.00033 -0.00034 1.85502

A31 1.88236 0.00056 0.00000 0.00108 0.00108 1.88344

A32 1.87888 -0.00016 0.00000 -0.00351 -0.00355 1.87533

A33 1.74210 0.00003 0.00000 -0.00371 -0.00369 1.73840

A34 1.56096 0.00010 0.00000 0.00291 0.00293 1.56388

A35 1.86636 0.00013 0.00000 0.00064 0.00063 1.86699

A36 2.20036 -0.00011 0.00000 -0.00159 -0.00159 2.19877

A37 2.09884 -0.00002 0.00000 0.00301 0.00301 2.10184

A38 1.87265 -0.00013 0.00000 0.00256 0.00253 1.87517

A39 1.73333 0.00014 0.00000 0.00410 0.00410 1.73744

A40 1.56794 0.00007 0.00000 -0.00393 -0.00391 1.56403

A41 1.86713 0.00012 0.00000 0.00033 0.00033 1.86746

A42 2.19776 0.00002 0.00000 0.00136 0.00136 2.19913

A43 2.10431 -0.00019 0.00000 -0.00287 -0.00288 2.10143

A44 1.90444 -0.00039 0.00000 -0.00099 -0.00098 1.90346

A45 2.02591 0.00030 0.00000 0.00009 0.00008 2.02599

A46 2.35283 0.00009 0.00000 0.00091 0.00091 2.35373

A47 1.90431 -0.00041 0.00000 -0.00105 -0.00104 1.90327

A48 2.02546 0.00039 0.00000 0.00107 0.00107 2.02652

A49 2.35342 0.00002 0.00000 -0.00002 -0.00003 2.35339

D1 -0.59544 -0.00010 0.00000 -0.00464 -0.00463 -0.60008

D2 2.95238 -0.00002 0.00000 -0.00353 -0.00353 2.94884

D3 1.19777 0.00000 0.00000 -0.00136 -0.00138 1.19639

D4 2.71377 -0.00008 0.00000 -0.00272 -0.00271 2.71107

D5 -0.02159 -0.00001 0.00000 -0.00160 -0.00160 -0.02320

D6 -1.77621 0.00001 0.00000 0.00056 0.00055 -1.77565

D7 0.00256 0.00002 0.00000 -0.00241 -0.00241 0.00015

D8 -2.96967 -0.00002 0.00000 -0.00215 -0.00215 -2.97182

D9 2.97739 -0.00003 0.00000 -0.00445 -0.00445 2.97294

D10 0.00516 -0.00007 0.00000 -0.00419 -0.00420 0.00096

D11 2.71906 0.00013 0.00000 0.01821 0.01820 2.73726

D12 -1.55191 0.00014 0.00000 0.01872 0.01872 -1.53319

D13 0.55587 0.00016 0.00000 0.01789 0.01788 0.57375

D14 -0.80974 0.00000 0.00000 0.01620 0.01619 -0.79355

D15 1.20247 0.00002 0.00000 0.01670 0.01671 1.21918

D16 -2.97294 0.00004 0.00000 0.01587 0.01587 -2.95706

D17 0.99702 -0.00003 0.00000 0.01461 0.01461 1.01163

D18 3.00923 -0.00002 0.00000 0.01511 0.01513 3.02436

D19 -1.16618 0.00000 0.00000 0.01429 0.01430 -1.15188

D20 -1.04802 0.00005 0.00000 0.01125 0.01126 -1.03676

D21 -2.98815 -0.00010 0.00000 0.00851 0.00850 -2.97964

D22 1.18337 0.00007 0.00000 0.01178 0.01179 1.19516

D23 1.06134 0.00002 0.00000 0.00940 0.00939 1.07074

D24 -0.87878 -0.00012 0.00000 0.00666 0.00663 -0.87215

D25 -2.99045 0.00004 0.00000 0.00993 0.00992 -2.98053

D26 3.11805 0.00014 0.00000 0.01248 0.01248 3.13053

D27 1.17793 0.00000 0.00000 0.00973 0.00972 1.18765

D28 -0.93374 0.00016 0.00000 0.01301 0.01301 -0.92073

D29 0.60379 0.00000 0.00000 -0.00355 -0.00356 0.60023

D30 -2.70786 0.00005 0.00000 -0.00376 -0.00377 -2.71162

D31 -2.95411 0.00003 0.00000 0.00447 0.00447 -2.94964

D32 0.01742 0.00008 0.00000 0.00426 0.00426 0.02169

D33 -1.19520 -0.00015 0.00000 -0.00118 -0.00117 -1.19637

D34 1.77634 -0.00010 0.00000 -0.00138 -0.00137 1.77496

D35 -0.59183 0.00011 0.00000 0.01699 0.01700 -0.57483

D36 -2.75312 -0.00008 0.00000 0.01524 0.01525 -2.73787

D37 1.51618 -0.00005 0.00000 0.01602 0.01602 1.53219

D38 2.94756 0.00008 0.00000 0.00925 0.00924 2.95681

D39 0.78627 -0.00011 0.00000 0.00749 0.00749 0.79377

D40 -1.22761 -0.00009 0.00000 0.00827 0.00826 -1.21935

D41 1.13491 0.00030 0.00000 0.01597 0.01596 1.15087

D42 -1.02638 0.00010 0.00000 0.01421 0.01421 -1.01217

D43 -3.04026 0.00013 0.00000 0.01499 0.01498 -3.02529

D44 1.02503 -0.00011 0.00000 0.01039 0.01038 1.03541

D45 2.96974 -0.00001 0.00000 0.00847 0.00848 2.97822

D46 -1.20787 0.00000 0.00000 0.01177 0.01177 -1.19610

D47 -1.08021 -0.00008 0.00000 0.00842 0.00844 -1.07177

D48 0.86450 0.00002 0.00000 0.00651 0.00654 0.87104

D49 2.97008 0.00003 0.00000 0.00981 0.00983 2.97991

D50 3.14136 -0.00006 0.00000 0.01024 0.01024 -3.13159

D51 -1.19712 0.00004 0.00000 0.00833 0.00834 -1.18878

D52 0.90845 0.00005 0.00000 0.01163 0.01163 0.92008

D53 0.02351 -0.00012 0.00000 -0.02268 -0.02268 0.00083

D54 2.18861 -0.00011 0.00000 -0.02266 -0.02267 2.16594

D55 -2.06494 -0.00004 0.00000 -0.02304 -0.02303 -2.08797

D56 -2.14135 -0.00014 0.00000 -0.02381 -0.02381 -2.16516

D57 0.02374 -0.00013 0.00000 -0.02380 -0.02380 -0.00005

D58 2.05339 -0.00006 0.00000 -0.02417 -0.02416 2.02923

D59 2.11322 -0.00005 0.00000 -0.02413 -0.02414 2.08909

D60 -2.00487 -0.00004 0.00000 -0.02411 -0.02412 -2.02899

D61 0.02477 0.00003 0.00000 -0.02449 -0.02449 0.00029

D62 -0.01679 0.00005 0.00000 0.00030 0.00031 -0.01648

D63 3.12042 0.00004 0.00000 0.00195 0.00196 3.12238

D64 0.01745 0.00001 0.00000 -0.00117 -0.00118 0.01627

D65 -3.12430 0.00001 0.00000 0.00108 0.00107 -3.12323

D66 0.01314 -0.00003 0.00000 -0.01252 -0.01251 0.00062

D67 1.85969 0.00012 0.00000 -0.00674 -0.00674 1.85296

D68 -1.78141 -0.00004 0.00000 -0.01005 -0.01004 -1.79145

D69 -1.84550 -0.00006 0.00000 -0.00716 -0.00716 -1.85266

D70 0.00105 0.00010 0.00000 -0.00138 -0.00138 -0.00033

D71 2.64314 -0.00006 0.00000 -0.00469 -0.00468 2.63845

D72 1.80475 -0.00008 0.00000 -0.01230 -0.01230 1.79245

D73 -2.63188 0.00008 0.00000 -0.00652 -0.00652 -2.63840

D74 0.01020 -0.00008 0.00000 -0.00982 -0.00982 0.00038

D75 -1.94485 0.00002 0.00000 0.00582 0.00585 -1.93901

D76 1.20229 0.00003 0.00000 0.00374 0.00376 1.20605

D77 0.00965 -0.00010 0.00000 0.00071 0.00071 0.01035

D78 -3.12640 -0.00009 0.00000 -0.00137 -0.00139 -3.12778

D79 2.67807 -0.00012 0.00000 0.00394 0.00395 2.68202

D80 -0.45797 -0.00010 0.00000 0.00185 0.00186 -0.45611

D81 1.93306 -0.00012 0.00000 0.00612 0.00609 1.93916

D82 -1.20833 -0.00012 0.00000 0.00327 0.00325 -1.20508

D83 -0.01143 -0.00007 0.00000 0.00163 0.00163 -0.00980

D84 3.13036 -0.00007 0.00000 -0.00122 -0.00121 3.12915

D85 -2.68569 0.00001 0.00000 0.00333 0.00332 -2.68237

D86 0.45610 0.00002 0.00000 0.00048 0.00048 0.45658

Item Value Threshold Converged?

Maximum Force 0.001499 0.000450 NO

RMS Force 0.000206 0.000300 YES

Maximum Displacement 0.048568 0.001800 NO

RMS Displacement 0.010676 0.001200 NO

Predicted change in Energy=-2.466803D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.138708 1.559427 0.440370

2 6 0 0.186144 1.280935 0.106373

3 6 0 -0.753576 3.779010 -0.370337

4 6 0 -1.622741 2.846301 0.194881

5 1 0 -1.733993 0.843839 1.025503

6 1 0 -2.602920 3.155695 0.585246

7 6 0 0.797476 1.928374 -1.088009

8 1 0 1.916830 1.951445 -0.988304

9 1 0 0.573308 1.272627 -1.975722

10 6 0 0.269482 3.330530 -1.356020

11 1 0 1.121925 4.062308 -1.391728

12 1 0 -0.211602 3.356220 -2.373912

13 1 0 -1.029575 4.845125 -0.415153

14 1 0 0.663141 0.346384 0.443907

15 8 0 2.755909 3.853851 0.822337

16 6 0 0.471959 3.875191 1.418073

17 6 0 0.960198 2.575837 1.666441

18 6 0 1.612501 4.675113 0.894728

19 8 0 1.759682 5.832604 0.536651

20 6 0 2.401425 2.574448 1.295869

21 8 0 3.294637 1.742929 1.316865

22 1 0 -0.350358 4.363751 1.946136

23 1 0 0.582455 1.881063 2.420261

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394398 0.000000

3 C 2.394185 2.711218 0.000000

4 C 1.396638 2.393798 1.394584 0.000000

5 H 1.099460 2.173196 3.394822 2.170752 0.000000

6 H 2.170939 3.394543 2.172956 1.099482 2.508693

7 C 2.494167 1.489782 2.519061 2.888918 3.471525

8 H 3.395747 2.154803 3.294381 3.837871 4.314014

9 H 2.975021 2.117802 3.258809 3.465631 3.809836

10 C 2.889087 2.519202 1.489749 2.494049 3.983616

11 H 3.838158 3.294849 2.154298 3.395466 4.935364

12 H 3.465281 3.258347 2.118206 2.974900 4.492856

13 H 3.397005 3.801764 1.102173 2.172391 4.310683

14 H 2.172130 1.102199 3.801710 3.396595 2.516340

15 O 4.536334 3.706237 3.707366 4.536677 5.409313

16 C 2.985450 2.921028 2.170161 2.634878 3.769540

17 C 2.634720 2.170194 2.921150 2.984998 3.266387

18 C 4.181279 3.765161 2.828730 3.781683 5.088692

19 O 5.164298 4.835167 3.369917 4.524996 6.110034

20 C 3.780832 2.827639 3.765799 4.180908 4.491078

21 O 4.522882 3.367707 4.835318 5.163030 5.116675

22 H 3.279186 3.629920 2.422923 2.643578 3.892530

23 H 2.643071 2.423075 3.629686 3.278245 2.896051

6 7 8 9 10

6 H 0.000000

7 C 3.983566 0.000000

8 H 4.935020 1.124023 0.000000

9 H 4.493654 1.126184 1.800234 0.000000

10 C 3.471279 1.522055 2.179643 2.170554 0.000000

11 H 4.313334 2.179722 2.291368 2.902473 1.124025

12 H 3.809886 2.170376 2.902331 2.261857 1.126147

13 H 2.516026 3.506892 4.169315 4.215133 2.206077

14 H 4.310379 2.206242 2.489816 2.592412 3.507112

15 O 5.409315 3.345496 2.757104 4.388120 3.346852

16 C 3.265909 3.190063 3.402807 4.278020 2.834298

17 C 3.768426 2.834199 2.890101 3.887595 3.190912

18 C 4.491569 3.484263 3.325175 4.571249 2.945754

19 O 5.118642 4.336862 4.172957 5.339746 3.473221

20 C 5.087859 2.944985 2.416694 3.967374 3.485592

21 O 6.108384 3.471832 2.693628 4.297435 4.337782

22 H 2.895765 4.056430 4.423834 5.078305 3.515108

23 H 3.890833 3.515171 3.661124 4.437899 4.056995

11 12 13 14 15

11 H 0.000000

12 H 1.800427 0.000000

13 H 2.489067 2.592808 0.000000

14 H 4.169908 4.214783 4.882821 0.000000

15 O 2.759609 4.389734 4.104132 4.101855 0.000000

16 C 2.890061 3.887896 2.560488 3.665792 2.360463

17 C 3.404138 4.278618 3.666320 2.559940 2.360172

18 C 2.417453 3.968733 2.953856 4.454483 1.409643

19 O 2.694313 4.299978 3.108215 5.595499 2.233729

20 C 3.327766 4.572348 4.455933 2.951566 1.409526

21 O 4.175724 5.340248 5.596635 3.104378 2.234005

22 H 3.660577 4.438151 2.503746 4.407167 3.342428

23 H 4.424943 5.078456 4.407254 2.503543 3.342029

16 17 18 19 20

16 C 0.000000

17 C 1.410101 0.000000

18 C 1.488154 2.329807 0.000000

19 O 2.503318 3.538663 1.220519 0.000000

20 C 2.330172 1.488107 2.279497 3.406439 0.000000

21 O 3.538967 2.503106 3.406682 4.437371 1.220529

22 H 1.092588 2.234374 2.248382 2.931969 3.346157

23 H 2.234533 1.092541 3.345887 4.533048 2.248042

21 22 23

21 O 0.000000

22 H 4.533286 0.000000

23 H 2.931295 2.694194 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306105 -0.698837 -0.663415

2 6 0 1.369881 -1.355395 0.134557

3 6 0 1.370607 1.355823 0.133665

4 6 0 2.306399 0.697801 -0.663934

5 1 0 2.914330 -1.255126 -1.391026

6 1 0 2.914071 1.253566 -1.392441

7 6 0 0.965812 -0.760202 1.439135

8 1 0 -0.045123 -1.144076 1.745855

9 1 0 1.692719 -1.130552 2.215496

10 6 0 0.966819 0.761853 1.438850

11 1 0 -0.043586 1.147292 1.745364

12 1 0 1.694467 1.131304 2.214892

13 1 0 1.212550 2.441676 0.030096

14 1 0 1.210727 -2.441145 0.031318

15 8 0 -2.076933 -0.000359 0.274365

16 6 0 -0.292158 0.705252 -1.099853

17 6 0 -0.292189 -0.704849 -1.099970

18 6 0 -1.425202 1.139577 -0.238358

19 8 0 -1.886886 2.218253 0.097757

20 6 0 -1.424770 -1.139920 -0.238324

21 8 0 -1.884979 -2.219118 0.098175

22 1 0 0.066128 1.347213 -1.908102

23 1 0 0.066266 -1.346981 -1.907944

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200519 0.8809445 0.6754970

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5674283202 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504193964268E-01 A.U. after 14 cycles

Convg = 0.4722D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000036966 0.000022178 0.000019869

2 6 0.000008973 0.000045384 -0.000002359

3 6 -0.000103550 -0.000249577 0.000031676

4 6 0.000031110 0.000226915 0.000018431

5 1 0.000019771 -0.000052339 0.000000068

6 1 -0.000034565 -0.000006619 -0.000037791

7 6 0.000030073 -0.000062375 -0.000027092

8 1 -0.000000253 -0.000016908 0.000049993

9 1 -0.000020241 0.000041538 -0.000026094

10 6 0.000064078 0.000046651 0.000018121

11 1 0.000010751 0.000009049 -0.000002552

12 1 -0.000008085 -0.000016185 0.000003559

13 1 0.000007633 0.000035512 0.000030176

14 1 0.000034707 -0.000022119 -0.000009114

15 8 0.000029534 0.000012772 -0.000011800

16 6 -0.000036706 0.000023277 -0.000065897

17 6 -0.000055358 -0.000153251 -0.000049720

18 6 0.000028651 0.000081867 0.000009661

19 8 -0.000036947 0.000050024 -0.000033909

20 6 0.000004847 -0.000037444 0.000013252

21 8 0.000046622 -0.000013218 -0.000000545

22 1 0.000031607 0.000015591 0.000019449

23 1 -0.000015688 0.000019279 0.000052617

-------------------------------------------------------------------

Cartesian Forces: Max 0.000249577 RMS 0.000056121

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000112425 RMS 0.000027105

Search for a saddle point.

Step number 65 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58 59 63 64

65

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0

Eigenvalues --- -0.07213 0.00144 0.00423 0.00747 0.00781

Eigenvalues --- 0.01069 0.01176 0.01254 0.01832 0.02396

Eigenvalues --- 0.02621 0.02828 0.02944 0.03271 0.03338

Eigenvalues --- 0.03573 0.03607 0.03795 0.03994 0.04096

Eigenvalues --- 0.04386 0.04558 0.04751 0.04931 0.06175

Eigenvalues --- 0.06544 0.06605 0.07019 0.07385 0.08515

Eigenvalues --- 0.08984 0.10040 0.10218 0.10402 0.10878

Eigenvalues --- 0.12722 0.13493 0.14688 0.16092 0.22665

Eigenvalues --- 0.26192 0.28416 0.29605 0.30037 0.31077

Eigenvalues --- 0.31399 0.31834 0.32019 0.32208 0.32493

Eigenvalues --- 0.33335 0.34259 0.36849 0.37980 0.39754

Eigenvalues --- 0.40271 0.40678 0.44607 0.48740 0.53306

Eigenvalues --- 0.62214 1.08665 1.11207

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 0.56886 0.51498 0.15491 -0.15165 -0.13921

R19 D4 D1 D79 D29

1 -0.13756 0.13269 0.13116 0.12872 -0.12458

RFO step: Lambda0=1.025230173D-08 Lambda=-9.52254258D-07.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00084779 RMS(Int)= 0.00000035

Iteration 2 RMS(Cart)= 0.00000042 RMS(Int)= 0.00000011

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63503 0.00005 0.00000 -0.00005 -0.00005 2.63498

R2 2.63926 0.00008 0.00000 0.00031 0.00031 2.63957

R3 2.07768 0.00002 0.00000 0.00007 0.00007 2.07774

R4 2.81528 -0.00002 0.00000 -0.00006 -0.00006 2.81522

R5 2.08285 0.00003 0.00000 0.00011 0.00011 2.08296

R6 4.10107 -0.00003 0.00000 0.00032 0.00032 4.10139

R7 2.63538 -0.00011 0.00000 -0.00046 -0.00046 2.63492

R8 2.81522 0.00003 0.00000 0.00004 0.00004 2.81526

R9 2.08281 0.00003 0.00000 0.00016 0.00016 2.08297

R10 4.10101 -0.00004 0.00000 0.00048 0.00048 4.10149

R11 2.07772 0.00002 0.00000 0.00001 0.00001 2.07773

R12 2.12409 0.00000 0.00000 0.00000 0.00000 2.12409

R13 2.12818 0.00000 0.00000 -0.00003 -0.00003 2.12815

R14 2.87627 0.00000 0.00000 0.00003 0.00003 2.87629

R15 2.12410 0.00001 0.00000 -0.00001 -0.00001 2.12409

R16 2.12811 0.00000 0.00000 0.00003 0.00003 2.12814

R17 2.66384 0.00005 0.00000 -0.00004 -0.00004 2.66379

R18 2.66362 0.00008 0.00000 0.00024 0.00024 2.66386

R19 2.66470 0.00007 0.00000 -0.00004 -0.00004 2.66466

R20 2.81220 0.00005 0.00000 0.00013 0.00013 2.81233

R21 2.06469 -0.00001 0.00000 -0.00002 -0.00002 2.06468

R22 2.81211 0.00006 0.00000 0.00018 0.00018 2.81229

R23 2.06460 0.00003 0.00000 0.00007 0.00007 2.06467

R24 2.30645 0.00005 0.00000 0.00003 0.00003 2.30648

R25 2.30647 0.00004 0.00000 0.00001 0.00001 2.30648

A1 2.06146 0.00000 0.00000 0.00003 0.00003 2.06148

A2 2.10821 -0.00005 0.00000 -0.00042 -0.00042 2.10780

A3 2.10088 0.00005 0.00000 0.00043 0.00043 2.10131

A4 2.08877 0.00001 0.00000 0.00022 0.00022 2.08899

A5 2.10270 0.00001 0.00000 0.00019 0.00019 2.10290

A6 1.61834 0.00001 0.00000 0.00019 0.00019 1.61854

A7 2.02240 -0.00002 0.00000 -0.00042 -0.00042 2.02199

A8 1.74229 -0.00003 0.00000 -0.00026 -0.00026 1.74203

A9 1.70260 0.00001 0.00000 0.00009 0.00009 1.70269

A10 2.08843 0.00005 0.00000 0.00069 0.00069 2.08911

A11 2.10289 -0.00004 0.00000 -0.00016 -0.00016 2.10273

A12 1.61841 0.00005 0.00000 0.00011 0.00011 1.61852

A13 2.02223 -0.00001 0.00000 -0.00018 -0.00018 2.02206

A14 1.74242 -0.00005 0.00000 -0.00052 -0.00052 1.74190

A15 1.70324 -0.00002 0.00000 -0.00047 -0.00047 1.70276

A16 2.06177 -0.00003 0.00000 -0.00029 -0.00029 2.06149

A17 2.10115 0.00002 0.00000 0.00009 0.00008 2.10124

A18 2.10751 0.00002 0.00000 0.00036 0.00036 2.10786

A19 1.92458 -0.00004 0.00000 -0.00051 -0.00051 1.92407

A20 1.87258 0.00004 0.00000 0.00045 0.00045 1.87302

A21 1.98141 -0.00001 0.00000 -0.00017 -0.00017 1.98124

A22 1.85469 0.00001 0.00000 0.00043 0.00043 1.85512

A23 1.92002 0.00004 0.00000 0.00034 0.00034 1.92036

A24 1.90557 -0.00004 0.00000 -0.00049 -0.00049 1.90508

A25 1.98127 0.00001 0.00000 -0.00004 -0.00004 1.98123

A26 1.92393 0.00000 0.00000 0.00025 0.00025 1.92417

A27 1.87319 0.00000 0.00000 -0.00014 -0.00014 1.87305

A28 1.92012 0.00001 0.00000 0.00011 0.00011 1.92023

A29 1.90537 -0.00002 0.00000 -0.00014 -0.00014 1.90523

A30 1.85502 0.00001 0.00000 -0.00004 -0.00004 1.85498

A31 1.88344 0.00003 0.00000 0.00005 0.00005 1.88349

A32 1.87533 -0.00001 0.00000 -0.00025 -0.00025 1.87508

A33 1.73840 -0.00001 0.00000 -0.00039 -0.00039 1.73801

A34 1.56388 0.00001 0.00000 0.00040 0.00040 1.56428

A35 1.86699 0.00003 0.00000 0.00034 0.00034 1.86734

A36 2.19877 0.00000 0.00000 0.00004 0.00004 2.19881

A37 2.10184 -0.00003 0.00000 -0.00032 -0.00032 2.10153

A38 1.87517 -0.00001 0.00000 0.00006 0.00006 1.87523

A39 1.73744 0.00000 0.00000 0.00063 0.00063 1.73807

A40 1.56403 0.00003 0.00000 0.00015 0.00015 1.56418

A41 1.86746 -0.00001 0.00000 -0.00027 -0.00027 1.86719

A42 2.19913 -0.00002 0.00000 -0.00041 -0.00041 2.19872

A43 2.10143 0.00002 0.00000 0.00029 0.00029 2.10172

A44 1.90346 -0.00003 0.00000 -0.00020 -0.00020 1.90326

A45 2.02599 0.00006 0.00000 0.00038 0.00038 2.02637

A46 2.35373 -0.00003 0.00000 -0.00017 -0.00017 2.35356

A47 1.90327 -0.00002 0.00000 0.00008 0.00008 1.90335

A48 2.02652 -0.00002 0.00000 -0.00033 -0.00033 2.02619

A49 2.35339 0.00003 0.00000 0.00025 0.00025 2.35364

D1 -0.60008 0.00001 0.00000 0.00024 0.00024 -0.59984

D2 2.94884 0.00001 0.00000 0.00035 0.00035 2.94919

D3 1.19639 -0.00001 0.00000 0.00009 0.00009 1.19648

D4 2.71107 0.00000 0.00000 -0.00010 -0.00010 2.71096

D5 -0.02320 0.00000 0.00000 0.00001 0.00001 -0.02319

D6 -1.77565 -0.00002 0.00000 -0.00025 -0.00025 -1.77590

D7 0.00015 0.00000 0.00000 -0.00031 -0.00031 -0.00015

D8 -2.97182 -0.00002 0.00000 -0.00136 -0.00136 -2.97317

D9 2.97294 0.00001 0.00000 -0.00006 -0.00006 2.97288

D10 0.00096 -0.00002 0.00000 -0.00111 -0.00111 -0.00014

D11 2.73726 0.00000 0.00000 0.00056 0.00056 2.73782

D12 -1.53319 0.00001 0.00000 0.00105 0.00105 -1.53215

D13 0.57375 -0.00002 0.00000 0.00063 0.00063 0.57438

D14 -0.79355 0.00000 0.00000 0.00059 0.00059 -0.79297

D15 1.21918 0.00002 0.00000 0.00107 0.00107 1.22025

D16 -2.95706 -0.00001 0.00000 0.00066 0.00066 -2.95640

D17 1.01163 -0.00001 0.00000 0.00043 0.00043 1.01206

D18 3.02436 0.00001 0.00000 0.00092 0.00092 3.02527

D19 -1.15188 -0.00002 0.00000 0.00050 0.00051 -1.15138

D20 -1.03676 0.00001 0.00000 0.00080 0.00080 -1.03596

D21 -2.97964 0.00003 0.00000 0.00082 0.00082 -2.97882

D22 1.19516 0.00000 0.00000 0.00043 0.00043 1.19560

D23 1.07074 0.00002 0.00000 0.00103 0.00103 1.07176

D24 -0.87215 0.00004 0.00000 0.00105 0.00105 -0.87110

D25 -2.98053 0.00001 0.00000 0.00066 0.00066 -2.97987

D26 3.13053 -0.00001 0.00000 0.00055 0.00055 3.13109

D27 1.18765 0.00001 0.00000 0.00057 0.00057 1.18822

D28 -0.92073 -0.00002 0.00000 0.00019 0.00019 -0.92054

D29 0.60023 -0.00002 0.00000 -0.00044 -0.00044 0.59979

D30 -2.71162 0.00000 0.00000 0.00058 0.00058 -2.71104

D31 -2.94964 0.00000 0.00000 0.00049 0.00049 -2.94915

D32 0.02169 0.00002 0.00000 0.00152 0.00152 0.02321

D33 -1.19637 0.00000 0.00000 -0.00002 -0.00002 -1.19639

D34 1.77496 0.00003 0.00000 0.00100 0.00100 1.77597

D35 -0.57483 0.00001 0.00000 0.00125 0.00125 -0.57359

D36 -2.73787 -0.00001 0.00000 0.00094 0.00095 -2.73693

D37 1.53219 -0.00001 0.00000 0.00095 0.00095 1.53314

D38 2.95681 0.00000 0.00000 0.00036 0.00036 2.95717

D39 0.79377 -0.00002 0.00000 0.00006 0.00006 0.79383

D40 -1.21935 -0.00002 0.00000 0.00006 0.00006 -1.21929

D41 1.15087 0.00005 0.00000 0.00124 0.00124 1.15211

D42 -1.01217 0.00003 0.00000 0.00094 0.00094 -1.01123

D43 -3.02529 0.00003 0.00000 0.00094 0.00094 -3.02435

D44 1.03541 0.00002 0.00000 0.00101 0.00101 1.03642

D45 2.97822 0.00005 0.00000 0.00115 0.00115 2.97937

D46 -1.19610 0.00003 0.00000 0.00087 0.00087 -1.19523

D47 -1.07177 -0.00003 0.00000 0.00036 0.00036 -1.07140

D48 0.87104 0.00000 0.00000 0.00050 0.00051 0.87155

D49 2.97991 -0.00003 0.00000 0.00022 0.00022 2.98013

D50 -3.13159 -0.00001 0.00000 0.00080 0.00080 -3.13079

D51 -1.18878 0.00002 0.00000 0.00094 0.00094 -1.18784

D52 0.92008 0.00000 0.00000 0.00066 0.00066 0.92074

D53 0.00083 -0.00002 0.00000 -0.00139 -0.00139 -0.00056

D54 2.16594 -0.00001 0.00000 -0.00101 -0.00101 2.16493

D55 -2.08797 -0.00001 0.00000 -0.00109 -0.00109 -2.08905

D56 -2.16516 0.00001 0.00000 -0.00085 -0.00085 -2.16601

D57 -0.00005 0.00002 0.00000 -0.00047 -0.00047 -0.00052

D58 2.02923 0.00002 0.00000 -0.00055 -0.00055 2.02868

D59 2.08909 0.00000 0.00000 -0.00128 -0.00128 2.08781

D60 -2.02899 0.00001 0.00000 -0.00090 -0.00090 -2.02989

D61 0.00029 0.00001 0.00000 -0.00097 -0.00097 -0.00069

D62 -0.01648 0.00000 0.00000 0.00032 0.00032 -0.01616

D63 3.12238 0.00001 0.00000 0.00069 0.00069 3.12308

D64 0.01627 0.00000 0.00000 -0.00023 -0.00023 0.01604

D65 -3.12323 0.00000 0.00000 -0.00007 -0.00007 -3.12330

D66 0.00062 0.00002 0.00000 -0.00089 -0.00089 -0.00026

D67 1.85296 0.00001 0.00000 -0.00026 -0.00026 1.85269

D68 -1.79145 -0.00001 0.00000 -0.00094 -0.00094 -1.79239

D69 -1.85266 0.00002 0.00000 -0.00049 -0.00049 -1.85315

D70 -0.00033 0.00001 0.00000 0.00013 0.00013 -0.00020

D71 2.63845 0.00000 0.00000 -0.00054 -0.00054 2.63791

D72 1.79245 0.00002 0.00000 -0.00055 -0.00055 1.79190

D73 -2.63840 0.00001 0.00000 0.00008 0.00008 -2.63832

D74 0.00038 0.00000 0.00000 -0.00060 -0.00060 -0.00022

D75 -1.93901 0.00000 0.00000 0.00004 0.00004 -1.93897

D76 1.20605 -0.00001 0.00000 -0.00044 -0.00044 1.20560

D77 0.01035 -0.00001 0.00000 -0.00028 -0.00028 0.01007

D78 -3.12778 -0.00002 0.00000 -0.00076 -0.00076 -3.12854

D79 2.68202 0.00000 0.00000 -0.00012 -0.00012 2.68189

D80 -0.45611 -0.00001 0.00000 -0.00060 -0.00060 -0.45672

D81 1.93916 -0.00002 0.00000 0.00029 0.00029 1.93945

D82 -1.20508 -0.00002 0.00000 0.00008 0.00008 -1.20500

D83 -0.00980 -0.00001 0.00000 0.00006 0.00006 -0.00974

D84 3.12915 -0.00001 0.00000 -0.00015 -0.00015 3.12900

D85 -2.68237 0.00002 0.00000 0.00092 0.00092 -2.68145

D86 0.45658 0.00002 0.00000 0.00071 0.00071 0.45729

Item Value Threshold Converged?

Maximum Force 0.000112 0.000450 YES

RMS Force 0.000027 0.000300 YES

Maximum Displacement 0.003836 0.001800 NO

RMS Displacement 0.000848 0.001200 YES

Predicted change in Energy=-4.709972D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.139211 1.559594 0.440546

2 6 0 0.185485 1.280640 0.106425

3 6 0 -0.753438 3.778679 -0.370400

4 6 0 -1.623003 2.846679 0.194768

5 1 0 -1.734368 0.843889 1.025732

6 1 0 -2.603593 3.156101 0.584095

7 6 0 0.797176 1.927644 -1.087967

8 1 0 1.916528 1.949415 -0.987954

9 1 0 0.572051 1.272801 -1.976083

10 6 0 0.270328 3.330349 -1.355447

11 1 0 1.123219 4.061643 -1.390166

12 1 0 -0.209980 3.356873 -2.373700

13 1 0 -1.028905 4.845028 -0.415033

14 1 0 0.662374 0.345903 0.443783

15 8 0 2.755727 3.854929 0.822090

16 6 0 0.472038 3.874916 1.418353

17 6 0 0.960606 2.575602 1.666150

18 6 0 1.612000 4.675675 0.894832

19 8 0 1.758065 5.833271 0.536578

20 6 0 2.401823 2.575053 1.295162

21 8 0 3.295666 1.744190 1.315569

22 1 0 -0.350226 4.363160 1.946777

23 1 0 0.583239 1.880971 2.420345

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394372 0.000000

3 C 2.393907 2.710930 0.000000

4 C 1.396800 2.393933 1.394339 0.000000

5 H 1.099495 2.172950 3.394761 2.171192 0.000000

6 H 2.171142 3.394773 2.172956 1.099488 2.509367

7 C 2.494274 1.489748 2.519055 2.889169 3.471449

8 H 3.395602 2.154398 3.294890 3.838254 4.313485

9 H 2.975023 2.118097 3.258001 3.465249 3.809781

10 C 2.889283 2.519042 1.489770 2.494354 3.983880

11 H 3.838013 3.294406 2.154492 3.395569 4.935211

12 H 3.466073 3.258551 2.118131 2.975560 4.493884

13 H 3.396802 3.801517 1.102259 2.172144 4.310754

14 H 2.172272 1.102255 3.801496 3.396886 2.516152

15 O 4.537035 3.707464 3.707032 4.536891 5.410063

16 C 2.985456 2.921222 2.170412 2.635077 3.769549

17 C 2.635073 2.170364 2.921109 2.985546 3.266779

18 C 4.181567 3.766005 2.828553 3.781608 5.088998

19 O 5.164082 4.835751 3.369214 4.524178 6.109852

20 C 3.781594 2.828561 3.765433 4.181372 4.491948

21 O 4.524144 3.368996 4.834965 5.163815 5.118182

22 H 3.278904 3.629850 2.423531 2.643712 3.892228

23 H 2.643808 2.423393 3.629912 3.279221 2.896857

6 7 8 9 10

6 H 0.000000

7 C 3.983733 0.000000

8 H 4.935476 1.124022 0.000000

9 H 4.492889 1.126166 1.800507 0.000000

10 C 3.471542 1.522069 2.179909 2.170191 0.000000

11 H 4.313565 2.179812 2.291859 2.902538 1.124020

12 H 3.810281 2.170292 2.902286 2.261201 1.126161

13 H 2.516024 3.506928 4.169938 4.214350 2.206045

14 H 4.310851 2.205977 2.488779 2.592885 3.506828

15 O 5.409928 3.346441 2.758894 4.389260 3.345752

16 C 3.266832 3.190490 3.403589 4.278224 2.833938

17 C 3.769793 2.834029 2.889665 3.887689 3.190011

18 C 4.491869 3.485270 3.327178 4.572002 2.945122

19 O 5.117964 4.337785 4.175362 5.340223 3.472426

20 C 5.088952 2.945053 2.416517 3.967994 3.484174

21 O 6.109812 3.471757 2.692649 4.298286 4.336231

22 H 2.896819 4.056838 4.424588 5.078360 3.515176

23 H 3.892772 3.515139 3.660443 4.438308 4.056503

11 12 13 14 15

11 H 0.000000

12 H 1.800405 0.000000

13 H 2.489220 2.592608 0.000000

14 H 4.169229 4.214873 4.882634 0.000000

15 O 2.757152 4.388228 4.102951 4.103475 0.000000

16 C 2.889063 3.887567 2.560323 3.666053 2.360332

17 C 3.402327 4.277972 3.666030 2.560210 2.360419

18 C 2.416021 3.967637 2.952762 4.455576 1.409619

19 O 2.693332 4.298309 3.106346 5.596459 2.233984

20 C 3.325021 4.570919 4.455048 2.952903 1.409655

21 O 4.172663 5.338633 5.595721 3.106356 2.233893

22 H 3.660210 4.438333 2.504186 4.407119 3.342179

23 H 4.423450 5.078420 4.407269 2.503895 3.342250

16 17 18 19 20

16 C 0.000000

17 C 1.410078 0.000000

18 C 1.488222 2.330140 0.000000

19 O 2.503307 3.538966 1.220536 0.000000

20 C 2.329998 1.488200 2.279627 3.406737 0.000000

21 O 3.538846 2.503329 3.406663 4.437525 1.220534

22 H 1.092580 2.234367 2.248240 2.931685 3.345998

23 H 2.234317 1.092579 3.346030 4.533153 2.248341

21 22 23

21 O 0.000000

22 H 4.533205 0.000000

23 H 2.931979 2.693861 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306829 -0.697375 -0.663818

2 6 0 1.371090 -1.355170 0.133661

3 6 0 1.369996 1.355760 0.134791

4 6 0 2.306316 0.699425 -0.663151

5 1 0 2.915352 -1.253124 -1.391644

6 1 0 2.914557 1.256242 -1.390386

7 6 0 0.966373 -0.761458 1.438675

8 1 0 -0.044047 -1.147208 1.744739

9 1 0 1.693899 -1.130724 2.214948

10 6 0 0.965346 0.760611 1.439195

11 1 0 -0.045799 1.144651 1.745006

12 1 0 1.691801 1.130475 2.216177

13 1 0 1.210877 2.441605 0.031853

14 1 0 1.212649 -2.441029 0.029873

15 8 0 -2.077189 -0.000564 0.274011

16 6 0 -0.292328 0.705219 -1.099780

17 6 0 -0.291866 -0.704859 -1.100094

18 6 0 -1.425490 1.139537 -0.238320

19 8 0 -1.886726 2.218324 0.098114

20 6 0 -1.424609 -1.140090 -0.238579

21 8 0 -1.885028 -2.219200 0.097930

22 1 0 0.065796 1.347447 -1.907878

23 1 0 0.066523 -1.346414 -1.908607

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200710 0.8808853 0.6754434

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5621562651 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504198187362E-01 A.U. after 11 cycles

Convg = 0.7008D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000009572 0.000019343 0.000008660

2 6 -0.000020223 -0.000029471 -0.000014514

3 6 -0.000009968 0.000033014 -0.000040109

4 6 -0.000002530 -0.000059443 0.000030384

5 1 0.000000016 0.000005877 -0.000006488

6 1 0.000001432 0.000002625 -0.000002669

7 6 0.000010929 0.000008893 -0.000003218

8 1 -0.000001589 0.000004999 -0.000008299

9 1 0.000006115 -0.000005565 0.000003622

10 6 0.000015029 0.000013160 0.000011508

11 1 -0.000002288 0.000006877 -0.000000653

12 1 -0.000004675 -0.000006854 0.000002231

13 1 0.000010557 0.000000653 0.000006038

14 1 -0.000006409 0.000003989 0.000010844

15 8 -0.000016410 -0.000005767 0.000004388

16 6 -0.000008995 0.000045322 -0.000011974

17 6 0.000027931 0.000002454 -0.000011592

18 6 -0.000017495 -0.000013407 0.000013268

19 8 -0.000000084 -0.000008149 -0.000000406

20 6 0.000019099 -0.000002020 0.000001803

21 8 -0.000004951 -0.000011595 0.000007805

22 1 0.000001890 -0.000000665 0.000000771

23 1 0.000012191 -0.000004269 -0.000001401

-------------------------------------------------------------------

Cartesian Forces: Max 0.000059443 RMS 0.000015116

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000037480 RMS 0.000006840

Search for a saddle point.

Step number 66 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58 59 63 64

65 66

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0

Eigenvalues --- -0.07166 -0.00003 0.00393 0.00741 0.00777

Eigenvalues --- 0.00969 0.01181 0.01328 0.01839 0.02176

Eigenvalues --- 0.02459 0.02808 0.02874 0.03210 0.03332

Eigenvalues --- 0.03580 0.03603 0.03789 0.04021 0.04093

Eigenvalues --- 0.04371 0.04398 0.04694 0.04845 0.06191

Eigenvalues --- 0.06561 0.06635 0.07047 0.07376 0.08513

Eigenvalues --- 0.08870 0.10091 0.10340 0.10694 0.10864

Eigenvalues --- 0.12732 0.13392 0.14649 0.15982 0.22667

Eigenvalues --- 0.26195 0.28438 0.29612 0.30057 0.31073

Eigenvalues --- 0.31412 0.31844 0.32021 0.32226 0.32508

Eigenvalues --- 0.33389 0.34679 0.36855 0.38008 0.39757

Eigenvalues --- 0.40288 0.40722 0.44786 0.48782 0.53451

Eigenvalues --- 0.62396 1.08670 1.11218

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 -0.56392 -0.51486 -0.15337 0.14734 0.14360

D1 R19 D4 D29 D13

1 -0.13519 0.13481 -0.13310 0.13141 0.12807

RFO step: Lambda0=5.684078208D-12 Lambda=-3.19255889D-05.

Linear search not attempted -- option 19 set.

Maximum step size ( 0.300) exceeded in Quadratic search.

-- Step size scaled by 0.146

Iteration 1 RMS(Cart)= 0.10703714 RMS(Int)= 0.07959285

Iteration 2 RMS(Cart)= 0.06813836 RMS(Int)= 0.01594465

Iteration 3 RMS(Cart)= 0.01328750 RMS(Int)= 0.00537673

Iteration 4 RMS(Cart)= 0.00028066 RMS(Int)= 0.00536891

Iteration 5 RMS(Cart)= 0.00000038 RMS(Int)= 0.00536891

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63498 0.00001 0.00000 -0.00862 -0.00863 2.62636

R2 2.63957 -0.00002 0.00000 0.02038 0.02146 2.66103

R3 2.07774 -0.00001 0.00000 0.00475 0.00475 2.08249

R4 2.81522 0.00002 0.00000 -0.00779 -0.00847 2.80675

R5 2.08296 0.00000 0.00000 0.00625 0.00625 2.08921

R6 4.10139 0.00001 0.00000 -0.00048 -0.00103 4.10037

R7 2.63492 0.00004 0.00000 -0.02854 -0.02753 2.60739

R8 2.81526 0.00000 0.00000 0.00952 0.01043 2.82569

R9 2.08297 0.00000 0.00000 0.00316 0.00316 2.08613

R10 4.10149 0.00000 0.00000 -0.00798 -0.00834 4.09314

R11 2.07773 0.00000 0.00000 -0.00413 -0.00413 2.07360

R12 2.12409 0.00000 0.00000 0.00496 0.00496 2.12905

R13 2.12815 0.00000 0.00000 0.00318 0.00318 2.13133

R14 2.87629 0.00001 0.00000 -0.00761 -0.00714 2.86915

R15 2.12409 0.00000 0.00000 -0.00442 -0.00442 2.11967

R16 2.12814 0.00000 0.00000 -0.00032 -0.00032 2.12782

R17 2.66379 0.00001 0.00000 -0.00774 -0.00925 2.65454

R18 2.66386 -0.00001 0.00000 0.02578 0.02372 2.68758

R19 2.66466 0.00002 0.00000 -0.01399 -0.01320 2.65146

R20 2.81233 -0.00003 0.00000 0.03471 0.03586 2.84819

R21 2.06468 0.00000 0.00000 0.00311 0.00311 2.06779

R22 2.81229 -0.00001 0.00000 0.00071 0.00083 2.81312

R23 2.06467 0.00000 0.00000 0.00063 0.00063 2.06530

R24 2.30648 -0.00001 0.00000 0.00037 0.00037 2.30685

R25 2.30648 0.00000 0.00000 -0.00120 -0.00120 2.30528

A1 2.06148 0.00000 0.00000 0.01137 0.00375 2.06524

A2 2.10780 0.00000 0.00000 -0.00930 -0.00697 2.10083

A3 2.10131 -0.00001 0.00000 0.00982 0.01242 2.11373

A4 2.08899 0.00000 0.00000 0.05570 0.04512 2.13411

A5 2.10290 0.00000 0.00000 -0.01947 -0.01881 2.08409

A6 1.61854 0.00000 0.00000 0.01003 0.01688 1.63542

A7 2.02199 0.00001 0.00000 -0.01469 -0.00629 2.01569

A8 1.74203 -0.00001 0.00000 -0.09252 -0.09850 1.64353

A9 1.70269 0.00000 0.00000 0.02696 0.02667 1.72936

A10 2.08911 0.00000 0.00000 -0.02519 -0.03419 2.05492

A11 2.10273 0.00001 0.00000 -0.00528 -0.00435 2.09838

A12 1.61852 0.00000 0.00000 -0.01295 -0.00710 1.61142

A13 2.02206 0.00000 0.00000 0.01877 0.02665 2.04871

A14 1.74190 0.00000 0.00000 0.06408 0.05830 1.80020

A15 1.70276 0.00000 0.00000 -0.02148 -0.02277 1.67999

A16 2.06149 0.00000 0.00000 -0.01927 -0.02705 2.03444

A17 2.10124 0.00000 0.00000 -0.01098 -0.00843 2.09281

A18 2.10786 -0.00001 0.00000 0.01663 0.01833 2.12619

A19 1.92407 0.00001 0.00000 -0.01250 -0.00382 1.92025

A20 1.87302 0.00000 0.00000 0.03884 0.05072 1.92375

A21 1.98124 0.00000 0.00000 0.00043 -0.03233 1.94890

A22 1.85512 0.00000 0.00000 -0.05075 -0.05558 1.79954

A23 1.92036 0.00000 0.00000 0.01958 0.02954 1.94990

A24 1.90508 0.00000 0.00000 0.00123 0.01098 1.91607

A25 1.98123 0.00000 0.00000 -0.00362 -0.03474 1.94650

A26 1.92417 0.00000 0.00000 0.00331 0.01500 1.93917

A27 1.87305 0.00000 0.00000 -0.01987 -0.01284 1.86021

A28 1.92023 0.00001 0.00000 -0.01057 -0.00019 1.92004

A29 1.90523 0.00000 0.00000 0.00659 0.01392 1.91915

A30 1.85498 0.00000 0.00000 0.02620 0.02161 1.87658

A31 1.88349 0.00001 0.00000 -0.01200 -0.01374 1.86976

A32 1.87508 0.00000 0.00000 0.03717 0.03239 1.90747

A33 1.73801 0.00000 0.00000 0.01813 0.01822 1.75624

A34 1.56428 0.00000 0.00000 -0.01116 -0.00858 1.55570

A35 1.86734 -0.00001 0.00000 0.02707 0.02479 1.89213

A36 2.19881 0.00000 0.00000 -0.02067 -0.01704 2.18177

A37 2.10153 0.00001 0.00000 -0.02931 -0.03121 2.07032

A38 1.87523 0.00000 0.00000 -0.03689 -0.04204 1.83319

A39 1.73807 0.00000 0.00000 0.03099 0.03149 1.76956

A40 1.56418 0.00000 0.00000 0.02542 0.02664 1.59082

A41 1.86719 0.00001 0.00000 -0.02728 -0.02873 1.83847

A42 2.19872 0.00000 0.00000 -0.01903 -0.01454 2.18418

A43 2.10172 -0.00001 0.00000 0.03915 0.03665 2.13837

A44 1.90326 0.00000 0.00000 -0.01405 -0.01260 1.89065

A45 2.02637 0.00000 0.00000 0.02876 0.02767 2.05404

A46 2.35356 0.00000 0.00000 -0.01481 -0.01599 2.33757

A47 1.90335 -0.00002 0.00000 0.02516 0.02529 1.92864

A48 2.02619 0.00002 0.00000 -0.05527 -0.05535 1.97084

A49 2.35364 -0.00001 0.00000 0.03007 0.02992 2.38357

D1 -0.59984 0.00000 0.00000 0.03820 0.04378 -0.55606

D2 2.94919 0.00000 0.00000 -0.01900 -0.01643 2.93276

D3 1.19648 0.00000 0.00000 -0.05360 -0.05439 1.14208

D4 2.71096 0.00000 0.00000 -0.04207 -0.03804 2.67292

D5 -0.02319 0.00000 0.00000 -0.09927 -0.09825 -0.12145

D6 -1.77590 0.00000 0.00000 -0.13387 -0.13622 -1.91212

D7 -0.00015 0.00000 0.00000 0.12905 0.12907 0.12892

D8 -2.97317 0.00000 0.00000 0.21782 0.21535 -2.75783

D9 2.97288 0.00000 0.00000 0.20708 0.20957 -3.10073

D10 -0.00014 0.00000 0.00000 0.29585 0.29585 0.29570

D11 2.73782 0.00000 0.00000 -0.34038 -0.34472 2.39310

D12 -1.53215 -0.00001 0.00000 -0.38547 -0.38496 -1.91711

D13 0.57438 0.00000 0.00000 -0.35681 -0.35687 0.21752

D14 -0.79297 0.00000 0.00000 -0.28781 -0.29015 -1.08311

D15 1.22025 0.00000 0.00000 -0.33290 -0.33038 0.88987

D16 -2.95640 0.00000 0.00000 -0.30424 -0.30229 3.02449

D17 1.01206 0.00000 0.00000 -0.31104 -0.31267 0.69939

D18 3.02527 -0.00001 0.00000 -0.35613 -0.35290 2.67237

D19 -1.15138 -0.00001 0.00000 -0.32747 -0.32481 -1.47619

D20 -1.03596 0.00000 0.00000 -0.07029 -0.07234 -1.10830

D21 -2.97882 -0.00001 0.00000 -0.04180 -0.04025 -3.01907

D22 1.19560 0.00000 0.00000 -0.08945 -0.08768 1.10792

D23 1.07176 0.00000 0.00000 -0.02544 -0.03736 1.03441

D24 -0.87110 -0.00001 0.00000 0.00304 -0.00526 -0.87636

D25 -2.97987 0.00000 0.00000 -0.04460 -0.05269 -3.03256

D26 3.13109 0.00001 0.00000 -0.05599 -0.06064 3.07044

D27 1.18822 0.00000 0.00000 -0.02751 -0.02855 1.15968

D28 -0.92054 0.00001 0.00000 -0.07515 -0.07598 -0.99652

D29 0.59979 -0.00001 0.00000 0.00530 0.00034 0.60013

D30 -2.71104 0.00000 0.00000 -0.08662 -0.09052 -2.80156

D31 -2.94915 0.00000 0.00000 -0.02327 -0.02504 -2.97418

D32 0.02321 0.00000 0.00000 -0.11520 -0.11589 -0.09269

D33 -1.19639 0.00000 0.00000 -0.05711 -0.05652 -1.25291

D34 1.77597 0.00000 0.00000 -0.14904 -0.14738 1.62859

D35 -0.57359 0.00001 0.00000 -0.32749 -0.32482 -0.89840

D36 -2.73693 0.00000 0.00000 -0.31346 -0.31051 -3.04744

D37 1.53314 0.00000 0.00000 -0.33520 -0.33678 1.19636

D38 2.95717 0.00000 0.00000 -0.29532 -0.29367 2.66350

D39 0.79383 -0.00001 0.00000 -0.28129 -0.27936 0.51447

D40 -1.21929 -0.00001 0.00000 -0.30304 -0.30564 -1.52492

D41 1.15211 0.00000 0.00000 -0.31071 -0.30897 0.84314

D42 -1.01123 0.00000 0.00000 -0.29668 -0.29467 -1.30589

D43 -3.02435 0.00000 0.00000 -0.31843 -0.32094 2.93790

D44 1.03642 0.00000 0.00000 -0.06068 -0.05881 0.97761

D45 2.97937 -0.00001 0.00000 -0.01254 -0.01277 2.96660

D46 -1.19523 -0.00001 0.00000 -0.04286 -0.04467 -1.23990

D47 -1.07140 0.00000 0.00000 -0.04199 -0.03140 -1.10281

D48 0.87155 -0.00001 0.00000 0.00615 0.01464 0.88618

D49 2.98013 0.00000 0.00000 -0.02416 -0.01726 2.96287

D50 -3.13079 0.00000 0.00000 -0.07137 -0.06725 3.08514

D51 -1.18784 0.00000 0.00000 -0.02323 -0.02122 -1.20905

D52 0.92074 0.00000 0.00000 -0.05355 -0.05312 0.86763

D53 -0.00056 0.00000 0.00000 0.46287 0.45708 0.45652

D54 2.16493 0.00000 0.00000 0.45640 0.45149 2.61641

D55 -2.08905 0.00001 0.00000 0.48581 0.48590 -1.60316

D56 -2.16601 -0.00001 0.00000 0.46387 0.46360 -1.70241

D57 -0.00052 0.00000 0.00000 0.45741 0.45801 0.45749

D58 2.02868 0.00000 0.00000 0.48682 0.49242 2.52111

D59 2.08781 0.00000 0.00000 0.51327 0.50774 2.59554

D60 -2.02989 0.00000 0.00000 0.50680 0.50215 -1.52775

D61 -0.00069 0.00000 0.00000 0.53621 0.53656 0.53587

D62 -0.01616 0.00000 0.00000 -0.04105 -0.03894 -0.05511

D63 3.12308 0.00000 0.00000 -0.07785 -0.07632 3.04676

D64 0.01604 0.00000 0.00000 0.07834 0.07753 0.09357

D65 -3.12330 0.00000 0.00000 0.09282 0.09040 -3.03290

D66 -0.00026 -0.00001 0.00000 0.09726 0.09693 0.09666

D67 1.85269 0.00000 0.00000 0.10570 0.10447 1.95716

D68 -1.79239 0.00000 0.00000 0.10281 0.10214 -1.69024

D69 -1.85315 -0.00001 0.00000 0.05040 0.05077 -1.80239

D70 -0.00020 0.00000 0.00000 0.05884 0.05831 0.05811

D71 2.63791 0.00000 0.00000 0.05595 0.05599 2.69389

D72 1.79190 0.00000 0.00000 0.10271 0.10312 1.89502

D73 -2.63832 0.00000 0.00000 0.11115 0.11066 -2.52767

D74 -0.00022 0.00000 0.00000 0.10826 0.10833 0.10811

D75 -1.93897 0.00000 0.00000 -0.06879 -0.06558 -2.00454

D76 1.20560 0.00000 0.00000 -0.02227 -0.01970 1.18590

D77 0.01007 0.00000 0.00000 -0.01294 -0.01402 -0.00395

D78 -3.12854 0.00000 0.00000 0.03358 0.03185 -3.09669

D79 2.68189 0.00000 0.00000 -0.06003 -0.05902 2.62287

D80 -0.45672 0.00000 0.00000 -0.01351 -0.01315 -0.46987

D81 1.93945 0.00000 0.00000 -0.12272 -0.12793 1.81151

D82 -1.20500 0.00000 0.00000 -0.14122 -0.14534 -1.35034

D83 -0.00974 0.00000 0.00000 -0.08655 -0.08544 -0.09518

D84 3.12900 0.00000 0.00000 -0.10505 -0.10284 3.02615

D85 -2.68145 0.00000 0.00000 -0.06520 -0.06619 -2.74764

D86 0.45729 0.00000 0.00000 -0.08370 -0.08359 0.37370

Item Value Threshold Converged?

Maximum Force 0.000037 0.000450 YES

RMS Force 0.000007 0.000300 YES

Maximum Displacement 0.937807 0.001800 NO

RMS Displacement 0.171804 0.001200 NO

Predicted change in Energy= 5.642566D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.168335 1.577354 0.372370

2 6 0 0.157093 1.311024 0.050074

3 6 0 -0.776262 3.800721 -0.353853

4 6 0 -1.635840 2.898949 0.239195

5 1 0 -1.807159 0.787832 0.800127

6 1 0 -2.519808 3.225858 0.801157

7 6 0 0.882011 2.060175 -1.007887

8 1 0 1.922019 2.314222 -0.656920

9 1 0 1.068317 1.394401 -1.898999

10 6 0 0.117480 3.297964 -1.442134

11 1 0 0.833681 4.093806 -1.776596

12 1 0 -0.547996 3.051668 -2.316399

13 1 0 -1.011379 4.879305 -0.347606

14 1 0 0.599265 0.337687 0.331791

15 8 0 2.812595 3.734367 0.797820

16 6 0 0.525438 3.832856 1.377069

17 6 0 0.941491 2.524939 1.668484

18 6 0 1.702793 4.595084 0.825264

19 8 0 1.871409 5.749656 0.466485

20 6 0 2.400412 2.500923 1.373491

21 8 0 3.319689 1.711340 1.513662

22 1 0 -0.244920 4.383394 1.925511

23 1 0 0.481604 1.869482 2.412350

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.389808 0.000000

3 C 2.371599 2.689406 0.000000

4 C 1.408158 2.402474 1.379773 0.000000

5 H 1.102006 2.166701 3.387022 2.191074 0.000000

6 H 2.174374 3.375872 2.168978 1.097302 2.540047

7 C 2.518362 1.485267 2.491412 2.932291 3.481294

8 H 3.339566 2.149701 3.095521 3.715278 4.284813

9 H 3.192992 2.153176 3.402988 3.761383 3.990184

10 C 2.811805 2.485194 1.495291 2.461749 3.877207

11 H 3.867642 3.396818 2.168413 3.404355 4.954089

12 H 3.128562 3.021124 2.113000 2.781687 4.052552

13 H 3.383176 3.775726 1.103930 2.157799 4.323275

14 H 2.159358 1.105561 3.788771 3.400636 2.492558

15 O 4.547694 3.671976 3.769702 4.560544 5.479435

16 C 2.994257 2.873366 2.165998 2.614969 3.878922

17 C 2.651262 2.169820 2.944171 2.970755 3.365510

18 C 4.189891 3.711491 2.857805 3.790360 5.178375

19 O 5.163042 4.776372 3.388431 4.525371 6.185699

20 C 3.819840 2.863525 3.842454 4.211458 4.578983

21 O 4.632802 3.507757 4.962856 5.252804 5.258001

22 H 3.337485 3.621924 2.411914 2.642328 4.078621

23 H 2.639916 2.448985 3.600526 3.204055 3.001277

6 7 8 9 10

6 H 0.000000

7 C 4.025399 0.000000

8 H 4.763077 1.126647 0.000000

9 H 4.849713 1.127849 1.765683 0.000000

10 C 3.463068 1.518289 2.200153 2.176321 0.000000

11 H 4.317874 2.174604 2.367503 2.712347 1.121683

12 H 3.692903 2.177196 3.065725 2.352281 1.125992

13 H 2.515731 3.459536 3.908983 4.344711 2.230011

14 H 4.276734 2.200374 2.575640 2.512583 3.484561

15 O 5.356596 3.129002 2.219506 3.973761 3.531499

16 C 3.158108 2.992918 2.897205 4.119879 2.898352

17 C 3.636501 2.717076 2.532457 3.744480 3.309457

18 C 4.439113 3.234176 2.728967 4.250711 3.055623

19 O 5.075859 4.094503 3.614803 5.020828 3.567896

20 C 5.006162 2.858454 2.094347 3.702439 3.711441

21 O 6.074632 3.524510 2.651109 4.100656 4.637699

22 H 2.789118 3.907959 3.955508 5.028473 3.556757

23 H 3.666629 3.448871 3.419505 4.376947 4.126766

11 12 13 14 15

11 H 0.000000

12 H 1.812863 0.000000

13 H 2.462370 2.726009 0.000000

14 H 4.313777 3.961667 4.866420 0.000000

15 O 3.266942 4.632279 4.152789 4.080864 0.000000

16 C 3.179420 3.924821 2.536014 3.648871 2.361423

17 C 3.787022 4.286642 3.663517 2.586105 2.392029

18 C 2.788603 4.161518 2.970376 4.425689 1.404723

19 O 2.974917 4.569146 3.119410 5.561106 2.248778

20 C 3.861990 4.755178 4.501021 3.001477 1.422208

21 O 4.762581 5.605786 5.679654 3.268708 2.205043

22 H 3.866889 4.456360 2.449580 4.429485 3.322848

23 H 4.755927 4.981837 4.348032 2.586304 3.393822

16 17 18 19 20

16 C 0.000000

17 C 1.403093 0.000000

18 C 1.507199 2.361378 0.000000

19 O 2.512951 3.564877 1.220733 0.000000

20 C 2.299909 1.488640 2.274365 3.414201 0.000000

21 O 3.511029 2.518281 3.377014 4.416117 1.219902

22 H 1.094227 2.219795 2.246985 2.911060 3.293357

23 H 2.220037 1.092912 3.382167 4.557817 2.271513

21 22 23

21 O 0.000000

22 H 4.473916 0.000000

23 H 2.981170 2.661692 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.259832 -0.948783 -0.550111

2 6 0 1.250866 -1.419039 0.282002

3 6 0 1.531952 1.240600 -0.001223

4 6 0 2.356530 0.439627 -0.764300

5 1 0 2.910305 -1.654984 -1.091019

6 1 0 2.870848 0.821276 -1.655307

7 6 0 0.746638 -0.635049 1.438346

8 1 0 -0.377715 -0.692016 1.482159

9 1 0 1.065126 -1.118935 2.406056

10 6 0 1.235279 0.801870 1.397131

11 1 0 0.482019 1.477475 1.881207

12 1 0 2.197051 0.897497 1.974807

13 1 0 1.440461 2.317597 -0.225650

14 1 0 1.029757 -2.501935 0.308645

15 8 0 -2.064927 0.158197 0.317401

16 6 0 -0.230935 0.620674 -1.096426

17 6 0 -0.338514 -0.777469 -1.048553

18 6 0 -1.316253 1.211433 -0.233444

19 8 0 -1.668957 2.351966 0.021450

20 6 0 -1.544303 -1.051428 -0.219658

21 8 0 -2.197983 -2.031708 0.096435

22 1 0 0.123408 1.193829 -1.958555

23 1 0 0.007121 -1.462075 -1.827210

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2422903 0.8649372 0.6681089

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5294474082 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.400987508554E-01 A.U. after 16 cycles

Convg = 0.6268D-08 -V/T = 0.9991

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.006209330 -0.000213429 -0.004562781

2 6 0.001348307 -0.009475182 0.001241989

3 6 0.002884885 0.014307035 -0.009483262

4 6 0.000960115 -0.016592714 0.011684020

5 1 0.001938845 0.003497290 0.003773074

6 1 -0.003836760 -0.000499494 -0.003313786

7 6 0.000861237 -0.002835036 -0.009192683

8 1 -0.002397452 0.000941593 -0.008173903

9 1 -0.005116330 -0.000352474 0.000800114

10 6 0.003163218 0.004523631 0.003699845

11 1 -0.000183419 0.000123425 0.001042098

12 1 0.001790138 -0.000176729 -0.000728164

13 1 0.001846081 -0.000733678 -0.001591758

14 1 -0.000360638 0.001214150 -0.000348381

15 8 -0.008464537 0.002852524 0.006257839

16 6 0.002032501 0.015442762 0.000521099

17 6 0.007637914 0.008238134 0.003059775

18 6 -0.008410674 -0.006592471 0.005654170

19 8 0.000420509 -0.003802562 -0.000996662

20 6 0.011024403 -0.002394997 0.000920761

21 8 -0.002375636 -0.006091378 0.002508488

22 1 -0.001464001 0.000036751 -0.001854260

23 1 0.002910624 -0.001417151 -0.000917632

-------------------------------------------------------------------

Cartesian Forces: Max 0.016592714 RMS 0.005422228

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.013397393 RMS 0.003392953

Search for a saddle point.

Step number 67 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 66 67

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0

Eigenvalues --- -0.07154 0.00100 0.00506 0.00758 0.00816

Eigenvalues --- 0.01009 0.01180 0.01334 0.01834 0.02189

Eigenvalues --- 0.02466 0.02791 0.02882 0.03194 0.03343

Eigenvalues --- 0.03563 0.03604 0.03782 0.04003 0.04087

Eigenvalues --- 0.04380 0.04385 0.04683 0.04848 0.06211

Eigenvalues --- 0.06514 0.06663 0.07095 0.07399 0.08521

Eigenvalues --- 0.08742 0.10049 0.10242 0.10753 0.10932

Eigenvalues --- 0.12135 0.13464 0.14447 0.15813 0.22747

Eigenvalues --- 0.26235 0.28329 0.29362 0.30061 0.30957

Eigenvalues --- 0.31387 0.31841 0.32020 0.32227 0.32500

Eigenvalues --- 0.33362 0.34839 0.36484 0.37684 0.39709

Eigenvalues --- 0.40174 0.40665 0.44510 0.48616 0.53392

Eigenvalues --- 0.62288 1.08681 1.11222

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 0.56203 0.51658 0.15253 -0.14528 -0.14321

D1 D4 R19 D29 D13

1 0.14040 0.13565 -0.13435 -0.12991 -0.12986

RFO step: Lambda0=1.873735666D-04 Lambda=-1.29316095D-02.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.05722072 RMS(Int)= 0.00176840

Iteration 2 RMS(Cart)= 0.00219022 RMS(Int)= 0.00043346

Iteration 3 RMS(Cart)= 0.00000249 RMS(Int)= 0.00043345

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00043345

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62636 0.00202 0.00000 0.00962 0.00928 2.63564

R2 2.66103 -0.00600 0.00000 -0.02412 -0.02429 2.63674

R3 2.08249 -0.00216 0.00000 -0.00625 -0.00625 2.07624

R4 2.80675 0.00893 0.00000 0.01423 0.01391 2.82066

R5 2.08921 -0.00130 0.00000 -0.00627 -0.00627 2.08294

R6 4.10037 0.01268 0.00000 0.04369 0.04356 4.14392

R7 2.60739 0.01340 0.00000 0.04437 0.04454 2.65193

R8 2.82569 0.00088 0.00000 -0.00741 -0.00680 2.81889

R9 2.08613 -0.00112 0.00000 -0.00653 -0.00653 2.07960

R10 4.09314 0.00432 0.00000 -0.04691 -0.04694 4.04620

R11 2.07360 0.00124 0.00000 0.00295 0.00295 2.07655

R12 2.12905 -0.00455 0.00000 -0.01045 -0.01045 2.11861

R13 2.13133 -0.00127 0.00000 -0.00575 -0.00575 2.12558

R14 2.86915 0.00043 0.00000 0.00193 0.00240 2.87155

R15 2.11967 -0.00034 0.00000 -0.00057 -0.00057 2.11910

R16 2.12782 -0.00045 0.00000 0.00188 0.00188 2.12970

R17 2.65454 -0.00129 0.00000 0.00698 0.00685 2.66139

R18 2.68758 -0.00300 0.00000 -0.02048 -0.02064 2.66694

R19 2.65146 0.00977 0.00000 0.02280 0.02274 2.67420

R20 2.84819 -0.01335 0.00000 -0.04057 -0.04049 2.80770

R21 2.06779 0.00012 0.00000 0.00060 0.00060 2.06839

R22 2.81312 -0.00095 0.00000 -0.00517 -0.00512 2.80800

R23 2.06530 -0.00100 0.00000 -0.00261 -0.00261 2.06269

R24 2.30685 -0.00325 0.00000 -0.00128 -0.00128 2.30557

R25 2.30528 0.00244 0.00000 0.00080 0.00080 2.30608

A1 2.06524 0.00175 0.00000 0.00748 0.00657 2.07181

A2 2.10083 0.00032 0.00000 0.00098 0.00108 2.10191

A3 2.11373 -0.00211 0.00000 -0.01156 -0.01143 2.10230

A4 2.13411 -0.00202 0.00000 -0.01985 -0.02003 2.11408

A5 2.08409 -0.00026 0.00000 0.00842 0.00819 2.09227

A6 1.63542 -0.00487 0.00000 -0.04455 -0.04335 1.59207

A7 2.01569 0.00160 0.00000 0.00483 0.00504 2.02073

A8 1.64353 0.00738 0.00000 0.06448 0.06334 1.70687

A9 1.72936 -0.00033 0.00000 0.00082 0.00052 1.72988

A10 2.05492 -0.00273 0.00000 -0.01758 -0.01789 2.03704

A11 2.09838 0.00279 0.00000 0.02293 0.02266 2.12104

A12 1.61142 -0.00550 0.00000 -0.00803 -0.00764 1.60378

A13 2.04871 -0.00050 0.00000 -0.01696 -0.01682 2.03189

A14 1.80020 0.00776 0.00000 0.02652 0.02636 1.82656

A15 1.67999 -0.00096 0.00000 0.01120 0.01131 1.69130

A16 2.03444 0.00096 0.00000 0.01195 0.01131 2.04575

A17 2.09281 -0.00013 0.00000 0.01399 0.01383 2.10664

A18 2.12619 -0.00042 0.00000 -0.01400 -0.01440 2.11179

A19 1.92025 0.00386 0.00000 0.01615 0.01667 1.93692

A20 1.92375 -0.00111 0.00000 -0.01121 -0.01040 1.91335

A21 1.94890 0.00035 0.00000 0.01520 0.01316 1.96207

A22 1.79954 0.00018 0.00000 0.02248 0.02210 1.82163

A23 1.94990 -0.00509 0.00000 -0.04469 -0.04397 1.90594

A24 1.91607 0.00179 0.00000 0.00211 0.00274 1.91880

A25 1.94650 0.00146 0.00000 0.02001 0.01870 1.96519

A26 1.93917 0.00118 0.00000 0.00057 0.00082 1.93999

A27 1.86021 -0.00147 0.00000 -0.01506 -0.01484 1.84537

A28 1.92004 -0.00036 0.00000 0.01221 0.01230 1.93234

A29 1.91915 -0.00109 0.00000 -0.02601 -0.02547 1.89367

A30 1.87658 0.00019 0.00000 0.00633 0.00624 1.88283

A31 1.86976 0.00490 0.00000 0.01660 0.01615 1.88591

A32 1.90747 0.00043 0.00000 0.00632 0.00634 1.91381

A33 1.75624 0.00316 0.00000 0.02740 0.02750 1.78374

A34 1.55570 -0.00237 0.00000 -0.01741 -0.01730 1.53841

A35 1.89213 -0.00388 0.00000 -0.03095 -0.03113 1.86100

A36 2.18177 0.00293 0.00000 0.00871 0.00890 2.19067

A37 2.07032 0.00063 0.00000 0.01685 0.01681 2.08712

A38 1.83319 -0.00219 0.00000 -0.00242 -0.00313 1.83007

A39 1.76956 0.00371 0.00000 0.00111 0.00135 1.77091

A40 1.59082 -0.00149 0.00000 -0.00830 -0.00825 1.58257

A41 1.83847 0.00348 0.00000 0.03314 0.03283 1.87130

A42 2.18418 0.00167 0.00000 0.01818 0.01881 2.20299

A43 2.13837 -0.00520 0.00000 -0.04779 -0.04804 2.09033

A44 1.89065 0.00253 0.00000 0.01570 0.01560 1.90625

A45 2.05404 -0.00288 0.00000 -0.03136 -0.03133 2.02271

A46 2.33757 0.00034 0.00000 0.01616 0.01616 2.35373

A47 1.92864 -0.00692 0.00000 -0.03090 -0.03108 1.89755

A48 1.97084 0.01101 0.00000 0.06726 0.06735 2.03819

A49 2.38357 -0.00410 0.00000 -0.03629 -0.03620 2.34737

D1 -0.55606 -0.00176 0.00000 -0.01447 -0.01414 -0.57020

D2 2.93276 0.00028 0.00000 0.00693 0.00706 2.93982

D3 1.14208 0.00360 0.00000 0.03074 0.03072 1.17280

D4 2.67292 -0.00116 0.00000 0.02600 0.02624 2.69916

D5 -0.12145 0.00088 0.00000 0.04740 0.04743 -0.07401

D6 -1.91212 0.00420 0.00000 0.07121 0.07109 -1.84103

D7 0.12892 -0.00110 0.00000 -0.04752 -0.04749 0.08143

D8 -2.75783 -0.00277 0.00000 -0.09547 -0.09614 -2.85397

D9 -3.10073 -0.00158 0.00000 -0.08764 -0.08722 3.09523

D10 0.29570 -0.00325 0.00000 -0.13559 -0.13587 0.15984

D11 2.39310 0.00082 0.00000 0.05392 0.05349 2.44659

D12 -1.91711 0.00256 0.00000 0.08368 0.08361 -1.83350

D13 0.21752 0.00430 0.00000 0.08894 0.08877 0.30629

D14 -1.08311 -0.00146 0.00000 0.03421 0.03397 -1.04915

D15 0.88987 0.00029 0.00000 0.06397 0.06408 0.95395

D16 3.02449 0.00203 0.00000 0.06923 0.06924 3.09374

D17 0.69939 0.00217 0.00000 0.06844 0.06843 0.76782

D18 2.67237 0.00391 0.00000 0.09820 0.09855 2.77092

D19 -1.47619 0.00565 0.00000 0.10346 0.10371 -1.37248

D20 -1.10830 -0.00079 0.00000 -0.02174 -0.02173 -1.13003

D21 -3.01907 -0.00519 0.00000 -0.05720 -0.05675 -3.07582

D22 1.10792 -0.00004 0.00000 -0.00593 -0.00538 1.10254

D23 1.03441 -0.00254 0.00000 -0.03953 -0.04116 0.99325

D24 -0.87636 -0.00695 0.00000 -0.07498 -0.07618 -0.95254

D25 -3.03256 -0.00179 0.00000 -0.02372 -0.02482 -3.05737

D26 3.07044 0.00063 0.00000 -0.02055 -0.02102 3.04943

D27 1.15968 -0.00378 0.00000 -0.05601 -0.05604 1.10364

D28 -0.99652 0.00138 0.00000 -0.00474 -0.00467 -1.00119

D29 0.60013 0.00142 0.00000 0.03201 0.03197 0.63210

D30 -2.80156 0.00317 0.00000 0.08545 0.08522 -2.71634

D31 -2.97418 0.00015 0.00000 -0.00171 -0.00203 -2.97621

D32 -0.09269 0.00190 0.00000 0.05173 0.05123 -0.04146

D33 -1.25291 -0.00388 0.00000 0.00952 0.00955 -1.24336

D34 1.62859 -0.00213 0.00000 0.06296 0.06280 1.69139

D35 -0.89840 0.00184 0.00000 0.04807 0.04823 -0.85017

D36 -3.04744 0.00042 0.00000 0.01748 0.01769 -3.02975

D37 1.19636 0.00043 0.00000 0.01839 0.01843 1.21478

D38 2.66350 0.00223 0.00000 0.07080 0.07049 2.73399

D39 0.51447 0.00080 0.00000 0.04021 0.03996 0.55442

D40 -1.52492 0.00081 0.00000 0.04112 0.04069 -1.48423

D41 0.84314 -0.00107 0.00000 0.04809 0.04806 0.89120

D42 -1.30589 -0.00250 0.00000 0.01750 0.01753 -1.28837

D43 2.93790 -0.00248 0.00000 0.01841 0.01826 2.95616

D44 0.97761 0.00081 0.00000 -0.02107 -0.02079 0.95682

D45 2.96660 -0.00190 0.00000 -0.04065 -0.04043 2.92617

D46 -1.23990 -0.00147 0.00000 -0.02466 -0.02461 -1.26451

D47 -1.10281 0.00388 0.00000 -0.00512 -0.00446 -1.10727

D48 0.88618 0.00117 0.00000 -0.02470 -0.02410 0.86208

D49 2.96287 0.00160 0.00000 -0.00871 -0.00828 2.95458

D50 3.08514 0.00269 0.00000 0.00218 0.00225 3.08739

D51 -1.20905 -0.00002 0.00000 -0.01740 -0.01739 -1.22645

D52 0.86763 0.00041 0.00000 -0.00141 -0.00157 0.86605

D53 0.45652 -0.00295 0.00000 -0.08959 -0.09020 0.36632

D54 2.61641 -0.00068 0.00000 -0.06604 -0.06634 2.55007

D55 -1.60316 -0.00133 0.00000 -0.06668 -0.06690 -1.67005

D56 -1.70241 -0.00449 0.00000 -0.08881 -0.08894 -1.79134

D57 0.45749 -0.00221 0.00000 -0.06527 -0.06508 0.39241

D58 2.52111 -0.00287 0.00000 -0.06591 -0.06564 2.45547

D59 2.59554 -0.00287 0.00000 -0.09203 -0.09251 2.50303

D60 -1.52775 -0.00060 0.00000 -0.06849 -0.06866 -1.59640

D61 0.53587 -0.00125 0.00000 -0.06913 -0.06921 0.46666

D62 -0.05511 0.00141 0.00000 0.04555 0.04662 -0.00848

D63 3.04676 0.00100 0.00000 0.05681 0.05764 3.10440

D64 0.09357 -0.00154 0.00000 -0.04551 -0.04508 0.04849

D65 -3.03290 -0.00097 0.00000 -0.04866 -0.04864 -3.08154

D66 0.09666 -0.00202 0.00000 0.01343 0.01310 0.10976

D67 1.95716 0.00252 0.00000 0.02576 0.02547 1.98263

D68 -1.69024 0.00090 0.00000 0.01826 0.01827 -1.67198

D69 -1.80239 -0.00401 0.00000 -0.00637 -0.00648 -1.80886

D70 0.05811 0.00052 0.00000 0.00596 0.00589 0.06400

D71 2.69389 -0.00109 0.00000 -0.00153 -0.00131 2.69259

D72 1.89502 -0.00329 0.00000 -0.00010 -0.00019 1.89483

D73 -2.52767 0.00125 0.00000 0.01223 0.01218 -2.51549

D74 0.10811 -0.00037 0.00000 0.00474 0.00498 0.11310

D75 -2.00454 -0.00178 0.00000 -0.04089 -0.04012 -2.04466

D76 1.18590 -0.00118 0.00000 -0.05317 -0.05254 1.13337

D77 -0.00395 -0.00127 0.00000 -0.03258 -0.03241 -0.03636

D78 -3.09669 -0.00067 0.00000 -0.04485 -0.04483 -3.14151

D79 2.62287 -0.00096 0.00000 -0.04004 -0.03989 2.58298

D80 -0.46987 -0.00036 0.00000 -0.05231 -0.05231 -0.52218

D81 1.81151 0.00086 0.00000 0.03182 0.03117 1.84268

D82 -1.35034 0.00028 0.00000 0.03739 0.03695 -1.31338

D83 -0.09518 0.00081 0.00000 0.02379 0.02363 -0.07155

D84 3.02615 0.00023 0.00000 0.02936 0.02942 3.05558

D85 -2.74764 -0.00003 0.00000 0.00796 0.00814 -2.73950

D86 0.37370 -0.00060 0.00000 0.01353 0.01393 0.38763

Item Value Threshold Converged?

Maximum Force 0.013397 0.000450 NO

RMS Force 0.003393 0.000300 NO

Maximum Displacement 0.332046 0.001800 NO

RMS Displacement 0.056918 0.001200 NO

Predicted change in Energy=-8.063961D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.124806 1.570977 0.395489

2 6 0 0.196953 1.307691 0.036500

3 6 0 -0.762346 3.811344 -0.350476

4 6 0 -1.613226 2.869703 0.248423

5 1 0 -1.729108 0.802170 0.896376

6 1 0 -2.535597 3.183152 0.756831

7 6 0 0.853096 2.042858 -1.084633

8 1 0 1.916518 2.292926 -0.832632

9 1 0 0.929750 1.370906 -1.983407

10 6 0 0.113504 3.318237 -1.452693

11 1 0 0.832680 4.112243 -1.784101

12 1 0 -0.576925 3.095052 -2.315016

13 1 0 -1.009412 4.883644 -0.363875

14 1 0 0.661743 0.348656 0.317867

15 8 0 2.822231 3.741324 0.915763

16 6 0 0.509895 3.861835 1.370978

17 6 0 0.940894 2.550524 1.682889

18 6 0 1.699966 4.590399 0.860646

19 8 0 1.907527 5.722128 0.454889

20 6 0 2.407639 2.502513 1.449785

21 8 0 3.275032 1.662994 1.628745

22 1 0 -0.278315 4.413188 1.893246

23 1 0 0.485903 1.878543 2.412864

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394719 0.000000

3 C 2.388951 2.708927 0.000000

4 C 1.395304 2.400321 1.403340 0.000000

5 H 1.098696 2.169021 3.397705 2.169785 0.000000

6 H 2.172558 3.391616 2.182927 1.098862 2.517732

7 C 2.515060 1.492627 2.505232 2.922919 3.483028

8 H 3.358444 2.164020 3.116791 3.736368 4.301443

9 H 3.149662 2.149654 3.389010 3.700565 3.960572

10 C 2.828799 2.503389 1.491694 2.465071 3.904349

11 H 3.878195 3.403565 2.165624 3.414310 4.970342

12 H 3.157502 3.053388 2.099256 2.774153 4.110703

13 H 3.400546 3.795136 1.100476 2.189853 4.331816

14 H 2.166068 1.102245 3.803277 3.396466 2.501303

15 O 4.534335 3.686158 3.802296 4.569282 5.417905

16 C 2.978566 2.898692 2.141156 2.598479 3.820986

17 C 2.623744 2.192870 2.936880 2.946709 3.286984

18 C 4.160843 3.703301 2.852494 3.783233 5.109844

19 O 5.141072 4.752722 3.380522 4.535929 6.134005

20 C 3.802298 2.883073 3.873343 4.212535 4.506674

21 O 4.570335 3.483684 4.983287 5.220776 5.130186

22 H 3.322347 3.649315 2.372928 2.621025 4.017214

23 H 2.599766 2.460989 3.595816 3.173884 2.892160

6 7 8 9 10

6 H 0.000000

7 C 4.021753 0.000000

8 H 4.810428 1.121118 0.000000

9 H 4.775119 1.124806 1.774293 0.000000

10 C 3.452243 1.519558 2.164855 2.177157 0.000000

11 H 4.320282 2.184497 2.321619 2.750286 1.121379

12 H 3.644229 2.160073 3.009673 2.313593 1.126990

13 H 2.544974 3.472535 3.936067 4.326957 2.212909

14 H 4.295351 2.207700 2.584239 2.532327 3.500551

15 O 5.389168 3.280833 2.444393 4.195897 3.622953

16 C 3.180064 3.075141 3.048928 4.199155 2.902713

17 C 3.652916 2.815069 2.710358 3.851408 3.332541

18 C 4.464428 3.315308 2.862249 4.364287 3.080064

19 O 5.126297 4.125407 3.662952 5.082762 3.554726

20 C 5.037761 3.008515 2.344046 3.905317 3.788514

21 O 6.069145 3.656842 2.881102 4.316631 4.714907

22 H 2.810650 3.970683 4.091847 5.073789 3.542279

23 H 3.684279 3.520556 3.570940 4.447683 4.141730

11 12 13 14 15

11 H 0.000000

12 H 1.817563 0.000000

13 H 2.450593 2.681988 0.000000

14 H 4.314171 4.001133 4.880947 0.000000

15 O 3.374190 4.733906 4.198078 4.066372 0.000000

16 C 3.181418 3.918633 2.522321 3.670766 2.359797

17 C 3.804036 4.310862 3.665567 2.605654 2.354976

18 C 2.824093 4.183913 2.987670 4.400556 1.408348

19 O 2.959747 4.554822 3.143559 5.517694 2.229948

20 C 3.940780 4.840708 4.542619 2.994744 1.411283

21 O 4.859158 5.695754 5.718355 3.205490 2.243396

22 H 3.853278 4.419968 2.418765 4.459366 3.319677

23 H 4.766989 4.996233 4.356246 2.600093 3.342109

16 17 18 19 20

16 C 0.000000

17 C 1.415127 0.000000

18 C 1.485770 2.326663 0.000000

19 O 2.500657 3.535736 1.220054 0.000000

20 C 2.335680 1.485929 2.281919 3.406736 0.000000

21 O 3.542221 2.497767 3.411819 4.441235 1.220323

22 H 1.094545 2.236121 2.238584 2.925764 3.325912

23 H 2.240435 1.091531 3.352237 4.541787 2.238287

21 22 23

21 O 0.000000

22 H 4.501089 0.000000

23 H 2.905262 2.697862 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.188938 -1.010657 -0.587341

2 6 0 1.218422 -1.429755 0.322437

3 6 0 1.543132 1.230681 -0.071176

4 6 0 2.329243 0.355139 -0.835912

5 1 0 2.745993 -1.745486 -1.184710

6 1 0 2.875812 0.711213 -1.720203

7 6 0 0.854945 -0.592348 1.503355

8 1 0 -0.250897 -0.615070 1.686392

9 1 0 1.301286 -1.038317 2.434526

10 6 0 1.306899 0.850503 1.351782

11 1 0 0.577980 1.548000 1.841340

12 1 0 2.300987 0.970061 1.869083

13 1 0 1.479996 2.303444 -0.308328

14 1 0 0.958044 -2.498399 0.394176

15 8 0 -2.094477 0.186336 0.295701

16 6 0 -0.241121 0.635461 -1.094263

17 6 0 -0.388315 -0.769815 -1.016054

18 6 0 -1.304433 1.222581 -0.238593

19 8 0 -1.641647 2.356884 0.058349

20 6 0 -1.592241 -1.040556 -0.188258

21 8 0 -2.204394 -2.048017 0.127142

22 1 0 0.117240 1.189638 -1.967472

23 1 0 -0.075109 -1.494118 -1.770194

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2254408 0.8590886 0.6642633

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 469.2395877009 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.463549852080E-01 A.U. after 15 cycles

Convg = 0.7517D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.003456869 -0.000918099 -0.003105562

2 6 0.004934133 0.001333540 0.000382701

3 6 -0.001969766 -0.003489007 0.003260546

4 6 0.004349922 0.002971338 0.000882689

5 1 0.000475239 0.000185372 0.002578836

6 1 -0.001197918 -0.000616042 -0.002135874

7 6 -0.000442234 0.000349503 0.000157453

8 1 0.002451947 -0.000617620 0.001648260

9 1 -0.003806075 -0.000812263 0.000349592

10 6 -0.000787330 0.000151173 0.000478900

11 1 0.000252214 -0.000660504 0.001195122

12 1 0.001690856 0.001601504 -0.002214860

13 1 -0.000909152 0.000069137 0.000217895

14 1 0.000543230 0.000418003 0.000364015

15 8 0.002855500 -0.002150462 0.000516571

16 6 -0.002015254 -0.001426821 -0.000603380

17 6 -0.002713214 -0.000667756 -0.001245175

18 6 0.002173829 0.001655101 0.001220576

19 8 -0.000344162 0.000974238 -0.001656413

20 6 -0.001972783 0.000378337 -0.001851677

21 8 0.000401802 0.001514018 -0.001296039

22 1 0.000230029 -0.000394443 0.000498062

23 1 -0.000743944 0.000151753 0.000357762

-------------------------------------------------------------------

Cartesian Forces: Max 0.004934133 RMS 0.001748412

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.003297148 RMS 0.000917107

Search for a saddle point.

Step number 68 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 67 68

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07217 -0.00246 0.00457 0.00757 0.00813

Eigenvalues --- 0.00937 0.01186 0.01331 0.01835 0.02180

Eigenvalues --- 0.02461 0.02799 0.02883 0.03213 0.03340

Eigenvalues --- 0.03590 0.03615 0.03800 0.04038 0.04099

Eigenvalues --- 0.04385 0.04445 0.04718 0.04878 0.06300

Eigenvalues --- 0.06547 0.06662 0.07119 0.07490 0.08557

Eigenvalues --- 0.08771 0.10092 0.10308 0.10823 0.10926

Eigenvalues --- 0.12317 0.13855 0.14997 0.15890 0.22791

Eigenvalues --- 0.26275 0.28472 0.29436 0.30121 0.31011

Eigenvalues --- 0.31405 0.31852 0.32038 0.32229 0.32538

Eigenvalues --- 0.33435 0.35186 0.36657 0.37812 0.39729

Eigenvalues --- 0.40222 0.40698 0.44652 0.48777 0.53437

Eigenvalues --- 0.62338 1.08701 1.11239

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D30 D73

1 0.56038 0.51764 0.15258 -0.14829 -0.14435

D1 D13 R19 D29 D4

1 0.13871 -0.13565 -0.13469 -0.13152 0.13055

RFO step: Lambda0=4.298441906D-05 Lambda=-6.75930021D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.09075801 RMS(Int)= 0.00930573

Iteration 2 RMS(Cart)= 0.00812728 RMS(Int)= 0.00104772

Iteration 3 RMS(Cart)= 0.00011957 RMS(Int)= 0.00104121

Iteration 4 RMS(Cart)= 0.00000006 RMS(Int)= 0.00104121

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63564 0.00179 0.00000 0.00567 0.00573 2.64137

R2 2.63674 0.00041 0.00000 0.00626 0.00633 2.64307

R3 2.07624 0.00078 0.00000 0.00420 0.00420 2.08044

R4 2.82066 -0.00295 0.00000 -0.00705 -0.00690 2.81375

R5 2.08294 -0.00004 0.00000 -0.00137 -0.00137 2.08157

R6 4.14392 -0.00309 0.00000 -0.01996 -0.01919 4.12474

R7 2.65193 -0.00290 0.00000 -0.02659 -0.02659 2.62534

R8 2.81889 0.00083 0.00000 -0.00054 -0.00115 2.81774

R9 2.07960 0.00027 0.00000 0.00326 0.00326 2.08286

R10 4.04620 -0.00133 0.00000 0.05323 0.05273 4.09893

R11 2.07655 -0.00016 0.00000 0.00214 0.00214 2.07869

R12 2.11861 0.00256 0.00000 0.01632 0.01632 2.13493

R13 2.12558 -0.00005 0.00000 -0.00060 -0.00060 2.12498

R14 2.87155 0.00002 0.00000 0.00270 0.00224 2.87379

R15 2.11910 -0.00066 0.00000 0.00001 0.00001 2.11911

R16 2.12970 0.00034 0.00000 0.00131 0.00131 2.13101

R17 2.66139 0.00141 0.00000 0.00809 0.00820 2.66960

R18 2.66694 -0.00074 0.00000 -0.00492 -0.00532 2.66162

R19 2.67420 -0.00164 0.00000 -0.01713 -0.01653 2.65768

R20 2.80770 0.00330 0.00000 0.02039 0.02086 2.82856

R21 2.06839 -0.00013 0.00000 -0.00411 -0.00411 2.06428

R22 2.80800 0.00063 0.00000 0.00914 0.00877 2.81677

R23 2.06269 0.00046 0.00000 0.00231 0.00231 2.06500

R24 2.30557 0.00140 0.00000 0.00133 0.00133 2.30690

R25 2.30608 -0.00095 0.00000 -0.00039 -0.00039 2.30568

A1 2.07181 -0.00090 0.00000 -0.00815 -0.01000 2.06181

A2 2.10191 0.00042 0.00000 0.00765 0.00719 2.10910

A3 2.10230 0.00038 0.00000 -0.00804 -0.00827 2.09403

A4 2.11408 -0.00017 0.00000 -0.01217 -0.01316 2.10092

A5 2.09227 0.00032 0.00000 0.00665 0.00674 2.09902

A6 1.59207 0.00058 0.00000 0.01076 0.01147 1.60354

A7 2.02073 -0.00006 0.00000 0.00310 0.00411 2.02484

A8 1.70687 -0.00103 0.00000 0.00407 0.00272 1.70958

A9 1.72988 0.00020 0.00000 -0.00877 -0.00848 1.72140

A10 2.03704 0.00023 0.00000 0.03062 0.02951 2.06654

A11 2.12104 -0.00033 0.00000 -0.01203 -0.01208 2.10895

A12 1.60378 0.00115 0.00000 0.02538 0.02664 1.63042

A13 2.03189 0.00014 0.00000 -0.00063 -0.00034 2.03155

A14 1.82656 -0.00136 0.00000 -0.05916 -0.06064 1.76593

A15 1.69130 0.00005 0.00000 -0.00782 -0.00749 1.68381

A16 2.04575 0.00076 0.00000 0.02052 0.01893 2.06468

A17 2.10664 -0.00043 0.00000 -0.01207 -0.01205 2.09458

A18 2.11179 -0.00023 0.00000 0.00216 0.00223 2.11403

A19 1.93692 -0.00166 0.00000 -0.04321 -0.04234 1.89457

A20 1.91335 -0.00087 0.00000 -0.04906 -0.04708 1.86627

A21 1.96207 0.00097 0.00000 0.02883 0.02364 1.98571

A22 1.82163 0.00126 0.00000 0.05856 0.05692 1.87856

A23 1.90594 0.00080 0.00000 0.02048 0.02234 1.92827

A24 1.91880 -0.00048 0.00000 -0.01388 -0.01218 1.90663

A25 1.96519 -0.00073 0.00000 0.01558 0.00883 1.97402

A26 1.93999 0.00033 0.00000 0.00021 0.00297 1.94296

A27 1.84537 0.00093 0.00000 0.02681 0.02780 1.87317

A28 1.93234 0.00009 0.00000 -0.01307 -0.01152 1.92082

A29 1.89367 0.00007 0.00000 0.00830 0.01001 1.90368

A30 1.88283 -0.00068 0.00000 -0.03835 -0.03929 1.84353

A31 1.88591 -0.00099 0.00000 -0.00609 -0.00613 1.87978

A32 1.91381 -0.00053 0.00000 -0.03647 -0.03767 1.87613

A33 1.78374 -0.00042 0.00000 -0.03097 -0.03049 1.75326

A34 1.53841 0.00072 0.00000 0.02120 0.02170 1.56011

A35 1.86100 0.00033 0.00000 0.01084 0.00970 1.87070

A36 2.19067 -0.00047 0.00000 -0.00138 -0.00100 2.18967

A37 2.08712 0.00022 0.00000 0.01495 0.01474 2.10186

A38 1.83007 0.00113 0.00000 0.04559 0.04492 1.87499

A39 1.77091 -0.00146 0.00000 -0.05824 -0.05754 1.71337

A40 1.58257 -0.00008 0.00000 -0.02321 -0.02206 1.56050

A41 1.87130 -0.00050 0.00000 -0.00868 -0.00841 1.86289

A42 2.20299 -0.00038 0.00000 -0.01075 -0.01038 2.19261

A43 2.09033 0.00108 0.00000 0.03757 0.03634 2.12667

A44 1.90625 -0.00055 0.00000 -0.00703 -0.00682 1.89943

A45 2.02271 0.00065 0.00000 0.01198 0.01100 2.03371

A46 2.35373 -0.00007 0.00000 -0.00311 -0.00406 2.34967

A47 1.89755 0.00174 0.00000 0.01454 0.01406 1.91162

A48 2.03819 -0.00283 0.00000 -0.03362 -0.03338 2.00480

A49 2.34737 0.00109 0.00000 0.01903 0.01926 2.36662

D1 -0.57020 0.00012 0.00000 0.00230 0.00325 -0.56694

D2 2.93982 -0.00014 0.00000 0.00924 0.00958 2.94940

D3 1.17280 -0.00075 0.00000 0.01218 0.01167 1.18447

D4 2.69916 0.00101 0.00000 0.07863 0.07963 2.77879

D5 -0.07401 0.00075 0.00000 0.08557 0.08596 0.01194

D6 -1.84103 0.00013 0.00000 0.08851 0.08804 -1.75299

D7 0.08143 -0.00019 0.00000 -0.05713 -0.05726 0.02416

D8 -2.85397 -0.00069 0.00000 -0.11433 -0.11449 -2.96846

D9 3.09523 -0.00108 0.00000 -0.13229 -0.13178 2.96344

D10 0.15984 -0.00157 0.00000 -0.18949 -0.18901 -0.02918

D11 2.44659 0.00053 0.00000 0.14501 0.14392 2.59051

D12 -1.83350 0.00059 0.00000 0.16264 0.16293 -1.67057

D13 0.30629 0.00002 0.00000 0.12944 0.12970 0.43599

D14 -1.04915 0.00086 0.00000 0.13922 0.13857 -0.91057

D15 0.95395 0.00093 0.00000 0.15684 0.15759 1.11154

D16 3.09374 0.00035 0.00000 0.12365 0.12436 -3.06509

D17 0.76782 0.00052 0.00000 0.13219 0.13142 0.89924

D18 2.77092 0.00059 0.00000 0.14982 0.15043 2.92135

D19 -1.37248 0.00001 0.00000 0.11662 0.11720 -1.25528

D20 -1.13003 0.00038 0.00000 0.03576 0.03521 -1.09482

D21 -3.07582 0.00109 0.00000 0.05172 0.05266 -3.02316

D22 1.10254 0.00020 0.00000 0.02647 0.02615 1.12869

D23 0.99325 0.00020 0.00000 0.02572 0.02420 1.01745

D24 -0.95254 0.00091 0.00000 0.04168 0.04166 -0.91089

D25 -3.05737 0.00002 0.00000 0.01643 0.01514 -3.04223

D26 3.04943 -0.00008 0.00000 0.02788 0.02712 3.07655

D27 1.10364 0.00063 0.00000 0.04385 0.04458 1.14821

D28 -1.00119 -0.00026 0.00000 0.01860 0.01806 -0.98313

D29 0.63210 -0.00005 0.00000 -0.00930 -0.01019 0.62191

D30 -2.71634 0.00043 0.00000 0.04631 0.04595 -2.67039

D31 -2.97621 0.00011 0.00000 0.03328 0.03264 -2.94357

D32 -0.04146 0.00058 0.00000 0.08889 0.08878 0.04732

D33 -1.24336 0.00084 0.00000 0.03835 0.03858 -1.20478

D34 1.69139 0.00131 0.00000 0.09395 0.09472 1.78611

D35 -0.85017 0.00033 0.00000 0.14812 0.14798 -0.70219

D36 -3.02975 0.00050 0.00000 0.15340 0.15420 -2.87555

D37 1.21478 0.00060 0.00000 0.18340 0.18346 1.39824

D38 2.73399 0.00032 0.00000 0.11142 0.11070 2.84469

D39 0.55442 0.00049 0.00000 0.11670 0.11691 0.67134

D40 -1.48423 0.00059 0.00000 0.14670 0.14617 -1.33806

D41 0.89120 0.00101 0.00000 0.15582 0.15426 1.04547

D42 -1.28837 0.00118 0.00000 0.16109 0.16048 -1.12789

D43 2.95616 0.00128 0.00000 0.19109 0.18974 -3.13729

D44 0.95682 -0.00017 0.00000 0.01716 0.01682 0.97364

D45 2.92617 -0.00020 0.00000 0.00054 0.00065 2.92682

D46 -1.26451 0.00016 0.00000 0.01810 0.01770 -1.24682

D47 -1.10727 -0.00053 0.00000 -0.01241 -0.01067 -1.11794

D48 0.86208 -0.00056 0.00000 -0.02903 -0.02683 0.83525

D49 2.95458 -0.00020 0.00000 -0.01147 -0.00979 2.94479

D50 3.08739 -0.00031 0.00000 0.00822 0.00804 3.09543

D51 -1.22645 -0.00034 0.00000 -0.00841 -0.00812 -1.23457

D52 0.86605 0.00002 0.00000 0.00915 0.00892 0.87498

D53 0.36632 -0.00046 0.00000 -0.19139 -0.19230 0.17402

D54 2.55007 -0.00049 0.00000 -0.18947 -0.19070 2.35938

D55 -1.67005 -0.00122 0.00000 -0.23872 -0.23888 -1.90893

D56 -1.79134 0.00043 0.00000 -0.17074 -0.17070 -1.96204

D57 0.39241 0.00039 0.00000 -0.16882 -0.16909 0.22331

D58 2.45547 -0.00033 0.00000 -0.21807 -0.21727 2.23820

D59 2.50303 -0.00125 0.00000 -0.24442 -0.24524 2.25779

D60 -1.59640 -0.00129 0.00000 -0.24251 -0.24364 -1.84004

D61 0.46666 -0.00201 0.00000 -0.29176 -0.29182 0.17484

D62 -0.00848 -0.00008 0.00000 0.00922 0.00954 0.00105

D63 3.10440 0.00075 0.00000 0.06232 0.06327 -3.11551

D64 0.04849 -0.00019 0.00000 -0.03395 -0.03417 0.01432

D65 -3.08154 -0.00009 0.00000 -0.03006 -0.03051 -3.11206

D66 0.10976 0.00031 0.00000 -0.03721 -0.03670 0.07305

D67 1.98263 -0.00104 0.00000 -0.08665 -0.08619 1.89644

D68 -1.67198 -0.00033 0.00000 -0.03891 -0.03909 -1.71107

D69 -1.80886 0.00087 0.00000 0.00950 0.00999 -1.79888

D70 0.06400 -0.00048 0.00000 -0.03995 -0.03950 0.02451

D71 2.69259 0.00023 0.00000 0.00779 0.00760 2.70018

D72 1.89483 0.00059 0.00000 -0.03911 -0.03866 1.85617

D73 -2.51549 -0.00076 0.00000 -0.08855 -0.08815 -2.60363

D74 0.11310 -0.00005 0.00000 -0.04081 -0.04105 0.07204

D75 -2.04466 0.00097 0.00000 0.06960 0.07055 -1.97411

D76 1.13337 -0.00009 0.00000 0.00186 0.00265 1.13602

D77 -0.03636 0.00033 0.00000 0.01986 0.01963 -0.01673

D78 -3.14151 -0.00073 0.00000 -0.04787 -0.04827 3.09340

D79 2.58298 0.00031 0.00000 0.05882 0.05939 2.64236

D80 -0.52218 -0.00075 0.00000 -0.00891 -0.00851 -0.53070

D81 1.84268 0.00086 0.00000 0.07042 0.07058 1.91325

D82 -1.31338 0.00070 0.00000 0.06503 0.06531 -1.24807

D83 -0.07155 0.00036 0.00000 0.04665 0.04666 -0.02489

D84 3.05558 0.00020 0.00000 0.04126 0.04139 3.09697

D85 -2.73950 0.00018 0.00000 0.01826 0.01737 -2.72213

D86 0.38763 0.00002 0.00000 0.01287 0.01211 0.39973

Item Value Threshold Converged?

Maximum Force 0.003297 0.000450 NO

RMS Force 0.000917 0.000300 NO

Maximum Displacement 0.436597 0.001800 NO

RMS Displacement 0.093612 0.001200 NO

Predicted change in Energy=-6.841978D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.133059 1.551525 0.416766

2 6 0 0.196642 1.287523 0.076312

3 6 0 -0.770431 3.790321 -0.347988

4 6 0 -1.622181 2.845536 0.210560

5 1 0 -1.718741 0.829511 1.006426

6 1 0 -2.604205 3.133304 0.614048

7 6 0 0.836258 1.996390 -1.066246

8 1 0 1.936683 2.119643 -0.842153

9 1 0 0.744406 1.323041 -1.962147

10 6 0 0.203903 3.342421 -1.384036

11 1 0 1.001934 4.111888 -1.553064

12 1 0 -0.355503 3.265482 -2.360158

13 1 0 -1.041447 4.858621 -0.359403

14 1 0 0.672267 0.343680 0.386603

15 8 0 2.790189 3.779793 0.836741

16 6 0 0.496263 3.878083 1.410593

17 6 0 0.936954 2.569967 1.679911

18 6 0 1.666403 4.635365 0.864947

19 8 0 1.831776 5.766784 0.437408

20 6 0 2.386282 2.525660 1.334531

21 8 0 3.272373 1.689310 1.398109

22 1 0 -0.300816 4.400728 1.944239

23 1 0 0.497647 1.888430 2.412458

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.397751 0.000000

3 C 2.393441 2.716479 0.000000

4 C 1.398652 2.398654 1.389271 0.000000

5 H 1.100921 2.177976 3.391184 2.169582 0.000000

6 H 2.169151 3.397176 2.172536 1.099993 2.499094

7 C 2.505083 1.488973 2.513072 2.897448 3.490788

8 H 3.366148 2.136293 3.219291 3.781618 4.294626

9 H 3.039129 2.111072 3.314772 3.555191 3.888842

10 C 2.870133 2.520967 1.491085 2.474714 3.965550

11 H 3.872194 3.358631 2.167231 3.405877 4.972632

12 H 3.354631 3.186467 2.120483 2.896449 4.373358

13 H 3.398193 3.804661 1.102200 2.171317 4.307893

14 H 2.172326 1.101518 3.807931 3.399230 2.517366

15 O 4.531383 3.676431 3.752560 4.553454 5.391049

16 C 3.009195 2.929347 2.169060 2.644624 3.789906

17 C 2.630155 2.182717 2.918356 2.963799 3.245842

18 C 4.189024 3.740346 2.850170 3.800854 5.095463

19 O 5.153551 4.782032 3.360764 4.529345 6.107915

20 C 3.765235 2.812582 3.794084 4.175333 4.453739

21 O 4.515512 3.371751 4.879279 5.167571 5.079753

22 H 3.338228 3.664513 2.418148 2.677736 3.955199

23 H 2.599133 2.430898 3.584030 3.202823 2.830303

6 7 8 9 10

6 H 0.000000

7 C 3.994089 0.000000

8 H 4.875213 1.129754 0.000000

9 H 4.596415 1.124489 1.819474 0.000000

10 C 3.452758 1.520744 2.188915 2.168929 0.000000

11 H 4.319519 2.177101 2.312616 2.830431 1.121385

12 H 3.730956 2.169124 2.978490 2.267442 1.127683

13 H 2.523200 3.495392 4.074839 4.272983 2.213511

14 H 4.309177 2.206607 2.502526 2.545777 3.513827

15 O 5.437557 3.258792 2.510629 4.249074 3.436861

16 C 3.286652 3.129072 3.200279 4.238536 2.860482

17 C 3.740752 2.807225 2.750102 3.854412 3.243736

18 C 4.534008 3.373845 3.052229 4.451295 2.978008

19 O 5.161817 4.179462 3.866513 5.165955 3.441680

20 C 5.078709 2.906274 2.259412 3.874291 3.580570

21 O 6.101970 3.478793 2.643488 4.220911 4.459665

22 H 2.946417 4.017064 4.239545 5.081782 3.528763

23 H 3.795454 3.496812 3.566059 4.417887 4.075995

11 12 13 14 15

11 H 0.000000

12 H 1.791770 0.000000

13 H 2.481501 2.647948 0.000000

14 H 4.250927 4.139799 4.886516 0.000000

15 O 3.003216 4.514428 4.156448 4.061415 0.000000

16 C 3.015564 3.913994 2.541435 3.683957 2.366656

17 C 3.582439 4.298412 3.648398 2.588255 2.368352

18 C 2.561703 4.045490 2.980156 4.431217 1.412690

19 O 2.718326 4.343625 3.116903 5.545909 2.241909

20 C 3.573617 4.659984 4.479000 2.932141 1.408469

21 O 4.442206 5.456223 5.634041 3.097485 2.217601

22 H 3.743223 4.451922 2.462715 4.453399 3.341620

23 H 4.574214 5.040039 4.344428 2.553592 3.363909

16 17 18 19 20

16 C 0.000000

17 C 1.406381 0.000000

18 C 1.496808 2.337120 0.000000

19 O 2.509557 3.544596 1.220757 0.000000

20 C 2.325297 1.490571 2.278067 3.408401 0.000000

21 O 3.535204 2.511802 3.397446 4.429905 1.220115

22 H 1.092370 2.225675 2.256076 2.946965 3.332885

23 H 2.227656 1.092752 3.362503 4.552181 2.266038

21 22 23

21 O 0.000000

22 H 4.518598 0.000000

23 H 2.961023 2.677389 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.271193 -0.850242 -0.591983

2 6 0 1.290196 -1.396123 0.240704

3 6 0 1.449571 1.308005 0.036874

4 6 0 2.339716 0.542110 -0.705499

5 1 0 2.841275 -1.487443 -1.285531

6 1 0 2.984383 1.000741 -1.469730

7 6 0 0.854511 -0.671442 1.466289

8 1 0 -0.233917 -0.907644 1.655701

9 1 0 1.448470 -1.091613 2.323694

10 6 0 1.068527 0.832609 1.397808

11 1 0 0.159152 1.368091 1.777018

12 1 0 1.903885 1.118271 2.099408

13 1 0 1.337376 2.387682 -0.154320

14 1 0 1.083450 -2.477864 0.219877

15 8 0 -2.083623 0.064340 0.263907

16 6 0 -0.267890 0.673837 -1.126304

17 6 0 -0.309087 -0.731411 -1.087719

18 6 0 -1.381871 1.172833 -0.260001

19 8 0 -1.768036 2.277032 0.089099

20 6 0 -1.467745 -1.103374 -0.226931

21 8 0 -1.994759 -2.146944 0.122209

22 1 0 0.092721 1.274464 -1.964444

23 1 0 0.071822 -1.400914 -1.862819

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2233604 0.8806067 0.6757845

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6714519518 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.488254346930E-01 A.U. after 16 cycles

Convg = 0.2789D-08 -V/T = 0.9990

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.006440647 -0.000798576 0.000326101

2 6 -0.009384469 0.001398600 0.001723381

3 6 0.001603860 0.002697141 -0.004722976

4 6 -0.004136161 -0.003133624 0.001888464

5 1 0.000461355 -0.000188824 -0.001779101

6 1 0.000590259 0.000491436 0.000718246

7 6 0.001225851 -0.002287328 0.001757282

8 1 -0.002789995 -0.000490916 -0.006306172

9 1 0.001683158 0.000603983 -0.001182101

10 6 0.001129090 -0.000015631 -0.000288837

11 1 0.000970576 0.001275852 0.002431005

12 1 -0.000557830 -0.000038432 0.000861580

13 1 -0.000032186 -0.000268264 -0.000719542

14 1 0.000541526 0.000171819 0.000439105

15 8 -0.005988813 0.005771664 0.000141627

16 6 0.004050289 0.003529763 -0.000202109

17 6 0.004622707 0.001285116 0.000111833

18 6 -0.003172043 -0.004047906 -0.001748386

19 8 0.000654249 -0.002075778 0.002069657

20 6 0.000776195 -0.000356690 0.004459910

21 8 -0.000362125 -0.004111100 0.000894211

22 1 -0.000518533 0.000735754 -0.000950512

23 1 0.002192392 -0.000148061 0.000077335

-------------------------------------------------------------------

Cartesian Forces: Max 0.009384469 RMS 0.002640978

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.006410478 RMS 0.001488652

Search for a saddle point.

Step number 69 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 49 63 68 69

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07103 -0.00032 0.00331 0.00737 0.00877

Eigenvalues --- 0.01153 0.01188 0.01321 0.01840 0.02188

Eigenvalues --- 0.02486 0.02787 0.02862 0.03203 0.03327

Eigenvalues --- 0.03604 0.03619 0.03793 0.04020 0.04086

Eigenvalues --- 0.04356 0.04423 0.04708 0.04857 0.06317

Eigenvalues --- 0.06601 0.06678 0.07097 0.07446 0.08558

Eigenvalues --- 0.08815 0.10080 0.10358 0.10765 0.10832

Eigenvalues --- 0.12610 0.13844 0.15170 0.15908 0.22759

Eigenvalues --- 0.26292 0.28498 0.29568 0.30135 0.31050

Eigenvalues --- 0.31424 0.31850 0.32043 0.32225 0.32546

Eigenvalues --- 0.33426 0.35168 0.36838 0.37967 0.39755

Eigenvalues --- 0.40278 0.40728 0.44818 0.48893 0.53458

Eigenvalues --- 0.62405 1.08711 1.11242

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D71 D73

1 0.56161 0.51724 -0.15513 0.15006 -0.14308

D29 R19 D1 D13 D79

1 -0.13494 -0.13475 0.13350 -0.13020 0.12494

RFO step: Lambda0=4.561384100D-05 Lambda=-3.60041574D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.09590203 RMS(Int)= 0.00635269

Iteration 2 RMS(Cart)= 0.00640557 RMS(Int)= 0.00107282

Iteration 3 RMS(Cart)= 0.00005425 RMS(Int)= 0.00107137

Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00107137

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.64137 -0.00546 0.00000 -0.02177 -0.02137 2.62000

R2 2.64307 -0.00005 0.00000 0.00636 0.00690 2.64997

R3 2.08044 -0.00107 0.00000 -0.00180 -0.00180 2.07863

R4 2.81375 0.00390 0.00000 -0.00471 -0.00438 2.80937

R5 2.08157 0.00021 0.00000 0.00472 0.00472 2.08629

R6 4.12474 0.00409 0.00000 -0.01430 -0.01444 4.11030

R7 2.62534 0.00334 0.00000 -0.00183 -0.00172 2.62362

R8 2.81774 -0.00150 0.00000 -0.00122 -0.00126 2.81648

R9 2.08286 -0.00024 0.00000 0.00139 0.00139 2.08424

R10 4.09893 0.00104 0.00000 0.04003 0.03963 4.13856

R11 2.07869 -0.00013 0.00000 -0.00439 -0.00439 2.07430

R12 2.13493 -0.00402 0.00000 -0.01332 -0.01332 2.12161

R13 2.12498 0.00044 0.00000 0.00701 0.00701 2.13198

R14 2.87379 0.00012 0.00000 0.00500 0.00535 2.87914

R15 2.11911 0.00120 0.00000 0.00547 0.00547 2.12458

R16 2.13101 -0.00047 0.00000 -0.00426 -0.00426 2.12675

R17 2.66960 -0.00396 0.00000 -0.01713 -0.01739 2.65221

R18 2.66162 0.00211 0.00000 0.01286 0.01258 2.67420

R19 2.65768 0.00220 0.00000 0.00291 0.00237 2.66004

R20 2.82856 -0.00641 0.00000 -0.02250 -0.02238 2.80617

R21 2.06428 0.00027 0.00000 -0.00036 -0.00036 2.06392

R22 2.81677 -0.00363 0.00000 -0.01788 -0.01780 2.79897

R23 2.06500 -0.00074 0.00000 0.00009 0.00009 2.06509

R24 2.30690 -0.00256 0.00000 -0.00003 -0.00003 2.30686

R25 2.30568 0.00260 0.00000 0.00278 0.00278 2.30847

A1 2.06181 0.00183 0.00000 0.00239 0.00146 2.06327

A2 2.10910 -0.00141 0.00000 -0.01062 -0.01098 2.09813

A3 2.09403 -0.00026 0.00000 0.01869 0.01844 2.11247

A4 2.10092 0.00053 0.00000 -0.00064 -0.00276 2.09816

A5 2.09902 -0.00042 0.00000 0.00261 0.00289 2.10191

A6 1.60354 -0.00063 0.00000 0.03291 0.03314 1.63668

A7 2.02484 -0.00033 0.00000 -0.01377 -0.01253 2.01231

A8 1.70958 0.00190 0.00000 0.02834 0.02703 1.73661

A9 1.72140 -0.00061 0.00000 -0.02884 -0.02800 1.69340

A10 2.06654 -0.00019 0.00000 0.03314 0.03165 2.09819

A11 2.10895 0.00041 0.00000 -0.00962 -0.00973 2.09922

A12 1.63042 -0.00139 0.00000 -0.03109 -0.03073 1.59970

A13 2.03155 -0.00022 0.00000 -0.00802 -0.00707 2.02448

A14 1.76593 0.00159 0.00000 -0.01431 -0.01528 1.75065

A15 1.68381 -0.00014 0.00000 0.00769 0.00835 1.69216

A16 2.06468 -0.00160 0.00000 -0.01156 -0.01239 2.05229

A17 2.09458 0.00115 0.00000 0.00809 0.00820 2.10278

A18 2.11403 0.00043 0.00000 -0.00025 0.00003 2.11406

A19 1.89457 0.00303 0.00000 0.05212 0.05387 1.94844

A20 1.86627 0.00170 0.00000 0.02141 0.02222 1.88849

A21 1.98571 -0.00186 0.00000 -0.00925 -0.01353 1.97218

A22 1.87856 -0.00195 0.00000 -0.04497 -0.04637 1.83219

A23 1.92827 -0.00123 0.00000 -0.01301 -0.01227 1.91601

A24 1.90663 0.00036 0.00000 -0.00774 -0.00617 1.90045

A25 1.97402 0.00130 0.00000 0.01329 0.00848 1.98251

A26 1.94296 -0.00078 0.00000 -0.02481 -0.02371 1.91925

A27 1.87317 -0.00143 0.00000 -0.00307 -0.00135 1.87182

A28 1.92082 -0.00003 0.00000 -0.00770 -0.00602 1.91481

A29 1.90368 -0.00017 0.00000 0.00666 0.00777 1.91144

A30 1.84353 0.00106 0.00000 0.01678 0.01604 1.85957

A31 1.87978 0.00172 0.00000 0.00328 0.00315 1.88293

A32 1.87613 0.00090 0.00000 0.00426 0.00033 1.87647

A33 1.75326 0.00020 0.00000 -0.04800 -0.04603 1.70722

A34 1.56011 -0.00100 0.00000 0.00178 0.00291 1.56302

A35 1.87070 -0.00043 0.00000 -0.00006 -0.00039 1.87031

A36 2.18967 0.00070 0.00000 0.01978 0.02063 2.21029

A37 2.10186 -0.00026 0.00000 0.00001 -0.00116 2.10070

A38 1.87499 -0.00196 0.00000 -0.00629 -0.00964 1.86535

A39 1.71337 0.00173 0.00000 0.04393 0.04493 1.75830

A40 1.56050 0.00046 0.00000 0.01595 0.01826 1.57877

A41 1.86289 0.00115 0.00000 0.00446 0.00447 1.86736

A42 2.19261 0.00069 0.00000 0.01094 0.01081 2.20342

A43 2.12667 -0.00204 0.00000 -0.04215 -0.04334 2.08333

A44 1.89943 0.00071 0.00000 0.00309 0.00304 1.90247

A45 2.03371 -0.00114 0.00000 -0.00548 -0.00590 2.02781

A46 2.34967 0.00047 0.00000 0.00356 0.00312 2.35279

A47 1.91162 -0.00316 0.00000 -0.01001 -0.01010 1.90151

A48 2.00480 0.00538 0.00000 0.02683 0.02643 2.03123

A49 2.36662 -0.00220 0.00000 -0.01615 -0.01648 2.35015

D1 -0.56694 -0.00050 0.00000 -0.04320 -0.04306 -0.61001

D2 2.94940 0.00026 0.00000 -0.00389 -0.00399 2.94541

D3 1.18447 0.00141 0.00000 0.00960 0.00824 1.19271

D4 2.77879 -0.00137 0.00000 -0.10328 -0.10250 2.67629

D5 0.01194 -0.00061 0.00000 -0.06397 -0.06343 -0.05149

D6 -1.75299 0.00054 0.00000 -0.05047 -0.05119 -1.80419

D7 0.02416 -0.00020 0.00000 -0.01093 -0.01125 0.01291

D8 -2.96846 -0.00002 0.00000 0.01692 0.01716 -2.95130

D9 2.96344 0.00052 0.00000 0.04508 0.04512 3.00856

D10 -0.02918 0.00070 0.00000 0.07293 0.07353 0.04435

D11 2.59051 0.00065 0.00000 0.15550 0.15500 2.74550

D12 -1.67057 0.00078 0.00000 0.14024 0.14055 -1.53002

D13 0.43599 0.00126 0.00000 0.13968 0.13968 0.57568

D14 -0.91057 -0.00011 0.00000 0.12103 0.12091 -0.78966

D15 1.11154 0.00002 0.00000 0.10578 0.10646 1.21799

D16 -3.06509 0.00050 0.00000 0.10521 0.10560 -2.95949

D17 0.89924 0.00012 0.00000 0.09964 0.09986 0.99910

D18 2.92135 0.00025 0.00000 0.08438 0.08541 3.00676

D19 -1.25528 0.00073 0.00000 0.08382 0.08455 -1.17073

D20 -1.09482 -0.00050 0.00000 0.10833 0.10792 -0.98690

D21 -3.02316 -0.00189 0.00000 0.08813 0.08817 -2.93498

D22 1.12869 -0.00003 0.00000 0.12482 0.12435 1.25304

D23 1.01745 0.00016 0.00000 0.11716 0.11612 1.13357

D24 -0.91089 -0.00123 0.00000 0.09696 0.09637 -0.81451

D25 -3.04223 0.00063 0.00000 0.13365 0.13255 -2.90968

D26 3.07655 0.00013 0.00000 0.10293 0.10260 -3.10403

D27 1.14821 -0.00126 0.00000 0.08273 0.08286 1.23107

D28 -0.98313 0.00060 0.00000 0.11942 0.11903 -0.86409

D29 0.62191 0.00006 0.00000 -0.03466 -0.03506 0.58685

D30 -2.67039 -0.00005 0.00000 -0.06210 -0.06295 -2.73333

D31 -2.94357 0.00001 0.00000 0.00466 0.00521 -2.93836

D32 0.04732 -0.00010 0.00000 -0.02279 -0.02268 0.02464

D33 -1.20478 -0.00094 0.00000 -0.00700 -0.00502 -1.20980

D34 1.78611 -0.00105 0.00000 -0.03444 -0.03290 1.75321

D35 -0.70219 0.00077 0.00000 0.13138 0.13226 -0.56993

D36 -2.87555 0.00043 0.00000 0.15094 0.15224 -2.72331

D37 1.39824 0.00039 0.00000 0.14574 0.14631 1.54455

D38 2.84469 0.00067 0.00000 0.09475 0.09481 2.93950

D39 0.67134 0.00033 0.00000 0.11431 0.11479 0.78613

D40 -1.33806 0.00029 0.00000 0.10911 0.10886 -1.22920

D41 1.04547 0.00001 0.00000 0.09633 0.09574 1.14120

D42 -1.12789 -0.00033 0.00000 0.11589 0.11572 -1.01217

D43 -3.13729 -0.00037 0.00000 0.11069 0.10978 -3.02750

D44 0.97364 0.00021 0.00000 0.12119 0.12176 1.09540

D45 2.92682 0.00011 0.00000 0.10264 0.10295 3.02977

D46 -1.24682 -0.00035 0.00000 0.09832 0.09838 -1.14843

D47 -1.11794 0.00049 0.00000 0.09763 0.09919 -1.01874

D48 0.83525 0.00038 0.00000 0.07908 0.08038 0.91563

D49 2.94479 -0.00008 0.00000 0.07476 0.07582 3.02061

D50 3.09543 0.00038 0.00000 0.10721 0.10786 -3.07989

D51 -1.23457 0.00027 0.00000 0.08866 0.08905 -1.14552

D52 0.87498 -0.00019 0.00000 0.08434 0.08449 0.95946

D53 0.17402 -0.00093 0.00000 -0.17492 -0.17423 -0.00021

D54 2.35938 -0.00102 0.00000 -0.20373 -0.20378 2.15559

D55 -1.90893 0.00015 0.00000 -0.18407 -0.18341 -2.09234

D56 -1.96204 -0.00262 0.00000 -0.22663 -0.22562 -2.18766

D57 0.22331 -0.00271 0.00000 -0.25544 -0.25517 -0.03186

D58 2.23820 -0.00154 0.00000 -0.23579 -0.23480 2.00339

D59 2.25779 0.00027 0.00000 -0.15915 -0.15913 2.09866

D60 -1.84004 0.00019 0.00000 -0.18796 -0.18868 -2.02872

D61 0.17484 0.00135 0.00000 -0.16830 -0.16831 0.00653

D62 0.00105 0.00041 0.00000 -0.02095 -0.02023 -0.01918

D63 -3.11551 -0.00077 0.00000 -0.06034 -0.05914 3.10853

D64 0.01432 -0.00002 0.00000 0.00189 0.00109 0.01541

D65 -3.11206 -0.00059 0.00000 -0.03407 -0.03639 3.13474

D66 0.07305 -0.00056 0.00000 -0.13149 -0.13075 -0.05770

D67 1.89644 0.00107 0.00000 -0.08301 -0.08243 1.81401

D68 -1.71107 0.00007 0.00000 -0.15271 -0.15233 -1.86340

D69 -1.79888 -0.00098 0.00000 -0.07902 -0.07890 -1.87777

D70 0.02451 0.00065 0.00000 -0.03054 -0.03057 -0.00606

D71 2.70018 -0.00035 0.00000 -0.10024 -0.10047 2.59971

D72 1.85617 -0.00084 0.00000 -0.11634 -0.11660 1.73956

D73 -2.60363 0.00079 0.00000 -0.06786 -0.06827 -2.67191

D74 0.07204 -0.00021 0.00000 -0.13756 -0.13818 -0.06614

D75 -1.97411 -0.00157 0.00000 0.04807 0.05053 -1.92358

D76 1.13602 -0.00011 0.00000 0.09740 0.09956 1.23558

D77 -0.01673 -0.00065 0.00000 0.03309 0.03254 0.01581

D78 3.09340 0.00081 0.00000 0.08242 0.08157 -3.10822

D79 2.64236 -0.00044 0.00000 0.07514 0.07507 2.71743

D80 -0.53070 0.00102 0.00000 0.12447 0.12410 -0.40659

D81 1.91325 -0.00151 0.00000 0.03002 0.02778 1.94104

D82 -1.24807 -0.00068 0.00000 0.07722 0.07556 -1.17252

D83 -0.02489 -0.00036 0.00000 0.01902 0.01939 -0.00550

D84 3.09697 0.00046 0.00000 0.06622 0.06716 -3.11905

D85 -2.72213 -0.00026 0.00000 0.06881 0.06711 -2.65502

D86 0.39973 0.00057 0.00000 0.11601 0.11488 0.51461

Item Value Threshold Converged?

Maximum Force 0.006410 0.000450 NO

RMS Force 0.001489 0.000300 NO

Maximum Displacement 0.397165 0.001800 NO

RMS Displacement 0.096675 0.001200 NO

Predicted change in Energy=-3.495573D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.154299 1.577815 0.439977

2 6 0 0.160815 1.281580 0.116027

3 6 0 -0.738124 3.778726 -0.384645

4 6 0 -1.622730 2.875557 0.189202

5 1 0 -1.761935 0.854586 1.003576

6 1 0 -2.590499 3.205102 0.588835

7 6 0 0.794737 1.900012 -1.078051

8 1 0 1.914270 1.909472 -0.994214

9 1 0 0.574788 1.247336 -1.971618

10 6 0 0.286856 3.308659 -1.359219

11 1 0 1.152131 4.026134 -1.382322

12 1 0 -0.184173 3.341604 -2.380805

13 1 0 -0.988267 4.852115 -0.426206

14 1 0 0.623544 0.340721 0.461744

15 8 0 2.730939 3.897985 0.809596

16 6 0 0.466098 3.857693 1.442884

17 6 0 0.983132 2.567531 1.665570

18 6 0 1.577414 4.690260 0.916646

19 8 0 1.695525 5.860589 0.590172

20 6 0 2.410105 2.598834 1.269877

21 8 0 3.310215 1.773612 1.236907

22 1 0 -0.372679 4.322876 1.965301

23 1 0 0.655738 1.864208 2.435222

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.386442 0.000000

3 C 2.386884 2.700834 0.000000

4 C 1.402301 2.393146 1.388360 0.000000

5 H 1.099966 2.160332 3.394988 2.183324 0.000000

6 H 2.175521 3.390164 2.169792 1.097671 2.526549

7 C 2.491377 1.486653 2.521912 2.898579 3.458707

8 H 3.403383 2.168292 3.301648 3.852812 4.314908

9 H 2.985757 2.128570 3.263458 3.485589 3.803460

10 C 2.882682 2.510237 1.490417 2.496339 3.975276

11 H 3.825527 3.280295 2.151659 3.390188 4.923719

12 H 3.465387 3.255286 2.117214 2.981876 4.486494

13 H 3.391000 3.789872 1.102933 2.165191 4.315446

14 H 2.166010 1.104017 3.793467 3.397855 2.499630

15 O 4.540361 3.732580 3.670808 4.514940 5.430085

16 C 2.971423 2.913779 2.190034 2.626692 3.765073

17 C 2.655226 2.175077 2.938213 3.010823 3.302697

18 C 4.168546 3.777147 2.808196 3.750099 5.086374

19 O 5.146475 4.852574 3.347696 4.481296 6.097950

20 C 3.799499 2.850585 3.747124 4.184279 4.529816

21 O 4.539308 3.378933 4.799891 5.161967 5.160015

22 H 3.236186 3.599154 2.439650 2.609959 3.857976

23 H 2.709106 2.441939 3.682374 3.355420 2.985647

6 7 8 9 10

6 H 0.000000

7 C 3.992691 0.000000

8 H 4.947488 1.122707 0.000000

9 H 4.517500 1.128196 1.785484 0.000000

10 C 3.476321 1.523577 2.177023 2.169561 0.000000

11 H 4.308925 2.177316 2.282924 2.898674 1.124279

12 H 3.824630 2.175688 2.894321 2.264821 1.125429

13 H 2.511992 3.509831 4.172110 4.222070 2.208780

14 H 4.307076 2.198105 2.499353 2.597225 3.498275

15 O 5.370896 3.362140 2.806218 4.405687 3.320332

16 C 3.240071 3.208681 3.439799 4.299373 2.861005

17 C 3.786382 2.829935 2.893875 3.890861 3.191147

18 C 4.436738 3.518079 3.390817 4.604460 2.958702

19 O 5.041985 4.390963 4.262565 5.394528 3.506682

20 C 5.083052 2.934371 2.418095 3.962604 3.453142

21 O 6.106355 3.420911 2.635341 4.249019 4.270473

22 H 2.839507 4.061418 4.451223 5.084877 3.537804

23 H 3.968022 3.516203 3.653351 4.450541 4.076799

11 12 13 14 15

11 H 0.000000

12 H 1.803124 0.000000

13 H 2.485500 2.597820 0.000000

14 H 4.154787 4.211626 4.872275 0.000000

15 O 2.704360 4.357303 4.033617 4.149246 0.000000

16 C 2.912182 3.912774 2.568570 3.654657 2.352060

17 C 3.383154 4.281932 3.671684 2.556791 2.357463

18 C 2.430470 3.974323 2.900374 4.476080 1.403489

19 O 2.747952 4.324957 3.041839 5.624463 2.229809

20 C 3.264023 4.539765 4.416210 2.990644 1.415127

21 O 4.073271 5.268508 5.542569 3.142014 2.243014

22 H 3.690486 4.459491 2.525539 4.371579 3.338957

23 H 4.415198 5.107079 4.451753 2.493323 3.329469

16 17 18 19 20

16 C 0.000000

17 C 1.407633 0.000000

18 C 1.484963 2.328097 0.000000

19 O 2.500040 3.536696 1.220740 0.000000

20 C 2.322460 1.481150 2.278642 3.407590 0.000000

21 O 3.531971 2.495871 3.407638 4.441719 1.221587

22 H 1.092182 2.238146 2.244440 2.921131 3.346614

23 H 2.234878 1.092800 3.337982 4.522878 2.230584

21 22 23

21 O 0.000000

22 H 4.537952 0.000000

23 H 2.913831 2.706199 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.321323 -0.615251 -0.696704

2 6 0 1.411927 -1.334020 0.063948

3 6 0 1.332422 1.362058 0.203040

4 6 0 2.278142 0.784969 -0.633694

5 1 0 2.959475 -1.130547 -1.429613

6 1 0 2.851830 1.392311 -1.345663

7 6 0 0.990793 -0.832106 1.398439

8 1 0 -0.001585 -1.257344 1.706383

9 1 0 1.723138 -1.215367 2.166298

10 6 0 0.946225 0.688871 1.475445

11 1 0 -0.080182 1.022687 1.790180

12 1 0 1.657452 1.046072 2.271155

13 1 0 1.126784 2.444198 0.146937

14 1 0 1.286117 -2.419556 -0.093021

15 8 0 -2.071360 -0.010255 0.279616

16 6 0 -0.306431 0.713024 -1.096639

17 6 0 -0.299301 -0.694450 -1.116564

18 6 0 -1.433398 1.133178 -0.225702

19 8 0 -1.905595 2.207056 0.111973

20 6 0 -1.414730 -1.145228 -0.252606

21 8 0 -1.844729 -2.234218 0.095930

22 1 0 0.063162 1.377870 -1.880376

23 1 0 0.025446 -1.327266 -1.946200

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2178928 0.8831727 0.6773150

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.6976929852 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.498398770689E-01 A.U. after 16 cycles

Convg = 0.4022D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.005566859 0.000569437 0.000526494

2 6 0.006031713 -0.007095968 -0.002806701

3 6 -0.001166837 0.003096241 -0.003030740

4 6 0.001571661 -0.004563853 0.001078703

5 1 -0.000503885 0.001775754 0.001205854

6 1 -0.001082661 0.000002326 0.000107637

7 6 -0.000751291 0.003473242 -0.004649017

8 1 0.000631820 -0.000281423 0.002435401

9 1 -0.001476041 -0.000317565 0.001714378

10 6 0.000494288 0.000926749 0.001905741

11 1 -0.000136551 0.000214965 -0.000381793

12 1 0.000127047 -0.000272609 -0.000100002

13 1 0.000453589 -0.000089051 -0.000547853

14 1 -0.000458879 0.000364605 0.000116670

15 8 0.005186974 -0.005882137 0.000766191

16 6 -0.000630664 -0.000793403 0.002782501

17 6 -0.004367281 0.003701713 0.005850842

18 6 -0.000975981 0.003026914 0.000299293

19 8 -0.000364005 0.000909339 -0.000770757

20 6 0.006519563 -0.000834308 -0.005958547

21 8 -0.000870887 0.003607649 0.000841161

22 1 -0.000308725 -0.000614944 0.000019454

23 1 -0.002356110 -0.000923675 -0.001404906

-------------------------------------------------------------------

Cartesian Forces: Max 0.007095968 RMS 0.002638335

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.007224757 RMS 0.001161953

Search for a saddle point.

Step number 70 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 33 34 37

41 43 45 46 50

51 52 55 56 57

58 59 64 65 66

69 70

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07197 0.00178 0.00373 0.00711 0.00853

Eigenvalues --- 0.00964 0.01170 0.01304 0.01802 0.02176

Eigenvalues --- 0.02472 0.02783 0.02891 0.03188 0.03319

Eigenvalues --- 0.03564 0.03616 0.03798 0.04040 0.04106

Eigenvalues --- 0.04382 0.04429 0.04722 0.04819 0.06374

Eigenvalues --- 0.06614 0.06639 0.07098 0.07454 0.08524

Eigenvalues --- 0.08919 0.10122 0.10348 0.10816 0.10955

Eigenvalues --- 0.12707 0.13834 0.15204 0.15930 0.22799

Eigenvalues --- 0.26394 0.28630 0.29607 0.30149 0.31077

Eigenvalues --- 0.31437 0.31858 0.32046 0.32222 0.32550

Eigenvalues --- 0.33411 0.35187 0.36993 0.38054 0.39789

Eigenvalues --- 0.40384 0.40784 0.45017 0.48977 0.53502

Eigenvalues --- 0.62624 1.08736 1.11246

Eigenvectors required to have negative eigenvalues:

R6 R10 D30 D73 D71

1 0.55427 0.53322 -0.15443 -0.14981 0.14268

D29 R19 D1 D13 D79

1 -0.13861 -0.13463 0.12928 -0.12759 0.12612

RFO step: Lambda0=1.205947109D-04 Lambda=-1.20252686D-03.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.02433061 RMS(Int)= 0.00028443

Iteration 2 RMS(Cart)= 0.00034467 RMS(Int)= 0.00011432

Iteration 3 RMS(Cart)= 0.00000005 RMS(Int)= 0.00011432

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.62000 0.00515 0.00000 0.01485 0.01475 2.63475

R2 2.64997 -0.00165 0.00000 -0.01028 -0.01038 2.63959

R3 2.07863 -0.00027 0.00000 -0.00102 -0.00102 2.07762

R4 2.80937 0.00076 0.00000 0.00604 0.00611 2.81548

R5 2.08629 -0.00047 0.00000 -0.00331 -0.00331 2.08298

R6 4.11030 0.00195 0.00000 -0.01249 -0.01246 4.09784

R7 2.62362 0.00312 0.00000 0.01158 0.01159 2.63521

R8 2.81648 -0.00051 0.00000 -0.00150 -0.00151 2.81497

R9 2.08424 -0.00017 0.00000 -0.00130 -0.00130 2.08295

R10 4.13856 0.00225 0.00000 -0.03297 -0.03299 4.10557

R11 2.07430 0.00099 0.00000 0.00350 0.00350 2.07780

R12 2.12161 0.00081 0.00000 0.00210 0.00210 2.12371

R13 2.13198 -0.00089 0.00000 -0.00381 -0.00381 2.12817

R14 2.87914 0.00026 0.00000 -0.00275 -0.00267 2.87648

R15 2.12458 0.00004 0.00000 -0.00029 -0.00029 2.12429

R16 2.12675 0.00003 0.00000 0.00131 0.00131 2.12806

R17 2.65221 0.00523 0.00000 0.01194 0.01191 2.66412

R18 2.67420 -0.00308 0.00000 -0.01093 -0.01096 2.66324

R19 2.66004 -0.00046 0.00000 0.00485 0.00490 2.66494

R20 2.80617 0.00328 0.00000 0.00539 0.00541 2.81159

R21 2.06392 -0.00002 0.00000 0.00070 0.00070 2.06463

R22 2.79897 0.00722 0.00000 0.01444 0.01443 2.81340

R23 2.06509 0.00031 0.00000 -0.00017 -0.00017 2.06492

R24 2.30686 0.00104 0.00000 -0.00045 -0.00045 2.30641

R25 2.30847 -0.00310 0.00000 -0.00204 -0.00204 2.30643

A1 2.06327 -0.00097 0.00000 -0.00169 -0.00181 2.06147

A2 2.09813 0.00207 0.00000 0.00987 0.00979 2.10791

A3 2.11247 -0.00115 0.00000 -0.01106 -0.01109 2.10138

A4 2.09816 -0.00081 0.00000 -0.00975 -0.00971 2.08846

A5 2.10191 0.00003 0.00000 0.00062 0.00063 2.10253

A6 1.63668 -0.00011 0.00000 -0.01384 -0.01387 1.62281

A7 2.01231 0.00102 0.00000 0.00964 0.00961 2.02192

A8 1.73661 -0.00093 0.00000 0.00403 0.00374 1.74035

A9 1.69340 0.00040 0.00000 0.00890 0.00901 1.70242

A10 2.09819 -0.00026 0.00000 -0.00828 -0.00824 2.08995

A11 2.09922 0.00057 0.00000 0.00446 0.00420 2.10342

A12 1.59970 -0.00006 0.00000 0.01489 0.01482 1.61452

A13 2.02448 -0.00025 0.00000 -0.00255 -0.00250 2.02198

A14 1.75065 -0.00035 0.00000 -0.00764 -0.00776 1.74288

A15 1.69216 0.00030 0.00000 0.00992 0.01004 1.70219

A16 2.05229 0.00137 0.00000 0.00917 0.00922 2.06151

A17 2.10278 -0.00087 0.00000 -0.00113 -0.00120 2.10157

A18 2.11406 -0.00048 0.00000 -0.00665 -0.00668 2.10738

A19 1.94844 -0.00164 0.00000 -0.02363 -0.02362 1.92482

A20 1.88849 -0.00135 0.00000 -0.01502 -0.01507 1.87342

A21 1.97218 0.00116 0.00000 0.00865 0.00867 1.98085

A22 1.83219 0.00111 0.00000 0.02217 0.02197 1.85415

A23 1.91601 0.00035 0.00000 0.00465 0.00457 1.92058

A24 1.90045 0.00039 0.00000 0.00446 0.00456 1.90501

A25 1.98251 -0.00007 0.00000 -0.00081 -0.00094 1.98156

A26 1.91925 -0.00003 0.00000 0.00407 0.00407 1.92332

A27 1.87182 0.00023 0.00000 0.00082 0.00086 1.87268

A28 1.91481 0.00037 0.00000 0.00577 0.00577 1.92058

A29 1.91144 -0.00039 0.00000 -0.00677 -0.00671 1.90474

A30 1.85957 -0.00011 0.00000 -0.00352 -0.00353 1.85604

A31 1.88293 -0.00053 0.00000 0.00066 0.00069 1.88362

A32 1.87647 -0.00018 0.00000 -0.00116 -0.00158 1.87489

A33 1.70722 0.00016 0.00000 0.02596 0.02625 1.73347

A34 1.56302 -0.00002 0.00000 0.00257 0.00259 1.56561

A35 1.87031 -0.00022 0.00000 -0.00241 -0.00253 1.86778

A36 2.21029 -0.00021 0.00000 -0.01172 -0.01162 2.19867

A37 2.10070 0.00049 0.00000 0.00237 0.00205 2.10275

A38 1.86535 0.00078 0.00000 0.01015 0.00987 1.87523

A39 1.75830 -0.00028 0.00000 -0.01299 -0.01300 1.74531

A40 1.57877 -0.00106 0.00000 -0.01511 -0.01479 1.56398

A41 1.86736 -0.00043 0.00000 -0.00088 -0.00077 1.86660

A42 2.20342 -0.00007 0.00000 -0.00469 -0.00475 2.19867

A43 2.08333 0.00088 0.00000 0.01585 0.01566 2.09899

A44 1.90247 0.00027 0.00000 0.00072 0.00077 1.90324

A45 2.02781 0.00024 0.00000 -0.00163 -0.00170 2.02612

A46 2.35279 -0.00050 0.00000 0.00110 0.00103 2.35382

A47 1.90151 0.00091 0.00000 0.00199 0.00191 1.90343

A48 2.03123 -0.00237 0.00000 -0.00451 -0.00463 2.02660

A49 2.35015 0.00148 0.00000 0.00314 0.00301 2.35316

D1 -0.61001 0.00089 0.00000 0.00882 0.00876 -0.60125

D2 2.94541 -0.00003 0.00000 0.00518 0.00509 2.95049

D3 1.19271 -0.00044 0.00000 0.00306 0.00286 1.19556

D4 2.67629 0.00140 0.00000 0.03199 0.03212 2.70840

D5 -0.05149 0.00047 0.00000 0.02835 0.02845 -0.02304

D6 -1.80419 0.00007 0.00000 0.02623 0.02622 -1.77797

D7 0.01291 -0.00012 0.00000 -0.01301 -0.01300 -0.00009

D8 -2.95130 -0.00023 0.00000 -0.02097 -0.02091 -2.97221

D9 3.00856 -0.00035 0.00000 -0.03455 -0.03447 2.97409

D10 0.04435 -0.00047 0.00000 -0.04251 -0.04237 0.00198

D11 2.74550 -0.00029 0.00000 -0.00241 -0.00247 2.74304

D12 -1.53002 -0.00065 0.00000 0.00253 0.00256 -1.52746

D13 0.57568 -0.00036 0.00000 0.00329 0.00334 0.57902

D14 -0.78966 0.00039 0.00000 -0.00071 -0.00074 -0.79040

D15 1.21799 0.00003 0.00000 0.00423 0.00429 1.22228

D16 -2.95949 0.00032 0.00000 0.00498 0.00507 -2.95442

D17 0.99910 0.00064 0.00000 0.01421 0.01428 1.01339

D18 3.00676 0.00028 0.00000 0.01914 0.01931 3.02607

D19 -1.17073 0.00057 0.00000 0.01990 0.02009 -1.15063

D20 -0.98690 0.00009 0.00000 -0.03510 -0.03512 -1.02202

D21 -2.93498 0.00042 0.00000 -0.03222 -0.03218 -2.96716

D22 1.25304 -0.00021 0.00000 -0.04354 -0.04364 1.20940

D23 1.13357 -0.00094 0.00000 -0.04770 -0.04770 1.08587

D24 -0.81451 -0.00061 0.00000 -0.04481 -0.04476 -0.85927

D25 -2.90968 -0.00124 0.00000 -0.05613 -0.05622 -2.96590

D26 -3.10403 0.00002 0.00000 -0.03454 -0.03451 -3.13854

D27 1.23107 0.00035 0.00000 -0.03165 -0.03157 1.19950

D28 -0.86409 -0.00029 0.00000 -0.04298 -0.04303 -0.90712

D29 0.58685 -0.00024 0.00000 0.01098 0.01105 0.59790

D30 -2.73333 -0.00016 0.00000 0.01961 0.01958 -2.71376

D31 -2.93836 -0.00014 0.00000 -0.00869 -0.00860 -2.94696

D32 0.02464 -0.00006 0.00000 -0.00007 -0.00007 0.02457

D33 -1.20980 0.00024 0.00000 0.01227 0.01260 -1.19719

D34 1.75321 0.00032 0.00000 0.02090 0.02113 1.77434

D35 -0.56993 0.00052 0.00000 0.00144 0.00145 -0.56848

D36 -2.72331 0.00012 0.00000 -0.00862 -0.00856 -2.73187

D37 1.54455 0.00014 0.00000 -0.00701 -0.00697 1.53758

D38 2.93950 0.00025 0.00000 0.01875 0.01871 2.95822

D39 0.78613 -0.00016 0.00000 0.00868 0.00870 0.79483

D40 -1.22920 -0.00013 0.00000 0.01029 0.01029 -1.21891

D41 1.14120 0.00018 0.00000 0.01223 0.01210 1.15331

D42 -1.01217 -0.00023 0.00000 0.00216 0.00209 -1.01008

D43 -3.02750 -0.00021 0.00000 0.00378 0.00368 -3.02382

D44 1.09540 -0.00044 0.00000 -0.04525 -0.04515 1.05025

D45 3.02977 -0.00067 0.00000 -0.03804 -0.03797 2.99180

D46 -1.14843 -0.00016 0.00000 -0.03338 -0.03330 -1.18173

D47 -1.01874 -0.00011 0.00000 -0.03907 -0.03894 -1.05768

D48 0.91563 -0.00033 0.00000 -0.03186 -0.03176 0.88387

D49 3.02061 0.00017 0.00000 -0.02720 -0.02708 2.99352

D50 -3.07989 0.00015 0.00000 -0.03730 -0.03718 -3.11707

D51 -1.14552 -0.00007 0.00000 -0.03009 -0.03000 -1.17552

D52 0.95946 0.00044 0.00000 -0.02543 -0.02533 0.93414

D53 -0.00021 -0.00016 0.00000 -0.00644 -0.00641 -0.00662

D54 2.15559 0.00003 0.00000 0.00269 0.00266 2.15826

D55 -2.09234 -0.00012 0.00000 -0.00216 -0.00218 -2.09452

D56 -2.18766 0.00087 0.00000 0.01463 0.01471 -2.17295

D57 -0.03186 0.00106 0.00000 0.02375 0.02379 -0.00807

D58 2.00339 0.00091 0.00000 0.01890 0.01895 2.02234

D59 2.09866 -0.00086 0.00000 -0.01675 -0.01671 2.08195

D60 -2.02872 -0.00067 0.00000 -0.00762 -0.00764 -2.03636

D61 0.00653 -0.00081 0.00000 -0.01247 -0.01248 -0.00595

D62 -0.01918 0.00016 0.00000 0.00415 0.00424 -0.01494

D63 3.10853 0.00043 0.00000 0.01523 0.01531 3.12384

D64 0.01541 -0.00033 0.00000 -0.00238 -0.00245 0.01296

D65 3.13474 0.00054 0.00000 0.02116 0.02091 -3.12754

D66 -0.05770 -0.00008 0.00000 0.04133 0.04158 -0.01612

D67 1.81401 -0.00025 0.00000 0.03057 0.03072 1.84473

D68 -1.86340 0.00073 0.00000 0.05536 0.05546 -1.80794

D69 -1.87777 -0.00010 0.00000 0.01364 0.01376 -1.86401

D70 -0.00606 -0.00027 0.00000 0.00288 0.00290 -0.00316

D71 2.59971 0.00071 0.00000 0.02766 0.02764 2.62735

D72 1.73956 -0.00037 0.00000 0.03801 0.03803 1.77759

D73 -2.67191 -0.00053 0.00000 0.02725 0.02717 -2.64474

D74 -0.06614 0.00044 0.00000 0.05203 0.05191 -0.01423

D75 -1.92358 0.00026 0.00000 -0.01258 -0.01234 -1.93592

D76 1.23558 -0.00010 0.00000 -0.02656 -0.02634 1.20924

D77 0.01581 0.00007 0.00000 -0.00450 -0.00456 0.01125

D78 -3.10822 -0.00029 0.00000 -0.01848 -0.01856 -3.12678

D79 2.71743 0.00010 0.00000 -0.03152 -0.03158 2.68585

D80 -0.40659 -0.00026 0.00000 -0.04550 -0.04558 -0.45218

D81 1.94104 0.00096 0.00000 0.00514 0.00492 1.94596

D82 -1.17252 -0.00006 0.00000 -0.02436 -0.02450 -1.19702

D83 -0.00550 0.00036 0.00000 -0.00045 -0.00042 -0.00591

D84 -3.11905 -0.00066 0.00000 -0.02994 -0.02984 3.13429

D85 -2.65502 -0.00022 0.00000 -0.01620 -0.01642 -2.67144

D86 0.51461 -0.00125 0.00000 -0.04569 -0.04584 0.46877

Item Value Threshold Converged?

Maximum Force 0.007225 0.000450 NO

RMS Force 0.001162 0.000300 NO

Maximum Displacement 0.108240 0.001800 NO

RMS Displacement 0.024313 0.001200 NO

Predicted change in Energy=-5.786928D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.143569 1.563275 0.442061

2 6 0 0.180287 1.278965 0.109644

3 6 0 -0.749260 3.779323 -0.373534

4 6 0 -1.622619 2.851530 0.193088

5 1 0 -1.742104 0.850589 1.027359

6 1 0 -2.602009 3.165898 0.581573

7 6 0 0.794021 1.920266 -1.086948

8 1 0 1.913571 1.934630 -0.990127

9 1 0 0.563069 1.265948 -1.973973

10 6 0 0.275542 3.326077 -1.355015

11 1 0 1.132188 4.053326 -1.385470

12 1 0 -0.201417 3.355383 -2.374721

13 1 0 -1.019388 4.846982 -0.419192

14 1 0 0.652901 0.342611 0.448568

15 8 0 2.752771 3.867871 0.822009

16 6 0 0.470222 3.870791 1.422176

17 6 0 0.966678 2.572813 1.662021

18 6 0 1.604270 4.681518 0.902281

19 8 0 1.743378 5.842387 0.552055

20 6 0 2.406990 2.582585 1.285337

21 8 0 3.304283 1.755281 1.294185

22 1 0 -0.356324 4.349893 1.952231

23 1 0 0.600116 1.875063 2.418849

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394248 0.000000

3 C 2.394065 2.710961 0.000000

4 C 1.396810 2.393825 1.394495 0.000000

5 H 1.099427 2.172854 3.394956 2.171187 0.000000

6 H 2.171384 3.394761 2.172831 1.099523 2.509745

7 C 2.493906 1.489889 2.519280 2.888926 3.470797

8 H 3.396347 2.154916 3.297537 3.839966 4.313856

9 H 2.972917 2.118526 3.255867 3.462291 3.807143

10 C 2.889781 2.518922 1.489617 2.494962 3.984300

11 H 3.836574 3.292197 2.153821 3.394867 4.933643

12 H 3.468943 3.260257 2.117690 2.977806 4.496872

13 H 3.397045 3.801267 1.102247 2.172695 4.311147

14 H 2.171950 1.102267 3.801697 3.396755 2.515768

15 O 4.542795 3.718544 3.701538 4.535695 5.417570

16 C 2.981540 2.919652 2.172574 2.632401 3.764558

17 C 2.638297 2.168485 2.922943 2.989968 3.272056

18 C 4.181610 3.772714 2.825025 3.776854 5.088211

19 O 5.163077 4.843945 3.365441 4.517081 6.106763

20 C 3.789008 2.835469 3.761110 4.183670 4.503482

21 O 4.532810 3.374812 4.827965 5.166095 5.133779

22 H 3.265825 3.621281 2.426753 2.634991 3.875682

23 H 2.654306 2.421573 3.639289 3.293639 2.910634

6 7 8 9 10

6 H 0.000000

7 C 3.983538 0.000000

8 H 4.937278 1.123821 0.000000

9 H 4.489804 1.126181 1.799707 0.000000

10 C 3.472223 1.522165 2.180001 2.170233 0.000000

11 H 4.312889 2.180234 2.292537 2.905117 1.124126

12 H 3.812928 2.169980 2.899795 2.260702 1.126121

13 H 2.516399 3.507138 4.172530 4.212519 2.205847

14 H 4.310810 2.206065 2.488706 2.594095 3.506621

15 O 5.405945 3.357676 2.779480 4.402535 3.342100

16 C 3.262222 3.194543 3.413382 4.281082 2.836795

17 C 3.775532 2.830629 2.887520 3.884746 3.185528

18 C 4.482493 3.498293 3.349965 4.585091 2.949258

19 O 5.103612 4.355531 4.204504 5.358893 3.481849

20 C 5.091719 2.944159 2.416825 3.969468 3.473803

21 O 6.114076 3.463875 2.680359 4.293548 4.319598

22 H 2.885073 4.057461 4.432086 5.076522 3.519280

23 H 3.910939 3.511447 3.653741 4.435006 4.056210

11 12 13 14 15

11 H 0.000000

12 H 1.801178 0.000000

13 H 2.488547 2.591918 0.000000

14 H 4.166872 4.216351 4.882512 0.000000

15 O 2.744749 4.382801 4.090039 4.120239 0.000000

16 C 2.890398 3.890138 2.561743 3.664607 2.360135

17 C 3.392126 4.274594 3.667118 2.558266 2.360704

18 C 2.418945 3.969620 2.942321 4.465095 1.409794

19 O 2.707083 4.305048 3.093062 5.607797 2.233934

20 C 3.304756 4.560376 4.446682 2.965551 1.409325

21 O 4.144823 5.320820 5.584658 3.120982 2.233865

22 H 3.666588 4.442472 2.512051 4.397482 3.343085

23 H 4.415968 5.080563 4.416965 2.496638 3.339926

16 17 18 19 20

16 C 0.000000

17 C 1.410228 0.000000

18 C 1.487829 2.330315 0.000000

19 O 2.503044 3.539125 1.220502 0.000000

20 C 2.330080 1.488787 2.279608 3.406522 0.000000

21 O 3.538879 2.503609 3.406831 4.437523 1.220510

22 H 1.092554 2.234406 2.248622 2.932026 3.347242

23 H 2.234538 1.092708 3.344323 4.531184 2.247272

21 22 23

21 O 0.000000

22 H 4.534873 0.000000

23 H 2.931166 2.693937 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.313112 -0.674462 -0.674028

2 6 0 1.383607 -1.351150 0.114669

3 6 0 1.359100 1.359423 0.153450

4 6 0 2.300598 0.722150 -0.654065

5 1 0 2.926734 -1.214889 -1.408973

6 1 0 2.902795 1.294502 -1.374288

7 6 0 0.976382 -0.779237 1.428767

8 1 0 -0.027975 -1.180624 1.733935

9 1 0 1.710570 -1.149859 2.198111

10 6 0 0.957883 0.742686 1.448679

11 1 0 -0.058583 1.111604 1.755856

12 1 0 1.678509 1.110361 2.232044

13 1 0 1.188616 2.444784 0.064705

14 1 0 1.235580 -2.437026 -0.003460

15 8 0 -2.079440 -0.005763 0.272187

16 6 0 -0.294310 0.708433 -1.096561

17 6 0 -0.290180 -0.701780 -1.101507

18 6 0 -1.430060 1.137483 -0.236548

19 8 0 -1.895610 2.214008 0.101065

20 6 0 -1.421803 -1.142107 -0.240097

21 8 0 -1.876469 -2.223472 0.096907

22 1 0 0.066753 1.354111 -1.900557

23 1 0 0.063183 -1.339783 -1.915200

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2201790 0.8803405 0.6750798

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5193155347 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504109098639E-01 A.U. after 15 cycles

Convg = 0.2699D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000226421 0.000149065 0.000043624

2 6 0.000422975 -0.000077632 -0.000190119

3 6 -0.000100231 -0.000153671 0.000385258

4 6 0.000150675 0.000099255 -0.000086442

5 1 -0.000008152 0.000004866 0.000060969

6 1 -0.000004680 -0.000047375 -0.000041544

7 6 -0.000082924 0.000070348 -0.000041087

8 1 0.000091862 0.000028416 0.000085947

9 1 -0.000065865 -0.000022441 0.000025637

10 6 0.000013791 -0.000025403 0.000046702

11 1 -0.000022923 -0.000073980 -0.000045759

12 1 0.000056170 0.000053864 -0.000046007

13 1 -0.000058395 -0.000021551 -0.000000563

14 1 0.000006840 0.000005371 -0.000007179

15 8 -0.000009974 0.000094382 -0.000110600

16 6 0.000025787 -0.000089973 -0.000094222

17 6 0.000077971 0.000085757 0.000149303

18 6 0.000094686 -0.000029533 0.000032819

19 8 -0.000016117 0.000051790 -0.000059075

20 6 -0.000332453 -0.000122798 -0.000066475

21 8 0.000073912 0.000002704 0.000094640

22 1 0.000079610 0.000046924 0.000003772

23 1 -0.000166142 -0.000028384 -0.000139598

-------------------------------------------------------------------

Cartesian Forces: Max 0.000422975 RMS 0.000112814

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000217845 RMS 0.000049308

Search for a saddle point.

Step number 71 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 43 45 46 50

51 52 55 56 57

58 59 63 64 65

66 70 71

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07028 0.00204 0.00333 0.00799 0.00803

Eigenvalues --- 0.01005 0.01217 0.01291 0.01864 0.02186

Eigenvalues --- 0.02484 0.02793 0.02892 0.03206 0.03335

Eigenvalues --- 0.03559 0.03610 0.03799 0.04029 0.04127

Eigenvalues --- 0.04381 0.04412 0.04735 0.04824 0.06382

Eigenvalues --- 0.06576 0.06621 0.07054 0.07435 0.08503

Eigenvalues --- 0.08983 0.10119 0.10373 0.10759 0.10923

Eigenvalues --- 0.12750 0.13791 0.15047 0.15925 0.22798

Eigenvalues --- 0.26432 0.28642 0.29598 0.30149 0.31083

Eigenvalues --- 0.31440 0.31868 0.32045 0.32223 0.32557

Eigenvalues --- 0.33398 0.35218 0.37031 0.38104 0.39794

Eigenvalues --- 0.40434 0.40884 0.45079 0.49021 0.53593

Eigenvalues --- 0.62817 1.08754 1.11256

Eigenvectors required to have negative eigenvalues:

R6 R10 D73 D71 D30

1 -0.56112 -0.52774 0.14945 -0.14398 0.14380

R19 D1 D79 D29 D13

1 0.13499 -0.13295 -0.12921 0.12843 0.12667

RFO step: Lambda0=7.791663149D-08 Lambda=-2.16998315D-05.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.01074664 RMS(Int)= 0.00004184

Iteration 2 RMS(Cart)= 0.00005664 RMS(Int)= 0.00001540

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001540

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63475 0.00022 0.00000 0.00040 0.00040 2.63514

R2 2.63959 -0.00008 0.00000 0.00003 0.00003 2.63962

R3 2.07762 0.00003 0.00000 0.00021 0.00021 2.07783

R4 2.81548 -0.00012 0.00000 -0.00018 -0.00018 2.81530

R5 2.08298 0.00000 0.00000 0.00003 0.00003 2.08301

R6 4.09784 -0.00011 0.00000 0.00371 0.00371 4.10155

R7 2.63521 -0.00019 0.00000 -0.00080 -0.00080 2.63441

R8 2.81497 0.00010 0.00000 0.00035 0.00035 2.81532

R9 2.08295 -0.00001 0.00000 -0.00003 -0.00003 2.08292

R10 4.10557 -0.00012 0.00000 -0.00322 -0.00322 4.10235

R11 2.07780 -0.00002 0.00000 -0.00023 -0.00023 2.07757

R12 2.12371 0.00010 0.00000 0.00043 0.00043 2.12414

R13 2.12817 0.00001 0.00000 -0.00005 -0.00005 2.12812

R14 2.87648 -0.00005 0.00000 -0.00012 -0.00011 2.87636

R15 2.12429 -0.00006 0.00000 -0.00023 -0.00023 2.12406

R16 2.12806 0.00002 0.00000 0.00007 0.00007 2.12813

R17 2.66412 -0.00006 0.00000 -0.00111 -0.00111 2.66301

R18 2.66324 0.00012 0.00000 0.00142 0.00142 2.66466

R19 2.66494 -0.00010 0.00000 -0.00011 -0.00012 2.66482

R20 2.81159 0.00005 0.00000 0.00045 0.00045 2.81204

R21 2.06463 -0.00004 0.00000 -0.00005 -0.00005 2.06458

R22 2.81340 -0.00018 0.00000 -0.00216 -0.00216 2.81124

R23 2.06492 -0.00002 0.00000 -0.00026 -0.00026 2.06466

R24 2.30641 0.00006 0.00000 0.00014 0.00014 2.30656

R25 2.30643 0.00005 0.00000 0.00013 0.00013 2.30656

A1 2.06147 -0.00001 0.00000 0.00013 0.00013 2.06159

A2 2.10791 0.00002 0.00000 -0.00025 -0.00024 2.10767

A3 2.10138 -0.00001 0.00000 -0.00021 -0.00021 2.10117

A4 2.08846 -0.00001 0.00000 0.00053 0.00054 2.08899

A5 2.10253 0.00001 0.00000 0.00049 0.00049 2.10302

A6 1.62281 -0.00005 0.00000 -0.00524 -0.00525 1.61756

A7 2.02192 0.00002 0.00000 -0.00041 -0.00041 2.02150

A8 1.74035 0.00000 0.00000 0.00264 0.00262 1.74298

A9 1.70242 0.00003 0.00000 0.00122 0.00125 1.70366

A10 2.08995 0.00001 0.00000 -0.00045 -0.00044 2.08951

A11 2.10342 -0.00002 0.00000 -0.00114 -0.00115 2.10227

A12 1.61452 0.00007 0.00000 0.00512 0.00510 1.61962

A13 2.02198 0.00000 0.00000 0.00032 0.00031 2.02229

A14 1.74288 -0.00005 0.00000 -0.00212 -0.00214 1.74075

A15 1.70219 0.00000 0.00000 0.00009 0.00012 1.70231

A16 2.06151 0.00002 0.00000 -0.00020 -0.00020 2.06130

A17 2.10157 -0.00004 0.00000 -0.00041 -0.00041 2.10116

A18 2.10738 0.00002 0.00000 0.00081 0.00081 2.10819

A19 1.92482 -0.00002 0.00000 -0.00029 -0.00029 1.92453

A20 1.87342 -0.00003 0.00000 -0.00057 -0.00056 1.87285

A21 1.98085 -0.00001 0.00000 0.00032 0.00031 1.98116

A22 1.85415 0.00004 0.00000 0.00150 0.00150 1.85565

A23 1.92058 0.00001 0.00000 -0.00107 -0.00108 1.91950

A24 1.90501 0.00001 0.00000 0.00023 0.00024 1.90525

A25 1.98156 0.00001 0.00000 -0.00041 -0.00041 1.98115

A26 1.92332 0.00003 0.00000 0.00092 0.00092 1.92424

A27 1.87268 0.00002 0.00000 0.00085 0.00085 1.87353

A28 1.92058 -0.00004 0.00000 -0.00044 -0.00045 1.92013

A29 1.90474 0.00001 0.00000 0.00062 0.00064 1.90537

A30 1.85604 -0.00003 0.00000 -0.00160 -0.00160 1.85444

A31 1.88362 -0.00004 0.00000 -0.00013 -0.00013 1.88349

A32 1.87489 -0.00003 0.00000 -0.00008 -0.00015 1.87474

A33 1.73347 -0.00001 0.00000 0.00583 0.00586 1.73934

A34 1.56561 0.00001 0.00000 -0.00251 -0.00248 1.56313

A35 1.86778 0.00004 0.00000 -0.00075 -0.00075 1.86703

A36 2.19867 -0.00001 0.00000 0.00077 0.00077 2.19944

A37 2.10275 -0.00001 0.00000 -0.00135 -0.00136 2.10139

A38 1.87523 0.00007 0.00000 0.00023 0.00016 1.87538

A39 1.74531 -0.00011 0.00000 -0.00859 -0.00856 1.73675

A40 1.56398 -0.00001 0.00000 0.00080 0.00083 1.56481

A41 1.86660 0.00001 0.00000 0.00100 0.00100 1.86759

A42 2.19867 -0.00003 0.00000 -0.00025 -0.00025 2.19842

A43 2.09899 0.00005 0.00000 0.00284 0.00283 2.10181

A44 1.90324 -0.00004 0.00000 0.00025 0.00025 1.90349

A45 2.02612 0.00004 0.00000 -0.00001 -0.00001 2.02610

A46 2.35382 0.00001 0.00000 -0.00023 -0.00023 2.35359

A47 1.90343 0.00003 0.00000 -0.00038 -0.00039 1.90304

A48 2.02660 -0.00003 0.00000 0.00002 0.00002 2.02662

A49 2.35316 0.00000 0.00000 0.00036 0.00036 2.35352

D1 -0.60125 0.00001 0.00000 0.00227 0.00227 -0.59898

D2 2.95049 -0.00003 0.00000 0.00066 0.00064 2.95114

D3 1.19556 -0.00002 0.00000 0.00233 0.00230 1.19786

D4 2.70840 0.00003 0.00000 0.00445 0.00446 2.71286

D5 -0.02304 -0.00001 0.00000 0.00283 0.00283 -0.02021

D6 -1.77797 -0.00001 0.00000 0.00450 0.00448 -1.77349

D7 -0.00009 -0.00002 0.00000 -0.00148 -0.00148 -0.00157

D8 -2.97221 -0.00003 0.00000 -0.00289 -0.00288 -2.97509

D9 2.97409 -0.00004 0.00000 -0.00364 -0.00366 2.97044

D10 0.00198 -0.00004 0.00000 -0.00506 -0.00506 -0.00308

D11 2.74304 -0.00005 0.00000 -0.00539 -0.00540 2.73764

D12 -1.52746 -0.00003 0.00000 -0.00408 -0.00409 -1.53155

D13 0.57902 -0.00004 0.00000 -0.00399 -0.00399 0.57503

D14 -0.79040 -0.00002 0.00000 -0.00365 -0.00365 -0.79406

D15 1.22228 0.00000 0.00000 -0.00234 -0.00234 1.21994

D16 -2.95442 0.00000 0.00000 -0.00225 -0.00224 -2.95666

D17 1.01339 0.00002 0.00000 -0.00095 -0.00093 1.01246

D18 3.02607 0.00004 0.00000 0.00037 0.00039 3.02646

D19 -1.15063 0.00003 0.00000 0.00046 0.00049 -1.15015

D20 -1.02202 -0.00001 0.00000 -0.01671 -0.01671 -1.03873

D21 -2.96716 0.00000 0.00000 -0.01439 -0.01438 -2.98154

D22 1.20940 -0.00003 0.00000 -0.01661 -0.01662 1.19279

D23 1.08587 -0.00004 0.00000 -0.01694 -0.01694 1.06892

D24 -0.85927 -0.00002 0.00000 -0.01462 -0.01462 -0.87389

D25 -2.96590 -0.00006 0.00000 -0.01684 -0.01685 -2.98275

D26 -3.13854 -0.00001 0.00000 -0.01641 -0.01641 3.12823

D27 1.19950 0.00000 0.00000 -0.01408 -0.01408 1.18542

D28 -0.90712 -0.00003 0.00000 -0.01631 -0.01631 -0.92344

D29 0.59790 0.00001 0.00000 0.00249 0.00250 0.60039

D30 -2.71376 0.00001 0.00000 0.00379 0.00378 -2.70998

D31 -2.94696 -0.00002 0.00000 -0.00106 -0.00104 -2.94800

D32 0.02457 -0.00002 0.00000 0.00024 0.00024 0.02481

D33 -1.19719 0.00002 0.00000 0.00199 0.00202 -1.19517

D34 1.77434 0.00002 0.00000 0.00328 0.00330 1.77764

D35 -0.56848 -0.00003 0.00000 -0.00419 -0.00419 -0.57267

D36 -2.73187 -0.00002 0.00000 -0.00402 -0.00401 -2.73588

D37 1.53758 0.00000 0.00000 -0.00307 -0.00306 1.53452

D38 2.95822 0.00000 0.00000 -0.00048 -0.00050 2.95772

D39 0.79483 0.00001 0.00000 -0.00031 -0.00031 0.79451

D40 -1.21891 0.00002 0.00000 0.00063 0.00063 -1.21828

D41 1.15331 0.00002 0.00000 0.00046 0.00043 1.15373

D42 -1.01008 0.00004 0.00000 0.00063 0.00061 -1.00947

D43 -3.02382 0.00005 0.00000 0.00157 0.00156 -3.02226

D44 1.05025 -0.00003 0.00000 -0.01652 -0.01652 1.03373

D45 2.99180 -0.00001 0.00000 -0.01503 -0.01503 2.97677

D46 -1.18173 -0.00002 0.00000 -0.01633 -0.01634 -1.19807

D47 -1.05768 -0.00005 0.00000 -0.01690 -0.01690 -1.07458

D48 0.88387 -0.00002 0.00000 -0.01541 -0.01540 0.86846

D49 2.99352 -0.00004 0.00000 -0.01672 -0.01672 2.97681

D50 -3.11707 -0.00004 0.00000 -0.01674 -0.01674 -3.13381

D51 -1.17552 -0.00001 0.00000 -0.01525 -0.01525 -1.19077

D52 0.93414 -0.00003 0.00000 -0.01656 -0.01656 0.91758

D53 -0.00662 0.00000 0.00000 0.00452 0.00452 -0.00210

D54 2.15826 0.00003 0.00000 0.00509 0.00508 2.16334

D55 -2.09452 -0.00003 0.00000 0.00327 0.00327 -2.09125

D56 -2.17295 0.00003 0.00000 0.00550 0.00551 -2.16744

D57 -0.00807 0.00005 0.00000 0.00606 0.00606 -0.00200

D58 2.02234 0.00000 0.00000 0.00425 0.00425 2.02659

D59 2.08195 -0.00003 0.00000 0.00417 0.00417 2.08612

D60 -2.03636 0.00000 0.00000 0.00473 0.00473 -2.03163

D61 -0.00595 -0.00006 0.00000 0.00292 0.00292 -0.00303

D62 -0.01494 -0.00001 0.00000 -0.00062 -0.00060 -0.01554

D63 3.12384 0.00002 0.00000 0.00046 0.00049 3.12433

D64 0.01296 0.00002 0.00000 0.00289 0.00288 0.01584

D65 -3.12754 0.00004 0.00000 0.00455 0.00452 -3.12301

D66 -0.01612 0.00009 0.00000 0.01902 0.01901 0.00289

D67 1.84473 0.00000 0.00000 0.00985 0.00986 1.85459

D68 -1.80794 0.00006 0.00000 0.01789 0.01790 -1.79004

D69 -1.86401 0.00010 0.00000 0.01280 0.01279 -1.85122

D70 -0.00316 0.00001 0.00000 0.00364 0.00364 0.00048

D71 2.62735 0.00008 0.00000 0.01167 0.01168 2.63903

D72 1.77759 0.00007 0.00000 0.01599 0.01597 1.79357

D73 -2.64474 -0.00002 0.00000 0.00683 0.00682 -2.63792

D74 -0.01423 0.00004 0.00000 0.01486 0.01486 0.00063

D75 -1.93592 0.00003 0.00000 -0.00398 -0.00393 -1.93984

D76 1.20924 -0.00001 0.00000 -0.00535 -0.00531 1.20393

D77 0.01125 0.00000 0.00000 -0.00199 -0.00200 0.00925

D78 -3.12678 -0.00004 0.00000 -0.00337 -0.00338 -3.13016

D79 2.68585 0.00003 0.00000 -0.00425 -0.00425 2.68160

D80 -0.45218 -0.00001 0.00000 -0.00563 -0.00563 -0.45781

D81 1.94596 0.00001 0.00000 -0.00702 -0.00706 1.93889

D82 -1.19702 -0.00002 0.00000 -0.00911 -0.00915 -1.20617

D83 -0.00591 -0.00002 0.00000 -0.00415 -0.00414 -0.01005

D84 3.13429 -0.00005 0.00000 -0.00625 -0.00623 3.12807

D85 -2.67144 -0.00005 0.00000 -0.01059 -0.01060 -2.68204

D86 0.46877 -0.00008 0.00000 -0.01269 -0.01269 0.45608

Item Value Threshold Converged?

Maximum Force 0.000218 0.000450 YES

RMS Force 0.000049 0.000300 YES

Maximum Displacement 0.045028 0.001800 NO

RMS Displacement 0.010747 0.001200 NO

Predicted change in Energy=-1.090013D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.137956 1.558978 0.441734

2 6 0 0.186656 1.281136 0.105994

3 6 0 -0.755244 3.778174 -0.369357

4 6 0 -1.623522 2.845405 0.195855

5 1 0 -1.731223 0.843352 1.029013

6 1 0 -2.604644 3.153280 0.584821

7 6 0 0.796461 1.928881 -1.089015

8 1 0 1.915960 1.951940 -0.990671

9 1 0 0.570193 1.274242 -1.976976

10 6 0 0.268753 3.331585 -1.355006

11 1 0 1.121261 4.063338 -1.388933

12 1 0 -0.211041 3.359228 -2.373469

13 1 0 -1.031955 4.844218 -0.412947

14 1 0 0.664502 0.346259 0.441694

15 8 0 2.756742 3.852758 0.821619

16 6 0 0.473323 3.875799 1.417754

17 6 0 0.960593 2.576076 1.666439

18 6 0 1.614088 4.674396 0.893117

19 8 0 1.761336 5.831125 0.532413

20 6 0 2.401366 2.573298 1.295974

21 8 0 3.294196 1.741328 1.318012

22 1 0 -0.348188 4.365851 1.945568

23 1 0 0.581942 1.882362 2.420823

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394459 0.000000

3 C 2.393568 2.710782 0.000000

4 C 1.396827 2.394109 1.394069 0.000000

5 H 1.099538 2.172989 3.394283 2.171167 0.000000

6 H 2.171048 3.394932 2.172839 1.099402 2.509171

7 C 2.494392 1.489793 2.519044 2.889156 3.471830

8 H 3.395968 2.154795 3.294919 3.838496 4.313934

9 H 2.974727 2.117997 3.257437 3.464409 3.810269

10 C 2.889505 2.519048 1.489804 2.494443 3.984313

11 H 3.837606 3.293773 2.154560 3.395401 4.934718

12 H 3.467771 3.259504 2.118523 2.976666 4.496384

13 H 3.396251 3.801298 1.102233 2.171600 4.309890

14 H 2.172450 1.102282 3.801516 3.397237 2.516256

15 O 4.535902 3.705496 3.709182 4.537957 5.407529

16 C 2.986050 2.921501 2.170869 2.636572 3.769202

17 C 2.634065 2.170446 2.921233 2.985432 3.264126

18 C 4.181306 3.764484 2.830334 3.783319 5.087875

19 O 5.163852 4.833617 3.370605 4.526043 6.109212

20 C 3.779599 2.826778 3.766861 4.181390 4.488014

21 O 4.521624 3.367130 4.836727 5.163542 5.113190

22 H 3.280821 3.631192 2.422794 2.645699 3.893695

23 H 2.641859 2.424079 3.628674 3.277500 2.892648

6 7 8 9 10

6 H 0.000000

7 C 3.983516 0.000000

8 H 4.935712 1.124046 0.000000

9 H 4.491456 1.126154 1.800878 0.000000

10 C 3.471474 1.522106 2.179323 2.170339 0.000000

11 H 4.313500 2.179760 2.290886 2.903192 1.124003

12 H 3.810936 2.170432 2.901159 2.261570 1.126159

13 H 2.515584 3.507045 4.170040 4.213999 2.206212

14 H 4.311284 2.205714 2.489182 2.592298 3.506696

15 O 5.412006 3.345822 2.757611 4.388835 3.346551

16 C 3.269510 3.190423 3.403372 4.278046 2.833057

17 C 3.770143 2.835195 2.891800 3.888658 3.190386

18 C 4.495169 3.483563 3.324387 4.570361 2.943997

19 O 5.122049 4.334458 4.170345 5.336764 3.469561

20 C 5.089426 2.946043 2.418771 3.968998 3.485790

21 O 6.109623 3.473851 2.697019 4.300618 4.339038

22 H 2.900612 4.056814 4.424345 5.078170 3.513418

23 H 3.891075 3.516696 3.663705 4.439661 4.056503

11 12 13 14 15

11 H 0.000000

12 H 1.800031 0.000000

13 H 2.489711 2.592825 0.000000

14 H 4.168513 4.215412 4.882623 0.000000

15 O 2.757840 4.388610 4.106260 4.100895 0.000000

16 C 2.886605 3.886975 2.560306 3.667001 2.360065

17 C 3.401920 4.278658 3.665865 2.561202 2.360040

18 C 2.413301 3.966276 2.955704 4.454016 1.409205

19 O 2.688186 4.294730 3.109690 5.594196 2.233475

20 C 3.326802 4.572436 4.457037 2.950626 1.410079

21 O 4.176234 5.341472 5.598190 3.103134 2.234592

22 H 3.656459 4.436911 2.501792 4.409568 3.341724

23 H 4.422868 5.078897 4.405395 2.506668 3.342106

16 17 18 19 20

16 C 0.000000

17 C 1.410162 0.000000

18 C 1.488068 2.329813 0.000000

19 O 2.503219 3.538722 1.220579 0.000000

20 C 2.329954 1.487642 2.279629 3.406772 0.000000

21 O 3.538819 2.502780 3.406785 4.437710 1.220577

22 H 1.092529 2.234752 2.247973 2.931574 3.345932

23 H 2.234219 1.092571 3.345843 4.533188 2.247884

21 22 23

21 O 0.000000

22 H 4.533090 0.000000

23 H 2.931280 2.694202 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.304970 -0.702181 -0.662262

2 6 0 1.368201 -1.355889 0.137515

3 6 0 1.373032 1.354880 0.130935

4 6 0 2.308044 0.694640 -0.664845

5 1 0 2.910789 -1.261072 -1.390004

6 1 0 2.918482 1.248086 -1.392682

7 6 0 0.965197 -0.757668 1.441049

8 1 0 -0.045943 -1.140111 1.748966

9 1 0 1.692776 -1.125772 2.217805

10 6 0 0.966368 0.764432 1.436888

11 1 0 -0.044520 1.150760 1.740596

12 1 0 1.692134 1.135794 2.213797

13 1 0 1.216197 2.440684 0.024394

14 1 0 1.208181 -2.441915 0.037680

15 8 0 -2.077253 0.000937 0.273768

16 6 0 -0.292262 0.704519 -1.100527

17 6 0 -0.292575 -0.705642 -1.099352

18 6 0 -1.424773 1.139881 -0.239002

19 8 0 -1.884720 2.219134 0.097859

20 6 0 -1.425169 -1.139748 -0.238039

21 8 0 -1.886306 -2.218576 0.098546

22 1 0 0.065874 1.346224 -1.908965

23 1 0 0.066066 -1.347977 -1.907122

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200220 0.8809524 0.6754800

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5669129392 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504180446795E-01 A.U. after 14 cycles

Convg = 0.5147D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000152637 -0.000095977 0.000020279

2 6 -0.000189922 -0.000073991 -0.000071460

3 6 0.000099464 0.000223494 -0.000249510

4 6 -0.000026475 -0.000214018 0.000107317

5 1 -0.000009026 -0.000008544 -0.000079109

6 1 -0.000028474 0.000044186 0.000059885

7 6 -0.000014825 0.000115294 0.000042360

8 1 -0.000021446 -0.000078718 0.000029533

9 1 0.000033670 0.000004669 0.000003444

10 6 -0.000021454 0.000003993 0.000001415

11 1 0.000005981 0.000028190 -0.000008432

12 1 -0.000050178 -0.000027908 0.000030581

13 1 0.000028802 0.000036589 -0.000047039

14 1 -0.000006815 0.000050536 0.000085143

15 8 0.000269383 -0.000499725 0.000058747

16 6 -0.000055775 -0.000148198 0.000070819

17 6 -0.000371615 0.000107252 0.000124083

18 6 -0.000106789 0.000237945 -0.000086887

19 8 -0.000032960 0.000059456 0.000038074

20 6 0.000442775 0.000130912 -0.000105992

21 8 -0.000068371 0.000172764 -0.000061934

22 1 -0.000023896 -0.000034491 0.000037582

23 1 -0.000004690 -0.000033710 0.000001100

-------------------------------------------------------------------

Cartesian Forces: Max 0.000499725 RMS 0.000131098

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000394728 RMS 0.000061879

Search for a saddle point.

Step number 72 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58 59 63 64

65 66 70 71 72

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07062 0.00184 0.00332 0.00777 0.00805

Eigenvalues --- 0.01129 0.01197 0.01276 0.01886 0.02174

Eigenvalues --- 0.02501 0.02795 0.02899 0.03205 0.03314

Eigenvalues --- 0.03560 0.03622 0.03799 0.04036 0.04164

Eigenvalues --- 0.04377 0.04423 0.04728 0.04840 0.06373

Eigenvalues --- 0.06568 0.06608 0.07019 0.07426 0.08492

Eigenvalues --- 0.09002 0.10094 0.10367 0.10747 0.10945

Eigenvalues --- 0.12761 0.13733 0.14957 0.15921 0.22844

Eigenvalues --- 0.26628 0.28781 0.29590 0.30199 0.31090

Eigenvalues --- 0.31443 0.31872 0.32046 0.32222 0.32565

Eigenvalues --- 0.33393 0.35288 0.37053 0.38137 0.39803

Eigenvalues --- 0.40467 0.40954 0.45202 0.49136 0.53684

Eigenvalues --- 0.62984 1.08793 1.11273

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 -0.56408 -0.52445 -0.14746 0.14539 0.14294

R19 D1 D13 D29 D79

1 0.13646 -0.13411 0.12934 0.12857 -0.12427

RFO step: Lambda0=8.639555765D-08 Lambda=-3.79931583D-06.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00169879 RMS(Int)= 0.00000117

Iteration 2 RMS(Cart)= 0.00000149 RMS(Int)= 0.00000038

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000038

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63514 -0.00016 0.00000 -0.00017 -0.00017 2.63498

R2 2.63962 0.00002 0.00000 -0.00018 -0.00018 2.63944

R3 2.07783 -0.00003 0.00000 -0.00011 -0.00011 2.07771

R4 2.81530 0.00000 0.00000 -0.00005 -0.00005 2.81525

R5 2.08301 -0.00002 0.00000 -0.00007 -0.00007 2.08294

R6 4.10155 0.00003 0.00000 -0.00045 -0.00045 4.10110

R7 2.63441 0.00022 0.00000 0.00064 0.00064 2.63505

R8 2.81532 -0.00009 0.00000 -0.00008 -0.00008 2.81524

R9 2.08292 0.00003 0.00000 0.00002 0.00002 2.08294

R10 4.10235 0.00007 0.00000 -0.00069 -0.00069 4.10166

R11 2.07757 0.00006 0.00000 0.00019 0.00019 2.07776

R12 2.12414 -0.00002 0.00000 -0.00006 -0.00006 2.12408

R13 2.12812 -0.00001 0.00000 0.00003 0.00003 2.12816

R14 2.87636 0.00003 0.00000 -0.00006 -0.00006 2.87631

R15 2.12406 0.00002 0.00000 0.00002 0.00002 2.12408

R16 2.12813 -0.00001 0.00000 0.00001 0.00001 2.12814

R17 2.66301 0.00034 0.00000 0.00097 0.00097 2.66398

R18 2.66466 -0.00027 0.00000 -0.00095 -0.00095 2.66371

R19 2.66482 -0.00006 0.00000 -0.00007 -0.00007 2.66475

R20 2.81204 0.00016 0.00000 0.00029 0.00029 2.81233

R21 2.06458 0.00002 0.00000 0.00009 0.00009 2.06467

R22 2.81124 0.00039 0.00000 0.00116 0.00116 2.81240

R23 2.06466 0.00002 0.00000 0.00001 0.00001 2.06467

R24 2.30656 0.00004 0.00000 -0.00009 -0.00009 2.30647

R25 2.30656 -0.00017 0.00000 -0.00008 -0.00008 2.30647

A1 2.06159 -0.00001 0.00000 -0.00007 -0.00007 2.06152

A2 2.10767 0.00000 0.00000 0.00010 0.00010 2.10777

A3 2.10117 0.00001 0.00000 0.00013 0.00013 2.10130

A4 2.08899 0.00002 0.00000 -0.00002 -0.00002 2.08898

A5 2.10302 -0.00003 0.00000 -0.00024 -0.00024 2.10278

A6 1.61756 0.00003 0.00000 0.00091 0.00091 1.61846

A7 2.02150 0.00003 0.00000 0.00066 0.00066 2.02217

A8 1.74298 -0.00004 0.00000 -0.00093 -0.00094 1.74204

A9 1.70366 -0.00002 0.00000 -0.00106 -0.00106 1.70260

A10 2.08951 -0.00003 0.00000 -0.00048 -0.00048 2.08903

A11 2.10227 0.00005 0.00000 0.00054 0.00054 2.10281

A12 1.61962 -0.00006 0.00000 -0.00108 -0.00108 1.61855

A13 2.02229 -0.00001 0.00000 -0.00011 -0.00011 2.02218

A14 1.74075 0.00001 0.00000 0.00095 0.00095 1.74170

A15 1.70231 0.00003 0.00000 0.00031 0.00031 1.70263

A16 2.06130 0.00001 0.00000 0.00027 0.00027 2.06157

A17 2.10116 0.00001 0.00000 0.00012 0.00012 2.10128

A18 2.10819 -0.00002 0.00000 -0.00045 -0.00045 2.10774

A19 1.92453 -0.00005 0.00000 -0.00036 -0.00036 1.92417

A20 1.87285 -0.00003 0.00000 0.00010 0.00010 1.87296

A21 1.98116 0.00006 0.00000 0.00013 0.00013 1.98129

A22 1.85565 -0.00001 0.00000 -0.00069 -0.00069 1.85497

A23 1.91950 0.00003 0.00000 0.00085 0.00085 1.92035

A24 1.90525 -0.00001 0.00000 -0.00012 -0.00012 1.90513

A25 1.98115 -0.00003 0.00000 0.00011 0.00011 1.98125

A26 1.92424 -0.00001 0.00000 -0.00010 -0.00010 1.92414

A27 1.87353 0.00001 0.00000 -0.00049 -0.00049 1.87304

A28 1.92013 0.00003 0.00000 0.00015 0.00015 1.92028

A29 1.90537 0.00001 0.00000 -0.00023 -0.00023 1.90515

A30 1.85444 0.00001 0.00000 0.00058 0.00058 1.85503

A31 1.88349 -0.00002 0.00000 0.00003 0.00003 1.88351

A32 1.87474 0.00002 0.00000 0.00037 0.00037 1.87511

A33 1.73934 -0.00002 0.00000 -0.00094 -0.00094 1.73840

A34 1.56313 0.00002 0.00000 0.00100 0.00100 1.56413

A35 1.86703 0.00001 0.00000 0.00029 0.00029 1.86732

A36 2.19944 -0.00003 0.00000 -0.00062 -0.00062 2.19881

A37 2.10139 0.00001 0.00000 0.00004 0.00004 2.10143

A38 1.87538 0.00001 0.00000 -0.00013 -0.00013 1.87525

A39 1.73675 0.00002 0.00000 0.00130 0.00130 1.73805

A40 1.56481 -0.00003 0.00000 -0.00041 -0.00041 1.56440

A41 1.86759 -0.00003 0.00000 -0.00040 -0.00040 1.86719

A42 2.19842 0.00002 0.00000 0.00037 0.00037 2.19879

A43 2.10181 0.00001 0.00000 -0.00028 -0.00028 2.10153

A44 1.90349 -0.00002 0.00000 -0.00025 -0.00025 1.90324

A45 2.02610 0.00007 0.00000 0.00031 0.00031 2.02641

A46 2.35359 -0.00005 0.00000 -0.00007 -0.00007 2.35353

A47 1.90304 0.00007 0.00000 0.00032 0.00032 1.90336

A48 2.02662 -0.00014 0.00000 -0.00036 -0.00036 2.02626

A49 2.35352 0.00008 0.00000 0.00004 0.00004 2.35356

D1 -0.59898 0.00001 0.00000 -0.00076 -0.00076 -0.59974

D2 2.95114 -0.00002 0.00000 -0.00205 -0.00205 2.94909

D3 1.19786 -0.00002 0.00000 -0.00132 -0.00132 1.19654

D4 2.71286 0.00000 0.00000 -0.00185 -0.00185 2.71101

D5 -0.02021 -0.00003 0.00000 -0.00314 -0.00314 -0.02335

D6 -1.77349 -0.00003 0.00000 -0.00241 -0.00241 -1.77589

D7 -0.00157 0.00003 0.00000 0.00152 0.00152 -0.00005

D8 -2.97509 0.00003 0.00000 0.00198 0.00198 -2.97311

D9 2.97044 0.00004 0.00000 0.00260 0.00260 2.97304

D10 -0.00308 0.00003 0.00000 0.00306 0.00306 -0.00002

D11 2.73764 0.00004 0.00000 0.00001 0.00001 2.73765

D12 -1.53155 0.00000 0.00000 -0.00093 -0.00093 -1.53248

D13 0.57503 0.00000 0.00000 -0.00093 -0.00093 0.57410

D14 -0.79406 0.00006 0.00000 0.00104 0.00104 -0.79301

D15 1.21994 0.00001 0.00000 0.00010 0.00010 1.22004

D16 -2.95666 0.00002 0.00000 0.00010 0.00010 -2.95656

D17 1.01246 0.00003 0.00000 -0.00049 -0.00049 1.01197

D18 3.02646 -0.00002 0.00000 -0.00143 -0.00143 3.02503

D19 -1.15015 -0.00001 0.00000 -0.00143 -0.00143 -1.15158

D20 -1.03873 -0.00003 0.00000 0.00226 0.00226 -1.03647

D21 -2.98154 0.00000 0.00000 0.00221 0.00221 -2.97933

D22 1.19279 -0.00001 0.00000 0.00246 0.00246 1.19524

D23 1.06892 -0.00001 0.00000 0.00230 0.00230 1.07123

D24 -0.87389 0.00001 0.00000 0.00226 0.00226 -0.87163

D25 -2.98275 0.00001 0.00000 0.00250 0.00250 -2.98024

D26 3.12823 0.00000 0.00000 0.00248 0.00248 3.13072

D27 1.18542 0.00003 0.00000 0.00244 0.00244 1.18786

D28 -0.92344 0.00002 0.00000 0.00268 0.00268 -0.92075

D29 0.60039 -0.00003 0.00000 -0.00072 -0.00072 0.59967

D30 -2.70998 -0.00002 0.00000 -0.00112 -0.00112 -2.71110

D31 -2.94800 -0.00001 0.00000 -0.00090 -0.00090 -2.94890

D32 0.02481 -0.00001 0.00000 -0.00130 -0.00130 0.02351

D33 -1.19517 0.00000 0.00000 -0.00110 -0.00110 -1.19627

D34 1.77764 0.00000 0.00000 -0.00150 -0.00150 1.77614

D35 -0.57267 0.00003 0.00000 -0.00097 -0.00097 -0.57364

D36 -2.73588 0.00003 0.00000 -0.00116 -0.00116 -2.73704

D37 1.53452 0.00002 0.00000 -0.00152 -0.00152 1.53299

D38 2.95772 0.00000 0.00000 -0.00095 -0.00095 2.95677

D39 0.79451 0.00000 0.00000 -0.00114 -0.00114 0.79337

D40 -1.21828 -0.00001 0.00000 -0.00151 -0.00151 -1.21978

D41 1.15373 -0.00004 0.00000 -0.00179 -0.00179 1.15194

D42 -1.00947 -0.00004 0.00000 -0.00198 -0.00199 -1.01146

D43 -3.02226 -0.00004 0.00000 -0.00235 -0.00235 -3.02461

D44 1.03373 -0.00003 0.00000 0.00206 0.00206 1.03579

D45 2.97677 -0.00002 0.00000 0.00211 0.00211 2.97888

D46 -1.19807 -0.00001 0.00000 0.00225 0.00225 -1.19582

D47 -1.07458 0.00001 0.00000 0.00265 0.00265 -1.07193

D48 0.86846 0.00002 0.00000 0.00270 0.00270 0.87117

D49 2.97681 0.00003 0.00000 0.00284 0.00284 2.97965

D50 -3.13381 0.00001 0.00000 0.00245 0.00245 -3.13136

D51 -1.19077 0.00002 0.00000 0.00250 0.00250 -1.18826

D52 0.91758 0.00003 0.00000 0.00265 0.00265 0.92022

D53 -0.00210 0.00003 0.00000 0.00181 0.00181 -0.00029

D54 2.16334 0.00001 0.00000 0.00186 0.00186 2.16520

D55 -2.09125 0.00004 0.00000 0.00252 0.00252 -2.08873

D56 -2.16744 0.00003 0.00000 0.00153 0.00153 -2.16591

D57 -0.00200 0.00001 0.00000 0.00158 0.00158 -0.00042

D58 2.02659 0.00004 0.00000 0.00224 0.00224 2.02883

D59 2.08612 0.00003 0.00000 0.00194 0.00194 2.08806

D60 -2.03163 0.00001 0.00000 0.00200 0.00200 -2.02963

D61 -0.00303 0.00003 0.00000 0.00265 0.00265 -0.00038

D62 -0.01554 -0.00001 0.00000 -0.00073 -0.00073 -0.01628

D63 3.12433 -0.00002 0.00000 -0.00153 -0.00153 3.12280

D64 0.01584 0.00000 0.00000 0.00042 0.00042 0.01626

D65 -3.12301 -0.00001 0.00000 -0.00018 -0.00018 -3.12319

D66 0.00289 -0.00004 0.00000 -0.00254 -0.00254 0.00035

D67 1.85459 -0.00002 0.00000 -0.00130 -0.00130 1.85330

D68 -1.79004 -0.00001 0.00000 -0.00206 -0.00206 -1.79211

D69 -1.85122 -0.00003 0.00000 -0.00175 -0.00175 -1.85297

D70 0.00048 -0.00001 0.00000 -0.00051 -0.00051 -0.00003

D71 2.63903 0.00000 0.00000 -0.00128 -0.00128 2.63775

D72 1.79357 -0.00002 0.00000 -0.00122 -0.00122 1.79235

D73 -2.63792 0.00000 0.00000 0.00003 0.00003 -2.63789

D74 0.00063 0.00001 0.00000 -0.00074 -0.00074 -0.00011

D75 -1.93984 0.00000 0.00000 0.00066 0.00066 -1.93918

D76 1.20393 0.00002 0.00000 0.00167 0.00167 1.20560

D77 0.00925 0.00001 0.00000 0.00078 0.00078 0.01003

D78 -3.13016 0.00003 0.00000 0.00179 0.00179 -3.12837

D79 2.68160 -0.00001 0.00000 0.00004 0.00004 2.68165

D80 -0.45781 0.00000 0.00000 0.00105 0.00105 -0.45676

D81 1.93889 0.00001 0.00000 0.00032 0.00032 1.93921

D82 -1.20617 0.00002 0.00000 0.00108 0.00108 -1.20509

D83 -0.01005 0.00000 0.00000 0.00007 0.00007 -0.00998

D84 3.12807 0.00001 0.00000 0.00083 0.00083 3.12890

D85 -2.68204 -0.00001 0.00000 0.00056 0.00056 -2.68148

D86 0.45608 0.00000 0.00000 0.00132 0.00132 0.45740

Item Value Threshold Converged?

Maximum Force 0.000395 0.000450 YES

RMS Force 0.000062 0.000300 YES

Maximum Displacement 0.006676 0.001800 NO

RMS Displacement 0.001699 0.001200 NO

Predicted change in Energy=-1.856465D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.138990 1.559509 0.441221

2 6 0 0.185556 1.280765 0.106338

3 6 0 -0.754089 3.778794 -0.369780

4 6 0 -1.623106 2.846485 0.195896

5 1 0 -1.733721 0.843628 1.026596

6 1 0 -2.603510 3.155763 0.585849

7 6 0 0.796540 1.928104 -1.088258

8 1 0 1.915932 1.950191 -0.988867

9 1 0 0.571273 1.273196 -1.976299

10 6 0 0.269158 3.330671 -1.355445

11 1 0 1.121799 4.062221 -1.390753

12 1 0 -0.211841 3.356940 -2.373380

13 1 0 -1.029641 4.845124 -0.413924

14 1 0 0.662665 0.346068 0.443456

15 8 0 2.756372 3.854244 0.821135

16 6 0 0.472811 3.874935 1.418116

17 6 0 0.961158 2.575470 1.665818

18 6 0 1.612810 4.675361 0.894167

19 8 0 1.759063 5.832939 0.535946

20 6 0 2.402360 2.574612 1.294542

21 8 0 3.295984 1.743514 1.314889

22 1 0 -0.348998 4.363501 1.946946

23 1 0 0.584015 1.880972 2.420248

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394369 0.000000

3 C 2.393971 2.711046 0.000000

4 C 1.396733 2.393900 1.394409 0.000000

5 H 1.099479 2.172921 3.394811 2.171114 0.000000

6 H 2.171120 3.394766 2.172958 1.099503 2.509334

7 C 2.494283 1.489769 2.519070 2.889146 3.471443

8 H 3.395634 2.154485 3.294855 3.838202 4.313530

9 H 2.975126 2.118068 3.258145 3.465396 3.809843

10 C 2.889274 2.519109 1.489760 2.494345 3.983845

11 H 3.838081 3.294591 2.154454 3.395581 4.935272

12 H 3.465883 3.258440 2.118115 2.975468 4.493628

13 H 3.396837 3.801583 1.102242 2.172242 4.310777

14 H 2.172189 1.102243 3.801599 3.396781 2.516006

15 O 4.536958 3.707132 3.707737 4.537216 5.409895

16 C 2.985536 2.921129 2.170506 2.635223 3.769734

17 C 2.634851 2.170207 2.921254 2.985388 3.266536

18 C 4.181638 3.765768 2.829064 3.781999 5.089104

19 O 5.164290 4.835574 3.369835 4.524777 6.110114

20 C 3.781501 2.828443 3.766058 4.181545 4.491689

21 O 4.523953 3.368901 4.835656 5.163927 5.117699

22 H 3.279279 3.629993 2.423469 2.644025 3.892815

23 H 2.643602 2.423467 3.629946 3.278924 2.896592

6 7 8 9 10

6 H 0.000000

7 C 3.983732 0.000000

8 H 4.935432 1.124013 0.000000

9 H 4.493095 1.126173 1.800403 0.000000

10 C 3.471517 1.522076 2.179901 2.170238 0.000000

11 H 4.313530 2.179852 2.291906 2.902517 1.124015

12 H 3.810195 2.170241 2.902281 2.261179 1.126163

13 H 2.516058 3.506946 4.169844 4.214571 2.206107

14 H 4.310750 2.206107 2.489063 2.592900 3.506957

15 O 5.410321 3.346153 2.758236 4.388861 3.346321

16 C 3.267052 3.190120 3.403058 4.277942 2.833785

17 C 3.769607 2.833923 2.889623 3.887537 3.190176

18 C 4.492392 3.484785 3.326297 4.571553 2.945224

19 O 5.118769 4.337307 4.174374 5.339801 3.472539

20 C 5.089078 2.945228 2.416706 3.967992 3.484911

21 O 6.109826 3.472234 2.693427 4.298507 4.337214

22 H 2.897247 4.056585 4.424135 5.078261 3.514917

23 H 3.892355 3.515253 3.660718 4.438375 4.056675

11 12 13 14 15

11 H 0.000000

12 H 1.800437 0.000000

13 H 2.489142 2.592867 0.000000

14 H 4.169523 4.214817 4.882674 0.000000

15 O 2.758176 4.388910 4.103793 4.102871 0.000000

16 C 2.888945 3.887481 2.560273 3.665912 2.360395

17 C 3.402773 4.278054 3.666053 2.559980 2.360412

18 C 2.416173 3.967927 2.953383 4.455187 1.409717

19 O 2.693273 4.298746 3.107234 5.596105 2.234098

20 C 3.326203 4.571623 4.455639 2.952506 1.409573

21 O 4.174205 5.339598 5.596411 3.105900 2.233865

22 H 3.659816 4.438153 2.503786 4.407234 3.342173

23 H 4.423888 5.078458 4.407110 2.503961 3.342170

16 17 18 19 20

16 C 0.000000

17 C 1.410124 0.000000

18 C 1.488221 2.330159 0.000000

19 O 2.503287 3.538978 1.220532 0.000000

20 C 2.330080 1.488257 2.279657 3.406757 0.000000

21 O 3.538915 2.503340 3.406730 4.437598 1.220533

22 H 1.092579 2.234412 2.248175 2.931568 3.346002

23 H 2.234396 1.092579 3.346035 4.533142 2.248272

21 22 23

21 O 0.000000

22 H 4.533180 0.000000

23 H 2.931806 2.693971 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306506 -0.698465 -0.663545

2 6 0 1.370479 -1.355418 0.134284

3 6 0 1.370830 1.355628 0.134146

4 6 0 2.306709 0.698268 -0.663592

5 1 0 2.914754 -1.254883 -1.391066

6 1 0 2.915157 1.254451 -1.391162

7 6 0 0.966002 -0.760793 1.438980

8 1 0 -0.044651 -1.145730 1.745261

9 1 0 1.693194 -1.130260 2.215479

10 6 0 0.965982 0.761282 1.438844

11 1 0 -0.044837 1.146175 1.744640

12 1 0 1.692860 1.130918 2.215542

13 1 0 1.212095 2.441446 0.030516

14 1 0 1.211533 -2.441228 0.030874

15 8 0 -2.077252 -0.000269 0.274100

16 6 0 -0.292167 0.705132 -1.099708

17 6 0 -0.291966 -0.704992 -1.099823

18 6 0 -1.425284 1.139751 -0.238341

19 8 0 -1.886412 2.218671 0.097803

20 6 0 -1.425004 -1.139906 -0.238438

21 8 0 -1.885674 -2.218927 0.098011

22 1 0 0.065886 1.347186 -1.907974

23 1 0 0.066189 -1.346785 -1.908251

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200682 0.8808243 0.6753903

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5564880480 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the read-write file.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504198155634E-01 A.U. after 12 cycles

Convg = 0.5045D-08 -V/T = 0.9989

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000027223 0.000001919 0.000004435

2 6 0.000025946 0.000009671 0.000000860

3 6 0.000004295 -0.000033449 0.000030327

4 6 -0.000007314 0.000043003 -0.000001065

5 1 -0.000007043 -0.000004478 0.000002092

6 1 0.000007509 -0.000003461 -0.000005011

7 6 0.000006411 -0.000017664 -0.000006405

8 1 0.000002911 0.000007867 0.000009735

9 1 -0.000002271 0.000001589 -0.000000167

10 6 0.000002248 0.000006369 0.000003367

11 1 0.000001755 0.000003493 -0.000002125

12 1 -0.000001979 -0.000000924 -0.000000251

13 1 0.000000639 -0.000001327 -0.000004597

14 1 0.000006972 -0.000003402 -0.000004897

15 8 -0.000053343 0.000085031 -0.000005474

16 6 -0.000000174 0.000014441 -0.000021175

17 6 0.000056574 0.000017413 -0.000022192

18 6 0.000011854 -0.000052982 0.000024882

19 8 0.000012489 -0.000028260 -0.000007465

20 6 -0.000043769 -0.000021790 -0.000007533

21 8 0.000005125 -0.000018952 0.000011247

22 1 -0.000001663 -0.000005499 0.000001338

23 1 0.000000052 0.000001392 0.000000075

-------------------------------------------------------------------

Cartesian Forces: Max 0.000085031 RMS 0.000020412

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000070103 RMS 0.000010198

Search for a saddle point.

Step number 73 out of a maximum of 138

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Update second derivatives using D2CorX and points 26 27 34 36 37

41 42 43 45 46

50 51 52 55 56

57 58 59 63 64

65 66 70 71 72

73

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

ITU= 0 0 0 0 0 0 0 0 0 0 0 0 0

Eigenvalues --- -0.07167 0.00144 0.00344 0.00758 0.00794

Eigenvalues --- 0.01093 0.01194 0.01375 0.01848 0.02170

Eigenvalues --- 0.02526 0.02783 0.02897 0.03225 0.03304

Eigenvalues --- 0.03549 0.03645 0.03782 0.04023 0.04142

Eigenvalues --- 0.04312 0.04453 0.04705 0.04857 0.06371

Eigenvalues --- 0.06555 0.06635 0.07001 0.07428 0.08505

Eigenvalues --- 0.08972 0.10140 0.10405 0.10901 0.10986

Eigenvalues --- 0.12790 0.13599 0.14837 0.15916 0.22857

Eigenvalues --- 0.26921 0.28809 0.29604 0.30251 0.31101

Eigenvalues --- 0.31449 0.31878 0.32049 0.32226 0.32574

Eigenvalues --- 0.33387 0.35404 0.37062 0.38193 0.39813

Eigenvalues --- 0.40494 0.41070 0.45317 0.49345 0.53844

Eigenvalues --- 0.63103 1.08827 1.11318

Eigenvectors required to have negative eigenvalues:

R6 R10 D71 D73 D30

1 -0.56555 -0.52663 -0.14930 0.14480 0.14075

R19 D1 D13 D29 R7

1 0.13678 -0.13338 0.12751 0.12674 0.12462

RFO step: Lambda0=2.508810243D-09 Lambda=-1.03016694D-07.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00044960 RMS(Int)= 0.00000008

Iteration 2 RMS(Cart)= 0.00000011 RMS(Int)= 0.00000003

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63498 0.00004 0.00000 0.00008 0.00008 2.63505

R2 2.63944 0.00001 0.00000 0.00004 0.00004 2.63948

R3 2.07771 0.00001 0.00000 0.00002 0.00002 2.07773

R4 2.81525 -0.00001 0.00000 0.00001 0.00001 2.81526

R5 2.08294 0.00000 0.00000 0.00001 0.00001 2.08295

R6 4.10110 -0.00001 0.00000 0.00015 0.00015 4.10124

R7 2.63505 -0.00002 0.00000 -0.00008 -0.00008 2.63497

R8 2.81524 0.00000 0.00000 0.00002 0.00002 2.81525

R9 2.08294 0.00000 0.00000 0.00001 0.00001 2.08295

R10 4.10166 -0.00002 0.00000 -0.00002 -0.00002 4.10164

R11 2.07776 -0.00001 0.00000 -0.00004 -0.00004 2.07772

R12 2.12408 0.00000 0.00000 0.00001 0.00001 2.12409

R13 2.12816 0.00000 0.00000 -0.00001 -0.00001 2.12815

R14 2.87631 0.00000 0.00000 0.00002 0.00002 2.87632

R15 2.12408 0.00000 0.00000 0.00000 0.00000 2.12408

R16 2.12814 0.00000 0.00000 0.00001 0.00001 2.12815

R17 2.66398 -0.00007 0.00000 -0.00024 -0.00024 2.66374

R18 2.66371 0.00003 0.00000 0.00017 0.00017 2.66387

R19 2.66475 -0.00001 0.00000 -0.00002 -0.00002 2.66473

R20 2.81233 -0.00004 0.00000 -0.00011 -0.00011 2.81222

R21 2.06467 0.00000 0.00000 -0.00001 -0.00001 2.06466

R22 2.81240 -0.00004 0.00000 -0.00014 -0.00014 2.81225

R23 2.06467 0.00000 0.00000 0.00001 0.00001 2.06468

R24 2.30647 -0.00002 0.00000 0.00001 0.00001 2.30648

R25 2.30647 0.00002 0.00000 0.00000 0.00000 2.30648

A1 2.06152 -0.00001 0.00000 -0.00001 -0.00001 2.06151

A2 2.10777 0.00001 0.00000 0.00007 0.00007 2.10785

A3 2.10130 0.00000 0.00000 -0.00004 -0.00004 2.10126

A4 2.08898 0.00000 0.00000 0.00006 0.00006 2.08904

A5 2.10278 0.00000 0.00000 0.00001 0.00001 2.10279

A6 1.61846 0.00000 0.00000 0.00027 0.00027 1.61873

A7 2.02217 -0.00001 0.00000 -0.00006 -0.00006 2.02211

A8 1.74204 -0.00001 0.00000 -0.00029 -0.00029 1.74175

A9 1.70260 0.00000 0.00000 -0.00001 -0.00001 1.70259

A10 2.08903 0.00001 0.00000 0.00007 0.00007 2.08910

A11 2.10281 -0.00001 0.00000 0.00004 0.00004 2.10285

A12 1.61855 0.00001 0.00000 -0.00013 -0.00013 1.61841

A13 2.02218 0.00000 0.00000 -0.00010 -0.00010 2.02208

A14 1.74170 -0.00001 0.00000 0.00016 0.00016 1.74186

A15 1.70263 0.00000 0.00000 -0.00005 -0.00005 1.70258

A16 2.06157 0.00000 0.00000 -0.00005 -0.00005 2.06152

A17 2.10128 0.00000 0.00000 0.00000 0.00000 2.10128

A18 2.10774 0.00000 0.00000 0.00006 0.00006 2.10780

A19 1.92417 0.00000 0.00000 0.00001 0.00001 1.92418

A20 1.87296 0.00000 0.00000 0.00003 0.00003 1.87299

A21 1.98129 0.00000 0.00000 -0.00007 -0.00007 1.98123

A22 1.85497 0.00000 0.00000 0.00008 0.00008 1.85505

A23 1.92035 0.00000 0.00000 -0.00003 -0.00003 1.92032

A24 1.90513 0.00000 0.00000 -0.00001 -0.00001 1.90512

A25 1.98125 0.00000 0.00000 0.00002 0.00002 1.98127

A26 1.92414 0.00000 0.00000 0.00001 0.00001 1.92415

A27 1.87304 0.00000 0.00000 -0.00004 -0.00004 1.87299

A28 1.92028 0.00000 0.00000 0.00002 0.00002 1.92030

A29 1.90515 0.00000 0.00000 -0.00002 -0.00002 1.90512

A30 1.85503 0.00000 0.00000 0.00001 0.00001 1.85504

A31 1.88351 0.00000 0.00000 -0.00001 -0.00001 1.88350

A32 1.87511 0.00000 0.00000 0.00002 0.00002 1.87513

A33 1.73840 0.00000 0.00000 -0.00041 -0.00041 1.73799

A34 1.56413 0.00000 0.00000 0.00015 0.00015 1.56428

A35 1.86732 -0.00001 0.00000 -0.00008 -0.00008 1.86724

A36 2.19881 0.00000 0.00000 0.00001 0.00001 2.19883

A37 2.10143 0.00001 0.00000 0.00018 0.00018 2.10161

A38 1.87525 0.00000 0.00000 -0.00005 -0.00005 1.87519

A39 1.73805 -0.00001 0.00000 0.00034 0.00034 1.73839

A40 1.56440 0.00000 0.00000 -0.00017 -0.00017 1.56423

A41 1.86719 0.00001 0.00000 0.00008 0.00008 1.86727

A42 2.19879 0.00000 0.00000 -0.00006 -0.00006 2.19872

A43 2.10153 0.00000 0.00000 -0.00006 -0.00006 2.10147

A44 1.90324 0.00002 0.00000 0.00010 0.00010 1.90334

A45 2.02641 -0.00003 0.00000 -0.00018 -0.00018 2.02624

A46 2.35353 0.00001 0.00000 0.00007 0.00007 2.35360

A47 1.90336 -0.00002 0.00000 -0.00009 -0.00009 1.90327

A48 2.02626 0.00002 0.00000 0.00011 0.00011 2.02636

A49 2.35356 -0.00001 0.00000 -0.00001 -0.00001 2.35355

D1 -0.59974 0.00000 0.00000 -0.00004 -0.00004 -0.59978

D2 2.94909 0.00000 0.00000 -0.00006 -0.00006 2.94903

D3 1.19654 -0.00001 0.00000 -0.00021 -0.00021 1.19633

D4 2.71101 0.00000 0.00000 -0.00018 -0.00018 2.71083

D5 -0.02335 0.00000 0.00000 -0.00020 -0.00020 -0.02354

D6 -1.77589 0.00000 0.00000 -0.00035 -0.00035 -1.77624

D7 -0.00005 0.00000 0.00000 0.00010 0.00010 0.00005

D8 -2.97311 0.00000 0.00000 0.00006 0.00006 -2.97306

D9 2.97304 0.00000 0.00000 0.00025 0.00025 2.97329

D10 -0.00002 0.00000 0.00000 0.00021 0.00021 0.00018

D11 2.73765 -0.00001 0.00000 -0.00017 -0.00017 2.73748

D12 -1.53248 0.00000 0.00000 -0.00005 -0.00005 -1.53253

D13 0.57410 0.00000 0.00000 -0.00009 -0.00009 0.57402

D14 -0.79301 0.00000 0.00000 -0.00014 -0.00014 -0.79316

D15 1.22004 0.00000 0.00000 -0.00002 -0.00002 1.22002

D16 -2.95656 0.00000 0.00000 -0.00006 -0.00006 -2.95662

D17 1.01197 -0.00001 0.00000 -0.00033 -0.00033 1.01164

D18 3.02503 0.00000 0.00000 -0.00021 -0.00021 3.02482

D19 -1.15158 0.00000 0.00000 -0.00024 -0.00024 -1.15182

D20 -1.03647 0.00001 0.00000 0.00085 0.00085 -1.03562

D21 -2.97933 0.00000 0.00000 0.00064 0.00064 -2.97869

D22 1.19524 0.00000 0.00000 0.00071 0.00071 1.19595

D23 1.07123 0.00001 0.00000 0.00093 0.00093 1.07215

D24 -0.87163 0.00000 0.00000 0.00072 0.00072 -0.87091

D25 -2.98024 0.00000 0.00000 0.00078 0.00078 -2.97946

D26 3.13072 0.00000 0.00000 0.00080 0.00080 3.13152

D27 1.18786 0.00000 0.00000 0.00059 0.00059 1.18845

D28 -0.92075 0.00000 0.00000 0.00065 0.00065 -0.92010

D29 0.59967 0.00000 0.00000 -0.00006 -0.00006 0.59961

D30 -2.71110 0.00000 0.00000 -0.00002 -0.00002 -2.71112

D31 -2.94890 0.00000 0.00000 -0.00005 -0.00005 -2.94895

D32 0.02351 0.00000 0.00000 -0.00001 -0.00001 0.02351

D33 -1.19627 0.00000 0.00000 -0.00018 -0.00018 -1.19645

D34 1.77614 0.00000 0.00000 -0.00014 -0.00014 1.77600

D35 -0.57364 0.00000 0.00000 -0.00007 -0.00007 -0.57372

D36 -2.73704 0.00000 0.00000 -0.00013 -0.00013 -2.73717

D37 1.53299 0.00000 0.00000 -0.00012 -0.00012 1.53287

D38 2.95677 0.00000 0.00000 -0.00012 -0.00012 2.95665

D39 0.79337 0.00000 0.00000 -0.00017 -0.00017 0.79320

D40 -1.21978 0.00000 0.00000 -0.00017 -0.00017 -1.21995

D41 1.15194 0.00000 0.00000 -0.00012 -0.00012 1.15182

D42 -1.01146 0.00000 0.00000 -0.00017 -0.00017 -1.01163

D43 -3.02461 0.00000 0.00000 -0.00017 -0.00017 -3.02478

D44 1.03579 0.00001 0.00000 0.00087 0.00087 1.03666

D45 2.97888 0.00000 0.00000 0.00063 0.00063 2.97951

D46 -1.19582 0.00001 0.00000 0.00080 0.00080 -1.19502

D47 -1.07193 0.00000 0.00000 0.00080 0.00080 -1.07112

D48 0.87117 -0.00001 0.00000 0.00056 0.00056 0.87172

D49 2.97965 0.00000 0.00000 0.00073 0.00073 2.98038

D50 -3.13136 0.00001 0.00000 0.00088 0.00088 -3.13047

D51 -1.18826 0.00000 0.00000 0.00063 0.00063 -1.18763

D52 0.92022 0.00000 0.00000 0.00081 0.00081 0.92103

D53 -0.00029 0.00000 0.00000 0.00011 0.00011 -0.00018

D54 2.16520 0.00000 0.00000 0.00016 0.00016 2.16536

D55 -2.08873 0.00000 0.00000 0.00017 0.00017 -2.08856

D56 -2.16591 0.00000 0.00000 0.00017 0.00017 -2.16574

D57 -0.00042 0.00000 0.00000 0.00022 0.00022 -0.00020

D58 2.02883 0.00000 0.00000 0.00023 0.00023 2.02906

D59 2.08806 0.00000 0.00000 0.00010 0.00010 2.08816

D60 -2.02963 0.00000 0.00000 0.00014 0.00014 -2.02949

D61 -0.00038 0.00000 0.00000 0.00016 0.00016 -0.00022

D62 -0.01628 0.00000 0.00000 0.00008 0.00008 -0.01620

D63 3.12280 0.00001 0.00000 0.00029 0.00029 3.12308

D64 0.01626 0.00000 0.00000 -0.00011 -0.00011 0.01615

D65 -3.12319 0.00000 0.00000 0.00008 0.00008 -3.12312

D66 0.00035 0.00000 0.00000 -0.00093 -0.00093 -0.00057

D67 1.85330 -0.00001 0.00000 -0.00054 -0.00054 1.85276

D68 -1.79211 0.00000 0.00000 -0.00063 -0.00063 -1.79274

D69 -1.85297 0.00000 0.00000 -0.00044 -0.00044 -1.85342

D70 -0.00003 0.00000 0.00000 -0.00005 -0.00005 -0.00008

D71 2.63775 0.00000 0.00000 -0.00015 -0.00015 2.63761

D72 1.79235 0.00000 0.00000 -0.00071 -0.00071 1.79164

D73 -2.63789 0.00000 0.00000 -0.00032 -0.00032 -2.63821

D74 -0.00011 0.00000 0.00000 -0.00041 -0.00041 -0.00052

D75 -1.93918 0.00000 0.00000 0.00015 0.00015 -1.93904

D76 1.20560 -0.00001 0.00000 -0.00011 -0.00011 1.20548

D77 0.01003 0.00000 0.00000 -0.00002 -0.00002 0.01002

D78 -3.12837 0.00000 0.00000 -0.00028 -0.00028 -3.12865

D79 2.68165 0.00000 0.00000 0.00018 0.00018 2.68183

D80 -0.45676 0.00000 0.00000 -0.00008 -0.00008 -0.45684

D81 1.93921 0.00000 0.00000 0.00020 0.00020 1.93942

D82 -1.20509 0.00000 0.00000 -0.00004 -0.00004 -1.20513

D83 -0.00998 0.00000 0.00000 0.00010 0.00010 -0.00988

D84 3.12890 0.00000 0.00000 -0.00014 -0.00014 3.12876

D85 -2.68148 0.00000 0.00000 0.00020 0.00020 -2.68128

D86 0.45740 0.00000 0.00000 -0.00004 -0.00004 0.45736

Item Value Threshold Converged?

Maximum Force 0.000070 0.000450 YES

RMS Force 0.000010 0.000300 YES

Maximum Displacement 0.001631 0.001800 YES

RMS Displacement 0.000450 0.001200 YES

Predicted change in Energy=-5.025490D-08

Optimization completed.

-- Stationary point found.

----------------------------

! Optimized Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.3944 -DE/DX = 0.0 !

! R2 R(1,4) 1.3967 -DE/DX = 0.0 !

! R3 R(1,5) 1.0995 -DE/DX = 0.0 !

! R4 R(2,7) 1.4898 -DE/DX = 0.0 !

! R5 R(2,14) 1.1022 -DE/DX = 0.0 !

! R6 R(2,17) 2.1702 -DE/DX = 0.0 !

! R7 R(3,4) 1.3944 -DE/DX = 0.0 !

! R8 R(3,10) 1.4898 -DE/DX = 0.0 !

! R9 R(3,13) 1.1022 -DE/DX = 0.0 !

! R10 R(3,16) 2.1705 -DE/DX = 0.0 !

! R11 R(4,6) 1.0995 -DE/DX = 0.0 !

! R12 R(7,8) 1.124 -DE/DX = 0.0 !

! R13 R(7,9) 1.1262 -DE/DX = 0.0 !

! R14 R(7,10) 1.5221 -DE/DX = 0.0 !

! R15 R(10,11) 1.124 -DE/DX = 0.0 !

! R16 R(10,12) 1.1262 -DE/DX = 0.0 !

! R17 R(15,18) 1.4097 -DE/DX = -0.0001 !

! R18 R(15,20) 1.4096 -DE/DX = 0.0 !

! R19 R(16,17) 1.4101 -DE/DX = 0.0 !

! R20 R(16,18) 1.4882 -DE/DX = 0.0 !

! R21 R(16,22) 1.0926 -DE/DX = 0.0 !

! R22 R(17,20) 1.4883 -DE/DX = 0.0 !

! R23 R(17,23) 1.0926 -DE/DX = 0.0 !

! R24 R(18,19) 1.2205 -DE/DX = 0.0 !

! R25 R(20,21) 1.2205 -DE/DX = 0.0 !

! A1 A(2,1,4) 118.1164 -DE/DX = 0.0 !

! A2 A(2,1,5) 120.7666 -DE/DX = 0.0 !

! A3 A(4,1,5) 120.3959 -DE/DX = 0.0 !

! A4 A(1,2,7) 119.6897 -DE/DX = 0.0 !

! A5 A(1,2,14) 120.4804 -DE/DX = 0.0 !

! A6 A(1,2,17) 92.7311 -DE/DX = 0.0 !

! A7 A(7,2,14) 115.8617 -DE/DX = 0.0 !

! A8 A(7,2,17) 99.8117 -DE/DX = 0.0 !

! A9 A(14,2,17) 97.5519 -DE/DX = 0.0 !

! A10 A(4,3,10) 119.6925 -DE/DX = 0.0 !

! A11 A(4,3,13) 120.4821 -DE/DX = 0.0 !

! A12 A(4,3,16) 92.7358 -DE/DX = 0.0 !

! A13 A(10,3,13) 115.8624 -DE/DX = 0.0 !

! A14 A(10,3,16) 99.7919 -DE/DX = 0.0 !

! A15 A(13,3,16) 97.5533 -DE/DX = 0.0 !

! A16 A(1,4,3) 118.1193 -DE/DX = 0.0 !

! A17 A(1,4,6) 120.3946 -DE/DX = 0.0 !

! A18 A(3,4,6) 120.7647 -DE/DX = 0.0 !

! A19 A(2,7,8) 110.247 -DE/DX = 0.0 !

! A20 A(2,7,9) 107.3126 -DE/DX = 0.0 !

! A21 A(2,7,10) 113.5197 -DE/DX = 0.0 !

! A22 A(8,7,9) 106.2818 -DE/DX = 0.0 !

! A23 A(8,7,10) 110.028 -DE/DX = 0.0 !

! A24 A(9,7,10) 109.1561 -DE/DX = 0.0 !

! A25 A(3,10,7) 113.5175 -DE/DX = 0.0 !

! A26 A(3,10,11) 110.245 -DE/DX = 0.0 !

! A27 A(3,10,12) 107.3172 -DE/DX = 0.0 !

! A28 A(7,10,11) 110.0241 -DE/DX = 0.0 !

! A29 A(7,10,12) 109.1569 -DE/DX = 0.0 !

! A30 A(11,10,12) 106.2852 -DE/DX = 0.0 !

! A31 A(18,15,20) 107.9173 -DE/DX = 0.0 !

! A32 A(3,16,17) 107.4357 -DE/DX = 0.0 !

! A33 A(3,16,18) 99.6028 -DE/DX = 0.0 !

! A34 A(3,16,22) 89.618 -DE/DX = 0.0 !

! A35 A(17,16,18) 106.9894 -DE/DX = 0.0 !

! A36 A(17,16,22) 125.9828 -DE/DX = 0.0 !

! A37 A(18,16,22) 120.4029 -DE/DX = 0.0 !

! A38 A(2,17,16) 107.4438 -DE/DX = 0.0 !

! A39 A(2,17,20) 99.583 -DE/DX = 0.0 !

! A40 A(2,17,23) 89.6335 -DE/DX = 0.0 !

! A41 A(16,17,20) 106.9822 -DE/DX = 0.0 !

! A42 A(16,17,23) 125.9811 -DE/DX = 0.0 !

! A43 A(20,17,23) 120.4088 -DE/DX = 0.0 !

! A44 A(15,18,16) 109.0477 -DE/DX = 0.0 !

! A45 A(15,18,19) 116.105 -DE/DX = 0.0 !

! A46 A(16,18,19) 134.8471 -DE/DX = 0.0 !

! A47 A(15,20,17) 109.0546 -DE/DX = 0.0 !

! A48 A(15,20,21) 116.096 -DE/DX = 0.0 !

! A49 A(17,20,21) 134.8492 -DE/DX = 0.0 !

! D1 D(4,1,2,7) -34.3627 -DE/DX = 0.0 !

! D2 D(4,1,2,14) 168.9703 -DE/DX = 0.0 !

! D3 D(4,1,2,17) 68.5569 -DE/DX = 0.0 !

! D4 D(5,1,2,7) 155.3292 -DE/DX = 0.0 !

! D5 D(5,1,2,14) -1.3377 -DE/DX = 0.0 !

! D6 D(5,1,2,17) -101.7512 -DE/DX = 0.0 !

! D7 D(2,1,4,3) -0.0029 -DE/DX = 0.0 !

! D8 D(2,1,4,6) -170.3468 -DE/DX = 0.0 !

! D9 D(5,1,4,3) 170.3425 -DE/DX = 0.0 !

! D10 D(5,1,4,6) -0.0014 -DE/DX = 0.0 !

! D11 D(1,2,7,8) 156.8558 -DE/DX = 0.0 !

! D12 D(1,2,7,9) -87.8046 -DE/DX = 0.0 !

! D13 D(1,2,7,10) 32.8937 -DE/DX = 0.0 !

! D14 D(14,2,7,8) -45.4363 -DE/DX = 0.0 !

! D15 D(14,2,7,9) 69.9032 -DE/DX = 0.0 !

! D16 D(14,2,7,10) -169.3984 -DE/DX = 0.0 !

! D17 D(17,2,7,8) 57.9816 -DE/DX = 0.0 !

! D18 D(17,2,7,9) 173.3212 -DE/DX = 0.0 !

! D19 D(17,2,7,10) -65.9805 -DE/DX = 0.0 !

! D20 D(1,2,17,16) -59.3855 -DE/DX = 0.0 !

! D21 D(1,2,17,20) -170.7031 -DE/DX = 0.0 !

! D22 D(1,2,17,23) 68.4824 -DE/DX = 0.0 !

! D23 D(7,2,17,16) 61.3767 -DE/DX = 0.0 !

! D24 D(7,2,17,20) -49.9409 -DE/DX = 0.0 !

! D25 D(7,2,17,23) -170.7554 -DE/DX = 0.0 !

! D26 D(14,2,17,16) 179.377 -DE/DX = 0.0 !

! D27 D(14,2,17,20) 68.0594 -DE/DX = 0.0 !

! D28 D(14,2,17,23) -52.7551 -DE/DX = 0.0 !

! D29 D(10,3,4,1) 34.3587 -DE/DX = 0.0 !

! D30 D(10,3,4,6) -155.3347 -DE/DX = 0.0 !

! D31 D(13,3,4,1) -168.9594 -DE/DX = 0.0 !

! D32 D(13,3,4,6) 1.3472 -DE/DX = 0.0 !

! D33 D(16,3,4,1) -68.5411 -DE/DX = 0.0 !

! D34 D(16,3,4,6) 101.7655 -DE/DX = 0.0 !

! D35 D(4,3,10,7) -32.8672 -DE/DX = 0.0 !

! D36 D(4,3,10,11) -156.8209 -DE/DX = 0.0 !

! D37 D(4,3,10,12) 87.834 -DE/DX = 0.0 !

! D38 D(13,3,10,7) 169.4105 -DE/DX = 0.0 !

! D39 D(13,3,10,11) 45.4567 -DE/DX = 0.0 !

! D40 D(13,3,10,12) -69.8884 -DE/DX = 0.0 !

! D41 D(16,3,10,7) 66.0014 -DE/DX = 0.0 !

! D42 D(16,3,10,11) -57.9523 -DE/DX = 0.0 !

! D43 D(16,3,10,12) -173.2975 -DE/DX = 0.0 !

! D44 D(4,3,16,17) 59.3461 -DE/DX = 0.0 !

! D45 D(4,3,16,18) 170.6772 -DE/DX = 0.0 !

! D46 D(4,3,16,22) -68.5155 -DE/DX = 0.0 !

! D47 D(10,3,16,17) -61.4168 -DE/DX = 0.0 !

! D48 D(10,3,16,18) 49.9142 -DE/DX = 0.0 !

! D49 D(10,3,16,22) 170.7215 -DE/DX = 0.0 !

! D50 D(13,3,16,17) -179.4135 -DE/DX = 0.0 !

! D51 D(13,3,16,18) -68.0825 -DE/DX = 0.0 !

! D52 D(13,3,16,22) 52.7249 -DE/DX = 0.0 !

! D53 D(2,7,10,3) -0.0168 -DE/DX = 0.0 !

! D54 D(2,7,10,11) 124.0569 -DE/DX = 0.0 !

! D55 D(2,7,10,12) -119.6755 -DE/DX = 0.0 !

! D56 D(8,7,10,3) -124.0978 -DE/DX = 0.0 !

! D57 D(8,7,10,11) -0.024 -DE/DX = 0.0 !

! D58 D(8,7,10,12) 116.2435 -DE/DX = 0.0 !

! D59 D(9,7,10,3) 119.637 -DE/DX = 0.0 !

! D60 D(9,7,10,11) -116.2893 -DE/DX = 0.0 !

! D61 D(9,7,10,12) -0.0217 -DE/DX = 0.0 !

! D62 D(20,15,18,16) -0.9326 -DE/DX = 0.0 !

! D63 D(20,15,18,19) 178.9232 -DE/DX = 0.0 !

! D64 D(18,15,20,17) 0.9316 -DE/DX = 0.0 !

! D65 D(18,15,20,21) -178.9458 -DE/DX = 0.0 !

! D66 D(3,16,17,2) 0.0202 -DE/DX = 0.0 !

! D67 D(3,16,17,20) 106.186 -DE/DX = 0.0 !

! D68 D(3,16,17,23) -102.6801 -DE/DX = 0.0 !

! D69 D(18,16,17,2) -106.1676 -DE/DX = 0.0 !

! D70 D(18,16,17,20) -0.0018 -DE/DX = 0.0 !

! D71 D(18,16,17,23) 151.1321 -DE/DX = 0.0 !

! D72 D(22,16,17,2) 102.694 -DE/DX = 0.0 !

! D73 D(22,16,17,20) -151.1402 -DE/DX = 0.0 !

! D74 D(22,16,17,23) -0.0063 -DE/DX = 0.0 !

! D75 D(3,16,18,15) -111.107 -DE/DX = 0.0 !

! D76 D(3,16,18,19) 69.0756 -DE/DX = 0.0 !

! D77 D(17,16,18,15) 0.5749 -DE/DX = 0.0 !

! D78 D(17,16,18,19) -179.2425 -DE/DX = 0.0 !

! D79 D(22,16,18,15) 153.647 -DE/DX = 0.0 !

! D80 D(22,16,18,19) -26.1704 -DE/DX = 0.0 !

! D81 D(2,17,20,15) 111.1087 -DE/DX = 0.0 !

! D82 D(2,17,20,21) -69.0466 -DE/DX = 0.0 !

! D83 D(16,17,20,15) -0.572 -DE/DX = 0.0 !

! D84 D(16,17,20,21) 179.2727 -DE/DX = 0.0 !

! D85 D(23,17,20,15) -153.6375 -DE/DX = 0.0 !

! D86 D(23,17,20,21) 26.2072 -DE/DX = 0.0 !

--------------------------------------------------------------------------------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.138990 1.559509 0.441221

2 6 0 0.185556 1.280765 0.106338

3 6 0 -0.754089 3.778794 -0.369780

4 6 0 -1.623106 2.846485 0.195896

5 1 0 -1.733721 0.843628 1.026596

6 1 0 -2.603510 3.155763 0.585849

7 6 0 0.796540 1.928104 -1.088258

8 1 0 1.915932 1.950191 -0.988867

9 1 0 0.571273 1.273196 -1.976299

10 6 0 0.269158 3.330671 -1.355445

11 1 0 1.121799 4.062221 -1.390753

12 1 0 -0.211841 3.356940 -2.373380

13 1 0 -1.029641 4.845124 -0.413924

14 1 0 0.662665 0.346068 0.443456

15 8 0 2.756372 3.854244 0.821135

16 6 0 0.472811 3.874935 1.418116

17 6 0 0.961158 2.575470 1.665818

18 6 0 1.612810 4.675361 0.894167

19 8 0 1.759063 5.832939 0.535946

20 6 0 2.402360 2.574612 1.294542

21 8 0 3.295984 1.743514 1.314889

22 1 0 -0.348998 4.363501 1.946946

23 1 0 0.584015 1.880972 2.420248

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394369 0.000000

3 C 2.393971 2.711046 0.000000

4 C 1.396733 2.393900 1.394409 0.000000

5 H 1.099479 2.172921 3.394811 2.171114 0.000000

6 H 2.171120 3.394766 2.172958 1.099503 2.509334

7 C 2.494283 1.489769 2.519070 2.889146 3.471443

8 H 3.395634 2.154485 3.294855 3.838202 4.313530

9 H 2.975126 2.118068 3.258145 3.465396 3.809843

10 C 2.889274 2.519109 1.489760 2.494345 3.983845

11 H 3.838081 3.294591 2.154454 3.395581 4.935272

12 H 3.465883 3.258440 2.118115 2.975468 4.493628

13 H 3.396837 3.801583 1.102242 2.172242 4.310777

14 H 2.172189 1.102243 3.801599 3.396781 2.516006

15 O 4.536958 3.707132 3.707737 4.537216 5.409895

16 C 2.985536 2.921129 2.170506 2.635223 3.769734

17 C 2.634851 2.170207 2.921254 2.985388 3.266536

18 C 4.181638 3.765768 2.829064 3.781999 5.089104

19 O 5.164290 4.835574 3.369835 4.524777 6.110114

20 C 3.781501 2.828443 3.766058 4.181545 4.491689

21 O 4.523953 3.368901 4.835656 5.163927 5.117699

22 H 3.279279 3.629993 2.423469 2.644025 3.892815

23 H 2.643602 2.423467 3.629946 3.278924 2.896592

6 7 8 9 10

6 H 0.000000

7 C 3.983732 0.000000

8 H 4.935432 1.124013 0.000000

9 H 4.493095 1.126173 1.800403 0.000000

10 C 3.471517 1.522076 2.179901 2.170238 0.000000

11 H 4.313530 2.179852 2.291906 2.902517 1.124015

12 H 3.810195 2.170241 2.902281 2.261179 1.126163

13 H 2.516058 3.506946 4.169844 4.214571 2.206107

14 H 4.310750 2.206107 2.489063 2.592900 3.506957

15 O 5.410321 3.346153 2.758236 4.388861 3.346321

16 C 3.267052 3.190120 3.403058 4.277942 2.833785

17 C 3.769607 2.833923 2.889623 3.887537 3.190176

18 C 4.492392 3.484785 3.326297 4.571553 2.945224

19 O 5.118769 4.337307 4.174374 5.339801 3.472539

20 C 5.089078 2.945228 2.416706 3.967992 3.484911

21 O 6.109826 3.472234 2.693427 4.298507 4.337214

22 H 2.897247 4.056585 4.424135 5.078261 3.514917

23 H 3.892355 3.515253 3.660718 4.438375 4.056675

11 12 13 14 15

11 H 0.000000

12 H 1.800437 0.000000

13 H 2.489142 2.592867 0.000000

14 H 4.169523 4.214817 4.882674 0.000000

15 O 2.758176 4.388910 4.103793 4.102871 0.000000

16 C 2.888945 3.887481 2.560273 3.665912 2.360395

17 C 3.402773 4.278054 3.666053 2.559980 2.360412

18 C 2.416173 3.967927 2.953383 4.455187 1.409717

19 O 2.693273 4.298746 3.107234 5.596105 2.234098

20 C 3.326203 4.571623 4.455639 2.952506 1.409573

21 O 4.174205 5.339598 5.596411 3.105900 2.233865

22 H 3.659816 4.438153 2.503786 4.407234 3.342173

23 H 4.423888 5.078458 4.407110 2.503961 3.342170

16 17 18 19 20

16 C 0.000000

17 C 1.410124 0.000000

18 C 1.488221 2.330159 0.000000

19 O 2.503287 3.538978 1.220532 0.000000

20 C 2.330080 1.488257 2.279657 3.406757 0.000000

21 O 3.538915 2.503340 3.406730 4.437598 1.220533

22 H 1.092579 2.234412 2.248175 2.931568 3.346002

23 H 2.234396 1.092579 3.346035 4.533142 2.248272

21 22 23

21 O 0.000000

22 H 4.533180 0.000000

23 H 2.931806 2.693971 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306506 -0.698465 -0.663545

2 6 0 1.370479 -1.355418 0.134284

3 6 0 1.370830 1.355628 0.134146

4 6 0 2.306709 0.698268 -0.663592

5 1 0 2.914754 -1.254883 -1.391066

6 1 0 2.915157 1.254451 -1.391162

7 6 0 0.966002 -0.760793 1.438980

8 1 0 -0.044651 -1.145730 1.745261

9 1 0 1.693194 -1.130260 2.215479

10 6 0 0.965982 0.761282 1.438844

11 1 0 -0.044837 1.146175 1.744640

12 1 0 1.692860 1.130918 2.215542

13 1 0 1.212095 2.441446 0.030516

14 1 0 1.211533 -2.441228 0.030874

15 8 0 -2.077252 -0.000269 0.274100

16 6 0 -0.292167 0.705132 -1.099708

17 6 0 -0.291966 -0.704992 -1.099823

18 6 0 -1.425284 1.139751 -0.238341

19 8 0 -1.886412 2.218671 0.097803

20 6 0 -1.425004 -1.139906 -0.238438

21 8 0 -1.885674 -2.218927 0.098011

22 1 0 0.065886 1.347186 -1.907974

23 1 0 0.066189 -1.346785 -1.908251

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200682 0.8808243 0.6753903

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -1.55554 -1.45667 -1.44457 -1.36911 -1.23237

Alpha occ. eigenvalues -- -1.19012 -1.18108 -0.97163 -0.89235 -0.86948

Alpha occ. eigenvalues -- -0.83226 -0.81028 -0.67967 -0.66424 -0.65438

Alpha occ. eigenvalues -- -0.64681 -0.63204 -0.59050 -0.58329 -0.57026

Alpha occ. eigenvalues -- -0.55532 -0.54826 -0.54276 -0.52983 -0.52325

Alpha occ. eigenvalues -- -0.48019 -0.46964 -0.45537 -0.45530 -0.44546

Alpha occ. eigenvalues -- -0.43245 -0.42543 -0.36669 -0.34275

Alpha virt. eigenvalues -- -0.04044 -0.02012 0.03385 0.05260 0.06310

Alpha virt. eigenvalues -- 0.06701 0.09315 0.10606 0.11564 0.11890

Alpha virt. eigenvalues -- 0.12346 0.12754 0.13248 0.13832 0.14307

Alpha virt. eigenvalues -- 0.14673 0.14740 0.15450 0.15534 0.15769

Alpha virt. eigenvalues -- 0.15896 0.16387 0.17567 0.18171 0.19091

Alpha virt. eigenvalues -- 0.19532 0.22627 0.22979

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.148927 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 4.080721 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 4.080658 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 4.149016 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.859926 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.859929

7 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 4.151515 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.892498 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.897109 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 4.151501 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.892520 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.897099

13 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.861887 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.861878 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 6.264537 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 4.205290 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 4.205093 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 3.677288

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23

1 C 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 6.263230 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 3.677324 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 6.263282 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.829384 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.829387

Mulliken atomic charges:

1

1 C -0.148927

2 C -0.080721

3 C -0.080658

4 C -0.149016

5 H 0.140074

6 H 0.140071

7 C -0.151515

8 H 0.107502

9 H 0.102891

10 C -0.151501

11 H 0.107480

12 H 0.102901

13 H 0.138113

14 H 0.138122

15 O -0.264537

16 C -0.205290

17 C -0.205093

18 C 0.322712

19 O -0.263230

20 C 0.322676

21 O -0.263282

22 H 0.170616

23 H 0.170613

Sum of Mulliken atomic charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.008854

2 C 0.057401

3 C 0.057454

4 C -0.008944

7 C 0.058878

10 C 0.058880

15 O -0.264537

16 C -0.034674

17 C -0.034480

18 C 0.322712

19 O -0.263230

20 C 0.322676

21 O -0.263282

Sum of Mulliken charges with hydrogens summed into heavy atoms = 0.00000

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 5.2721 Y= 0.0008 Z= -1.7785 Tot= 5.5640

N-N= 4.705564880480D+02 E-N=-8.432647352171D+02 KE=-4.715035908992D+01

1|1|UNPC-CHWS-122|FTS|RAM1|ZDO|C10H10O3|MC1210|07-Feb-2013|0||# opt=(c

alcfc,ts,noeigen) freq am1 geom=connectivity||Title Card Required||0,1

|C,-1.1389899091,1.5595086484,0.4412210365|C,0.1855557178,1.2807649585

,0.1063383882|C,-0.7540894021,3.7787936567,-0.3697796388|C,-1.62310595

47,2.8464853371,0.1958957027|H,-1.7337211472,0.8436284038,1.0265963222

|H,-2.6035097899,3.1557631402,0.5858486694|C,0.796539999,1.9281038627,

-1.0882583299|H,1.9159316639,1.9501909666,-0.9888670162|H,0.5712731791

,1.2731963791,-1.9762988258|C,0.269157873,3.3306705847,-1.355444734|H,

1.1217986652,4.0622213143,-1.3907530527|H,-0.2118412109,3.3569400536,-

2.3733803017|H,-1.029641329,4.8451240023,-0.4139240095|H,0.6626653842,

0.3460679967,0.4434559164|O,2.7563722566,3.8542438521,0.8211350045|C,0

.472811123,3.8749354432,1.4181157834|C,0.961158348,2.5754696813,1.6658

183996|C,1.6128097641,4.6753608068,0.8941665835|O,1.7590629186,5.83293

89217,0.535946269|C,2.4023600689,2.5746118222,1.2945418966|O,3.2959839

52,1.7435139062,1.314888848|H,-0.3489980868,4.3635009145,1.9469464733|

H,0.5840152261,1.8809716474,2.4202477153||Version=EM64W-G09RevC.01|Sta

te=1-A|HF=-0.0504198|RMSD=5.045e-009|RMSF=2.041e-005|Dipole=-2.04919,-

0.7699162,0.0010702|PG=C01 [X(C10H10O3)]||@

In the beginning there was nothing, which exploded.

Job cpu time: 0 days 0 hours 1 minutes 59.0 seconds.

File lengths (MBytes): RWF= 36 Int= 0 D2E= 0 Chk= 4 Scr= 1

Normal termination of Gaussian 09 at Thu Feb 07 16:36:49 2013.

Link1: Proceeding to internal job step number 2.

-------------------------------------------------------------

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RAM1/ZDO Freq

-------------------------------------------------------------

1/5=1,10=4,11=1,29=7,30=1,38=1,40=1/1,3;

2/12=2,40=1/2;

3/5=2,14=-4,16=1,25=1,41=700000,70=2,71=2,116=1,135=40/1,2,3;

4/5=101,35=1/1;

5/5=2,35=1,98=1/2;

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1/2;

6/7=2,8=2,9=2,10=2,18=1,28=1/1;

7/8=1,10=1,25=1/1,2,3,16;

1/5=1,10=4,11=1,30=1/3;

99//99;

Structure from the checkpoint file: \\ic.ac.uk\homes\mc1210\Desktop\module 3\part\_2\exo endo\exo\exo\_opt\_fre.chk

-------------------

Title Card Required

-------------------

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,-1.1389899091,1.5595086484,0.4412210365

C,0,0.1855557178,1.2807649585,0.1063383882

C,0,-0.7540894021,3.7787936567,-0.3697796388

C,0,-1.6231059547,2.8464853371,0.1958957027

H,0,-1.7337211472,0.8436284038,1.0265963222

H,0,-2.6035097899,3.1557631402,0.5858486694

C,0,0.796539999,1.9281038627,-1.0882583299

H,0,1.9159316639,1.9501909666,-0.9888670162

H,0,0.5712731791,1.2731963791,-1.9762988258

C,0,0.269157873,3.3306705847,-1.355444734

H,0,1.1217986652,4.0622213143,-1.3907530527

H,0,-0.2118412109,3.3569400536,-2.3733803017

H,0,-1.029641329,4.8451240023,-0.4139240095

H,0,0.6626653842,0.3460679967,0.4434559164

O,0,2.7563722566,3.8542438521,0.8211350045

C,0,0.472811123,3.8749354432,1.4181157834

C,0,0.961158348,2.5754696813,1.6658183996

C,0,1.6128097641,4.6753608068,0.8941665835

O,0,1.7590629186,5.8329389217,0.535946269

C,0,2.4023600689,2.5746118222,1.2945418966

O,0,3.295983952,1.7435139062,1.314888848

H,0,-0.3489980868,4.3635009145,1.9469464733

H,0,0.5840152261,1.8809716474,2.4202477153

Recover connectivity data from disk.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

----------------------------

! Initial Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.3944 calculate D2E/DX2 analytically !

! R2 R(1,4) 1.3967 calculate D2E/DX2 analytically !

! R3 R(1,5) 1.0995 calculate D2E/DX2 analytically !

! R4 R(2,7) 1.4898 calculate D2E/DX2 analytically !

! R5 R(2,14) 1.1022 calculate D2E/DX2 analytically !

! R6 R(2,17) 2.1702 calculate D2E/DX2 analytically !

! R7 R(3,4) 1.3944 calculate D2E/DX2 analytically !

! R8 R(3,10) 1.4898 calculate D2E/DX2 analytically !

! R9 R(3,13) 1.1022 calculate D2E/DX2 analytically !

! R10 R(3,16) 2.1705 calculate D2E/DX2 analytically !

! R11 R(4,6) 1.0995 calculate D2E/DX2 analytically !

! R12 R(7,8) 1.124 calculate D2E/DX2 analytically !

! R13 R(7,9) 1.1262 calculate D2E/DX2 analytically !

! R14 R(7,10) 1.5221 calculate D2E/DX2 analytically !

! R15 R(10,11) 1.124 calculate D2E/DX2 analytically !

! R16 R(10,12) 1.1262 calculate D2E/DX2 analytically !

! R17 R(15,18) 1.4097 calculate D2E/DX2 analytically !

! R18 R(15,20) 1.4096 calculate D2E/DX2 analytically !

! R19 R(16,17) 1.4101 calculate D2E/DX2 analytically !

! R20 R(16,18) 1.4882 calculate D2E/DX2 analytically !

! R21 R(16,22) 1.0926 calculate D2E/DX2 analytically !

! R22 R(17,20) 1.4883 calculate D2E/DX2 analytically !

! R23 R(17,23) 1.0926 calculate D2E/DX2 analytically !

! R24 R(18,19) 1.2205 calculate D2E/DX2 analytically !

! R25 R(20,21) 1.2205 calculate D2E/DX2 analytically !

! A1 A(2,1,4) 118.1164 calculate D2E/DX2 analytically !

! A2 A(2,1,5) 120.7666 calculate D2E/DX2 analytically !

! A3 A(4,1,5) 120.3959 calculate D2E/DX2 analytically !

! A4 A(1,2,7) 119.6897 calculate D2E/DX2 analytically !

! A5 A(1,2,14) 120.4804 calculate D2E/DX2 analytically !

! A6 A(1,2,17) 92.7311 calculate D2E/DX2 analytically !

! A7 A(7,2,14) 115.8617 calculate D2E/DX2 analytically !

! A8 A(7,2,17) 99.8117 calculate D2E/DX2 analytically !

! A9 A(14,2,17) 97.5519 calculate D2E/DX2 analytically !

! A10 A(4,3,10) 119.6925 calculate D2E/DX2 analytically !

! A11 A(4,3,13) 120.4821 calculate D2E/DX2 analytically !

! A12 A(4,3,16) 92.7358 calculate D2E/DX2 analytically !

! A13 A(10,3,13) 115.8624 calculate D2E/DX2 analytically !

! A14 A(10,3,16) 99.7919 calculate D2E/DX2 analytically !

! A15 A(13,3,16) 97.5533 calculate D2E/DX2 analytically !

! A16 A(1,4,3) 118.1193 calculate D2E/DX2 analytically !

! A17 A(1,4,6) 120.3946 calculate D2E/DX2 analytically !

! A18 A(3,4,6) 120.7647 calculate D2E/DX2 analytically !

! A19 A(2,7,8) 110.247 calculate D2E/DX2 analytically !

! A20 A(2,7,9) 107.3126 calculate D2E/DX2 analytically !

! A21 A(2,7,10) 113.5197 calculate D2E/DX2 analytically !

! A22 A(8,7,9) 106.2818 calculate D2E/DX2 analytically !

! A23 A(8,7,10) 110.028 calculate D2E/DX2 analytically !

! A24 A(9,7,10) 109.1561 calculate D2E/DX2 analytically !

! A25 A(3,10,7) 113.5175 calculate D2E/DX2 analytically !

! A26 A(3,10,11) 110.245 calculate D2E/DX2 analytically !

! A27 A(3,10,12) 107.3172 calculate D2E/DX2 analytically !

! A28 A(7,10,11) 110.0241 calculate D2E/DX2 analytically !

! A29 A(7,10,12) 109.1569 calculate D2E/DX2 analytically !

! A30 A(11,10,12) 106.2852 calculate D2E/DX2 analytically !

! A31 A(18,15,20) 107.9173 calculate D2E/DX2 analytically !

! A32 A(3,16,17) 107.4357 calculate D2E/DX2 analytically !

! A33 A(3,16,18) 99.6028 calculate D2E/DX2 analytically !

! A34 A(3,16,22) 89.618 calculate D2E/DX2 analytically !

! A35 A(17,16,18) 106.9894 calculate D2E/DX2 analytically !

! A36 A(17,16,22) 125.9828 calculate D2E/DX2 analytically !

! A37 A(18,16,22) 120.4029 calculate D2E/DX2 analytically !

! A38 A(2,17,16) 107.4438 calculate D2E/DX2 analytically !

! A39 A(2,17,20) 99.583 calculate D2E/DX2 analytically !

! A40 A(2,17,23) 89.6335 calculate D2E/DX2 analytically !

! A41 A(16,17,20) 106.9822 calculate D2E/DX2 analytically !

! A42 A(16,17,23) 125.9811 calculate D2E/DX2 analytically !

! A43 A(20,17,23) 120.4088 calculate D2E/DX2 analytically !

! A44 A(15,18,16) 109.0477 calculate D2E/DX2 analytically !

! A45 A(15,18,19) 116.105 calculate D2E/DX2 analytically !

! A46 A(16,18,19) 134.8471 calculate D2E/DX2 analytically !

! A47 A(15,20,17) 109.0546 calculate D2E/DX2 analytically !

! A48 A(15,20,21) 116.096 calculate D2E/DX2 analytically !

! A49 A(17,20,21) 134.8492 calculate D2E/DX2 analytically !

! D1 D(4,1,2,7) -34.3627 calculate D2E/DX2 analytically !

! D2 D(4,1,2,14) 168.9703 calculate D2E/DX2 analytically !

! D3 D(4,1,2,17) 68.5569 calculate D2E/DX2 analytically !

! D4 D(5,1,2,7) 155.3292 calculate D2E/DX2 analytically !

! D5 D(5,1,2,14) -1.3377 calculate D2E/DX2 analytically !

! D6 D(5,1,2,17) -101.7512 calculate D2E/DX2 analytically !

! D7 D(2,1,4,3) -0.0029 calculate D2E/DX2 analytically !

! D8 D(2,1,4,6) -170.3468 calculate D2E/DX2 analytically !

! D9 D(5,1,4,3) 170.3425 calculate D2E/DX2 analytically !

! D10 D(5,1,4,6) -0.0014 calculate D2E/DX2 analytically !

! D11 D(1,2,7,8) 156.8558 calculate D2E/DX2 analytically !

! D12 D(1,2,7,9) -87.8046 calculate D2E/DX2 analytically !

! D13 D(1,2,7,10) 32.8937 calculate D2E/DX2 analytically !

! D14 D(14,2,7,8) -45.4363 calculate D2E/DX2 analytically !

! D15 D(14,2,7,9) 69.9032 calculate D2E/DX2 analytically !

! D16 D(14,2,7,10) -169.3984 calculate D2E/DX2 analytically !

! D17 D(17,2,7,8) 57.9816 calculate D2E/DX2 analytically !

! D18 D(17,2,7,9) 173.3212 calculate D2E/DX2 analytically !

! D19 D(17,2,7,10) -65.9805 calculate D2E/DX2 analytically !

! D20 D(1,2,17,16) -59.3855 calculate D2E/DX2 analytically !

! D21 D(1,2,17,20) -170.7031 calculate D2E/DX2 analytically !

! D22 D(1,2,17,23) 68.4824 calculate D2E/DX2 analytically !

! D23 D(7,2,17,16) 61.3767 calculate D2E/DX2 analytically !

! D24 D(7,2,17,20) -49.9409 calculate D2E/DX2 analytically !

! D25 D(7,2,17,23) -170.7554 calculate D2E/DX2 analytically !

! D26 D(14,2,17,16) 179.377 calculate D2E/DX2 analytically !

! D27 D(14,2,17,20) 68.0594 calculate D2E/DX2 analytically !

! D28 D(14,2,17,23) -52.7551 calculate D2E/DX2 analytically !

! D29 D(10,3,4,1) 34.3587 calculate D2E/DX2 analytically !

! D30 D(10,3,4,6) -155.3347 calculate D2E/DX2 analytically !

! D31 D(13,3,4,1) -168.9594 calculate D2E/DX2 analytically !

! D32 D(13,3,4,6) 1.3472 calculate D2E/DX2 analytically !

! D33 D(16,3,4,1) -68.5411 calculate D2E/DX2 analytically !

! D34 D(16,3,4,6) 101.7655 calculate D2E/DX2 analytically !

! D35 D(4,3,10,7) -32.8672 calculate D2E/DX2 analytically !

! D36 D(4,3,10,11) -156.8209 calculate D2E/DX2 analytically !

! D37 D(4,3,10,12) 87.834 calculate D2E/DX2 analytically !

! D38 D(13,3,10,7) 169.4105 calculate D2E/DX2 analytically !

! D39 D(13,3,10,11) 45.4567 calculate D2E/DX2 analytically !

! D40 D(13,3,10,12) -69.8884 calculate D2E/DX2 analytically !

! D41 D(16,3,10,7) 66.0014 calculate D2E/DX2 analytically !

! D42 D(16,3,10,11) -57.9523 calculate D2E/DX2 analytically !

! D43 D(16,3,10,12) -173.2975 calculate D2E/DX2 analytically !

! D44 D(4,3,16,17) 59.3461 calculate D2E/DX2 analytically !

! D45 D(4,3,16,18) 170.6772 calculate D2E/DX2 analytically !

! D46 D(4,3,16,22) -68.5155 calculate D2E/DX2 analytically !

! D47 D(10,3,16,17) -61.4168 calculate D2E/DX2 analytically !

! D48 D(10,3,16,18) 49.9142 calculate D2E/DX2 analytically !

! D49 D(10,3,16,22) 170.7215 calculate D2E/DX2 analytically !

! D50 D(13,3,16,17) -179.4135 calculate D2E/DX2 analytically !

! D51 D(13,3,16,18) -68.0825 calculate D2E/DX2 analytically !

! D52 D(13,3,16,22) 52.7249 calculate D2E/DX2 analytically !

! D53 D(2,7,10,3) -0.0168 calculate D2E/DX2 analytically !

! D54 D(2,7,10,11) 124.0569 calculate D2E/DX2 analytically !

! D55 D(2,7,10,12) -119.6755 calculate D2E/DX2 analytically !

! D56 D(8,7,10,3) -124.0978 calculate D2E/DX2 analytically !

! D57 D(8,7,10,11) -0.024 calculate D2E/DX2 analytically !

! D58 D(8,7,10,12) 116.2435 calculate D2E/DX2 analytically !

! D59 D(9,7,10,3) 119.637 calculate D2E/DX2 analytically !

! D60 D(9,7,10,11) -116.2893 calculate D2E/DX2 analytically !

! D61 D(9,7,10,12) -0.0217 calculate D2E/DX2 analytically !

! D62 D(20,15,18,16) -0.9326 calculate D2E/DX2 analytically !

! D63 D(20,15,18,19) 178.9232 calculate D2E/DX2 analytically !

! D64 D(18,15,20,17) 0.9316 calculate D2E/DX2 analytically !

! D65 D(18,15,20,21) -178.9458 calculate D2E/DX2 analytically !

! D66 D(3,16,17,2) 0.0202 calculate D2E/DX2 analytically !

! D67 D(3,16,17,20) 106.186 calculate D2E/DX2 analytically !

! D68 D(3,16,17,23) -102.6801 calculate D2E/DX2 analytically !

! D69 D(18,16,17,2) -106.1676 calculate D2E/DX2 analytically !

! D70 D(18,16,17,20) -0.0018 calculate D2E/DX2 analytically !

! D71 D(18,16,17,23) 151.1321 calculate D2E/DX2 analytically !

! D72 D(22,16,17,2) 102.694 calculate D2E/DX2 analytically !

! D73 D(22,16,17,20) -151.1402 calculate D2E/DX2 analytically !

! D74 D(22,16,17,23) -0.0063 calculate D2E/DX2 analytically !

! D75 D(3,16,18,15) -111.107 calculate D2E/DX2 analytically !

! D76 D(3,16,18,19) 69.0756 calculate D2E/DX2 analytically !

! D77 D(17,16,18,15) 0.5749 calculate D2E/DX2 analytically !

! D78 D(17,16,18,19) -179.2425 calculate D2E/DX2 analytically !

! D79 D(22,16,18,15) 153.647 calculate D2E/DX2 analytically !

! D80 D(22,16,18,19) -26.1704 calculate D2E/DX2 analytically !

! D81 D(2,17,20,15) 111.1087 calculate D2E/DX2 analytically !

! D82 D(2,17,20,21) -69.0466 calculate D2E/DX2 analytically !

! D83 D(16,17,20,15) -0.572 calculate D2E/DX2 analytically !

! D84 D(16,17,20,21) 179.2727 calculate D2E/DX2 analytically !

! D85 D(23,17,20,15) -153.6375 calculate D2E/DX2 analytically !

! D86 D(23,17,20,21) 26.2072 calculate D2E/DX2 analytically !

--------------------------------------------------------------------------------

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07

Number of steps in this run= 2 maximum allowed number of steps= 2.

Search for a saddle point of order 1.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -1.138990 1.559509 0.441221

2 6 0 0.185556 1.280765 0.106338

3 6 0 -0.754089 3.778794 -0.369780

4 6 0 -1.623106 2.846485 0.195896

5 1 0 -1.733721 0.843628 1.026596

6 1 0 -2.603510 3.155763 0.585849

7 6 0 0.796540 1.928104 -1.088258

8 1 0 1.915932 1.950191 -0.988867

9 1 0 0.571273 1.273196 -1.976299

10 6 0 0.269158 3.330671 -1.355445

11 1 0 1.121799 4.062221 -1.390753

12 1 0 -0.211841 3.356940 -2.373380

13 1 0 -1.029641 4.845124 -0.413924

14 1 0 0.662665 0.346068 0.443456

15 8 0 2.756372 3.854244 0.821135

16 6 0 0.472811 3.874935 1.418116

17 6 0 0.961158 2.575470 1.665818

18 6 0 1.612810 4.675361 0.894167

19 8 0 1.759063 5.832939 0.535946

20 6 0 2.402360 2.574612 1.294542

21 8 0 3.295984 1.743514 1.314889

22 1 0 -0.348998 4.363501 1.946946

23 1 0 0.584015 1.880972 2.420248

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394369 0.000000

3 C 2.393971 2.711046 0.000000

4 C 1.396733 2.393900 1.394409 0.000000

5 H 1.099479 2.172921 3.394811 2.171114 0.000000

6 H 2.171120 3.394766 2.172958 1.099503 2.509334

7 C 2.494283 1.489769 2.519070 2.889146 3.471443

8 H 3.395634 2.154485 3.294855 3.838202 4.313530

9 H 2.975126 2.118068 3.258145 3.465396 3.809843

10 C 2.889274 2.519109 1.489760 2.494345 3.983845

11 H 3.838081 3.294591 2.154454 3.395581 4.935272

12 H 3.465883 3.258440 2.118115 2.975468 4.493628

13 H 3.396837 3.801583 1.102242 2.172242 4.310777

14 H 2.172189 1.102243 3.801599 3.396781 2.516006

15 O 4.536958 3.707132 3.707737 4.537216 5.409895

16 C 2.985536 2.921129 2.170506 2.635223 3.769734

17 C 2.634851 2.170207 2.921254 2.985388 3.266536

18 C 4.181638 3.765768 2.829064 3.781999 5.089104

19 O 5.164290 4.835574 3.369835 4.524777 6.110114

20 C 3.781501 2.828443 3.766058 4.181545 4.491689

21 O 4.523953 3.368901 4.835656 5.163927 5.117699

22 H 3.279279 3.629993 2.423469 2.644025 3.892815

23 H 2.643602 2.423467 3.629946 3.278924 2.896592

6 7 8 9 10

6 H 0.000000

7 C 3.983732 0.000000

8 H 4.935432 1.124013 0.000000

9 H 4.493095 1.126173 1.800403 0.000000

10 C 3.471517 1.522076 2.179901 2.170238 0.000000

11 H 4.313530 2.179852 2.291906 2.902517 1.124015

12 H 3.810195 2.170241 2.902281 2.261179 1.126163

13 H 2.516058 3.506946 4.169844 4.214571 2.206107

14 H 4.310750 2.206107 2.489063 2.592900 3.506957

15 O 5.410321 3.346153 2.758236 4.388861 3.346321

16 C 3.267052 3.190120 3.403058 4.277942 2.833785

17 C 3.769607 2.833923 2.889623 3.887537 3.190176

18 C 4.492392 3.484785 3.326297 4.571553 2.945224

19 O 5.118769 4.337307 4.174374 5.339801 3.472539

20 C 5.089078 2.945228 2.416706 3.967992 3.484911

21 O 6.109826 3.472234 2.693427 4.298507 4.337214

22 H 2.897247 4.056585 4.424135 5.078261 3.514917

23 H 3.892355 3.515253 3.660718 4.438375 4.056675

11 12 13 14 15

11 H 0.000000

12 H 1.800437 0.000000

13 H 2.489142 2.592867 0.000000

14 H 4.169523 4.214817 4.882674 0.000000

15 O 2.758176 4.388910 4.103793 4.102871 0.000000

16 C 2.888945 3.887481 2.560273 3.665912 2.360395

17 C 3.402773 4.278054 3.666053 2.559980 2.360412

18 C 2.416173 3.967927 2.953383 4.455187 1.409717

19 O 2.693273 4.298746 3.107234 5.596105 2.234098

20 C 3.326203 4.571623 4.455639 2.952506 1.409573

21 O 4.174205 5.339598 5.596411 3.105900 2.233865

22 H 3.659816 4.438153 2.503786 4.407234 3.342173

23 H 4.423888 5.078458 4.407110 2.503961 3.342170

16 17 18 19 20

16 C 0.000000

17 C 1.410124 0.000000

18 C 1.488221 2.330159 0.000000

19 O 2.503287 3.538978 1.220532 0.000000

20 C 2.330080 1.488257 2.279657 3.406757 0.000000

21 O 3.538915 2.503340 3.406730 4.437598 1.220533

22 H 1.092579 2.234412 2.248175 2.931568 3.346002

23 H 2.234396 1.092579 3.346035 4.533142 2.248272

21 22 23

21 O 0.000000

22 H 4.533180 0.000000

23 H 2.931806 2.693971 0.000000

Stoichiometry C10H10O3

Framework group C1[X(C10H10O3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 2.306506 -0.698465 -0.663545

2 6 0 1.370479 -1.355418 0.134284

3 6 0 1.370830 1.355628 0.134146

4 6 0 2.306709 0.698268 -0.663592

5 1 0 2.914754 -1.254883 -1.391066

6 1 0 2.915157 1.254451 -1.391162

7 6 0 0.966002 -0.760793 1.438980

8 1 0 -0.044651 -1.145730 1.745261

9 1 0 1.693194 -1.130260 2.215479

10 6 0 0.965982 0.761282 1.438844

11 1 0 -0.044837 1.146175 1.744640

12 1 0 1.692860 1.130918 2.215542

13 1 0 1.212095 2.441446 0.030516

14 1 0 1.211533 -2.441228 0.030874

15 8 0 -2.077252 -0.000269 0.274100

16 6 0 -0.292167 0.705132 -1.099708

17 6 0 -0.291966 -0.704992 -1.099823

18 6 0 -1.425284 1.139751 -0.238341

19 8 0 -1.886412 2.218671 0.097803

20 6 0 -1.425004 -1.139906 -0.238438

21 8 0 -1.885674 -2.218927 0.098011

22 1 0 0.065886 1.347186 -1.907974

23 1 0 0.066189 -1.346785 -1.908251

---------------------------------------------------------------------

Rotational constants (GHZ): 1.2200682 0.8808243 0.6753903

Standard basis: VSTO-6G (5D, 7F)

There are 62 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned off.

62 basis functions, 372 primitive gaussians, 62 cartesian basis functions

34 alpha electrons 34 beta electrons

nuclear repulsion energy 470.5564880480 Hartrees.

Do NDO integrals.

One-electron integrals computed using PRISM.

NBasis= 62 RedAO= F NBF= 62

NBsUse= 62 1.00D-04 NBFU= 62

Initial guess read from the checkpoint file: \\ic.ac.uk\homes\mc1210\Desktop\module 3\part\_2\exo endo\exo\exo\_opt\_fre.chk

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Initial guess orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Overlap will be assumed to be unity.

Keep J ints in memory in canonical form, NReq=899243.

SCF Done: E(RAM1) = -0.504198155658E-01 A.U. after 2 cycles

Convg = 0.9675D-09 -V/T = 0.9989

Range of M.O.s used for correlation: 1 62

NBasis= 62 NAE= 34 NBE= 34 NFC= 0 NFV= 0

NROrb= 62 NOA= 34 NOB= 34 NVA= 28 NVB= 28

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

G2DrvN: will do 24 centers at a time, making 1 passes doing MaxLOS=1.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFDir/FoFCou used for L=0 through L=1.

End of G2Drv Frequency-dependent properties file 721 does not exist.

End of G2Drv Frequency-dependent properties file 722 does not exist.

IDoAtm=11111111111111111111111

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Electric field/nuclear overlap derivatives assumed to be zero.

Keep J ints in memory in canonical form, NReq=811133.

There are 72 degrees of freedom in the 1st order CPHF. IDoFFX=5.

LinEq1: Iter= 0 NonCon= 72 RMS=2.63D-01 Max=4.87D+00

AX will form 72 AO Fock derivatives at one time.

LinEq1: Iter= 1 NonCon= 72 RMS=4.14D-02 Max=3.57D-01

LinEq1: Iter= 2 NonCon= 72 RMS=9.46D-03 Max=1.23D-01

LinEq1: Iter= 3 NonCon= 72 RMS=3.03D-03 Max=5.10D-02

LinEq1: Iter= 4 NonCon= 72 RMS=6.10D-04 Max=5.65D-03

LinEq1: Iter= 5 NonCon= 72 RMS=8.57D-05 Max=1.06D-03

LinEq1: Iter= 6 NonCon= 72 RMS=1.37D-05 Max=1.50D-04

LinEq1: Iter= 7 NonCon= 72 RMS=2.10D-06 Max=2.11D-05

LinEq1: Iter= 8 NonCon= 51 RMS=2.78D-07 Max=1.61D-06

LinEq1: Iter= 9 NonCon= 9 RMS=4.77D-08 Max=5.30D-07

LinEq1: Iter= 10 NonCon= 1 RMS=9.41D-09 Max=1.08D-07

LinEq1: Iter= 11 NonCon= 0 RMS=1.39D-09 Max=8.76D-09

Linear equations converged to 1.000D-08 1.000D-07 after 11 iterations.

Isotropic polarizability for W= 0.000000 101.94 Bohr\*\*3.

End of Minotr Frequency-dependent properties file 721 does not exist.

End of Minotr Frequency-dependent properties file 722 does not exist.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -1.55554 -1.45667 -1.44457 -1.36911 -1.23237

Alpha occ. eigenvalues -- -1.19012 -1.18108 -0.97163 -0.89235 -0.86948

Alpha occ. eigenvalues -- -0.83226 -0.81028 -0.67967 -0.66424 -0.65438

Alpha occ. eigenvalues -- -0.64681 -0.63204 -0.59050 -0.58329 -0.57026

Alpha occ. eigenvalues -- -0.55532 -0.54826 -0.54276 -0.52983 -0.52325

Alpha occ. eigenvalues -- -0.48019 -0.46964 -0.45537 -0.45530 -0.44546

Alpha occ. eigenvalues -- -0.43245 -0.42543 -0.36669 -0.34275

Alpha virt. eigenvalues -- -0.04044 -0.02012 0.03385 0.05260 0.06310

Alpha virt. eigenvalues -- 0.06701 0.09315 0.10606 0.11564 0.11890

Alpha virt. eigenvalues -- 0.12346 0.12754 0.13248 0.13832 0.14307

Alpha virt. eigenvalues -- 0.14673 0.14740 0.15450 0.15534 0.15769

Alpha virt. eigenvalues -- 0.15896 0.16387 0.17567 0.18171 0.19091

Alpha virt. eigenvalues -- 0.19532 0.22627 0.22979

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.148927 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 4.080721 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 4.080658 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 4.149016 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.859926 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.859929

7 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 4.151515 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.892498 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.897109 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 4.151501 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.892520 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.897099

13 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.861887 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.861878 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 6.264537 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 4.205290 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 4.205093 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000 3.677288

19 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 20 21 22 23

1 C 0.000000 0.000000 0.000000 0.000000 0.000000

2 C 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000

5 H 0.000000 0.000000 0.000000 0.000000 0.000000

6 H 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000 0.000000 0.000000

8 H 0.000000 0.000000 0.000000 0.000000 0.000000

9 H 0.000000 0.000000 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000

11 H 0.000000 0.000000 0.000000 0.000000 0.000000

12 H 0.000000 0.000000 0.000000 0.000000 0.000000

13 H 0.000000 0.000000 0.000000 0.000000 0.000000

14 H 0.000000 0.000000 0.000000 0.000000 0.000000

15 O 0.000000 0.000000 0.000000 0.000000 0.000000

16 C 0.000000 0.000000 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000 0.000000 0.000000

18 C 0.000000 0.000000 0.000000 0.000000 0.000000

19 O 6.263230 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 3.677324 0.000000 0.000000 0.000000

21 O 0.000000 0.000000 6.263282 0.000000 0.000000

22 H 0.000000 0.000000 0.000000 0.829384 0.000000

23 H 0.000000 0.000000 0.000000 0.000000 0.829387

Mulliken atomic charges:

1

1 C -0.148927

2 C -0.080721

3 C -0.080658

4 C -0.149016

5 H 0.140074

6 H 0.140071

7 C -0.151515

8 H 0.107502

9 H 0.102891

10 C -0.151501

11 H 0.107480

12 H 0.102901

13 H 0.138113

14 H 0.138122

15 O -0.264537

16 C -0.205290

17 C -0.205093

18 C 0.322712

19 O -0.263230

20 C 0.322676

21 O -0.263282

22 H 0.170616

23 H 0.170613

Sum of Mulliken atomic charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.008854

2 C 0.057401

3 C 0.057454

4 C -0.008944

7 C 0.058878

10 C 0.058880

15 O -0.264537

16 C -0.034674

17 C -0.034480

18 C 0.322712

19 O -0.263230

20 C 0.322676

21 O -0.263282

Sum of Mulliken charges with hydrogens summed into heavy atoms = 0.00000

APT atomic charges:

1

1 C -0.156931

2 C -0.119552

3 C -0.119142

4 C -0.157270

5 H 0.140649

6 H 0.140640

7 C -0.063168

8 H 0.057119

9 H 0.058130

10 C -0.063193

11 H 0.057094

12 H 0.058151

13 H 0.098338

14 H 0.098383

15 O -0.819639

16 C -0.136391

17 C -0.135791

18 C 1.155179

19 O -0.718208

20 C 1.154868

21 O -0.718152

22 H 0.094450

23 H 0.094416

Sum of APT charges= -0.00002

APT Atomic charges with hydrogens summed into heavy atoms:

1

1 C -0.016282

2 C -0.021169

3 C -0.020804

4 C -0.016630

5 H 0.000000

6 H 0.000000

7 C 0.052082

8 H 0.000000

9 H 0.000000

10 C 0.052052

11 H 0.000000

12 H 0.000000

13 H 0.000000

14 H 0.000000

15 O -0.819639

16 C -0.041941

17 C -0.041376

18 C 1.155179

19 O -0.718208

20 C 1.154868

21 O -0.718152

22 H 0.000000

23 H 0.000000

Sum of APT charges= -0.00002

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 5.2721 Y= 0.0008 Z= -1.7785 Tot= 5.5640

N-N= 4.705564880480D+02 E-N=-8.432647351794D+02 KE=-4.715035909038D+01

Exact polarizability: 112.813 -0.008 122.738 -7.066 -0.002 70.266

Approx polarizability: 87.615 -0.012 117.865 -8.104 -0.002 51.676

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

Full mass-weighted force constant matrix:

Low frequencies --- -812.3128 -0.7385 -0.3078 -0.0047 1.3156 1.8993

Low frequencies --- 3.0495 60.8706 123.8838

\*\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*\*

Harmonic frequencies (cm\*\*-1), IR intensities (KM/Mole), Raman scattering

activities (A\*\*4/AMU), depolarization ratios for plane and unpolarized

incident light, reduced masses (AMU), force constants (mDyne/A),

and normal coordinates:

1 2 3

A A A

Frequencies -- -812.3128 60.8706 123.8838

Red. masses -- 7.0431 4.4896 7.1632

Frc consts -- 2.7382 0.0098 0.0648

IR Inten -- 96.8477 0.5530 0.0414

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 -0.09 0.05 -0.04 -0.10 0.07 0.08 0.15 0.02

2 6 0.32 -0.07 0.16 -0.09 0.04 0.12 0.15 0.06 0.03

3 6 0.32 0.07 0.16 0.09 0.04 -0.12 -0.15 0.06 -0.03

4 6 -0.05 0.09 0.05 0.04 -0.10 -0.07 -0.08 0.15 -0.02

5 1 -0.18 0.05 -0.18 -0.07 -0.20 0.13 0.15 0.21 0.04

6 1 -0.18 -0.05 -0.18 0.07 -0.20 -0.13 -0.15 0.21 -0.04

7 6 0.00 0.00 0.00 -0.10 0.18 0.05 0.05 0.04 0.00

8 1 -0.02 -0.01 -0.08 -0.16 0.33 0.02 0.05 -0.02 -0.06

9 1 -0.07 0.03 0.08 -0.19 0.15 0.12 0.02 0.09 0.05

10 6 0.00 0.00 0.00 0.10 0.18 -0.05 -0.05 0.04 0.00

11 1 -0.02 0.01 -0.08 0.16 0.33 -0.02 -0.05 -0.02 0.06

12 1 -0.07 -0.03 0.08 0.19 0.15 -0.12 -0.02 0.09 -0.05

13 1 0.04 0.02 0.05 0.16 0.04 -0.22 -0.30 0.04 -0.05

14 1 0.04 -0.02 0.05 -0.16 0.04 0.22 0.30 0.04 0.05

15 8 -0.01 0.00 0.03 0.00 -0.08 0.00 0.00 0.00 0.00

16 6 -0.25 -0.12 -0.23 -0.01 0.03 0.03 0.01 -0.18 -0.06

17 6 -0.25 0.13 -0.23 0.01 0.03 -0.03 -0.01 -0.18 0.06

18 6 -0.02 0.00 0.01 0.00 -0.04 0.09 0.11 -0.07 0.00

19 8 0.01 0.00 0.00 0.01 -0.07 0.19 0.33 -0.01 0.11

20 6 -0.02 0.00 0.01 0.00 -0.04 -0.09 -0.11 -0.07 0.00

21 8 0.01 0.00 0.00 -0.01 -0.07 -0.19 -0.33 -0.01 -0.11

22 1 0.28 0.12 0.21 -0.07 0.07 0.04 0.00 -0.26 -0.13

23 1 0.28 -0.12 0.21 0.07 0.07 -0.04 0.00 -0.26 0.13

4 5 6

A A A

Frequencies -- 139.2096 167.5353 218.8873

Red. masses -- 8.3655 14.3936 4.4306

Frc consts -- 0.0955 0.2380 0.1251

IR Inten -- 4.1549 0.3649 0.2165

Atom AN X Y Z X Y Z X Y Z

1 6 0.10 0.00 -0.06 -0.05 0.00 0.03 0.08 -0.09 0.07

2 6 0.17 0.00 0.02 -0.08 0.00 0.00 0.19 -0.11 0.15

3 6 0.17 0.00 0.02 -0.08 0.00 0.00 -0.19 -0.11 -0.15

4 6 0.10 0.00 -0.06 -0.05 0.00 0.03 -0.08 -0.09 -0.07

5 1 0.04 0.00 -0.10 -0.03 0.00 0.05 0.13 -0.09 0.10

6 1 0.04 0.00 -0.10 -0.03 0.00 0.05 -0.13 -0.09 -0.10

7 6 0.24 0.00 0.04 -0.10 0.00 -0.01 0.14 -0.04 0.10

8 1 0.24 0.01 0.05 -0.10 0.00 0.00 0.22 -0.20 0.16

9 1 0.26 -0.01 0.02 -0.10 0.00 0.00 0.24 0.18 0.11

10 6 0.24 0.00 0.04 -0.10 0.00 -0.01 -0.14 -0.04 -0.10

11 1 0.24 -0.01 0.05 -0.10 0.00 0.00 -0.22 -0.20 -0.16

12 1 0.26 0.01 0.02 -0.10 0.00 0.00 -0.24 0.18 -0.11

13 1 0.18 0.00 0.04 -0.08 0.00 -0.01 -0.17 -0.10 -0.16

14 1 0.18 0.00 0.04 -0.08 0.00 -0.01 0.17 -0.10 0.16

15 8 -0.14 0.00 0.00 0.52 0.00 0.59 0.00 0.04 0.00

16 6 0.03 0.00 0.20 -0.01 0.00 -0.09 -0.01 0.10 0.00

17 6 0.03 0.00 0.20 -0.01 0.00 -0.09 0.01 0.10 0.00

18 6 -0.11 0.00 0.03 0.11 0.00 0.06 -0.04 0.07 0.03

19 8 -0.29 -0.01 -0.19 -0.14 0.00 -0.29 -0.04 0.05 0.08

20 6 -0.11 0.00 0.03 0.11 0.00 0.06 0.04 0.07 -0.03

21 8 -0.29 0.01 -0.19 -0.14 0.00 -0.29 0.04 0.05 -0.08

22 1 0.04 -0.01 0.20 -0.05 0.00 -0.10 -0.15 0.09 -0.07

23 1 0.04 0.01 0.20 -0.05 0.00 -0.10 0.15 0.09 0.07

7 8 9

A A A

Frequencies -- 234.7434 257.7497 359.4292

Red. masses -- 3.8325 1.9115 3.0031

Frc consts -- 0.1244 0.0748 0.2286

IR Inten -- 3.3463 0.1319 2.8119

Atom AN X Y Z X Y Z X Y Z

1 6 0.22 0.00 0.08 -0.07 -0.02 -0.05 0.08 0.00 0.12

2 6 0.07 0.00 -0.10 -0.09 0.03 -0.03 -0.10 0.03 -0.04

3 6 0.07 0.00 -0.10 0.09 0.03 0.03 -0.10 -0.03 -0.04

4 6 0.22 0.00 0.08 0.07 -0.02 0.05 0.08 0.00 0.12

5 1 0.39 0.00 0.22 -0.16 -0.03 -0.12 0.20 -0.01 0.24

6 1 0.39 0.00 0.22 0.16 -0.03 0.12 0.20 0.01 0.24

7 6 -0.13 0.00 -0.16 0.13 0.04 0.04 0.14 0.00 0.05

8 1 -0.15 -0.01 -0.27 0.27 -0.11 0.28 0.20 0.00 0.24

9 1 -0.23 0.01 -0.05 0.41 0.20 -0.14 0.33 -0.01 -0.12

10 6 -0.13 0.00 -0.16 -0.13 0.04 -0.04 0.14 0.00 0.05

11 1 -0.15 0.01 -0.27 -0.27 -0.11 -0.28 0.20 0.00 0.24

12 1 -0.23 -0.01 -0.05 -0.41 0.20 0.14 0.33 0.01 -0.12

13 1 0.09 0.00 -0.13 0.15 0.03 0.02 -0.23 -0.06 -0.12

14 1 0.09 0.00 -0.13 -0.15 0.03 -0.02 -0.23 0.06 -0.12

15 8 -0.02 0.00 0.06 0.00 -0.01 0.00 0.02 0.00 0.01

16 6 -0.04 0.00 0.02 -0.01 -0.01 -0.01 -0.09 0.00 -0.13

17 6 -0.04 0.00 0.02 0.01 -0.01 0.01 -0.09 0.00 -0.13

18 6 -0.04 0.00 0.04 0.00 -0.01 -0.01 -0.04 0.00 -0.06

19 8 -0.06 -0.02 0.07 0.03 -0.01 0.03 -0.03 -0.02 0.03

20 6 -0.04 0.00 0.04 0.00 -0.01 0.01 -0.04 0.00 -0.06

21 8 -0.06 0.02 0.07 -0.03 -0.01 -0.03 -0.03 0.02 0.03

22 1 -0.04 0.00 0.02 0.04 -0.01 0.01 -0.08 0.01 -0.12

23 1 -0.04 0.00 0.02 -0.04 -0.01 -0.01 -0.08 -0.01 -0.12

10 11 12

A A A

Frequencies -- 390.6208 446.5835 500.8086

Red. masses -- 11.0303 7.0438 2.1243

Frc consts -- 0.9916 0.8277 0.3139

IR Inten -- 19.5821 0.0299 0.0483

Atom AN X Y Z X Y Z X Y Z

1 6 0.06 0.00 0.06 -0.04 0.00 -0.06 0.13 -0.02 0.13

2 6 -0.04 0.01 -0.05 0.10 -0.01 0.05 -0.08 0.03 -0.07

3 6 -0.04 -0.01 -0.05 -0.10 -0.01 -0.05 0.08 0.03 0.07

4 6 0.06 0.00 0.06 0.04 0.00 0.06 -0.13 -0.02 -0.13

5 1 0.15 0.00 0.14 -0.14 0.04 -0.18 0.42 -0.06 0.40

6 1 0.15 0.00 0.13 0.14 0.04 0.18 -0.42 -0.06 -0.40

7 6 0.03 0.00 -0.02 0.05 0.07 0.00 0.02 0.00 -0.02

8 1 0.06 -0.01 0.05 0.05 0.03 -0.05 0.08 -0.04 0.11

9 1 0.10 0.01 -0.08 0.04 0.14 0.04 0.17 0.01 -0.16

10 6 0.03 0.00 -0.02 -0.05 0.07 0.00 -0.02 0.00 0.02

11 1 0.06 0.01 0.05 -0.05 0.03 0.05 -0.08 -0.04 -0.11

12 1 0.10 -0.01 -0.08 -0.04 0.14 -0.04 -0.17 0.01 0.16

13 1 -0.12 -0.03 -0.10 -0.02 0.01 -0.05 0.10 0.03 0.08

14 1 -0.12 0.03 -0.10 0.02 0.01 0.05 -0.10 0.03 -0.08

15 8 -0.24 0.00 0.16 0.00 -0.06 0.00 0.00 -0.02 0.00

16 6 -0.16 -0.02 0.10 0.21 0.02 0.29 0.00 0.01 0.04

17 6 -0.16 0.02 0.10 -0.21 0.02 -0.29 0.00 0.01 -0.04

18 6 -0.13 -0.01 0.12 0.14 -0.07 0.26 0.01 -0.02 0.04

19 8 0.31 0.28 -0.25 0.02 0.01 -0.15 0.02 0.01 -0.03

20 6 -0.13 0.01 0.12 -0.14 -0.07 -0.26 -0.01 -0.02 -0.04

21 8 0.31 -0.28 -0.25 -0.02 0.01 0.15 -0.02 0.01 0.03

22 1 -0.20 0.02 0.12 0.10 0.17 0.34 0.02 0.07 0.09

23 1 -0.20 -0.02 0.12 -0.10 0.17 -0.34 -0.02 0.07 -0.09

13 14 15

A A A

Frequencies -- 554.9269 581.9230 601.5152

Red. masses -- 6.2299 5.5740 5.5633

Frc consts -- 1.1303 1.1121 1.1860

IR Inten -- 17.4634 0.4705 1.3391

Atom AN X Y Z X Y Z X Y Z

1 6 0.05 -0.02 0.00 -0.12 0.18 0.16 0.14 0.02 -0.16

2 6 0.01 0.00 -0.03 -0.10 0.07 0.12 0.03 0.31 0.04

3 6 -0.01 0.00 0.03 0.10 0.07 -0.12 0.03 -0.31 0.04

4 6 -0.05 -0.02 0.00 0.12 0.18 -0.16 0.14 -0.02 -0.16

5 1 0.15 0.00 0.08 -0.19 0.03 0.21 -0.03 -0.19 -0.13

6 1 -0.15 0.00 -0.08 0.19 0.03 -0.21 -0.03 0.19 -0.13

7 6 0.02 0.05 -0.05 -0.05 -0.21 0.21 -0.05 0.03 0.18

8 1 0.03 0.02 -0.04 -0.02 -0.19 0.32 -0.12 -0.02 -0.08

9 1 0.05 0.05 -0.07 0.01 -0.14 0.19 -0.22 -0.13 0.24

10 6 -0.02 0.05 0.05 0.05 -0.21 -0.21 -0.05 -0.03 0.18

11 1 -0.03 0.02 0.04 0.02 -0.19 -0.32 -0.12 0.02 -0.08

12 1 -0.05 0.05 0.07 -0.01 -0.14 -0.19 -0.22 0.13 0.24

13 1 -0.01 -0.01 -0.02 -0.01 0.07 0.10 0.03 -0.30 0.06

14 1 0.01 -0.01 0.02 0.01 0.07 -0.10 0.03 0.30 0.06

15 8 0.00 0.20 0.00 0.00 0.02 0.00 0.02 0.00 0.07

16 6 0.19 -0.14 -0.01 0.06 -0.01 0.02 -0.04 0.01 -0.04

17 6 -0.19 -0.14 0.01 -0.06 -0.01 -0.02 -0.04 -0.01 -0.04

18 6 0.23 0.13 -0.06 0.07 0.01 0.03 -0.09 0.00 -0.09

19 8 -0.18 -0.10 0.10 -0.02 -0.02 0.00 0.02 0.01 0.02

20 6 -0.23 0.13 0.06 -0.07 0.01 -0.03 -0.09 0.00 -0.09

21 8 0.18 -0.10 -0.10 0.02 -0.02 0.00 0.02 -0.01 0.02

22 1 0.35 -0.34 -0.10 0.04 -0.03 0.00 -0.03 0.00 -0.04

23 1 -0.35 -0.34 0.10 -0.04 -0.03 0.00 -0.03 0.00 -0.04

16 17 18

A A A

Frequencies -- 674.2543 698.0824 734.5366

Red. masses -- 6.7827 12.1770 6.0660

Frc consts -- 1.8168 3.4963 1.9283

IR Inten -- 9.2628 0.8763 4.8235

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 0.01 0.03 0.01 0.00 0.00 -0.01 0.00 -0.01

2 6 0.02 -0.13 0.02 0.01 0.02 0.00 -0.04 0.00 -0.02

3 6 0.02 0.13 0.02 0.01 -0.02 0.00 0.04 0.00 0.02

4 6 -0.05 -0.01 0.03 0.01 0.00 0.00 0.01 0.00 0.01

5 1 0.07 0.06 0.07 0.02 -0.01 0.01 -0.03 0.00 -0.03

6 1 0.07 -0.06 0.07 0.02 0.01 0.01 0.03 0.00 0.03

7 6 0.06 -0.01 -0.04 0.00 0.00 0.01 0.01 0.00 -0.01

8 1 -0.02 0.09 -0.14 0.00 0.00 0.00 0.01 -0.01 -0.01

9 1 -0.05 -0.02 0.04 -0.01 0.00 0.01 0.04 0.00 -0.04

10 6 0.06 0.01 -0.04 0.00 0.00 0.01 -0.01 0.00 0.01

11 1 -0.02 -0.09 -0.14 0.00 0.00 0.00 -0.01 -0.01 0.01

12 1 -0.05 0.02 0.04 -0.01 0.00 0.01 -0.04 0.00 0.04

13 1 0.23 0.17 0.13 0.01 -0.02 -0.01 -0.12 -0.04 -0.10

14 1 0.23 -0.17 0.13 0.01 0.02 -0.01 0.12 -0.04 0.10

15 8 0.13 0.00 0.16 0.31 0.00 -0.27 0.00 0.03 0.00

16 6 0.05 0.03 0.09 -0.11 0.03 0.05 -0.23 -0.20 -0.07

17 6 0.05 -0.03 0.09 -0.11 -0.03 0.05 0.23 -0.20 0.07

18 6 -0.27 0.03 -0.32 0.05 0.39 0.04 0.09 0.06 0.30

19 8 0.05 0.05 0.08 -0.13 0.37 0.07 -0.09 0.11 -0.02

20 6 -0.27 -0.03 -0.33 0.05 -0.39 0.05 -0.09 0.06 -0.30

21 8 0.05 -0.05 0.08 -0.13 -0.38 0.07 0.09 0.11 0.02

22 1 0.29 -0.08 0.12 0.01 -0.25 -0.13 -0.42 -0.22 -0.16

23 1 0.29 0.08 0.12 0.01 0.25 -0.13 0.42 -0.22 0.16

19 20 21

A A A

Frequencies -- 771.5411 802.3597 819.7415

Red. masses -- 5.8252 1.1456 1.2141

Frc consts -- 2.0431 0.4345 0.4807

IR Inten -- 7.5716 72.0784 0.3795

Atom AN X Y Z X Y Z X Y Z

1 6 0.04 -0.03 -0.02 -0.04 0.01 -0.05 0.01 -0.01 -0.01

2 6 0.02 0.03 0.00 0.01 -0.01 0.01 0.01 0.03 0.00

3 6 -0.02 0.03 0.00 0.01 0.01 0.01 0.01 -0.03 0.00

4 6 -0.04 -0.03 0.02 -0.04 -0.01 -0.05 0.01 0.01 -0.01

5 1 -0.01 -0.01 -0.07 0.33 -0.06 0.32 -0.05 -0.02 -0.04

6 1 0.01 -0.01 0.07 0.33 0.06 0.32 -0.05 0.03 -0.04

7 6 0.02 -0.01 0.00 -0.01 0.01 0.02 -0.08 0.00 -0.02

8 1 -0.01 -0.03 -0.10 0.03 -0.04 0.08 0.15 -0.27 0.31

9 1 -0.05 -0.02 0.06 0.06 0.03 -0.03 0.32 0.26 -0.24

10 6 -0.02 -0.01 0.00 -0.01 -0.01 0.02 -0.08 0.00 -0.02

11 1 0.01 -0.03 0.10 0.03 0.04 0.08 0.15 0.27 0.31

12 1 0.05 -0.02 -0.06 0.06 -0.03 -0.03 0.32 -0.26 -0.24

13 1 0.19 0.06 0.10 0.40 0.09 0.26 0.03 -0.03 0.01

14 1 -0.19 0.06 -0.10 0.40 -0.09 0.26 0.03 0.03 0.01

15 8 0.00 -0.02 0.00 -0.01 0.00 0.00 0.01 0.00 0.00

16 6 -0.02 0.24 -0.23 -0.02 0.01 -0.03 0.01 -0.01 0.02

17 6 0.02 0.24 0.23 -0.02 -0.01 -0.03 0.01 0.01 0.02

18 6 0.25 -0.05 0.08 0.01 0.00 0.01 -0.01 0.00 -0.01

19 8 0.03 -0.13 -0.08 0.00 0.00 0.00 0.00 0.00 0.00

20 6 -0.25 -0.05 -0.08 0.01 0.00 0.01 -0.01 0.00 -0.01

21 8 -0.03 -0.13 0.08 0.00 0.00 0.00 0.00 0.00 0.00

22 1 -0.24 0.22 -0.34 -0.14 0.00 -0.09 0.22 0.04 0.16

23 1 0.24 0.22 0.34 -0.14 0.00 -0.09 0.22 -0.04 0.16

22 23 24

A A A

Frequencies -- 877.5895 891.9282 971.0814

Red. masses -- 1.5091 1.1532 1.4851

Frc consts -- 0.6848 0.5405 0.8251

IR Inten -- 1.2848 13.6354 1.0160

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 0.04 0.02 0.05 0.01 0.04 0.00 0.03 0.09

2 6 -0.03 -0.08 -0.01 0.01 -0.02 0.01 0.01 -0.05 0.01

3 6 0.03 -0.08 0.01 0.01 0.02 0.01 -0.01 -0.05 -0.01

4 6 0.08 0.04 -0.02 0.05 -0.01 0.04 0.00 0.03 -0.09

5 1 0.05 0.01 0.15 -0.29 0.06 -0.28 -0.25 0.03 -0.13

6 1 -0.05 0.01 -0.15 -0.29 -0.06 -0.28 0.25 0.03 0.13

7 6 -0.03 0.02 -0.06 -0.02 -0.01 0.00 -0.02 0.02 -0.07

8 1 0.03 0.03 0.11 0.04 -0.08 0.07 0.02 0.02 0.05

9 1 0.14 0.03 -0.19 0.06 0.09 -0.02 0.11 0.00 -0.18

10 6 0.03 0.02 0.06 -0.02 0.01 0.00 0.02 0.02 0.07

11 1 -0.03 0.03 -0.11 0.04 0.08 0.07 -0.02 0.02 -0.05

12 1 -0.14 0.03 0.19 0.06 -0.09 -0.02 -0.11 0.00 0.18

13 1 -0.51 -0.18 -0.28 0.24 0.06 0.09 0.18 -0.01 0.15

14 1 0.51 -0.18 0.28 0.24 -0.06 0.09 -0.18 -0.01 -0.15

15 8 0.00 0.00 0.00 -0.01 0.00 0.01 0.00 0.00 0.00

16 6 0.00 0.04 -0.02 0.00 0.02 -0.01 0.06 0.01 0.02

17 6 0.00 0.04 0.02 0.00 -0.02 -0.01 -0.06 0.01 -0.02

18 6 0.02 0.00 0.00 -0.02 0.00 -0.01 -0.02 0.00 -0.01

19 8 0.01 -0.01 -0.01 0.00 0.00 0.00 0.00 0.01 0.00

20 6 -0.02 0.00 0.00 -0.02 0.00 -0.01 0.02 0.00 0.00

21 8 -0.01 -0.01 0.01 0.00 0.00 0.00 0.00 0.01 0.00

22 1 0.02 0.07 0.02 -0.38 -0.09 -0.28 -0.41 -0.16 -0.32

23 1 -0.02 0.07 -0.02 -0.38 0.09 -0.28 0.41 -0.16 0.32

25 26 27

A A A

Frequencies -- 976.7536 984.8532 996.8604

Red. masses -- 1.3221 1.4604 2.0542

Frc consts -- 0.7432 0.8346 1.2027

IR Inten -- 0.0539 2.7344 0.1073

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.01 -0.05 -0.10 0.01 -0.09 0.07 -0.07 -0.07

2 6 0.07 -0.04 0.03 0.01 -0.01 0.01 -0.02 0.14 -0.01

3 6 0.07 0.04 0.03 -0.01 -0.01 -0.01 0.02 0.14 0.01

4 6 -0.02 0.00 -0.05 0.10 0.01 0.09 -0.07 -0.07 0.07

5 1 0.20 0.00 0.14 0.41 -0.04 0.39 -0.02 -0.11 -0.11

6 1 0.20 0.00 0.13 -0.41 -0.04 -0.39 0.02 -0.11 0.11

7 6 -0.03 -0.03 0.03 0.01 0.00 0.00 -0.06 -0.05 0.03

8 1 0.04 -0.17 0.05 0.00 0.00 -0.04 0.02 -0.11 0.18

9 1 0.03 0.15 0.06 -0.03 -0.01 0.04 0.08 -0.14 -0.13

10 6 -0.03 0.03 0.03 -0.01 0.00 0.00 0.06 -0.05 -0.03

11 1 0.04 0.17 0.05 0.00 0.00 0.04 -0.02 -0.11 -0.18

12 1 0.03 -0.15 0.06 0.03 0.00 -0.04 -0.08 -0.14 0.13

13 1 -0.37 -0.05 -0.28 0.15 0.03 0.07 -0.34 0.05 -0.28

14 1 -0.37 0.05 -0.28 -0.15 0.03 -0.07 0.34 0.05 0.28

15 8 0.01 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

16 6 0.01 0.00 0.03 0.04 0.00 0.01 0.05 0.01 0.04

17 6 0.01 0.00 0.03 -0.04 0.00 -0.01 -0.05 0.01 -0.04

18 6 -0.01 0.00 -0.02 -0.02 0.00 0.00 -0.01 0.00 -0.01

19 8 0.01 -0.01 0.00 0.00 0.01 0.00 0.00 0.00 0.00

20 6 -0.01 0.00 -0.02 0.02 0.00 0.00 0.01 0.00 0.01

21 8 0.01 0.01 0.00 0.00 0.01 0.00 0.00 0.00 0.00

22 1 -0.26 -0.17 -0.23 -0.24 -0.13 -0.22 -0.28 -0.11 -0.22

23 1 -0.26 0.17 -0.23 0.24 -0.13 0.22 0.29 -0.11 0.22

28 29 30

A A A

Frequencies -- 1059.1181 1063.8518 1068.9476

Red. masses -- 1.6384 2.0732 2.1186

Frc consts -- 1.0828 1.3824 1.4263

IR Inten -- 0.0551 1.9108 19.0594

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 0.00 0.05 -0.01 -0.02 0.02 0.00 0.00 -0.02

2 6 -0.06 0.03 -0.03 0.01 0.06 0.07 0.01 -0.02 0.00

3 6 0.06 0.03 0.03 0.01 -0.06 0.07 -0.01 -0.02 0.00

4 6 0.02 0.00 -0.05 -0.01 0.02 0.02 0.00 0.00 0.02

5 1 -0.13 -0.15 0.07 -0.06 -0.16 0.09 0.08 0.08 -0.02

6 1 0.13 -0.15 -0.07 -0.06 0.16 0.09 -0.08 0.08 0.02

7 6 0.13 0.00 -0.02 0.03 0.14 -0.12 -0.03 0.00 0.02

8 1 0.01 -0.11 -0.45 0.01 0.18 -0.08 -0.01 0.07 0.14

9 1 -0.21 -0.04 0.24 0.04 0.18 -0.08 0.03 0.03 -0.02

10 6 -0.13 0.00 0.02 0.03 -0.14 -0.12 0.03 0.00 -0.02

11 1 -0.01 -0.11 0.45 0.01 -0.18 -0.08 0.01 0.07 -0.14

12 1 0.21 -0.05 -0.24 0.04 -0.18 -0.08 -0.03 0.04 0.02

13 1 -0.17 -0.03 -0.17 -0.30 -0.08 0.41 0.06 0.00 0.06

14 1 0.16 -0.03 0.17 -0.31 0.08 0.41 -0.06 0.00 -0.06

15 8 0.00 0.03 0.00 0.01 0.00 -0.01 0.00 0.18 0.00

16 6 0.00 0.00 0.04 -0.01 -0.01 0.03 -0.08 -0.03 0.08

17 6 0.00 0.00 -0.04 -0.01 0.01 0.04 0.08 -0.03 -0.08

18 6 0.00 0.00 -0.03 0.00 -0.01 -0.01 0.03 -0.03 -0.05

19 8 0.00 -0.01 0.00 0.01 -0.02 0.00 0.01 -0.07 0.00

20 6 0.00 0.00 0.02 0.00 0.01 -0.01 -0.03 -0.03 0.05

21 8 0.00 -0.01 0.00 0.01 0.02 0.00 -0.01 -0.07 0.00

22 1 -0.22 0.03 -0.04 -0.12 -0.17 -0.15 -0.46 0.38 0.23

23 1 0.22 0.03 0.04 -0.12 0.17 -0.15 0.46 0.38 -0.23

31 32 33

A A A

Frequencies -- 1095.9626 1099.4950 1101.8482

Red. masses -- 1.1778 5.0562 1.6994

Frc consts -- 0.8335 3.6013 1.2156

IR Inten -- 3.1741 2.8968 9.3795

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.01 0.00 0.00 0.02 0.05 0.00 -0.01

2 6 0.01 -0.01 0.02 -0.01 0.02 -0.02 -0.06 -0.08 -0.08

3 6 0.01 0.01 0.02 -0.01 -0.02 -0.02 0.06 -0.08 0.08

4 6 0.00 0.00 -0.01 0.00 0.00 0.02 -0.05 0.00 0.01

5 1 0.01 0.00 0.01 -0.02 0.02 -0.01 0.15 0.36 -0.20

6 1 0.01 0.00 0.01 -0.01 -0.03 -0.02 -0.15 0.36 0.20

7 6 0.00 0.02 -0.01 0.00 -0.02 0.01 0.02 0.01 0.10

8 1 0.02 -0.03 -0.03 -0.01 0.00 0.00 -0.07 0.26 0.12

9 1 -0.01 0.11 0.05 0.00 -0.10 -0.04 -0.12 0.17 0.27

10 6 0.00 -0.02 -0.01 0.00 0.02 0.01 -0.02 0.01 -0.10

11 1 0.02 0.03 -0.03 -0.01 0.00 0.01 0.07 0.26 -0.12

12 1 -0.01 -0.11 0.05 0.00 0.10 -0.04 0.12 0.17 -0.27

13 1 -0.13 -0.01 0.04 0.15 0.00 -0.08 -0.15 -0.11 0.02

14 1 -0.13 0.01 0.04 0.15 0.00 -0.08 0.15 -0.11 -0.02

15 8 0.02 0.00 -0.01 0.23 0.00 -0.17 0.00 -0.03 0.00

16 6 0.05 0.03 -0.03 -0.23 -0.01 0.19 0.03 0.02 0.01

17 6 0.05 -0.03 -0.03 -0.23 0.01 0.19 -0.04 0.02 -0.01

18 6 -0.03 0.00 0.00 0.01 -0.07 -0.04 0.00 0.01 0.00

19 8 -0.01 0.03 0.01 0.06 -0.13 -0.04 0.00 0.01 0.00

20 6 -0.03 0.00 0.00 0.01 0.07 -0.04 0.00 0.01 0.00

21 8 -0.01 -0.03 0.01 0.06 0.13 -0.04 0.00 0.01 0.00

22 1 -0.32 0.56 0.22 -0.36 0.23 0.33 -0.12 -0.09 -0.14

23 1 -0.32 -0.56 0.22 -0.37 -0.23 0.33 0.11 -0.09 0.14

34 35 36

A A A

Frequencies -- 1160.6073 1167.4946 1182.3614

Red. masses -- 1.1602 1.1565 1.2251

Frc consts -- 0.9208 0.9287 1.0091

IR Inten -- 1.3454 3.2338 0.6739

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 0.03 0.03 0.00 -0.01 0.00 0.04 -0.02 -0.03

2 6 -0.03 0.03 -0.01 -0.01 0.00 -0.01 -0.02 -0.04 -0.04

3 6 -0.03 -0.03 -0.01 0.01 0.00 0.01 -0.02 0.04 -0.04

4 6 -0.03 -0.03 0.03 0.00 -0.01 0.00 0.04 0.02 -0.03

5 1 -0.03 0.01 0.04 -0.01 -0.03 0.01 0.21 0.41 -0.22

6 1 -0.03 -0.01 0.04 0.01 -0.03 -0.01 0.21 -0.41 -0.22

7 6 0.05 0.00 -0.02 -0.08 0.00 -0.02 -0.01 0.02 0.05

8 1 0.09 -0.35 -0.30 0.07 -0.41 -0.08 0.02 -0.08 0.01

9 1 -0.09 0.38 0.29 -0.02 0.51 0.17 -0.05 0.10 0.12

10 6 0.05 0.00 -0.02 0.08 0.00 0.02 -0.01 -0.02 0.05

11 1 0.09 0.35 -0.30 -0.07 -0.41 0.08 0.02 0.08 0.01

12 1 -0.09 -0.39 0.29 0.01 0.51 -0.17 -0.05 -0.10 0.12

13 1 0.12 -0.02 -0.08 -0.06 0.00 0.12 -0.20 0.06 0.38

14 1 0.12 0.02 -0.08 0.06 0.00 -0.12 -0.20 -0.05 0.38

15 8 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 -0.01

16 6 -0.02 0.01 0.00 0.00 0.00 0.00 -0.02 0.01 0.00

17 6 -0.02 -0.01 0.00 0.00 0.00 0.00 -0.02 -0.01 0.00

18 6 0.01 0.00 0.01 0.00 0.01 0.00 0.00 0.00 0.00

19 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.01 0.00

20 6 0.01 0.00 0.01 0.00 0.01 0.00 0.00 0.00 0.00

21 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.00

22 1 0.09 -0.03 0.01 -0.02 0.00 -0.01 0.08 -0.03 0.02

23 1 0.09 0.03 0.01 0.02 0.00 0.01 0.08 0.03 0.02

37 38 39

A A A

Frequencies -- 1198.6640 1203.1012 1208.2204

Red. masses -- 1.4820 1.5010 2.0192

Frc consts -- 1.2546 1.2800 1.7367

IR Inten -- 92.7168 0.8605 162.0278

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.02 -0.01 -0.07 0.05 0.04 0.00 0.01 0.01

2 6 0.01 0.01 -0.02 0.03 0.09 0.02 -0.02 -0.01 0.01

3 6 -0.01 0.01 0.02 0.03 -0.09 0.02 0.02 -0.01 -0.01

4 6 0.00 -0.01 0.01 -0.07 -0.05 0.04 0.00 0.01 -0.01

5 1 -0.11 -0.27 0.09 0.21 0.55 -0.10 0.10 0.25 -0.09

6 1 0.11 -0.27 -0.09 0.21 -0.55 -0.10 -0.10 0.26 0.09

7 6 0.01 0.01 0.01 0.00 0.04 -0.03 -0.01 -0.01 -0.01

8 1 -0.03 0.18 0.06 -0.01 0.06 -0.04 0.04 -0.19 -0.07

9 1 -0.01 0.04 0.04 0.07 -0.10 -0.15 -0.01 0.02 0.01

10 6 -0.01 0.01 -0.01 0.00 -0.04 -0.03 0.01 -0.01 0.01

11 1 0.03 0.18 -0.06 -0.01 -0.06 -0.04 -0.04 -0.19 0.07

12 1 0.01 0.04 -0.04 0.07 0.10 -0.15 0.01 0.02 -0.01

13 1 -0.31 0.01 0.47 0.11 -0.10 -0.21 0.25 -0.01 -0.42

14 1 0.31 0.01 -0.47 0.11 0.10 -0.22 -0.25 -0.01 0.42

15 8 0.00 0.12 0.00 0.00 0.00 0.01 0.00 0.18 0.00

16 6 0.01 0.02 -0.02 0.02 -0.01 0.00 0.01 0.03 -0.02

17 6 -0.01 0.02 0.02 0.02 0.01 0.00 -0.01 0.03 0.02

18 6 -0.05 -0.07 0.05 0.00 0.00 0.00 -0.08 -0.10 0.07

19 8 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 -0.03 0.00

20 6 0.05 -0.07 -0.05 0.00 0.00 0.00 0.08 -0.10 -0.07

21 8 0.00 -0.02 0.00 0.00 -0.01 0.00 0.00 -0.03 0.00

22 1 0.11 -0.12 -0.08 -0.07 0.01 -0.03 0.21 -0.21 -0.11

23 1 -0.11 -0.12 0.08 -0.07 -0.01 -0.03 -0.21 -0.21 0.11

40 41 42

A A A

Frequencies -- 1242.7464 1303.9045 1335.8885

Red. masses -- 1.1072 2.6330 1.3207

Frc consts -- 1.0075 2.6375 1.3887

IR Inten -- 3.2021 0.0524 0.0014

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.01 -0.02 0.00 -0.01 0.00 -0.03 -0.06 0.02

2 6 -0.01 -0.02 0.00 -0.01 0.01 0.00 -0.04 0.02 0.07

3 6 -0.01 0.02 0.00 0.01 0.01 0.00 0.04 0.02 -0.07

4 6 0.02 -0.01 -0.02 0.00 -0.01 0.00 0.03 -0.06 -0.02

5 1 0.03 0.04 -0.04 0.03 0.07 -0.02 0.18 0.39 -0.14

6 1 0.03 -0.04 -0.04 -0.03 0.07 0.02 -0.18 0.39 0.14

7 6 0.00 0.05 0.00 0.00 0.01 0.00 0.01 0.05 0.01

8 1 -0.06 0.40 0.28 0.01 -0.05 -0.02 0.05 -0.23 -0.16

9 1 -0.07 0.36 0.22 -0.02 -0.03 0.00 0.02 -0.22 -0.12

10 6 0.00 -0.05 0.00 0.00 0.01 0.00 -0.01 0.05 -0.01

11 1 -0.06 -0.40 0.28 -0.01 -0.05 0.02 -0.05 -0.23 0.16

12 1 -0.07 -0.36 0.22 0.02 -0.03 0.00 -0.02 -0.22 0.12

13 1 0.12 0.01 -0.23 -0.03 0.00 0.00 -0.20 0.02 0.31

14 1 0.12 -0.01 -0.23 0.03 0.00 0.00 0.20 0.02 -0.31

15 8 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00

16 6 -0.01 0.01 0.00 0.17 -0.09 -0.16 -0.01 0.00 0.01

17 6 -0.01 -0.01 0.00 -0.17 -0.09 0.16 0.01 0.00 -0.01

18 6 0.00 0.00 0.00 -0.07 -0.03 0.05 0.00 0.00 0.00

19 8 0.00 0.00 0.00 -0.02 0.05 0.02 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.07 -0.03 -0.05 0.00 0.00 0.00

21 8 0.00 0.00 0.00 0.02 0.05 -0.02 0.00 0.00 0.00

22 1 0.05 0.00 0.02 -0.21 0.57 0.21 0.02 -0.03 0.00

23 1 0.05 0.00 0.02 0.21 0.57 -0.21 -0.02 -0.03 0.00

43 44 45

A A A

Frequencies -- 1391.4569 1401.5190 1409.4276

Red. masses -- 8.1527 1.1166 3.5012

Frc consts -- 9.3001 1.2922 4.0979

IR Inten -- 220.4932 5.3804 1.5336

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.00 0.00 0.01 0.01 0.00 0.02 -0.03 -0.01

2 6 0.01 0.00 -0.01 0.00 -0.02 -0.02 -0.01 -0.09 -0.04

3 6 0.01 0.00 -0.01 0.00 -0.02 0.02 -0.01 0.09 -0.04

4 6 -0.01 0.00 0.00 -0.01 0.01 0.00 0.02 0.03 -0.01

5 1 0.00 0.00 0.02 -0.03 -0.06 0.02 -0.04 -0.11 -0.01

6 1 0.00 0.00 0.02 0.03 -0.06 -0.02 -0.04 0.11 -0.01

7 6 0.00 0.02 -0.01 0.01 0.06 -0.03 -0.03 0.29 0.12

8 1 0.06 -0.04 0.13 0.23 -0.24 0.40 0.05 -0.27 -0.27

9 1 -0.10 -0.08 0.05 -0.35 -0.25 0.19 0.07 -0.19 -0.19

10 6 0.00 -0.02 -0.01 -0.01 0.06 0.03 -0.03 -0.29 0.12

11 1 0.06 0.04 0.13 -0.23 -0.24 -0.39 0.05 0.27 -0.27

12 1 -0.10 0.08 0.05 0.35 -0.25 -0.19 0.08 0.18 -0.19

13 1 0.01 -0.01 -0.02 0.00 -0.02 0.01 0.14 0.07 -0.35

14 1 0.01 0.01 -0.02 0.00 -0.02 -0.01 0.14 -0.07 -0.35

15 8 0.26 0.00 -0.20 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.11 -0.02 -0.09 0.00 0.00 0.00 0.00 0.00 0.00

17 6 0.11 0.02 -0.09 0.00 0.00 0.00 0.00 0.00 0.00

18 6 -0.33 -0.22 0.26 0.00 0.00 0.00 0.00 0.00 0.00

19 8 0.02 0.03 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

20 6 -0.33 0.22 0.26 0.00 0.00 0.00 0.00 0.00 0.00

21 8 0.02 -0.03 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

22 1 0.23 -0.25 -0.20 0.00 -0.01 0.00 0.01 0.01 0.02

23 1 0.23 0.25 -0.20 0.00 -0.01 0.00 0.01 -0.01 0.02

46 47 48

A A A

Frequencies -- 1415.1728 1442.3944 1470.6939

Red. masses -- 1.1213 2.2880 6.0518

Frc consts -- 1.3231 2.8046 7.7123

IR Inten -- 3.2308 2.8778 95.5692

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.01 0.01 0.03 0.05 -0.02 0.07 0.15 -0.06

2 6 0.00 0.01 0.00 0.02 -0.08 -0.08 -0.02 -0.06 0.18

3 6 0.00 -0.01 0.00 -0.02 -0.08 0.08 -0.02 0.06 0.18

4 6 -0.01 -0.01 0.01 -0.03 0.05 0.02 0.07 -0.15 -0.06

5 1 -0.01 0.00 0.01 -0.11 -0.23 0.07 -0.01 0.06 -0.06

6 1 -0.01 0.00 0.01 0.11 -0.23 -0.07 -0.01 -0.06 -0.06

7 6 0.01 0.04 -0.05 -0.05 0.10 0.17 0.00 0.01 -0.06

8 1 0.23 -0.23 0.40 -0.02 -0.33 -0.32 0.02 -0.11 -0.08

9 1 -0.35 -0.25 0.19 0.15 -0.28 -0.23 0.04 -0.19 -0.17

10 6 0.01 -0.04 -0.05 0.05 0.10 -0.17 0.00 -0.01 -0.06

11 1 0.23 0.24 0.40 0.02 -0.33 0.32 0.02 0.11 -0.08

12 1 -0.35 0.25 0.19 -0.15 -0.28 0.23 0.04 0.19 -0.17

13 1 0.00 -0.01 -0.01 0.05 -0.07 -0.02 -0.13 0.01 -0.11

14 1 0.00 0.01 -0.01 -0.05 -0.07 0.02 -0.13 -0.01 -0.11

15 8 -0.01 0.00 0.01 0.00 0.00 0.00 -0.01 0.00 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.10 0.38 -0.03

17 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.10 -0.38 -0.03

18 6 0.01 0.01 -0.01 0.00 0.00 0.00 0.01 -0.03 0.03

19 8 0.00 0.00 0.00 0.00 0.00 0.00 0.01 -0.01 -0.01

20 6 0.01 -0.01 -0.01 0.00 0.00 0.00 0.01 0.03 0.03

21 8 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.01 -0.01

22 1 -0.02 0.01 0.01 -0.02 0.00 -0.01 0.37 0.07 -0.07

23 1 -0.02 -0.01 0.01 0.02 0.00 0.01 0.37 -0.07 -0.07

49 50 51

A A A

Frequencies -- 1544.1423 1665.7189 1691.7261

Red. masses -- 4.5789 9.5866 8.3907

Frc consts -- 6.4326 15.6718 14.1484

IR Inten -- 1.9036 14.3438 17.1347

Atom AN X Y Z X Y Z X Y Z

1 6 -0.09 0.23 0.08 0.14 0.44 -0.12 -0.25 -0.19 0.23

2 6 0.17 0.01 -0.22 -0.11 -0.12 0.16 0.26 0.13 -0.31

3 6 0.17 -0.01 -0.22 -0.11 0.13 0.17 -0.26 0.13 0.31

4 6 -0.09 -0.23 0.08 0.14 -0.44 -0.12 0.25 -0.19 -0.23

5 1 -0.26 -0.15 0.23 -0.08 0.02 0.00 0.02 0.31 0.03

6 1 -0.26 0.15 0.23 -0.08 -0.02 0.00 -0.02 0.31 -0.03

7 6 -0.03 0.03 0.08 0.00 0.02 -0.02 -0.03 0.01 0.08

8 1 -0.03 0.12 0.13 -0.01 -0.08 -0.11 0.01 0.05 0.15

9 1 0.00 0.08 0.05 0.04 -0.08 -0.08 -0.03 0.01 0.04

10 6 -0.03 -0.03 0.08 0.00 -0.02 -0.03 0.03 0.01 -0.08

11 1 -0.03 -0.12 0.13 -0.01 0.08 -0.11 -0.01 0.05 -0.15

12 1 0.00 -0.08 0.05 0.04 0.08 -0.08 0.03 0.01 -0.04

13 1 -0.25 -0.05 0.29 -0.10 0.10 0.08 0.04 0.15 -0.13

14 1 -0.25 0.05 0.29 -0.10 -0.10 0.08 -0.04 0.15 0.13

15 8 0.00 0.00 0.00 0.01 0.00 -0.01 0.00 0.00 0.00

16 6 -0.01 0.07 0.00 -0.01 -0.33 -0.03 -0.01 0.00 -0.01

17 6 -0.01 -0.07 0.00 -0.01 0.33 -0.03 0.01 -0.01 0.01

18 6 0.00 0.00 0.00 0.01 0.01 0.00 0.01 0.00 0.00

19 8 0.00 0.00 0.00 -0.01 0.01 0.01 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.01 -0.01 0.00 -0.01 0.00 0.00

21 8 0.00 0.00 0.00 -0.01 -0.01 0.01 0.00 0.00 0.00

22 1 0.07 0.02 -0.01 -0.09 -0.05 0.18 -0.01 0.00 0.00

23 1 0.07 -0.02 -0.01 -0.09 0.05 0.18 0.01 0.00 0.00

52 53 54

A A A

Frequencies -- 2098.6266 2176.0039 2980.7336

Red. masses -- 13.1567 12.8712 1.0869

Frc consts -- 34.1403 35.9077 5.6898

IR Inten -- 632.3679 202.3611 0.0433

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00

3 6 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00

4 6 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00

5 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

6 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.06 0.00 -0.02

8 1 -0.01 0.00 0.01 -0.01 0.01 0.00 0.40 0.16 -0.14

9 1 0.00 0.00 0.01 0.00 0.01 0.00 0.34 -0.18 0.38

10 6 0.00 0.00 0.00 0.00 0.00 0.00 0.06 0.00 0.02

11 1 0.01 0.00 -0.01 -0.01 -0.01 0.00 -0.40 0.16 0.14

12 1 0.00 0.00 -0.01 0.00 -0.01 0.00 -0.34 -0.18 -0.38

13 1 -0.01 -0.01 0.00 0.01 0.00 0.00 0.00 -0.01 0.00

14 1 0.01 -0.01 0.00 0.01 0.00 0.00 0.00 -0.01 0.00

15 8 0.00 0.01 0.00 0.01 0.00 -0.01 0.00 0.00 0.00

16 6 0.03 -0.04 -0.03 -0.05 -0.01 0.04 0.00 0.00 0.00

17 6 -0.03 -0.04 0.03 -0.05 0.01 0.04 0.00 0.00 0.00

18 6 -0.26 0.49 0.19 0.23 -0.53 -0.17 0.00 0.00 0.00

19 8 0.15 -0.34 -0.11 -0.14 0.31 0.10 0.00 0.00 0.00

20 6 0.26 0.49 -0.19 0.23 0.53 -0.17 0.00 0.00 0.00

21 8 -0.15 -0.34 0.11 -0.14 -0.31 0.10 0.00 0.00 0.00

22 1 0.00 0.02 0.03 -0.02 -0.07 0.04 0.00 0.00 0.00

23 1 0.00 0.02 -0.03 -0.02 0.07 0.04 0.00 0.00 0.00

55 56 57

A A A

Frequencies -- 3003.4072 3071.9639 3073.1999

Red. masses -- 1.0939 1.0479 1.0517

Frc consts -- 5.8138 5.8263 5.8521

IR Inten -- 17.0951 11.7100 4.7061

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

3 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

5 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

6 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 -0.06 0.00 -0.02 -0.02 -0.02 0.03 -0.01 -0.03 0.03

8 1 0.38 0.16 -0.14 0.50 0.18 -0.14 0.49 0.18 -0.13

9 1 0.34 -0.19 0.39 -0.30 0.13 -0.30 -0.31 0.14 -0.31

10 6 -0.06 0.00 -0.02 -0.02 0.02 0.03 0.01 -0.03 -0.03

11 1 0.38 -0.16 -0.14 0.50 -0.18 -0.13 -0.49 0.18 0.13

12 1 0.34 0.19 0.39 -0.30 -0.13 -0.30 0.31 0.14 0.31

13 1 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.00 0.00

14 1 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

15 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

17 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

21 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

22 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

23 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

58 59 60

A A A

Frequencies -- 3165.2461 3166.4121 3186.6356

Red. masses -- 1.0789 1.0780 1.0773

Frc consts -- 6.3686 6.3682 6.4457

IR Inten -- 57.6544 4.6878 32.5761

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.01 0.01 0.00 -0.01 0.03 -0.03 -0.04

2 6 -0.01 -0.05 0.00 0.01 0.05 0.00 0.00 -0.01 0.00

3 6 0.01 -0.06 0.00 0.01 -0.05 0.00 0.00 -0.01 0.00

4 6 0.00 0.00 -0.01 0.01 0.00 -0.01 -0.03 -0.03 0.04

5 1 0.06 -0.06 -0.07 -0.08 0.08 0.10 -0.39 0.35 0.45

6 1 -0.06 -0.06 0.07 -0.08 -0.08 0.10 0.39 0.35 -0.46

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 1 0.01 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00

9 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

10 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

11 1 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00

12 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 1 -0.10 0.69 -0.07 -0.10 0.67 -0.07 -0.02 0.11 -0.01

14 1 0.10 0.68 0.07 -0.10 -0.68 -0.07 0.02 0.10 0.01

15 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

17 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

21 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

22 1 -0.01 -0.01 0.01 -0.01 -0.01 0.01 0.00 0.00 0.00

23 1 0.01 -0.01 -0.01 -0.01 0.01 0.01 0.00 0.00 0.00

61 62 63

A A A

Frequencies -- 3196.8398 3224.4918 3230.5868

Red. masses -- 1.0863 1.0806 1.0871

Frc consts -- 6.5410 6.6196 6.6846

IR Inten -- 59.2204 46.3226 82.8142

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.03 -0.04 0.00 0.00 0.00 0.00 0.00 0.00

2 6 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00

3 6 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.03 0.03 -0.04 0.00 0.00 0.00 0.00 0.00 0.00

5 1 -0.39 0.35 0.46 0.00 0.00 0.00 0.01 -0.01 -0.01

6 1 -0.38 -0.35 0.45 0.00 0.00 0.00 0.01 0.01 -0.01

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 1 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

10 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

11 1 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

12 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 1 0.02 -0.14 0.01 0.00 -0.01 0.00 0.00 0.02 0.00

14 1 0.02 0.14 0.01 0.00 -0.01 0.00 0.00 -0.02 0.00

15 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.00 0.00 0.00 0.02 0.04 -0.04 -0.02 -0.04 0.04

17 6 0.00 0.00 0.00 -0.02 0.04 0.04 -0.02 0.04 0.04

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

21 8 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

22 1 0.01 0.02 -0.02 -0.24 -0.41 0.52 0.23 0.41 -0.52

23 1 0.01 -0.02 -0.02 0.24 -0.41 -0.52 0.23 -0.41 -0.52

-------------------

- Thermochemistry -

-------------------

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 6 and mass 12.00000

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 1 and mass 1.00783

Atom 6 has atomic number 1 and mass 1.00783

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 1 and mass 1.00783

Atom 9 has atomic number 1 and mass 1.00783

Atom 10 has atomic number 6 and mass 12.00000

Atom 11 has atomic number 1 and mass 1.00783

Atom 12 has atomic number 1 and mass 1.00783

Atom 13 has atomic number 1 and mass 1.00783

Atom 14 has atomic number 1 and mass 1.00783

Atom 15 has atomic number 8 and mass 15.99491

Atom 16 has atomic number 6 and mass 12.00000

Atom 17 has atomic number 6 and mass 12.00000

Atom 18 has atomic number 6 and mass 12.00000

Atom 19 has atomic number 8 and mass 15.99491

Atom 20 has atomic number 6 and mass 12.00000

Atom 21 has atomic number 8 and mass 15.99491

Atom 22 has atomic number 1 and mass 1.00783

Atom 23 has atomic number 1 and mass 1.00783

Molecular mass: 178.06299 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- 1479.213372048.923052672.14576

X 1.00000 0.00001 -0.00254

Y -0.00001 1.00000 0.00000

Z 0.00254 0.00000 1.00000

This molecule is an asymmetric top.

Rotational symmetry number 1.

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.05855 0.04227 0.03241

Rotational constants (GHZ): 1.22007 0.88082 0.67539

1 imaginary frequencies ignored.

Zero-point vibrational energy 486502.6 (Joules/Mol)

116.27691 (Kcal/Mol)

Warning -- explicit consideration of 14 degrees of freedom as

vibrations may cause significant error

Vibrational temperatures: 87.58 178.24 200.29 241.05 314.93

(Kelvin) 337.74 370.84 517.14 562.02 642.53

720.55 798.41 837.26 865.45 970.10

1004.38 1056.83 1110.07 1154.42 1179.42

1262.65 1283.28 1397.17 1405.33 1416.98

1434.26 1523.83 1530.64 1537.98 1576.84

1581.93 1585.31 1669.85 1679.76 1701.15

1724.61 1730.99 1738.36 1788.03 1876.03

1922.04 2001.99 2016.47 2027.85 2036.12

2075.28 2116.00 2221.67 2396.59 2434.01

3019.45 3130.78 4288.61 4321.23 4419.87

4421.64 4554.08 4555.76 4584.85 4599.53

4639.32 4648.09

Zero-point correction= 0.185299 (Hartree/Particle)

Thermal correction to Energy= 0.195300

Thermal correction to Enthalpy= 0.196244

Thermal correction to Gibbs Free Energy= 0.149536

Sum of electronic and zero-point Energies= 0.134879

Sum of electronic and thermal Energies= 0.144880

Sum of electronic and thermal Enthalpies= 0.145824

Sum of electronic and thermal Free Energies= 0.099116

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 122.553 39.242 98.306

Electronic 0.000 0.000 0.000

Translational 0.889 2.981 41.438

Rotational 0.889 2.981 30.472

Vibrational 120.775 33.280 26.396

Vibration 1 0.597 1.973 4.429

Vibration 2 0.610 1.929 3.039

Vibration 3 0.615 1.914 2.815

Vibration 4 0.624 1.882 2.463

Vibration 5 0.647 1.812 1.968

Vibration 6 0.655 1.788 1.842

Vibration 7 0.667 1.750 1.677

Vibration 8 0.734 1.556 1.125

Vibration 9 0.758 1.490 0.998

Vibration 10 0.806 1.368 0.806

Vibration 11 0.856 1.248 0.656

Vibration 12 0.910 1.129 0.534

Vibration 13 0.939 1.070 0.482

Vibration 14 0.960 1.029 0.447

Q Log10(Q) Ln(Q)

Total Bot 0.165351D-68 -68.781593 -158.375470

Total V=0 0.281754D+17 16.449870 37.877225

Vib (Bot) 0.173795D-82 -82.759963 -190.561858

Vib (Bot) 1 0.339214D+01 0.530474 1.221462

Vib (Bot) 2 0.164808D+01 0.216979 0.499613

Vib (Bot) 3 0.146095D+01 0.164637 0.379090

Vib (Bot) 4 0.120385D+01 0.080571 0.185523

Vib (Bot) 5 0.904099D+00 -0.043784 -0.100816

Vib (Bot) 6 0.837281D+00 -0.077129 -0.177596

Vib (Bot) 7 0.754398D+00 -0.122399 -0.281835

Vib (Bot) 8 0.510143D+00 -0.292308 -0.673064

Vib (Bot) 9 0.459400D+00 -0.337809 -0.777833

Vib (Bot) 10 0.385061D+00 -0.414471 -0.954354

Vib (Bot) 11 0.327940D+00 -0.484206 -1.114925

Vib (Bot) 12 0.281460D+00 -0.550584 -1.267767

Vib (Bot) 13 0.261355D+00 -0.582769 -1.341875

Vib (Bot) 14 0.247852D+00 -0.605807 -1.394922

Vib (V=0) 0.296142D+03 2.471499 5.690837

Vib (V=0) 1 0.392880D+01 0.594259 1.368333

Vib (V=0) 2 0.222226D+01 0.346795 0.798525

Vib (V=0) 3 0.204415D+01 0.310512 0.714980

Vib (V=0) 4 0.180355D+01 0.256129 0.589758

Vib (V=0) 5 0.153315D+01 0.185584 0.427323

Vib (V=0) 6 0.147521D+01 0.168855 0.388802

Vib (V=0) 7 0.140505D+01 0.147692 0.340073

Vib (V=0) 8 0.121431D+01 0.084331 0.194180

Vib (V=0) 9 0.117901D+01 0.071516 0.164671

Vib (V=0) 10 0.113109D+01 0.053496 0.123180

Vib (V=0) 11 0.109795D+01 0.040583 0.093445

Vib (V=0) 12 0.107378D+01 0.030914 0.071182

Vib (V=0) 13 0.106419D+01 0.027018 0.062211

Vib (V=0) 14 0.105806D+01 0.024510 0.056437

Electronic 0.100000D+01 0.000000 0.000000

Translational 0.933933D+08 7.970316 18.352330

Rotational 0.101872D+07 6.008055 13.834057

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000027224 0.000001919 0.000004435

2 6 0.000025947 0.000009671 0.000000860

3 6 0.000004297 -0.000033449 0.000030328

4 6 -0.000007314 0.000043002 -0.000001065

5 1 -0.000007043 -0.000004478 0.000002092

6 1 0.000007509 -0.000003461 -0.000005012

7 6 0.000006411 -0.000017664 -0.000006405

8 1 0.000002911 0.000007867 0.000009735

9 1 -0.000002271 0.000001589 -0.000000167

10 6 0.000002247 0.000006369 0.000003367

11 1 0.000001755 0.000003493 -0.000002125

12 1 -0.000001979 -0.000000924 -0.000000251

13 1 0.000000639 -0.000001327 -0.000004597

14 1 0.000006972 -0.000003402 -0.000004897

15 8 -0.000053343 0.000085030 -0.000005474

16 6 -0.000000174 0.000014442 -0.000021173

17 6 0.000056574 0.000017412 -0.000022193

18 6 0.000011853 -0.000052982 0.000024882

19 8 0.000012490 -0.000028260 -0.000007465

20 6 -0.000043770 -0.000021787 -0.000007533

21 8 0.000005125 -0.000018953 0.000011247

22 1 -0.000001663 -0.000005499 0.000001338

23 1 0.000000053 0.000001392 0.000000075

-------------------------------------------------------------------

Cartesian Forces: Max 0.000085030 RMS 0.000020412

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Internal Forces: Max 0.000070103 RMS 0.000010198

Search for a saddle point.

Step number 1 out of a maximum of 2

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swaping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- -0.06894 0.00192 0.00418 0.00811 0.00833

Eigenvalues --- 0.01158 0.01209 0.01268 0.01802 0.01814

Eigenvalues --- 0.02283 0.02495 0.02720 0.03329 0.03389

Eigenvalues --- 0.03488 0.03513 0.03670 0.03787 0.03817

Eigenvalues --- 0.03883 0.04445 0.04966 0.04988 0.06276

Eigenvalues --- 0.06517 0.07151 0.07720 0.07986 0.08412

Eigenvalues --- 0.09240 0.11053 0.11084 0.11590 0.12002

Eigenvalues --- 0.13308 0.14380 0.16819 0.17315 0.25811

Eigenvalues --- 0.30816 0.31428 0.31613 0.32106 0.33618

Eigenvalues --- 0.34299 0.35235 0.35280 0.35699 0.36326

Eigenvalues --- 0.37292 0.38078 0.38873 0.39480 0.40224

Eigenvalues --- 0.40625 0.43477 0.50258 0.53253 0.60939

Eigenvalues --- 0.67504 1.17543 1.18483

Eigenvectors required to have negative eigenvalues:

R6 R10 R19 D73 D71

1 -0.56844 -0.56829 0.14909 0.13628 -0.13624

R7 R1 R2 D1 D29

1 0.13101 0.13100 -0.12989 -0.11395 0.11392

Angle between quadratic step and forces= 75.91 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.00019781 RMS(Int)= 0.00000002

Iteration 2 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000001

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.63498 0.00004 0.00000 0.00001 0.00001 2.63499

R2 2.63944 0.00001 0.00000 0.00005 0.00005 2.63950

R3 2.07771 0.00001 0.00000 0.00002 0.00002 2.07773

R4 2.81525 -0.00001 0.00000 -0.00001 -0.00001 2.81524

R5 2.08294 0.00000 0.00000 0.00001 0.00001 2.08295

R6 4.10110 -0.00001 0.00000 0.00036 0.00036 4.10145

R7 2.63505 -0.00002 0.00000 -0.00006 -0.00006 2.63499

R8 2.81524 0.00000 0.00000 0.00001 0.00001 2.81524

R9 2.08294 0.00000 0.00000 0.00001 0.00001 2.08295

R10 4.10166 -0.00002 0.00000 -0.00021 -0.00021 4.10145

R11 2.07776 -0.00001 0.00000 -0.00003 -0.00003 2.07773

R12 2.12408 0.00000 0.00000 0.00001 0.00001 2.12409

R13 2.12816 0.00000 0.00000 -0.00001 -0.00001 2.12815

R14 2.87631 0.00000 0.00000 0.00001 0.00001 2.87632

R15 2.12408 0.00000 0.00000 0.00001 0.00001 2.12409

R16 2.12814 0.00000 0.00000 0.00001 0.00001 2.12815

R17 2.66398 -0.00007 0.00000 -0.00016 -0.00016 2.66382

R18 2.66371 0.00003 0.00000 0.00011 0.00011 2.66382

R19 2.66475 -0.00001 0.00000 -0.00003 -0.00003 2.66472

R20 2.81233 -0.00004 0.00000 -0.00006 -0.00006 2.81227

R21 2.06467 0.00000 0.00000 0.00000 0.00000 2.06467

R22 2.81240 -0.00004 0.00000 -0.00013 -0.00013 2.81227

R23 2.06467 0.00000 0.00000 0.00000 0.00000 2.06467

R24 2.30647 -0.00002 0.00000 0.00001 0.00001 2.30648

R25 2.30647 0.00002 0.00000 0.00000 0.00000 2.30648

A1 2.06152 -0.00001 0.00000 0.00000 0.00000 2.06152

A2 2.10777 0.00001 0.00000 0.00002 0.00002 2.10780

A3 2.10130 0.00000 0.00000 -0.00002 -0.00002 2.10129

A4 2.08898 0.00000 0.00000 0.00009 0.00009 2.08907

A5 2.10278 0.00000 0.00000 0.00003 0.00003 2.10281

A6 1.61846 0.00000 0.00000 0.00006 0.00006 1.61852

A7 2.02217 -0.00001 0.00000 -0.00008 -0.00008 2.02209

A8 1.74204 -0.00001 0.00000 -0.00021 -0.00021 1.74184

A9 1.70260 0.00000 0.00000 0.00003 0.00003 1.70263

A10 2.08903 0.00001 0.00000 0.00004 0.00004 2.08907

A11 2.10281 -0.00001 0.00000 0.00000 0.00000 2.10281

A12 1.61855 0.00001 0.00000 -0.00002 -0.00002 1.61852

A13 2.02218 0.00000 0.00000 -0.00009 -0.00009 2.02209

A14 1.74170 -0.00001 0.00000 0.00014 0.00014 1.74184

A15 1.70263 0.00000 0.00000 0.00001 0.00001 1.70263

A16 2.06157 0.00000 0.00000 -0.00005 -0.00005 2.06152

A17 2.10128 0.00000 0.00000 0.00001 0.00001 2.10129

A18 2.10774 0.00000 0.00000 0.00005 0.00005 2.10780

A19 1.92417 0.00000 0.00000 -0.00002 -0.00002 1.92416

A20 1.87296 0.00000 0.00000 0.00004 0.00004 1.87300

A21 1.98129 0.00000 0.00000 -0.00004 -0.00004 1.98125

A22 1.85497 0.00000 0.00000 0.00006 0.00006 1.85503

A23 1.92035 0.00000 0.00000 -0.00004 -0.00004 1.92031

A24 1.90513 0.00000 0.00000 0.00000 0.00000 1.90514

A25 1.98125 0.00000 0.00000 0.00000 0.00000 1.98125

A26 1.92414 0.00000 0.00000 0.00002 0.00002 1.92416

A27 1.87304 0.00000 0.00000 -0.00004 -0.00004 1.87300

A28 1.92028 0.00000 0.00000 0.00003 0.00003 1.92031

A29 1.90515 0.00000 0.00000 -0.00001 -0.00001 1.90514

A30 1.85503 0.00000 0.00000 0.00000 0.00000 1.85503

A31 1.88351 0.00000 0.00000 0.00000 0.00000 1.88351

A32 1.87511 0.00000 0.00000 0.00006 0.00006 1.87516

A33 1.73840 0.00000 0.00000 -0.00024 -0.00024 1.73816

A34 1.56413 0.00000 0.00000 0.00010 0.00010 1.56423

A35 1.86732 -0.00001 0.00000 -0.00006 -0.00006 1.86726

A36 2.19881 0.00000 0.00000 -0.00003 -0.00003 2.19878

A37 2.10143 0.00001 0.00000 0.00013 0.00013 2.10155

A38 1.87525 0.00000 0.00000 -0.00008 -0.00008 1.87516

A39 1.73805 -0.00001 0.00000 0.00011 0.00011 1.73816

A40 1.56440 0.00000 0.00000 -0.00017 -0.00017 1.56423

A41 1.86719 0.00001 0.00000 0.00007 0.00007 1.86726

A42 2.19879 0.00000 0.00000 -0.00001 -0.00001 2.19878

A43 2.10153 0.00000 0.00000 0.00002 0.00002 2.10155

A44 1.90324 0.00002 0.00000 0.00006 0.00006 1.90330

A45 2.02641 -0.00003 0.00000 -0.00010 -0.00010 2.02631

A46 2.35353 0.00001 0.00000 0.00005 0.00005 2.35357

A47 1.90336 -0.00002 0.00000 -0.00007 -0.00007 1.90330

A48 2.02626 0.00002 0.00000 0.00006 0.00006 2.02631

A49 2.35356 -0.00001 0.00000 0.00001 0.00001 2.35357

D1 -0.59974 0.00000 0.00000 0.00006 0.00006 -0.59968

D2 2.94909 0.00000 0.00000 -0.00005 -0.00005 2.94904

D3 1.19654 -0.00001 0.00000 -0.00013 -0.00013 1.19642

D4 2.71101 0.00000 0.00000 0.00004 0.00004 2.71104

D5 -0.02335 0.00000 0.00000 -0.00007 -0.00007 -0.02342

D6 -1.77589 0.00000 0.00000 -0.00015 -0.00015 -1.77605

D7 -0.00005 0.00000 0.00000 0.00005 0.00005 0.00000

D8 -2.97311 0.00000 0.00000 -0.00001 -0.00001 -2.97312

D9 2.97304 0.00000 0.00000 0.00008 0.00008 2.97312

D10 -0.00002 0.00000 0.00000 0.00002 0.00002 0.00000

D11 2.73765 -0.00001 0.00000 -0.00035 -0.00035 2.73730

D12 -1.53248 0.00000 0.00000 -0.00026 -0.00026 -1.53274

D13 0.57410 0.00000 0.00000 -0.00026 -0.00026 0.57385

D14 -0.79301 0.00000 0.00000 -0.00023 -0.00023 -0.79324

D15 1.22004 0.00000 0.00000 -0.00014 -0.00014 1.21990

D16 -2.95656 0.00000 0.00000 -0.00013 -0.00013 -2.95669

D17 1.01197 -0.00001 0.00000 -0.00032 -0.00032 1.01165

D18 3.02503 0.00000 0.00000 -0.00023 -0.00023 3.02479

D19 -1.15158 0.00000 0.00000 -0.00023 -0.00023 -1.15180

D20 -1.03647 0.00001 0.00000 0.00032 0.00032 -1.03615

D21 -2.97933 0.00000 0.00000 0.00022 0.00022 -2.97911

D22 1.19524 0.00000 0.00000 0.00022 0.00022 1.19547

D23 1.07123 0.00001 0.00000 0.00039 0.00039 1.07162

D24 -0.87163 0.00000 0.00000 0.00030 0.00030 -0.87134

D25 -2.98024 0.00000 0.00000 0.00030 0.00030 -2.97995

D26 3.13072 0.00000 0.00000 0.00027 0.00027 3.13099

D27 1.18786 0.00000 0.00000 0.00017 0.00017 1.18803

D28 -0.92075 0.00000 0.00000 0.00017 0.00017 -0.92058

D29 0.59967 0.00000 0.00000 0.00001 0.00001 0.59968

D30 -2.71110 0.00000 0.00000 0.00006 0.00006 -2.71104

D31 -2.94890 0.00000 0.00000 -0.00015 -0.00015 -2.94904

D32 0.02351 0.00000 0.00000 -0.00009 -0.00009 0.02342

D33 -1.19627 0.00000 0.00000 -0.00015 -0.00015 -1.19642

D34 1.77614 0.00000 0.00000 -0.00010 -0.00010 1.77605

D35 -0.57364 0.00000 0.00000 -0.00021 -0.00021 -0.57385

D36 -2.73704 0.00000 0.00000 -0.00026 -0.00026 -2.73730

D37 1.53299 0.00000 0.00000 -0.00025 -0.00025 1.53274

D38 2.95677 0.00000 0.00000 -0.00008 -0.00008 2.95669

D39 0.79337 0.00000 0.00000 -0.00013 -0.00013 0.79324

D40 -1.21978 0.00000 0.00000 -0.00012 -0.00012 -1.21991

D41 1.15194 0.00000 0.00000 -0.00014 -0.00014 1.15180

D42 -1.01146 0.00000 0.00000 -0.00019 -0.00019 -1.01165

D43 -3.02461 0.00000 0.00000 -0.00018 -0.00018 -3.02479

D44 1.03579 0.00001 0.00000 0.00037 0.00037 1.03615

D45 2.97888 0.00000 0.00000 0.00023 0.00023 2.97911

D46 -1.19582 0.00001 0.00000 0.00035 0.00035 -1.19547

D47 -1.07193 0.00000 0.00000 0.00031 0.00031 -1.07162

D48 0.87117 -0.00001 0.00000 0.00017 0.00017 0.87133

D49 2.97965 0.00000 0.00000 0.00029 0.00029 2.97995

D50 -3.13136 0.00001 0.00000 0.00037 0.00037 -3.13099

D51 -1.18826 0.00000 0.00000 0.00023 0.00023 -1.18804

D52 0.92022 0.00000 0.00000 0.00035 0.00035 0.92058

D53 -0.00029 0.00000 0.00000 0.00029 0.00029 0.00000

D54 2.16520 0.00000 0.00000 0.00034 0.00034 2.16554

D55 -2.08873 0.00000 0.00000 0.00035 0.00035 -2.08838

D56 -2.16591 0.00000 0.00000 0.00038 0.00038 -2.16554

D57 -0.00042 0.00000 0.00000 0.00042 0.00042 0.00000

D58 2.02883 0.00000 0.00000 0.00043 0.00043 2.02927

D59 2.08806 0.00000 0.00000 0.00032 0.00032 2.08838

D60 -2.02963 0.00000 0.00000 0.00037 0.00037 -2.02927

D61 -0.00038 0.00000 0.00000 0.00038 0.00038 0.00000

D62 -0.01628 0.00000 0.00000 0.00015 0.00015 -0.01613

D63 3.12280 0.00001 0.00000 0.00036 0.00036 3.12316

D64 0.01626 0.00000 0.00000 -0.00013 -0.00013 0.01613

D65 -3.12319 0.00000 0.00000 0.00004 0.00004 -3.12316

D66 0.00035 0.00000 0.00000 -0.00035 -0.00035 0.00000

D67 1.85330 -0.00001 0.00000 -0.00024 -0.00024 1.85306

D68 -1.79211 0.00000 0.00000 -0.00005 -0.00005 -1.79216

D69 -1.85297 0.00000 0.00000 -0.00008 -0.00008 -1.85306

D70 -0.00003 0.00000 0.00000 0.00003 0.00003 0.00000

D71 2.63775 0.00000 0.00000 0.00022 0.00022 2.63797

D72 1.79235 0.00000 0.00000 -0.00019 -0.00019 1.79216

D73 -2.63789 0.00000 0.00000 -0.00008 -0.00008 -2.63797

D74 -0.00011 0.00000 0.00000 0.00011 0.00011 0.00000

D75 -1.93918 0.00000 0.00000 -0.00006 -0.00006 -1.93924

D76 1.20560 -0.00001 0.00000 -0.00033 -0.00033 1.20527

D77 0.01003 0.00000 0.00000 -0.00011 -0.00011 0.00992

D78 -3.12837 0.00000 0.00000 -0.00038 -0.00038 -3.12875

D79 2.68165 0.00000 0.00000 -0.00006 -0.00006 2.68159

D80 -0.45676 0.00000 0.00000 -0.00033 -0.00033 -0.45709

D81 1.93921 0.00000 0.00000 0.00003 0.00003 1.93924

D82 -1.20509 0.00000 0.00000 -0.00018 -0.00018 -1.20527

D83 -0.00998 0.00000 0.00000 0.00006 0.00006 -0.00992

D84 3.12890 0.00000 0.00000 -0.00015 -0.00015 3.12875

D85 -2.68148 0.00000 0.00000 -0.00010 -0.00010 -2.68159

D86 0.45740 0.00000 0.00000 -0.00032 -0.00032 0.45709

Item Value Threshold Converged?

Maximum Force 0.000070 0.000450 YES

RMS Force 0.000010 0.000300 YES

Maximum Displacement 0.000755 0.001800 YES

RMS Displacement 0.000198 0.001200 YES

Predicted change in Energy=-3.582496D-08

Optimization completed.

-- Stationary point found.

----------------------------

! Optimized Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.3944 -DE/DX = 0.0 !

! R2 R(1,4) 1.3967 -DE/DX = 0.0 !

! R3 R(1,5) 1.0995 -DE/DX = 0.0 !

! R4 R(2,7) 1.4898 -DE/DX = 0.0 !

! R5 R(2,14) 1.1022 -DE/DX = 0.0 !

! R6 R(2,17) 2.1702 -DE/DX = 0.0 !

! R7 R(3,4) 1.3944 -DE/DX = 0.0 !

! R8 R(3,10) 1.4898 -DE/DX = 0.0 !

! R9 R(3,13) 1.1022 -DE/DX = 0.0 !

! R10 R(3,16) 2.1705 -DE/DX = 0.0 !

! R11 R(4,6) 1.0995 -DE/DX = 0.0 !

! R12 R(7,8) 1.124 -DE/DX = 0.0 !

! R13 R(7,9) 1.1262 -DE/DX = 0.0 !

! R14 R(7,10) 1.5221 -DE/DX = 0.0 !

! R15 R(10,11) 1.124 -DE/DX = 0.0 !

! R16 R(10,12) 1.1262 -DE/DX = 0.0 !

! R17 R(15,18) 1.4097 -DE/DX = -0.0001 !

! R18 R(15,20) 1.4096 -DE/DX = 0.0 !

! R19 R(16,17) 1.4101 -DE/DX = 0.0 !

! R20 R(16,18) 1.4882 -DE/DX = 0.0 !

! R21 R(16,22) 1.0926 -DE/DX = 0.0 !

! R22 R(17,20) 1.4883 -DE/DX = 0.0 !

! R23 R(17,23) 1.0926 -DE/DX = 0.0 !

! R24 R(18,19) 1.2205 -DE/DX = 0.0 !

! R25 R(20,21) 1.2205 -DE/DX = 0.0 !

! A1 A(2,1,4) 118.1164 -DE/DX = 0.0 !

! A2 A(2,1,5) 120.7666 -DE/DX = 0.0 !

! A3 A(4,1,5) 120.3959 -DE/DX = 0.0 !

! A4 A(1,2,7) 119.6897 -DE/DX = 0.0 !

! A5 A(1,2,14) 120.4804 -DE/DX = 0.0 !

! A6 A(1,2,17) 92.7311 -DE/DX = 0.0 !

! A7 A(7,2,14) 115.8617 -DE/DX = 0.0 !

! A8 A(7,2,17) 99.8117 -DE/DX = 0.0 !

! A9 A(14,2,17) 97.5519 -DE/DX = 0.0 !

! A10 A(4,3,10) 119.6925 -DE/DX = 0.0 !

! A11 A(4,3,13) 120.4821 -DE/DX = 0.0 !

! A12 A(4,3,16) 92.7358 -DE/DX = 0.0 !

! A13 A(10,3,13) 115.8624 -DE/DX = 0.0 !

! A14 A(10,3,16) 99.7919 -DE/DX = 0.0 !

! A15 A(13,3,16) 97.5533 -DE/DX = 0.0 !

! A16 A(1,4,3) 118.1193 -DE/DX = 0.0 !

! A17 A(1,4,6) 120.3946 -DE/DX = 0.0 !

! A18 A(3,4,6) 120.7647 -DE/DX = 0.0 !

! A19 A(2,7,8) 110.247 -DE/DX = 0.0 !

! A20 A(2,7,9) 107.3126 -DE/DX = 0.0 !

! A21 A(2,7,10) 113.5197 -DE/DX = 0.0 !

! A22 A(8,7,9) 106.2818 -DE/DX = 0.0 !

! A23 A(8,7,10) 110.028 -DE/DX = 0.0 !

! A24 A(9,7,10) 109.1561 -DE/DX = 0.0 !

! A25 A(3,10,7) 113.5175 -DE/DX = 0.0 !

! A26 A(3,10,11) 110.245 -DE/DX = 0.0 !

! A27 A(3,10,12) 107.3172 -DE/DX = 0.0 !

! A28 A(7,10,11) 110.0241 -DE/DX = 0.0 !

! A29 A(7,10,12) 109.1569 -DE/DX = 0.0 !

! A30 A(11,10,12) 106.2852 -DE/DX = 0.0 !

! A31 A(18,15,20) 107.9173 -DE/DX = 0.0 !

! A32 A(3,16,17) 107.4357 -DE/DX = 0.0 !

! A33 A(3,16,18) 99.6028 -DE/DX = 0.0 !

! A34 A(3,16,22) 89.618 -DE/DX = 0.0 !

! A35 A(17,16,18) 106.9894 -DE/DX = 0.0 !

! A36 A(17,16,22) 125.9828 -DE/DX = 0.0 !

! A37 A(18,16,22) 120.4029 -DE/DX = 0.0 !

! A38 A(2,17,16) 107.4438 -DE/DX = 0.0 !

! A39 A(2,17,20) 99.583 -DE/DX = 0.0 !

! A40 A(2,17,23) 89.6335 -DE/DX = 0.0 !

! A41 A(16,17,20) 106.9822 -DE/DX = 0.0 !

! A42 A(16,17,23) 125.9811 -DE/DX = 0.0 !

! A43 A(20,17,23) 120.4088 -DE/DX = 0.0 !

! A44 A(15,18,16) 109.0477 -DE/DX = 0.0 !

! A45 A(15,18,19) 116.105 -DE/DX = 0.0 !

! A46 A(16,18,19) 134.8471 -DE/DX = 0.0 !

! A47 A(15,20,17) 109.0546 -DE/DX = 0.0 !

! A48 A(15,20,21) 116.096 -DE/DX = 0.0 !

! A49 A(17,20,21) 134.8492 -DE/DX = 0.0 !

! D1 D(4,1,2,7) -34.3627 -DE/DX = 0.0 !

! D2 D(4,1,2,14) 168.9703 -DE/DX = 0.0 !

! D3 D(4,1,2,17) 68.5569 -DE/DX = 0.0 !

! D4 D(5,1,2,7) 155.3292 -DE/DX = 0.0 !

! D5 D(5,1,2,14) -1.3377 -DE/DX = 0.0 !

! D6 D(5,1,2,17) -101.7512 -DE/DX = 0.0 !

! D7 D(2,1,4,3) -0.0029 -DE/DX = 0.0 !

! D8 D(2,1,4,6) -170.3468 -DE/DX = 0.0 !

! D9 D(5,1,4,3) 170.3425 -DE/DX = 0.0 !

! D10 D(5,1,4,6) -0.0014 -DE/DX = 0.0 !

! D11 D(1,2,7,8) 156.8558 -DE/DX = 0.0 !

! D12 D(1,2,7,9) -87.8046 -DE/DX = 0.0 !

! D13 D(1,2,7,10) 32.8937 -DE/DX = 0.0 !

! D14 D(14,2,7,8) -45.4363 -DE/DX = 0.0 !

! D15 D(14,2,7,9) 69.9032 -DE/DX = 0.0 !

! D16 D(14,2,7,10) -169.3984 -DE/DX = 0.0 !

! D17 D(17,2,7,8) 57.9816 -DE/DX = 0.0 !

! D18 D(17,2,7,9) 173.3212 -DE/DX = 0.0 !

! D19 D(17,2,7,10) -65.9805 -DE/DX = 0.0 !

! D20 D(1,2,17,16) -59.3855 -DE/DX = 0.0 !

! D21 D(1,2,17,20) -170.7031 -DE/DX = 0.0 !

! D22 D(1,2,17,23) 68.4824 -DE/DX = 0.0 !

! D23 D(7,2,17,16) 61.3767 -DE/DX = 0.0 !

! D24 D(7,2,17,20) -49.9409 -DE/DX = 0.0 !

! D25 D(7,2,17,23) -170.7554 -DE/DX = 0.0 !

! D26 D(14,2,17,16) 179.377 -DE/DX = 0.0 !

! D27 D(14,2,17,20) 68.0594 -DE/DX = 0.0 !

! D28 D(14,2,17,23) -52.7551 -DE/DX = 0.0 !

! D29 D(10,3,4,1) 34.3587 -DE/DX = 0.0 !

! D30 D(10,3,4,6) -155.3347 -DE/DX = 0.0 !

! D31 D(13,3,4,1) -168.9594 -DE/DX = 0.0 !

! D32 D(13,3,4,6) 1.3472 -DE/DX = 0.0 !

! D33 D(16,3,4,1) -68.5411 -DE/DX = 0.0 !

! D34 D(16,3,4,6) 101.7655 -DE/DX = 0.0 !

! D35 D(4,3,10,7) -32.8672 -DE/DX = 0.0 !

! D36 D(4,3,10,11) -156.8209 -DE/DX = 0.0 !

! D37 D(4,3,10,12) 87.834 -DE/DX = 0.0 !

! D38 D(13,3,10,7) 169.4105 -DE/DX = 0.0 !

! D39 D(13,3,10,11) 45.4567 -DE/DX = 0.0 !

! D40 D(13,3,10,12) -69.8884 -DE/DX = 0.0 !

! D41 D(16,3,10,7) 66.0014 -DE/DX = 0.0 !

! D42 D(16,3,10,11) -57.9523 -DE/DX = 0.0 !

! D43 D(16,3,10,12) -173.2975 -DE/DX = 0.0 !

! D44 D(4,3,16,17) 59.3461 -DE/DX = 0.0 !

! D45 D(4,3,16,18) 170.6772 -DE/DX = 0.0 !

! D46 D(4,3,16,22) -68.5155 -DE/DX = 0.0 !

! D47 D(10,3,16,17) -61.4168 -DE/DX = 0.0 !

! D48 D(10,3,16,18) 49.9142 -DE/DX = 0.0 !

! D49 D(10,3,16,22) 170.7215 -DE/DX = 0.0 !

! D50 D(13,3,16,17) -179.4135 -DE/DX = 0.0 !

! D51 D(13,3,16,18) -68.0825 -DE/DX = 0.0 !

! D52 D(13,3,16,22) 52.7249 -DE/DX = 0.0 !

! D53 D(2,7,10,3) -0.0168 -DE/DX = 0.0 !

! D54 D(2,7,10,11) 124.0569 -DE/DX = 0.0 !

! D55 D(2,7,10,12) -119.6755 -DE/DX = 0.0 !

! D56 D(8,7,10,3) -124.0978 -DE/DX = 0.0 !

! D57 D(8,7,10,11) -0.024 -DE/DX = 0.0 !

! D58 D(8,7,10,12) 116.2435 -DE/DX = 0.0 !

! D59 D(9,7,10,3) 119.637 -DE/DX = 0.0 !

! D60 D(9,7,10,11) -116.2893 -DE/DX = 0.0 !

! D61 D(9,7,10,12) -0.0217 -DE/DX = 0.0 !

! D62 D(20,15,18,16) -0.9326 -DE/DX = 0.0 !

! D63 D(20,15,18,19) 178.9232 -DE/DX = 0.0 !

! D64 D(18,15,20,17) 0.9316 -DE/DX = 0.0 !

! D65 D(18,15,20,21) -178.9458 -DE/DX = 0.0 !

! D66 D(3,16,17,2) 0.0202 -DE/DX = 0.0 !

! D67 D(3,16,17,20) 106.186 -DE/DX = 0.0 !

! D68 D(3,16,17,23) -102.6801 -DE/DX = 0.0 !

! D69 D(18,16,17,2) -106.1676 -DE/DX = 0.0 !

! D70 D(18,16,17,20) -0.0018 -DE/DX = 0.0 !

! D71 D(18,16,17,23) 151.1321 -DE/DX = 0.0 !

! D72 D(22,16,17,2) 102.694 -DE/DX = 0.0 !

! D73 D(22,16,17,20) -151.1402 -DE/DX = 0.0 !

! D74 D(22,16,17,23) -0.0063 -DE/DX = 0.0 !

! D75 D(3,16,18,15) -111.107 -DE/DX = 0.0 !

! D76 D(3,16,18,19) 69.0756 -DE/DX = 0.0 !

! D77 D(17,16,18,15) 0.5749 -DE/DX = 0.0 !

! D78 D(17,16,18,19) -179.2425 -DE/DX = 0.0 !

! D79 D(22,16,18,15) 153.647 -DE/DX = 0.0 !

! D80 D(22,16,18,19) -26.1704 -DE/DX = 0.0 !

! D81 D(2,17,20,15) 111.1087 -DE/DX = 0.0 !

! D82 D(2,17,20,21) -69.0466 -DE/DX = 0.0 !

! D83 D(16,17,20,15) -0.572 -DE/DX = 0.0 !

! D84 D(16,17,20,21) 179.2727 -DE/DX = 0.0 !

! D85 D(23,17,20,15) -153.6375 -DE/DX = 0.0 !

! D86 D(23,17,20,21) 26.2072 -DE/DX = 0.0 !

--------------------------------------------------------------------------------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-CHWS-122|Freq|RAM1|ZDO|C10H10O3|MC1210|07-Feb-2013|0||#N Geom

=AllCheck Guess=TCheck SCRF=Check GenChk RAM1/ZDO Freq||Title Card Req

uired||0,1|C,-1.1389899091,1.5595086484,0.4412210365|C,0.1855557178,1.

2807649585,0.1063383882|C,-0.7540894021,3.7787936567,-0.3697796388|C,-

1.6231059547,2.8464853371,0.1958957027|H,-1.7337211472,0.8436284038,1.

0265963222|H,-2.6035097899,3.1557631402,0.5858486694|C,0.796539999,1.9

281038627,-1.0882583299|H,1.9159316639,1.9501909666,-0.9888670162|H,0.

5712731791,1.2731963791,-1.9762988258|C,0.269157873,3.3306705847,-1.35

5444734|H,1.1217986652,4.0622213143,-1.3907530527|H,-0.2118412109,3.35

69400536,-2.3733803017|H,-1.029641329,4.8451240023,-0.4139240095|H,0.6

626653842,0.3460679967,0.4434559164|O,2.7563722566,3.8542438521,0.8211

350045|C,0.472811123,3.8749354432,1.4181157834|C,0.961158348,2.5754696

813,1.6658183996|C,1.6128097641,4.6753608068,0.8941665835|O,1.75906291

86,5.8329389217,0.535946269|C,2.4023600689,2.5746118222,1.2945418966|O

,3.295983952,1.7435139062,1.314888848|H,-0.3489980868,4.3635009145,1.9

469464733|H,0.5840152261,1.8809716474,2.4202477153||Version=EM64W-G09R

evC.01|State=1-A|HF=-0.0504198|RMSD=9.675e-010|RMSF=2.041e-005|ZeroPoi

nt=0.185299|Thermal=0.1952999|Dipole=-2.04919,-0.7699162,0.0010702|Dip

oleDeriv=0.147888,0.1689654,0.2989596,-0.2139623,-0.3705703,-0.3101509

,0.0128104,-0.2209427,-0.2481114,-0.3151142,-0.3406276,-0.4059557,-0.0

762052,-0.1017166,-0.0758376,-0.1189158,0.121967,0.0581751,-0.3793643,

-0.0555139,-0.4176759,-0.1870894,-0.1045866,-0.1878176,-0.0051598,-0.1

22368,0.1265252,-0.0789099,0.0593354,0.0324228,0.3371443,0.0573476,0.3

723916,-0.2343246,0.0753374,-0.4502483,0.125892,0.0832985,0.0079453,0.

0942377,0.1493774,-0.0019725,-0.0059396,-0.0062744,0.1466774,0.2223559

,-0.0155563,0.0202668,-0.0308149,0.0626238,0.0318701,0.0114111,0.02756

9,0.136941,-0.0634633,0.025764,0.0213492,0.0613987,-0.0724661,-0.00886

25,0.0653102,-0.0391612,-0.0535751,0.0899963,-0.0075994,-0.0080388,-0.

0074899,0.0368273,0.0131012,-0.0169393,0.0139893,0.0445348,0.0378671,0

.0063661,0.0037977,-0.0100251,0.073381,0.0480455,0.0146141,0.0136251,0

.0631429,-0.0290581,0.0099327,0.0109798,-0.0128492,-0.0769202,0.027531

5,0.0338596,0.0828923,-0.0836006,0.0605013,0.0296914,-0.0057271,0.0268

19,0.0547388,-0.0152721,-0.0113573,-0.0215944,0.0560433,0.0444871,-0.0

133964,0.0379764,0.0012662,0.0493294,-0.0282301,0.0182345,0.0028118,0.

0806361,0.067689,-0.017749,0.038638,-0.0638923,0.1749851,-0.0486006,0.

0262466,0.0009983,0.0523406,0.0693762,-0.0663702,0.0233312,-0.0210151,

0.1789634,0.0160748,0.0314775,-0.0351078,0.0468103,-0.8001829,0.254341

3,-0.0010938,0.2677982,-1.3354055,0.2195758,0.0677513,0.2455571,-0.323

33,-0.0285758,-0.1239012,0.2717109,-0.3753983,-0.5331007,-0.3265114,0.

3570938,0.1346552,0.1525045,-0.516255,0.1138217,-0.1276378,0.4336072,0

.1407255,0.4885524,0.1448573,0.1618406,-0.0318447,1.2374313,-0.101834,

0.183683,0.0227986,1.95179,-0.0281761,-0.2687262,-0.4620552,0.2763171,

-0.5090516,-0.1321812,0.0198087,-0.1053477,-1.328985,0.0540377,0.09762

09,0.3191502,-0.3165876,1.5211494,-0.1961662,0.3584287,-0.5126064,1.61

354,-0.3817189,-0.193796,-0.3254723,0.3299158,-0.9952575,0.4207299,-0.

1802111,0.4529859,-0.8430294,0.2134973,0.0521524,0.064803,-0.3161681,0

.0718409,-0.0915382,-0.1144979,-0.0719679,0.115663,0.0456185,-0.062920

1,0.0625425,0.0958449,0.0187367,-0.0097842,-0.06837,-0.0093623,0.10745

49,-0.1171023,-0.0152676,-0.0947172,0.157055|Polar=112.9475528,-1.7948

71,120.9283042,9.8600674,-5.9700094,71.9402385|HyperPolar=160.2776121,

144.8982208,43.0389041,-11.9067994,252.8045832,152.2916626,73.7470607,

222.4249239,144.4087178,289.007903|PG=C01 [X(C10H10O3)]|NImag=1||0.682

35714,-0.05598972,0.69808543,-0.18331441,-0.18373336,0.30653630,-0.361

68214,0.00284448,0.09956045,0.64119232,0.12698694,-0.11140263,-0.01624

565,-0.21611043,0.49645183,0.14079647,-0.03575930,-0.09046699,-0.22643

833,-0.19041610,0.39771757,0.08349377,-0.07778470,-0.00186133,-0.07248

995,-0.02379987,-0.02815472,0.44029209,0.02085380,-0.10761559,0.030355

68,-0.03415705,-0.02224216,-0.01118695,0.00691222,0.73026435,0.0276504

9,0.00586464,-0.00291260,-0.02588244,-0.01191207,-0.01641456,-0.309773

08,-0.12621696,0.36478214,-0.13340307,0.15647371,-0.02305235,-0.028597

76,0.05656282,0.00354414,-0.21069580,-0.17030690,0.13274664,0.69127755

,0.03077147,-0.33777994,0.07819793,0.14254107,0.00385054,0.03064320,-0

.06478344,-0.20775372,0.15442121,-0.06983234,0.70776875,0.01780905,0.0

3327241,-0.08606152,-0.03333929,-0.01884675,-0.00231051,0.07626843,0.0

9817770,-0.14502958,-0.19943833,-0.13554760,0.28778086,-0.12204959,-0.

09653099,0.07685166,-0.02458261,-0.01526102,0.02338835,0.00116748,0.00

287282,0.00203965,0.00755788,0.00270210,-0.00275130,0.14140842,-0.0996

6492,-0.15241553,0.09530957,0.00147750,0.00591300,0.00121862,0.0036356

7,-0.00135715,0.00232702,-0.01087616,-0.03278213,0.02030702,0.10525729

,0.18143560,0.07311657,0.09943475,-0.11896583,0.01741900,0.00702165,-0

.00021543,0.00410011,0.00342433,0.00481566,0.00420841,0.00749979,0.000

53138,-0.09759083,-0.11640390,0.11750330,-0.01526988,0.01622398,0.0039

4882,0.00233445,0.00189670,0.00225948,-0.02288411,-0.00061799,0.017033

90,-0.25859461,0.06529941,0.08643933,0.00007960,-0.00004605,-0.0007067

0,0.29567786,0.02965878,-0.01517097,-0.00771459,0.00198071,-0.00261262

,0.00247640,-0.01754804,0.00554763,0.01074805,0.06753270,-0.06203813,-

0.02945087,0.00016072,-0.00049896,-0.00041810,-0.08013104,0.07679328,-

0.00376681,0.00480515,0.00574540,0.00464387,0.00305162,0.00490353,0.02

199267,0.00456591,-0.00155308,0.08545285,-0.03535189,-0.07276823,-0.00

076357,-0.00037181,-0.00106678,-0.10747057,0.02379752,0.06784967,-0.03

890845,-0.00789432,0.03719128,-0.09764174,-0.03932813,0.07733880,-0.01

210500,0.03236997,0.00584861,-0.00278064,-0.00595066,0.00212146,-0.002

04231,0.00166618,0.00216463,-0.00007404,-0.00014922,-0.00044452,0.5607

0418,-0.01300597,0.01283783,0.00178899,-0.03160312,-0.10962312,0.08391

390,0.02699340,-0.02113894,-0.01106894,-0.00196474,-0.00840569,0.00081

281,0.00184485,0.00097229,0.00284109,-0.00009465,-0.00009967,-0.000010

30,-0.00319295,0.55767266,0.02040385,0.01063569,-0.01585116,0.08632596

,0.08909319,-0.20160675,0.01527749,-0.01685601,0.00741723,-0.00099433,

-0.00588097,0.00085743,0.00045524,0.00050913,0.00237958,-0.00030232,-0

.00015935,-0.00064233,-0.03423596,-0.03309629,0.54648994,-0.00023800,-

0.00104929,0.00048620,-0.02268170,-0.00709613,0.01220298,-0.00012616,0

.00035038,-0.00026572,0.00006274,-0.00007098,-0.00013147,-0.00013057,0

.00010512,0.00021685,0.00000901,0.00001189,0.00000905,-0.27369017,-0.0

0563176,-0.02257593,0.32867687,-0.00106766,0.00017387,0.00157617,-0.01

300182,0.00134012,0.00246601,0.00080964,-0.00179178,0.00059869,-0.0001

3598,-0.00055069,0.00014226,-0.00015947,0.00013363,0.00014160,-0.00003

729,-0.00002773,-0.00008575,-0.00673493,-0.03939194,0.00034905,0.00628

622,0.05177734,0.00182689,0.00132650,-0.00216321,0.02671022,0.00534266

,-0.00433561,-0.00055864,0.00000952,-0.00049899,0.00006515,0.00075933,

-0.00010072,0.00045648,-0.00028552,-0.00037934,0.00002990,0.00002084,0

.00006130,-0.02321377,-0.00041161,-0.03909023,0.02440848,-0.00221877,0

.05390761,0.00022731,-0.00070902,0.00062476,0.00360173,0.00288765,0.01

132192,-0.00070648,0.00040178,-0.00052933,0.00022255,0.00050529,-0.000

14833,-0.00012790,-0.00007570,-0.00035303,0.00003277,0.00000581,0.0000

7670,-0.04816938,-0.02928377,-0.03888887,-0.01446942,-0.01605979,-0.02

345540,0.05436757,0.00035941,-0.00078914,0.00080335,0.00050575,0.00693

527,0.00266603,-0.00024206,-0.00195828,0.00111326,0.00036739,0.0008554

4,-0.00000701,-0.00015246,-0.00005964,-0.00039138,0.00000040,-0.000024

50,0.00000382,-0.02850090,-0.11417927,-0.10534098,-0.00643284,-0.00000

398,-0.00678900,0.03099998,0.14442319,-0.00217064,0.00179103,-0.000491

49,0.00607172,-0.00646112,-0.03807628,0.00082543,0.00123798,-0.0001371

3,-0.00045738,-0.00182900,0.00047044,0.00017938,0.00019540,0.00057650,

-0.00001264,0.00001000,-0.00004739,-0.03931302,-0.10935391,-0.18301286

,-0.00981111,-0.00701346,-0.00536472,0.04463737,0.12603582,0.22500239,

-0.00857304,0.00498785,-0.00067242,0.01351941,-0.00636449,0.00018906,-

0.16711991,0.05462114,0.10538625,-0.03388652,-0.01627225,0.03459457,-0

.00012902,-0.00002717,-0.00029109,0.00045438,-0.00052149,0.00361677,-0

.09112487,0.05478590,-0.01038853,-0.01821327,0.02893143,-0.00534910,0.

00436322,0.00144440,0.00082925,0.56762863,-0.00057800,-0.00023204,0.00

113947,0.00102330,-0.03025084,0.02533787,0.05091367,-0.08798792,-0.042

35474,-0.01582948,0.00713532,0.01400502,-0.00005059,-0.00015350,-0.000

47033,-0.00152627,-0.00189092,0.00063502,0.05496740,-0.21647104,0.0275

1471,0.01284056,-0.00829923,0.00293749,0.00950849,-0.03266662,-0.00588

452,-0.01310696,0.56137206,-0.00583829,0.00472342,-0.00152276,0.001340

72,0.03510922,-0.00908459,0.11747931,-0.03960392,-0.15378070,0.0268730

3,-0.00406878,-0.01515621,-0.00026944,-0.00025969,-0.00053431,0.000992

36,0.00133689,0.00274748,-0.01110846,0.02933106,-0.07209661,-0.0043736

0,0.00528190,0.00339851,0.00536592,-0.01959335,0.00301867,-0.04296781,

-0.00549707,0.53586317,-0.00035513,0.00031934,-0.00015261,-0.00021798,

0.00100351,-0.00011705,-0.02658155,-0.01108723,0.01249036,-0.00156588,

0.00042813,0.00139614,-0.00001609,-0.00002326,-0.00005309,-0.00010382,

-0.00020591,0.00037910,0.00667781,0.00039189,0.00034285,0.00048743,0.0

0107781,-0.00023001,-0.00030406,0.00072906,0.00003768,-0.17643936,-0.1

1717007,0.00447265,0.21362988,0.00051891,-0.00037902,-0.00003215,0.000

40545,-0.00180064,-0.00012440,-0.00050351,0.00618526,0.00278086,0.0008

4952,0.00052875,-0.00165932,0.00004261,0.00003064,0.00008607,0.0000676

7,0.00016789,-0.00013780,-0.01530612,-0.03361374,0.00385659,0.00039617

,-0.00118823,0.00047604,0.00076677,-0.00155732,0.00035744,-0.11643325,

-0.13883086,0.00360893,0.13696753,0.17039642,0.00035761,-0.00038301,0.

00014416,-0.00054956,0.00019142,-0.00039612,0.02254795,0.00913477,-0.0

0528132,0.00216599,-0.00061556,-0.00118852,0.00001366,0.00001240,0.000

02797,0.00018728,0.00030741,-0.00044077,0.00336846,0.00697774,0.003819

46,0.00000596,0.00019326,0.00045245,-0.00017387,0.00048222,-0.00016226

,0.00318782,0.00364951,-0.03689220,-0.00817178,-0.00406873,0.05034226,

0.00110739,-0.00056833,0.00015363,-0.00134161,0.00036492,0.00004700,0.

00467068,0.00113992,0.01614641,-0.00042727,0.00164628,0.00049225,0.000

00422,0.00004727,0.00005513,-0.00016925,-0.00024553,-0.00056452,-0.004

02819,0.00881225,-0.01294026,-0.00013978,0.00052726,0.00000853,0.00047

488,0.00078089,-0.00026622,-0.08115446,0.00110898,-0.09031372,-0.01519

067,-0.00790707,-0.02216554,0.09579241,-0.00075991,0.00045726,-0.00018

964,0.00142328,-0.00180024,-0.00043117,0.00056937,0.00380446,-0.008637

69,-0.00014141,-0.00109315,0.00001588,0.00002419,0.00000383,0.00003486

,0.00007049,0.00008934,0.00022802,0.01657405,-0.01168449,0.02545387,0.

00061584,-0.00178350,0.00016191,0.00076079,-0.00123610,0.00097183,-0.0

0024991,-0.03635737,0.00135013,-0.01255259,-0.00018663,-0.01432673,-0.

00644002,0.04999073,-0.00127121,0.00098064,-0.00001577,0.00086455,0.00

026135,0.00033833,0.00587902,-0.00534245,-0.03601412,-0.00048098,-0.00

239045,0.00046692,-0.00000507,-0.00002757,-0.00004716,0.00015733,0.000

11310,0.00046867,-0.00995969,0.01115606,-0.00957157,0.00006393,0.00038

713,-0.00009895,0.00014327,-0.00010765,0.00077947,-0.09291984,0.004222

60,-0.22786267,-0.00966749,-0.00426953,-0.00445917,0.10733466,-0.00393

611,0.27801928,-0.00223438,0.00021687,0.00411044,0.00082341,0.00092703

,0.00104902,-0.05245612,0.06977557,0.00010879,0.00515550,-0.02167620,0

.00438509,0.00029043,-0.00060458,-0.00005671,-0.00038472,-0.00064420,-

0.00085113,-0.00121061,0.00107941,0.00139172,-0.00003558,0.00033351,-0

.00004252,0.00008600,0.00001917,-0.00008384,-0.00724816,0.02160574,0.0

0595971,-0.00054904,0.00041873,0.00007793,-0.00015223,0.00022155,0.000

16814,0.06293667,-0.00110867,-0.00121415,0.00146147,-0.00083680,-0.000

06827,-0.00073686,0.06403509,-0.29347207,0.01090716,-0.00166881,-0.029

54237,0.00680404,0.00017957,-0.00032932,0.00006816,-0.00046026,-0.0000

2479,-0.00004659,0.00055467,0.00059717,-0.00054621,0.00004928,-0.00009

161,-0.00000505,0.00000891,-0.00016620,0.00006572,0.01136389,-0.013661

94,-0.00623137,0.00022707,0.00012614,-0.00007922,0.00015301,-0.0001786

7,-0.00029845,-0.07479645,0.33771669,0.00086656,0.00279605,0.00387019,

0.00060859,0.00118395,0.00052658,0.00014834,0.01279439,-0.03323777,0.0

0059554,0.01201151,0.00182474,-0.00013743,-0.00006928,-0.00030718,-0.0

0052877,-0.00000779,-0.00122863,0.00195816,0.00075507,-0.00220064,0.00

001392,-0.00019601,0.00004235,0.00027532,-0.00057949,0.00018270,0.0116

0215,-0.01875963,-0.00000003,0.00027242,-0.00019424,0.00001886,0.00014

019,-0.00015894,-0.00017255,-0.00889418,-0.01371482,0.03972827,-0.0223

0753,0.02988033,-0.00524931,-0.08742452,0.09918407,-0.03371188,0.00031

293,-0.00026392,0.00041153,-0.00295195,0.00021808,0.00336297,-0.000654

76,-0.00015195,-0.00059407,-0.00015965,0.00069861,-0.00022154,0.006560

19,-0.00656501,0.00369715,0.00003710,-0.00048803,0.00018003,0.00002530

,-0.00008720,-0.00001132,-0.00002067,-0.00097180,0.00137276,0.00014662

,-0.00016397,0.00003232,0.00002051,0.00002430,-0.00005265,-0.00016554,

0.00008887,-0.00013555,0.10587743,0.01050893,-0.00491245,0.00160943,0.

10481733,-0.23286611,0.07438926,0.00148291,0.00055974,0.00144268,0.000

57625,-0.00063479,0.00333893,-0.00021536,-0.00007827,-0.00096937,-0.00

007986,0.00007548,-0.00023149,0.00334441,-0.01503881,0.01431241,-0.000

25903,-0.00031417,0.00019348,-0.00001505,-0.00016727,0.00033273,-0.000

13788,-0.00051634,0.00075476,0.00009750,-0.00018586,0.00006623,0.00007

182,0.00011625,-0.00007373,-0.00029388,-0.00005786,-0.00039999,-0.1179

4952,0.26364713,0.00189920,-0.00232901,0.00465349,-0.03433338,0.072279

86,-0.05886321,0.00076335,-0.00051037,0.00041181,0.00152049,0.00008744

,0.00400799,-0.00028461,-0.00077088,-0.00090546,-0.00011166,-0.0000833

5,-0.00026188,-0.00367941,0.02618941,-0.01243243,0.00018022,0.00038180

,-0.00012672,0.00003620,0.00020046,-0.00036198,0.00242816,0.00006403,-

0.00227752,-0.00014206,0.00021244,-0.00004545,-0.00021727,0.00064495,-

0.00003429,-0.00026481,0.00013759,-0.00028801,0.03271188,-0.08834900,0

.07086506,-0.00070321,-0.00035024,-0.00057881,-0.00061674,-0.00050807,

0.00022693,0.00177815,0.00080708,0.00187537,0.00020292,-0.00118352,0.0

0041975,0.00021980,0.00015808,-0.00006704,0.00010436,0.00002375,0.0000

9855,-0.00010602,-0.00026343,-0.00036991,-0.00050109,-0.00012843,-0.00

036912,0.00006174,0.00004776,-0.00001311,-0.00053927,-0.00005347,-0.00

066588,-0.00036273,0.00004237,-0.00021684,0.00010434,-0.00007246,0.000

00799,0.00015240,-0.00004967,-0.00002343,-0.00026017,0.00017857,0.0000

1090,0.50999367,-0.00058991,0.00244295,0.00077601,0.00382047,0.0025317

9,0.00252033,-0.00270471,-0.00056966,-0.00194426,-0.00135237,0.0002755

1,-0.00104715,-0.00015425,-0.00007686,0.00018501,0.00026835,-0.0000259

5,-0.00019705,-0.00056205,-0.00059646,-0.00058505,0.00029369,-0.000263

73,0.00020443,-0.00003957,0.00011821,-0.00003029,0.00015625,0.00000177

,-0.00001763,-0.00011790,-0.00060564,-0.00022350,-0.00001840,0.0000802

5,-0.00001819,-0.00033668,-0.00036367,0.00016772,0.00041456,-0.0000513

4,-0.00009925,-0.03978774,0.52023779,-0.00214542,0.00166775,0.00055981

,0.00273686,0.00042073,-0.00018918,0.00368896,0.00178433,0.00051257,-0

.00018052,-0.00275454,0.00182929,-0.00011361,-0.00008891,-0.00016853,-

0.00020966,-0.00005720,-0.00010352,-0.00062760,-0.00048304,-0.00064233

,0.00023429,0.00053513,-0.00004091,-0.00008507,-0.00006634,-0.00000530

,-0.00087720,-0.00029644,-0.00080717,0.00055227,-0.00003874,0.00016160

,-0.00009337,-0.00004746,-0.00000985,-0.00012027,0.00014017,-0.0000882

4,-0.00016726,-0.00017589,0.00001111,-0.11223340,-0.12781450,0.1104774

3,-0.04966928,0.03516273,-0.00042048,0.04738272,0.02047980,0.02380675,

0.06034841,0.03418948,0.03982065,-0.02653739,-0.07270615,0.01833881,-0

.00044368,-0.00059025,-0.00224297,-0.00170819,-0.00070206,-0.00238129,

-0.00185927,-0.00190266,-0.00457223,-0.00007752,-0.00008415,0.00026660

,0.00033027,0.00020459,-0.00065866,-0.00192759,-0.00218455,-0.00869791

,-0.00018515,0.00002806,0.00116964,0.00103703,-0.00028517,-0.00045580,

-0.00534557,0.00136463,-0.00711136,-0.00054354,-0.00142429,-0.00073531

,-0.08425877,0.01188482,0.02114455,0.59811944,0.04109354,-0.04043315,-

0.00578023,-0.05563335,-0.03400392,-0.03258733,-0.04577286,-0.03568511

,-0.02357976,0.00646070,0.04753118,-0.02230811,0.00129470,0.00139826,0

.00158323,0.00108886,0.00042458,0.00230961,0.00275674,0.00253938,0.005

51619,0.00005168,0.00005976,-0.00054370,-0.00057992,-0.00036025,0.0009

2159,0.00177058,0.00211845,0.00270030,-0.00008706,-0.00020453,-0.00015

464,-0.00020053,0.00003110,0.00035620,0.00471206,-0.00106969,0.0055870

8,0.00064908,0.00170149,0.00106883,0.00810066,0.00926732,0.00449864,-0

.12702670,0.67704185,-0.05963569,0.05048507,0.00323887,0.06440085,0.02

337141,0.03175470,0.08247553,0.03952714,0.03250481,-0.02928649,-0.0864

2133,0.02682646,-0.00124753,-0.00143007,-0.00261173,-0.00174093,-0.000

88596,-0.00329282,-0.00322225,-0.00370775,-0.00734131,-0.00007729,-0.0

0003569,0.00055492,0.00048274,0.00040815,-0.00094831,-0.00553617,-0.00

487647,-0.02203087,-0.00053043,0.00002013,0.00020148,0.00185855,-0.000

99310,-0.00161252,-0.00585414,0.00197446,-0.00644589,-0.00115622,-0.00

257041,-0.00196020,0.02464668,0.00198664,0.00781879,-0.24779208,-0.006

29313,0.20644871,-0.01824768,0.00090554,-0.00649526,0.00261246,0.00898

535,0.00923216,-0.01051735,-0.00054380,-0.00818366,-0.00604049,-0.0004

7795,-0.00530932,-0.00040411,-0.00012076,0.00005996,0.00092722,-0.0001

4345,-0.00023004,0.00070995,-0.00069416,-0.00201485,-0.00026442,0.0002

4091,0.00069609,0.00027094,0.00035432,-0.00000456,0.00084612,0.0003388

3,0.00099432,-0.00000026,-0.00006387,-0.00020333,-0.00023920,0.0000387

7,0.00017184,0.00026586,-0.00001273,0.00042468,-0.00005583,-0.00063636

,-0.00090609,-0.03983655,-0.04393539,0.02916944,-0.10345758,0.12652662

,-0.00982630,0.54797883,-0.09663252,0.06698159,0.00269122,0.10551337,0

.03749434,0.05667282,0.09081515,0.04207161,0.04864526,-0.01832965,-0.0

9614471,0.03591789,-0.00198340,-0.00218255,-0.00398095,-0.00195607,-0.

00084317,-0.00356716,-0.00430616,-0.00432390,-0.01458702,-0.00017815,0

.00003529,0.00094666,0.00085989,0.00091897,-0.00133580,-0.00471911,-0.

00269067,-0.00943724,-0.00024202,0.00023999,0.00066282,0.00108251,-0.0

0030975,-0.00121476,-0.00253583,0.00069698,-0.00253741,-0.00381255,-0.

01048640,-0.00811158,-0.03956276,-0.02990328,0.01892071,0.06248258,-0.

32703014,-0.02997175,-0.04760193,0.60918797,-0.05510344,0.03062665,-0.

00096222,0.05345462,0.02621394,0.01714499,0.03125788,0.02281953,0.0136

0382,-0.00880027,-0.04394715,0.01531800,-0.00095504,-0.00092590,-0.001

99246,-0.00084932,-0.00041374,-0.00174201,-0.00337126,-0.00633715,-0.0

1822248,-0.00041413,-0.00028571,0.00004587,0.00077721,0.00117689,-0.00

173567,-0.00244384,-0.00099546,-0.00482219,-0.00007601,0.00007422,0.00

029699,0.00038780,-0.00019038,-0.00042957,-0.00152049,0.00020815,-0.00

176321,-0.00125596,-0.00415427,-0.00233438,0.02879324,0.02259937,0.002

56226,-0.04875224,0.10605202,-0.11255337,-0.14428007,-0.30908621,0.324

32811,0.00025008,0.00207424,0.00142759,0.00538203,0.00297003,0.0026341

1,-0.01223229,-0.00436279,-0.01156596,-0.00179656,0.00161928,-0.000950

10,-0.00059506,-0.00041726,0.00036992,-0.00005316,0.00006234,-0.000080

64,-0.00047091,-0.00066853,-0.00050858,0.00059244,0.00031698,0.0004423

7,-0.00002292,0.00001668,-0.00011640,0.00052509,-0.00085084,-0.0001117

4,0.00118593,-0.00011479,-0.00144902,-0.00054145,0.00022604,0.00005614

,-0.00047776,0.00061305,0.00040828,0.00022454,-0.00051777,-0.00024574,

-0.26909089,0.07103062,0.03811748,-0.17226490,-0.07439474,0.06281144,-

0.00308614,-0.03326118,0.00634464,0.50829170,-0.00228100,0.00152764,0.

00034076,0.00380662,-0.00026763,0.00125505,-0.00323981,0.00031914,-0.0

0685322,0.00002512,-0.00300140,0.00233210,-0.00029801,-0.00045085,0.00

002182,-0.00042370,0.00014636,0.00006646,-0.00055693,-0.00060256,-0.00

060295,-0.00025703,-0.00039178,-0.00058820,0.00028878,-0.00013337,-0.0

0007249,-0.00005015,-0.00089665,0.00005973,0.00018926,0.00191569,-0.00

144160,-0.00034363,0.00026457,0.00007149,0.00126556,0.00187565,0.00079

357,-0.00031166,-0.00049951,-0.00021778,0.08962855,-0.07973586,-0.0172

4540,-0.09039151,-0.11219694,0.03744736,-0.02797793,-0.07727332,0.0296

5532,0.11631110,1.28835380,0.00948759,-0.01044652,-0.00189285,-0.01466

129,-0.00604837,-0.00637295,-0.01369423,-0.00738108,0.00071638,0.00293

609,0.01152771,-0.00570355,0.00057926,0.00058988,0.00025326,0.00031055

,0.00016026,0.00055565,0.00093318,0.00034874,0.00144413,0.00005414,-0.

00011838,-0.00016117,-0.00016973,0.00001705,0.00020036,-0.00060199,-0.

00069795,-0.00005760,-0.00089326,-0.00164020,-0.00572522,0.00031038,-0

.00013215,-0.00002285,-0.00039929,-0.00078513,-0.00041464,0.00028569,0

.00065943,0.00039327,0.03204551,-0.01031658,-0.05466982,0.06262641,0.0

1423480,-0.09181038,0.01105634,0.05021857,0.00267456,-0.12346075,-0.33

706882,0.30175729,0.00012700,-0.00050076,-0.00036155,-0.00069503,-0.00

038734,0.00004399,0.00001989,-0.00036571,0.00057978,0.00027560,-0.0001

3075,0.00000134,0.00013186,0.00009783,-0.00001084,0.00010095,0.0000252

1,0.00005224,0.00010135,-0.00003250,-0.00003138,-0.00014794,-0.0000604

7,-0.00004450,0.00001528,0.00003490,0.00000785,-0.00015994,-0.00035755

,-0.00023903,-0.00039536,-0.00012151,-0.00017568,0.00007337,-0.0000021

8,0.00001537,0.00061280,0.00033087,0.00024313,-0.00009506,0.00010117,-

0.00005880,0.00287454,0.04985339,-0.01176353,-0.00436448,-0.03319347,0

.01404341,-0.00237724,-0.00070153,0.00201136,-0.06788281,-0.12080676,0

.03665384,0.08021949,0.00219102,-0.00181340,-0.00048273,-0.00316190,-0

.00073928,-0.00075695,-0.00129440,-0.00166538,0.00230676,0.00017748,0.

00258657,-0.00166560,0.00023887,0.00031059,0.00004853,0.00034925,-0.00

007316,0.00004430,0.00019155,0.00006426,0.00020546,0.00008384,0.000156

17,0.00025155,-0.00012723,0.00009959,0.00005681,-0.00063278,-0.0000566

0,-0.00064079,-0.00040493,-0.00124003,-0.00073634,0.00017614,-0.000115

71,0.00001163,-0.00032091,-0.00105856,-0.00022387,0.00009715,0.0002998

5,0.00002115,0.04528906,-0.11032005,0.02250298,-0.01827781,-0.04382314

,0.02032837,-0.00497493,0.00351377,0.00327908,-0.14350540,-0.90335914,

0.27279191,0.10908449,1.04813014,-0.00245697,0.00242949,0.00054747,0.0

0338599,0.00125387,0.00114976,0.00238565,0.00123675,-0.00096331,-0.000

61342,-0.00300583,0.00163025,-0.00016205,-0.00018850,-0.00009102,-0.00

016608,-0.00003926,-0.00014918,-0.00035952,-0.00017309,-0.00037248,-0.

00001895,-0.00003896,-0.00006277,0.00007665,-0.00005111,-0.00003139,-0

.00056091,-0.00077176,-0.00034523,0.00023522,0.00069304,-0.00021998,-0

.00011566,0.00009469,0.00003877,0.00039994,0.00056716,0.00000529,-0.00

005536,-0.00017152,-0.00000745,-0.01070355,0.02085543,0.00785136,0.009

21392,0.02837194,0.00557809,0.00224211,-0.00404522,-0.00179508,0.04301

565,0.26484614,-0.13755889,-0.04403052,-0.30978519,0.12018801,-0.00281

075,0.00084243,0.00090086,-0.00717547,-0.00894107,-0.01197713,0.007669

74,0.00448822,0.00325603,0.00041564,-0.00371895,0.00296730,-0.00017684

,-0.00033545,0.00000026,-0.00100530,0.00010235,0.00011538,-0.00038436,

0.00106006,-0.00045889,0.00187133,-0.00063776,-0.00094557,-0.00029098,

-0.00064640,0.00028241,-0.00110937,-0.00018141,-0.00108948,0.00021799,

0.00016848,-0.00005111,0.00011419,0.00012023,-0.00019597,-0.00050825,0

.00039184,-0.00059873,0.00139217,-0.00063343,0.00132146,-0.11518115,-0

.09170415,0.04294145,-0.07075355,0.05019851,-0.00151054,-0.24212137,-0

.00774091,0.05952546,0.03024240,0.03496450,-0.01973236,-0.00906588,0.0

1263611,-0.00037955,1.01106423,0.00471542,-0.00624641,-0.00158361,-0.0

1074716,-0.00337426,-0.00276089,-0.00277925,-0.00302726,-0.00065336,0.

00166034,0.00527773,-0.00154216,0.00025875,0.00026567,0.00002902,0.000

12802,-0.00005923,0.00035955,0.00005893,0.00016850,-0.00019157,-0.0007

6814,0.00099748,-0.00232651,-0.00005474,0.00004778,-0.00004647,0.00029

591,0.00035727,0.00051657,0.00063879,0.00026884,0.00067303,-0.00014118

,-0.00023624,0.00010698,0.00047668,0.00016678,0.00013399,-0.00170117,-

0.00016291,-0.00062161,-0.11026434,-0.20548711,0.07652877,0.04927167,-

0.02583501,-0.00153023,0.00437619,-0.04682778,-0.00007136,0.09440636,-

0.12892460,0.00799993,-0.00616331,0.01913783,-0.00246300,-0.47296041,0

.86521068,0.00898323,-0.00628665,-0.00144369,-0.01344524,-0.00358650,-

0.00067110,-0.01321070,-0.00605190,-0.00590670,0.00029893,0.01128185,-

0.00581252,0.00017669,0.00014905,0.00056122,0.00066294,0.00007659,0.00

027291,-0.00102264,0.00016959,-0.00021268,-0.00058859,-0.00178444,-0.0

0548548,0.00014520,0.00020137,-0.00005608,0.00055948,0.00072697,0.0011

2423,-0.00020761,-0.00000147,-0.00044725,-0.00008843,0.00003804,0.0001

6591,0.00039851,-0.00016742,0.00045900,-0.00003743,0.00014318,-0.00024

664,0.04913280,0.06966912,-0.08320717,0.01660267,-0.01351791,0.0189004

4,0.03940848,0.01551013,-0.08726582,-0.03883483,0.02870629,-0.00267746

,0.00536868,-0.00870742,0.00505678,-0.07443509,-0.08860218,0.22247861,

0.00168054,-0.00149336,-0.00061061,-0.00204104,0.00099428,0.00155485,-

0.00276032,-0.00143762,-0.00048843,0.00027065,0.00221526,-0.00142085,0

.00021804,0.00024820,0.00003453,0.00039144,-0.00002132,0.00009435,-0.0

0041727,-0.00031969,-0.00052864,-0.00099343,0.00011456,-0.00078157,0.0

0008100,0.00018176,-0.00003688,0.00018973,0.00017860,0.00012540,-0.000

02190,-0.00003354,0.00015194,-0.00000402,-0.00010272,0.00008392,0.0001

8543,-0.00021400,0.00006520,-0.00015808,0.00049367,-0.00014591,0.00169

984,0.04665183,-0.01110078,-0.00305903,-0.00364688,0.00495097,-0.05118

156,0.03671405,0.00519370,0.00618283,-0.00536730,0.00042365,0.00003247

,0.00213876,-0.00068157,-0.58665697,0.46542375,-0.00326429,0.63724873,

-0.00214563,0.00245258,0.00067887,0.00232279,-0.00035105,-0.00123083,0

.00248821,0.00165482,0.00073937,-0.00063222,-0.00254981,0.00109971,-0.

00013683,-0.00020201,0.00000307,-0.00023156,0.00004143,-0.00011921,-0.

00018198,0.00046670,0.00001093,0.00068648,-0.00053228,0.00062457,-0.00

001762,-0.00014473,0.00006284,-0.00018366,-0.00012550,-0.00028324,-0.0

0019610,-0.00006223,-0.00024313,0.00005840,0.00010889,-0.00007767,-0.0

0023213,0.00002883,-0.00009788,0.00125381,-0.00021508,0.00057071,0.051

07132,-0.10879538,0.02207555,-0.00045158,0.00413926,-0.00317725,0.0221

2924,-0.00582743,0.00121948,-0.02411450,0.00684469,0.00639274,0.004391

29,-0.00775273,0.00068422,0.48782787,-0.46999714,-0.00043301,-0.544324

12,0.58129266,-0.00179787,0.00134232,0.00035944,0.00183336,0.00062226,

-0.00021801,0.00222910,0.00101088,0.00082288,-0.00015365,-0.00212480,0

.00114102,-0.00006655,-0.00003360,-0.00013782,-0.00011707,-0.00001850,

-0.00008172,-0.00092598,-0.00012827,-0.00061117,0.00032588,-0.00023317

,-0.00032684,-0.00001766,-0.00006240,0.00006005,-0.00027256,-0.0001779

1,-0.00027150,0.00003090,0.00001157,0.00002960,0.00001067,0.00002850,-

0.00002126,-0.00005635,0.00004981,-0.00001686,0.00025767,-0.00000993,-

0.00006697,-0.01288169,0.02343571,0.00739573,-0.00094000,0.00201715,-0

.00174413,0.01177467,-0.00616659,0.01441368,0.00647348,0.00026568,0.00

210894,-0.00149168,0.00169842,-0.00080791,-0.01123832,0.00692015,-0.05

214699,0.00812861,-0.02872204,0.03008188,0.00444400,-0.00397202,-0.000

23152,-0.00567091,-0.00270250,-0.00305120,-0.00510271,-0.00408836,-0.0

0642741,0.00112184,0.00493710,-0.00379999,0.00015740,0.00014013,0.0000

8841,0.00019818,0.00001712,0.00019646,0.00023395,0.00030610,0.00061424

,-0.00001094,-0.00000459,-0.00006261,-0.00006019,-0.00001946,0.0000971

4,-0.00008341,0.00026116,0.00025352,-0.00003519,-0.00001556,-0.0000577

6,0.00004147,-0.00006510,-0.00000366,0.00016271,-0.00014819,-0.0002944

8,0.00006689,0.00024941,0.00015973,-0.00249695,0.00057581,0.00010904,-

0.19127546,0.09233947,0.11396177,-0.00711496,0.02025828,0.00665812,-0.

02198926,0.00256060,0.01478710,-0.00014830,0.00015792,-0.00042609,0.00

000178,-0.00052899,0.00232373,-0.00009229,0.00031727,-0.00027153,0.227

94495,0.00122092,-0.00070494,0.00017336,-0.00063530,-0.00094524,-0.000

56630,-0.00269299,-0.00109527,-0.00587471,-0.00047779,0.00083509,-0.00

197584,-0.00003609,-0.00005741,0.00003125,0.00000870,0.00007969,0.0000

7062,0.00005686,0.00001590,0.00010668,-0.00000658,-0.00002929,-0.00002

044,-0.00001398,-0.00000849,0.00001601,0.00004286,-0.00001403,0.000226

49,-0.00000872,0.00002483,-0.00003188,-0.00003911,0.00002372,0.0000057

9,0.00017921,0.00014094,0.00045897,-0.00002923,-0.00003908,-0.00006001

,-0.00450484,0.00050029,0.00022490,0.10176651,-0.09561603,-0.05870894,

0.02403317,-0.01590823,-0.00974404,-0.00988109,0.00835457,0.00758083,-

0.00038112,-0.00169320,-0.00034395,0.00079245,-0.00417486,0.00128176,0

.00070891,0.00041102,-0.00024335,-0.10997721,0.10997117,0.00782865,-0.

00630795,-0.00017021,-0.00807883,-0.00381202,-0.00429565,-0.01287920,-

0.00963904,-0.01997105,0.00119094,0.00898884,-0.00577585,0.00006595,0.

00012986,0.00036661,0.00015693,0.00013113,0.00042830,0.00035391,0.0004

0136,0.00086035,0.00002658,0.00001482,-0.00009548,-0.00007440,-0.00005

008,0.00012081,0.00011621,0.00033615,0.00059828,-0.00000052,0.00000618

,-0.00015204,-0.00008595,-0.00000423,0.00000193,-0.00004442,0.00024175

,-0.00064559,0.00010222,0.00020365,0.00017063,0.00117539,-0.00045627,0

.00042317,0.12552291,-0.07081651,-0.08670442,-0.00458428,0.01390680,0.

00877567,0.01211377,-0.00315281,-0.00461235,-0.00035838,0.00023245,0.0

0037294,0.00297701,0.00300506,0.00151203,-0.00115352,0.00016252,-0.000

17858,-0.12352027,0.06751877,0.10992769,0.00276227,-0.00308625,-0.0022

5436,-0.00398600,-0.00274295,-0.00618459,-0.00397267,-0.00155045,-0.00

227855,0.00071413,0.00391643,-0.00130528,0.00011727,0.00010005,0.00013

235,0.00009652,0.00003261,0.00004648,0.00002430,-0.00005066,0.00030189

,-0.00001695,-0.00003768,-0.00003790,-0.00000868,0.00003480,-0.0000125

1,0.00020140,0.00011301,0.00044564,-0.00002130,-0.00000913,-0.00005179

,-0.00005214,0.00000316,0.00006606,0.00009664,-0.00006484,0.00010120,0

.00013365,0.00024024,0.00009288,-0.00324092,-0.00364775,0.00102593,0.0

1051185,0.00349449,-0.00221801,-0.06866771,-0.05416628,0.07341701,-0.0

0237181,0.00326676,0.00112324,0.00074746,-0.00011386,-0.00022600,-0.01

574375,-0.01560017,0.02107188,-0.00079830,0.00030164,-0.00083448,-0.00

029192,-0.00012527,-0.00084975,0.08376691,0.00494385,-0.00384948,-0.00

113932,-0.00659595,-0.00216828,-0.00700447,-0.00550864,-0.00304526,-0.

00279788,0.00086246,0.00563136,-0.00217550,0.00010251,0.00018050,0.000

18001,0.00020248,0.00002376,0.00018136,0.00012299,-0.00016492,0.000282

39,-0.00002103,-0.00001362,-0.00006585,-0.00001747,0.00005633,-0.00002

800,0.00029837,0.00011671,0.00063380,0.00002588,-0.00002989,-0.0000465

7,-0.00006551,0.00001127,0.00008347,0.00020985,-0.00005040,0.00025650,

-0.00001257,-0.00017401,-0.00070527,0.00138028,0.00134000,-0.00023109,

-0.00081114,-0.02999446,0.02505292,-0.06074320,-0.14138827,0.13222643,

0.00244948,-0.00186786,0.00211159,-0.00071799,-0.00058970,0.00004450,-

0.00609685,0.00245213,0.00118809,0.00089875,-0.00088440,0.00051593,-0.

00059849,-0.00007147,-0.00103981,0.06969262,0.17448002,0.00647884,-0.0

0693839,-0.00273501,-0.01263178,-0.00808913,-0.02002021,-0.00719026,-0

.00329312,-0.00388833,0.00186083,0.00852356,-0.00277885,0.00014044,0.0

0010767,0.00040811,0.00003672,0.00007070,0.00034598,0.00020512,0.00008

444,0.00063931,0.00002839,-0.00005761,-0.00013180,-0.00006762,-0.00006

937,0.00001931,0.00037131,0.00021330,0.00079219,0.00003233,-0.00001672

,-0.00008444,-0.00009418,0.00002480,0.00009300,0.00013905,-0.00001420,

0.00015180,0.00023451,-0.00034043,-0.00030042,-0.00031010,0.00034919,0

.00032590,0.00625087,0.00036270,0.00523124,0.07680840,0.14995193,-0.16

354381,0.00310828,0.00138026,0.00158040,-0.00045603,-0.00077930,-0.000

01817,0.00832519,0.00612293,-0.00494869,-0.00059452,0.00005641,0.00021

351,-0.00110312,-0.00012591,-0.00095685,-0.08157177,-0.14752334,0.1896

0623||0.00002722,-0.00000192,-0.00000444,-0.00002595,-0.00000967,-0.00

000086,-0.00000430,0.00003345,-0.00003033,0.00000731,-0.00004300,0.000

00107,0.00000704,0.00000448,-0.00000209,-0.00000751,0.00000346,0.00000

501,-0.00000641,0.00001766,0.00000641,-0.00000291,-0.00000787,-0.00000

973,0.00000227,-0.00000159,0.00000017,-0.00000225,-0.00000637,-0.00000

337,-0.00000175,-0.00000349,0.00000213,0.00000198,0.00000092,0.0000002

5,-0.00000064,0.00000133,0.00000460,-0.00000697,0.00000340,0.00000490,

0.00005334,-0.00008503,0.00000547,0.00000017,-0.00001444,0.00002117,-0

.00005657,-0.00001741,0.00002219,-0.00001185,0.00005298,-0.00002488,-0

.00001249,0.00002826,0.00000747,0.00004377,0.00002179,0.00000753,-0.00

000513,0.00001895,-0.00001125,0.00000166,0.00000550,-0.00000134,-0.000

00005,-0.00000139,-0.00000007|||@

In the beginning there was nothing, which exploded.

Job cpu time: 0 days 0 hours 0 minutes 4.0 seconds.

File lengths (MBytes): RWF= 40 Int= 0 D2E= 0 Chk= 4 Scr= 1

Normal termination of Gaussian 09 at Thu Feb 07 16:36:53 2013.