

B4Cl4

(Occupancy) Bond orbital/ Coefficients/ Hybrids

1. (1.99909) BD (1) B 1 -Cl 5

(34.31%) 0.5858* B 1 s(30.55%)p 2.26(69.11%)d 0.01(0.33%)

-0.0002 0.5452 -0.0913 -0.0040 -0.6779

-0.0413 -0.4588 -0.0280 -0.1359 -0.0083

0.0452 0.0134 0.0091 0.0181 -0.0266

(65.69%) 0.8105*Cl 5 s(32.72%)p 2.05(66.95%)d 0.01(0.33%)

0.0000 0.0000 0.5714 -0.0248 0.0022

0.0000 0.6680 -0.0251 0.0000 0.4522

-0.0170 0.0000 0.1339 -0.0050 0.0453

0.0134 0.0091 0.0181 -0.0266

2. (1.99399) BD (2) B 1 -Cl 5

(7.05%) 0.2655* B 1 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 0.0000 0.0000 0.0000 -0.5573

0.0437 0.8226 -0.0644 0.0029 -0.0002

-0.0263 0.0110 -0.0184 0.0742 0.0050

(92.95%) 0.9641*Cl 5 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 0.0000 0.0000 0.0000

0.0000 -0.5608 -0.0051 0.0000 0.8275

0.0076 0.0000 0.0029 0.0000 0.0096

-0.0023 0.0035 -0.0238 0.0001

3. (1.99399) BD (3) B 1 -Cl 5

(7.05%) 0.2655* B 1 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 0.0000 0.0000 0.0000 -0.1331

0.0104 -0.0937 0.0073 0.9802 -0.0768

0.0158 -0.0680 -0.0388 0.0071 -0.0158

(92.95%) 0.9641*Cl 5 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 0.0000 0.0000 0.0000

0.0000 -0.1339 -0.0012 0.0000 -0.0942

-0.0009 0.0000 0.9861 0.0090 -0.0039

0.0203 0.0138 -0.0015 0.0074

4. (1.99909) BD (1) B 2 -Cl 6

(34.31%) 0.5858* B 2 s(30.55%)p 2.26(69.11%)d 0.01(0.33%)

0.0002 -0.5452 0.0913 0.0040 0.0283

0.0017 -0.6818 -0.0416 0.4721 0.0288

0.0028 -0.0019 0.0468 0.0337 0.0008

(65.69%) 0.8105*Cl 6 s(32.72%)p 2.05(66.95%)d 0.01(0.33%)

0.0000 0.0000 -0.5714 0.0248 -0.0022

0.0000 -0.0282 0.0011 0.0000 0.6722

-0.0253 0.0000 -0.4646 0.0175 0.0028

-0.0020 0.0468 0.0338 0.0009

5. (1.99399) BD (2) B 2 -Cl 6

(7.05%) 0.2655* B 2 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 -0.0001 0.0000 0.0000 0.9930

-0.0778 0.0278 -0.0022 -0.0194 0.0015

0.0607 -0.0544 -0.0023 -0.0050 0.0023

(92.95%) 0.9641*Cl 6 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 -0.0001 0.0000 0.0000

0.0000 0.9990 0.0091 0.0000 0.0282

0.0003 0.0000 -0.0197 -0.0002 -0.0214

0.0146 0.0008 0.0015 -0.0005

6. (1.99398) BD (3) B 2 -Cl 6

(7.05%) 0.2655* B 2 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 0.0002 0.0000 0.0000 0.0001

0.0000 0.5656 -0.0443 0.8169 -0.0640

-0.0014 -0.0014 0.0333 -0.0447 -0.0597

(92.95%) 0.9641*Cl 6 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 0.0002 0.0000 0.0000

0.0000 0.0001 0.0000 0.0000 0.5685

0.0052 0.0000 0.8223 0.0075 0.0005

0.0007 -0.0091 0.0120 0.0211

7. (1.99909) BD (1) B 3 -Cl 7

(34.31%) 0.5858* B 3 s(30.55%)p 2.26(69.11%)d 0.01(0.33%)

0.0002 -0.5452 0.0913 0.0040 -0.6758

-0.0412 0.4416 0.0269 0.1921 0.0117

0.0434 0.0189 -0.0123 -0.0190 0.0242

(65.69%) 0.8105*Cl 7 s(32.71%)p 2.05(66.95%)d 0.01(0.33%)

0.0000 0.0000 -0.5714 0.0248 -0.0022

0.0000 0.6662 -0.0250 0.0000 -0.4346

0.0163 0.0000 -0.1894 0.0071 0.0434

0.0189 -0.0123 -0.0191 0.0243

8. (1.99399) BD (2) B 3 -Cl 7

(7.05%) 0.2655* B 3 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 0.0001 0.0000 0.0000 0.5441

-0.0426 0.8314 -0.0652 0.0037 -0.0003

0.0275 -0.0126 -0.0227 0.0722 0.0057

(92.95%) 0.9641*Cl 7 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 0.0002 0.0000 0.0000

0.0000 0.5471 0.0050 0.0000 0.8366

0.0076 0.0000 0.0038 0.0000 -0.0102

0.0032 0.0050 -0.0232 0.0001

9. (1.99399) BD (3) B 3 -Cl 7

(7.05%) 0.2655* B 3 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 0.0000 0.0000 0.0000 0.1905

-0.0149 -0.1290 0.0101 0.9666 -0.0757

-0.0197 0.0658 -0.0346 0.0101 -0.0257

(92.95%) 0.9641*Cl 7 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 -0.0001 0.0000 0.0000

0.0000 0.1918 0.0017 0.0000 -0.1298

-0.0012 0.0000 0.9724 0.0089 0.0054

-0.0194 0.0127 -0.0022 0.0102

10. (1.99909) BD (1) B 4 -Cl 8

(34.31%) 0.5858* B 4 s(30.56%)p 2.26(69.11%)d 0.01(0.33%)

-0.0002 0.5452 -0.0913 -0.0040 0.0304

0.0019 0.2184 0.0133 0.7999 0.0488

0.0010 0.0035 0.0254 -0.0034 0.0517

(65.69%) 0.8105*Cl 8 s(32.72%)p 2.05(66.95%)d 0.01(0.33%)

0.0000 0.0000 0.5714 -0.0248 0.0022

0.0000 -0.0300 0.0011 0.0000 -0.2149

0.0081 0.0000 -0.7883 0.0296 0.0010

0.0035 0.0254 -0.0034 0.0518

11. (1.99399) BD (2) B 4 -Cl 8

(7.05%) 0.2655* B 4 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)

0.0000 -0.0001 0.0000 0.0000 0.0004

0.0000 0.9585 -0.0751 -0.2617 0.0205

0.0023 -0.0002 0.0672 -0.0304 -0.0351
 (92.95%) 0.9641*Cl 8 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)
 0.0000 0.0000 -0.0001 0.0000 0.0000
 0.0000 0.0004 0.0000 0.0000 0.9644
 0.0088 0.0000 -0.2630 -0.0024 -0.0009
 0.0002 -0.0224 0.0065 0.0114

12. (1.99399) BD (3) B 4 -Cl 8

(7.05%) 0.2655* B 4 s(0.00%)p 1.00(99.33%)d 0.01(0.67%)
 0.0000 0.0000 0.0000 0.0000 0.9929
 -0.0778 -0.0099 0.0008 -0.0350 0.0027
 0.0114 0.0807 -0.0010 0.0038 -0.0050

(92.95%) 0.9641*Cl 8 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.9989 0.0091 0.0000 -0.0100
 -0.0001 0.0000 -0.0353 -0.0003 -0.0070
 -0.0250 0.0005 -0.0010 0.0015

13. (1.99711) CR (1) B 1 s(100.00%)p 0.00(0.00%)

1.0000 0.0001 0.0000 0.0000 -0.0001
 0.0000 -0.0001 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000 0.0000

B4Cl2F2

(Occupancy) Bond orbital/ Coefficients/ Hybrids

1. (1.99920) BD (1) B 1 - F 7

(16.86%) 0.4106* B 1 s(29.83%)p 2.34(69.78%)d 0.01(0.39%)

-0.0003 0.5402 -0.0796 -0.0103 0.0000

0.0000 0.4772 0.0208 -0.6847 -0.0297

0.0000 0.0000 -0.0504 -0.0171 0.0332

(83.14%) 0.9118* F 7 s(52.34%)p 0.91(47.50%)d 0.00(0.16%)

0.0000 0.7234 0.0070 0.0004 0.0000

0.0000 -0.3876 0.0031 0.5699 -0.0049

0.0000 0.0000 -0.0323 -0.0111 0.0211

2. (1.99823) BD (1) B 2 -Cl 5

(34.14%) 0.5843* B 2 s(31.35%)p 2.18(68.31%)d 0.01(0.34%)

-0.0001 0.5527 -0.0892 -0.0044 -0.7083

-0.0426 -0.4222 -0.0358 0.0000 0.0000

0.0469 0.0000 0.0000 0.0202 -0.0286

(65.86%) 0.8115*Cl 5 s(32.30%)p 2.09(67.37%)d 0.01(0.34%)

0.0000 0.0000 0.5677 -0.0261 0.0021

0.0000 0.6241 -0.0260 0.0000 0.5321

-0.0187 0.0000 0.0000 0.0000 0.0485

0.0000 0.0000 0.0134 -0.0288

3. (1.99515) BD (2) B 2 -Cl 5

(7.14%) 0.2673* B 2 s(0.00%)p 1.00(99.32%)d 0.01(0.68%)

0.0000 0.0000 0.0000 0.0000 0.0001

0.0000 -0.0002 0.0000 0.9943 -0.0671

0.0000 -0.0718 -0.0409 0.0000 0.0000

(92.86%) 0.9636*Cl 5 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)

0.0000 0.0000 0.0000 0.0000 0.0000

0.0000 0.0001 0.0000 0.0000 -0.0001

0.0000 0.0000 0.9996 0.0092 0.0000

0.0211 0.0158 0.0000 0.0000

4. (1.99414) BD (3) B 2 -Cl 5

(6.98%) 0.2641* B 2 s(0.07%)p99.99(99.24%)d 9.70(0.69%)

0.0001 -0.0265 -0.0002 -0.0025 -0.5240

0.0465 0.8445 -0.0508 0.0002 0.0000

-0.0237 0.0000 0.0000 0.0786 0.0118

(93.02%) 0.9645*Cl 5 s(0.16%)p99.99(99.77%)d 0.42(0.07%)

0.0000 0.0000 -0.0400 0.0010 -0.0002

0.0000 -0.6265 -0.0047 0.0000 0.7779

0.0079 0.0000 0.0002 0.0000 0.0048

0.0000 0.0000 -0.0253 0.0016

5. (1.99920) BD (1) B 3 - F 8

(16.86%) 0.4106* B 3 s(29.83%)p 2.34(69.78%)d 0.01(0.39%)

-0.0003 0.5402 -0.0796 -0.0103 0.0000

0.0000 0.4771 0.0208 0.6847 0.0297

0.0000 0.0000 0.0504 -0.0171 0.0332

(83.14%) 0.9118* F 8 s(52.34%)p 0.91(47.50%)d 0.00(0.16%)

0.0000 0.7234 0.0070 0.0004 0.0000

0.0000 -0.3875 0.0031 -0.5699 0.0049

0.0000 0.0000 0.0323 -0.0111 0.0211

6. (1.99823) BD (1) B 4 -Cl 6

(34.14%) 0.5843* B 4 s(31.35%)p 2.18(68.31%)d 0.01(0.34%)

0.0001 -0.5527 0.0892 0.0044 -0.7083

-0.0426 0.4222 0.0358 0.0001 0.0000

0.0469 0.0000 0.0000 -0.0202 0.0286

(65.86%) 0.8115*Cl 6 s(32.30%)p 2.09(67.37%)d 0.01(0.34%)

0.0000 0.0000 -0.5677 0.0261 -0.0021
 0.0000 0.6241 -0.0260 0.0000 -0.5321
 0.0187 0.0000 0.0000 0.0000 0.0485
 0.0000 0.0000 -0.0134 0.0288

7. (1.99515) BD (2) B 4 -Cl 6

(7.14%) 0.2673* B 4 s(0.00%)p 1.00(99.32%)d 0.01(0.68%)
 0.0000 0.0000 0.0000 0.0000 -0.0002
 0.0000 -0.0004 0.0000 0.9943 -0.0671
 0.0000 0.0718 -0.0409 0.0000 0.0000
 (92.86%) 0.9636*Cl 6 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0003 0.0000 0.0000 -0.0003
 0.0000 0.0000 0.9996 0.0092 0.0000
 -0.0211 0.0158 0.0000 0.0000

8. (1.99414) BD (3) B 4 -Cl 6

(6.98%) 0.2641* B 4 s(0.07%)p99.99(99.24%)d 9.72(0.69%)
 0.0001 -0.0265 -0.0002 -0.0025 0.5240
 -0.0465 0.8444 -0.0508 0.0005 0.0000
 0.0237 0.0000 0.0000 0.0786 0.0118
 (93.02%) 0.9645*Cl 6 s(0.16%)p99.99(99.77%)d 0.42(0.07%)
 0.0000 0.0000 -0.0400 0.0010 -0.0002
 0.0000 0.6265 0.0047 0.0000 0.7779
 0.0079 0.0000 0.0005 0.0000 -0.0048
 0.0000 0.0000 -0.0253 0.0016

9. (1.99730) CR (1) B 1 s(100.00%)p 0.00(0.00%)

1.0000 0.0002 0.0000 0.0000 0.0000
 0.0000 0.0001 0.0000 -0.0002 0.0000

0.0000 0.0000 0.0000 0.0000 0.0000

B4F4

1. (1.99938) BD (1) B 1 - F 5

(16.87%) 0.4108* B 1 s(30.85%)p 2.23(68.75%)d 0.01(0.40%)

-0.0002 0.5503 -0.0746 -0.0118 0.6867

0.0397 -0.3725 -0.0215 -0.2737 -0.0158

-0.0408 -0.0300 0.0163 0.0266 -0.0212

(83.13%) 0.9117* F 5 s(52.18%)p 0.91(47.66%)d 0.00(0.16%)

0.0000 0.7223 0.0070 0.0005 -0.5727

0.0050 0.3106 -0.0027 0.2283 -0.0020

-0.0258 -0.0190 0.0103 0.0168 -0.0134

2. (1.99938) BD (1) B 2 - F 8

(16.87%) 0.4108* B 2 s(30.85%)p 2.23(68.75%)d 0.01(0.40%)

-0.0002 0.5503 -0.0746 -0.0118 -0.6499

-0.0376 -0.4992 -0.0289 -0.1166 -0.0067

0.0518 0.0121 0.0093 0.0138 -0.0297

(83.13%) 0.9117* F 8 s(52.18%)p 0.91(47.66%)d 0.00(0.16%)

0.0000 0.7223 0.0070 0.0005 0.5421

-0.0048 0.4163 -0.0037 0.0971 -0.0009

0.0328 0.0077 0.0059 0.0088 -0.0188

3. (1.99938) BD (1) B 3 - F 6

(16.87%) 0.4107* B 3 s(30.85%)p 2.23(68.75%)d 0.01(0.40%)

-0.0002 0.5503 -0.0746 -0.0118 -0.1159

-0.0067 0.7058 0.0408 -0.4167 -0.0241

-0.0131 0.0077 -0.0469 -0.0387 -0.0076

(83.13%) 0.9117* F 6 s(52.18%)p 0.91(47.66%)d 0.00(0.16%)

0.0000 0.7223 0.0070 0.0005 0.0967

-0.0008 -0.5886 0.0052 0.3475 -0.0031

-0.0083 0.0049 -0.0297 -0.0245 -0.0048

4. (1.99938) BD (1) B 4 - F 7

(16.87%) 0.4107* B 4 s(30.85%)p 2.23(68.75%)d 0.01(0.40%)

-0.0002 0.5503 -0.0746 -0.0118 0.0792

0.0046 0.1660 0.0096 0.8071 0.0467

0.0021 0.0102 0.0214 -0.0017 0.0585

(83.13%) 0.9117* F 7 s(52.18%)p 0.91(47.66%)d 0.00(0.16%)

0.0000 0.7223 0.0070 0.0005 -0.0661

0.0006 -0.1384 0.0012 -0.6731 0.0059

0.0013 0.0065 0.0135 -0.0011 0.0370

5. (1.99764) CR (1) B 1 s(100.00%)p 0.00(0.00%)

1.0000 0.0001 0.0000 0.0000 0.0002

0.0000 -0.0001 0.0000 -0.0001 0.0000

0.0000 0.0000 0.0000 0.0000 0.0000