```
EMIM-ALCl4 - JPCB 2002 v.106 p.3546
units kJ
molecules 2
EMIM
nummols 128
atoms 19
CR     12.011000000  -0.11000 1
NA     14.006740000   0.15000 1
CW     12.011000000  -0.13000 1
CW     12.011000000  -0.13000 1
NA     14.006740000   0.15000 1
HCR     1.007940000   0.21000 1
HCW     1.007940000   0.21000 1
HCW     1.007940000   0.21000 1
C1     12.011000000  -0.17000 1
H1      1.007940000   0.13000 1
H1      1.007940000   0.13000 1
H1      1.007940000   0.13000 1
C1     12.011000000  -0.17000 1
H1      1.007940000   0.13000 1
H1      1.007940000   0.13000 1
C2     12.011000000  -0.05000 1
HC      1.007940000   0.06000 1
HC      1.007940000   0.06000 1
HC      1.007940000   0.06000 1
bonds 8
harm    1     2     3992.00000   1.3150
harm    1     5     3992.00000   1.3150
harm    2     3     3574.00000   1.3780
harm    5     4     3574.00000   1.3780
harm    2     9     2820.00000   1.4660
harm    5    13     2820.00000   1.4660
harm    3     4     4352.00000   1.3410
harm    13   16     2242.00000   1.5290
constrains 11
   1     6     1.080000
   4     8     1.080000
   3     7     1.080000
   9    10     1.090000
   9    11     1.090000
   9    12     1.090000
  13    14     1.090000
  13    15     1.090000
  16    17     1.090000
  16    18     1.090000
  16    19     1.090000
angles 33
harm   5   1   2   585.20   109.8000
harm   6   1   2   292.60   125.1000
harm   6   1   5   292.60   125.1000
harm   1   2   3   585.20   108.0000
harm   1   5   4   585.20   108.0000
harm   2   3   7   292.60   122.0000
harm   5   4   8   292.60   122.0000
```

```
harm   2   3   4   585.20   107.1000
harm   5   4   3   585.20   107.1000
harm   8   4   3   292.60   130.9000
harm   7   3   4   292.60   130.9000
harm   9   2   1   585.20   126.4000
harm  13   5   1   585.20   126.4000
harm   9   2   3   585.20   125.6000
harm  13   5   4   585.20   125.6000
harm  10   9   2   313.20   110.7000
harm  11   9   2   313.20   110.7000
harm  12   9   2   313.20   110.7000
harm  10   9  11   276.20   107.8000
harm  10   9  12   276.20   107.8000
harm  11   9  12   276.20   107.8000
harm  14  13   5   313.20   110.7000
harm  15  13   5   313.20   110.7000
harm  16  13   5   488.30   112.7000
harm  14  13  15   276.20   107.8000
harm  17  16  13   313.20   110.7000
harm  18  16  13   313.20   110.7000
harm  19  16  13   313.20   110.7000
harm  14  13  16   313.20   110.7000
harm  15  13  16   313.20   110.7000
harm  17  16  18   276.20   107.8000
harm  17  16  19   276.20   107.8000
harm  18  16  19   276.20   107.8000
dihedrals 46
cos3     6     1     2     9    0.000000   19.460000   0.000000
0.500000   0.500000
cos3     6     1     5    13    0.000000   19.460000   0.000000
0.500000   0.500000
cos3     6     1     2     3    0.000000   19.460000   0.000000
0.500000   0.500000
cos3     6     1     5     4    0.000000   19.460000   0.000000
0.500000   0.500000
cos3     1     2     3     7    0.000000   12.550000   0.000000
0.500000   0.500000
cos3     1     5     4     8    0.000000   12.550000   0.000000
0.500000   0.500000
cos3     1     2     3     4    0.000000   12.550000   0.000000
0.000000   0.000000
cos3     1     5     4     3    0.000000   12.550000   0.000000
0.000000   0.000000
cos3     2     3     4     8    0.000000   44.980000   0.000000
0.500000   0.500000
cos3     5     4     3     7    0.000000   44.980000   0.000000
0.500000   0.500000
cos3     2     3     4     5    0.000000   44.980000   0.000000
0.000000   0.000000
cos3     2     1     5     4    0.000000   19.460000   0.000000
0.000000   0.000000
cos3     5     1     2     3    0.000000   19.460000   0.000000
0.000000   0.000000
cos3     2     1     5    13    0.000000   19.460000   0.000000
```

```
0.500000   0.500000
cos3     5     1     2     9    0.000000   19.460000   0.000000
0.500000   0.500000
cos3     7     3     4     8    0.000000   44.980000   0.000000
0.500000   0.500000
cos3     3     4     5    13    0.000000   12.550000   0.000000
0.500000   0.500000
cos3     4     3     2     9    0.000000   12.550000   0.000000
0.500000   0.500000
cos3     7     3     2     9    0.000000   12.550000   0.000000
0.500000   0.500000
cos3     8     4     5    13    0.000000   12.550000   0.000000
0.500000   0.500000
cos3    10     9     2     1    0.000000    0.000000   0.000000
0.500000   0.500000
cos3    11     9     2     1    0.000000    0.000000   0.000000
0.500000   0.500000
cos3    12     9     2     1    0.000000    0.000000   0.000000
0.500000   0.500000
cos3    10     9     2     3    0.000000    0.000000   0.519000
0.500000   0.500000
cos3    11     9     2     3    0.000000    0.000000   0.519000
0.500000   0.500000
cos3    12     9     2     3    0.000000    0.000000   0.519000
0.500000   0.500000
cos3    14    13     5     1    0.000000    0.000000   0.000000
0.500000   0.500000
cos3    15    13     5     1    0.000000    0.000000   0.000000
0.500000   0.500000
cos3    14    13     5     4    0.000000    0.000000   0.519000
0.500000   0.500000
cos3    15    13     5     4    0.000000    0.000000   0.519000
0.500000   0.500000
cos3    14    13    16    17    0.000000    0.000000   1.330500
0.500000   0.500000
cos3    14    13    16    18    0.000000    0.000000   1.330500
0.500000   0.500000
cos3    14    13    16    19    0.000000    0.000000   1.330500
0.500000   0.500000
cos3    15    13    16    17    0.000000    0.000000   1.330500
0.500000   0.500000
cos3    15    13    16    18    0.000000    0.000000   1.330500
0.500000   0.500000
cos3    15    13    16    19    0.000000    0.000000   1.330500
0.500000   0.500000
cos3    16    13     5     1   -5.269100    0.000000   0.000000
0.500000   0.500000
cos3    16    13     5     4   -7.153500    6.106400   0.793900
0.500000   0.500000
cos3    17    16    13     5    0.000000    0.000000   0.367000
0.500000   0.500000
cos3    18    16    13     5    0.000000    0.000000   0.367000
0.500000   0.500000
cos3    19    16    13     5    0.000000    0.000000   0.367000
```

```
0.500000   0.500000
cos3     1     3     2     9    0.000000    8.370000   0.000000
0.500000   0.500000
cos3     1     4     5    13    0.000000    8.370000   0.000000
0.500000   0.500000
cos3     2     5     1     6    0.000000    9.200000   0.000000
0.500000   0.500000
cos3     5     3     4     8    0.000000    9.200000   0.000000
0.500000   0.500000
cos3     2     4     3     7    0.000000    9.200000   0.000000
0.500000   0.500000
finish
alumcl
nummols 128
atoms 5
AL     26.9815400000   0.90920 1
CL     35.4530000000  -0.47730 4
bonds 4
harm    1     2      485.34000   2.1700
harm    1     3      485.34000   2.1700
harm    1     4      485.34000   2.1700
harm    1     5      485.34000   2.1700
angles 6
harm   3   1   2   209.20   109.5000
harm   4   1   2   209.20   109.5000
harm   5   1   2   209.20   109.5000
harm   4   1   3   209.20   109.5000
harm   5   1   3   209.20   109.5000
harm   5   1   4   209.20   109.5000
finish
vdW 66
CR    CR    lj    0.29288000 3.55000000
CR    NA    lj    0.45642051 3.39669000
CR    CW    lj    0.29288000 3.55000000
CR    HCR   lj    0.19173497 2.93104100
CR    HCW   lj    0.19173497 2.93104100
CR    C1    lj    0.28438685 3.52491100
CR    H1    lj    0.19173497 2.97909400
CR    C2    lj    0.28438685 3.52491100
CR    HC    lj    0.19173497 2.97909400
CR    AL    lj    0.61633218 3.72613070
CR    CL    lj    0.56991571 3.51027777
NA    NA    lj    0.71128000 3.25000000
NA    CW    lj    0.45642051 3.39669000
NA    HCR   lj    0.29879737 2.80446100
NA    HCW   lj    0.29879737 2.80446100
NA    C1    lj    0.44318490 3.37268400
NA    H1    lj    0.29879737 2.85043900
NA    C2    lj    0.44318490 3.37268400
NA    HC    lj    0.29879737 2.85043900
NA    AL    lj    0.96048434 3.56521388
NA    CL    lj    0.88814949 3.35868278
CW    CW    lj    0.29288000 3.55000000
CW    HCR   lj    0.19173497 2.93104100
```

```
CW    HCW   lj    0.19173497 2.93104100
CW    C1    lj    0.28438685 3.52491100
CW    H1    lj    0.19173497 2.97909400
CW    C2    lj    0.28438685 3.52491100
CW    HC    lj    0.19173497 2.97909400
CW    AL    lj    0.61633218 3.72613070
CW    CL    lj    0.56991571 3.35102777
HCR   HCR   lj    0.12552000 2.42000000
HCR   HCW   lj    0.12552000 2.42000000
HCR   C1    lj    0.18617490 2.91032600
HCR   H1    lj    0.12552000 2.45967500
HCR   C2    lj    0.18617490 2.91032600
HCR   HC    lj    0.12552000 2.45967500
HCR   AL    lj    0.40348413 3.07646225
HCR   CL    lj    0.37309741 2.89824430
HCW   HCW   lj    0.12552000 2.42000000
HCW   C1    lj    0.18617490 2.91032600
HCW   H1    lj    0.12552000 2.45967500
HCW   C2    lj    0.18617490 2.91032600
HCW   HC    lj    0.12552000 2.45967500
HCW   AL    lj    0.40348413 3.07646225
HCW   CL    lj    0.37309741 2.89824430
C1    C1    lj    0.27614000 3.50000000
C1    H1    lj    0.18617490 2.95804000
C1    C2    lj    0.27614000 3.50000000
C1    HC    lj    0.18617490 2.95804000
C1    AL    lj    0.59845934 3.69979729
C1    CL    lj    0.55338889 3.48546984
H1    H1    lj    0.12552000 2.50000000
H1    C2    lj    0.18617490 2.95804000
H1    HC    lj    0.12552000 2.50000000
H1    AL    lj    0.40348413 3.12689942
H1    CL    lj    0.37309741 2.94575966
C2    C2    lj    0.27614000 3.50000000
C2    HC    lj    0.18617490 2.95804000
C2    AL    lj    0.59845934 3.69979729
C2    CL    lj    0.55338889 3.48546984
HC    HC    lj    0.12552000 2.50000000
HC    AL    lj    0.40348413 3.12689942
HC    CL    lj    0.37309741 2.94575966
AL    AL    lj    1.29700000 3.91100000
AL    CL    lj    1.19932189 3.68443768
CL    CL    lj    1.10900000 3.47100000
close
```