Global optimization of clusters of rigid molecules by the artificial bee colony algorithm Electronic Supplementary Information

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In this Electronic Supplementary Information, we give the geometries and force field parameters of the molecules considered in this work.

For each species, we list its geometry and force field parameters in the format that can be used by ABCluster without modification. First the geometry is given in standard XYZ format (unit: Å). After a comment line, each atom's q (no unit), ε (unit: kJ mol^{-1}) and σ (unit: Å) parameter in Equation (3) are given followed by a comment after "#".

All the parameters are taken from CHARMM36 force field:

http://mackerell.umaryland.edu/charmm_ff.shtml

Note that since CHARMM and ABCluster used different unit and formulae, the parameters from CHARMM36 force field have to be transformed for ABCluster;

$$\varepsilon_{\mathrm{ABCluster}} = \varepsilon_{\mathrm{CHARMM}} \times (-4.184)$$

$$\sigma_{\mathrm{ABCluster}} = \sigma_{\mathrm{CHARMM}} \times 2^{\frac{5}{6}}$$

For instance, if you want to find the parameters for K^+, you can find its parameters from CHARMM36 as:

```
POT     0.0      -0.0870    1.76375   ! Potassium
```

then:

$$\varepsilon_{\mathrm{ABCluster}} = -0.087 \times (-4.184) = 0.3640$$

$$\sigma_{\mathrm{ABCluster}} = 1.76375 \times 2^{\frac{5}{6}} = 3.14265$$

which is exactly what we give below.

TIP4P Water

```
4
H2O
O               0.00000000   0.00000000   0.21451132
qLP             0.00000000   0.00000000   0.06451132
H              -0.00000000   0.75695033  -0.37137096
H               0.00000000  -0.75695033  -0.37137096
TIP4P q  epsilon (kJ/mol) sigma (AA)
 0.000 0.64852 3.1536 # OT
-1.040 0.00000 0.0000 # LP
+0.520 0.00000 0.0000 # HT
+0.520 0.00000 0.0000 # HT
```

Na^+

```
1
Na(+)
Na 0.0 0.0 0.0
water_ions_tip4p  q   epsilon (kJ/mol) sigma (AA)
+1.00 0.1962 2.5137 # SOD
```

K^+

```
1
K(+)
K 0.0 0.0 0.0
water_ions_tip4p  q   epsilon (kJ/mol) sigma (AA)
+1.00 0.3640 3.14265 # POT
```

Cs^+

```
1
Cs(+)
Cs 0.0 0.0 0.0
top_all36_cgenff   q   epsilon (kJ/mol) sigma (AA)
+1.00 0.7945 3.7418  # CES
```

Gmd^+

```
10
```

```
guanidinium(+)
 C               0.00000000    0.00000000    0.00000000
 N               0.00000000    1.32851100    0.00000000
 H               0.84344100    1.85336400    0.17097300
 H              -0.84344100    1.85336400   -0.17097300
 N              -1.15052400   -0.66425600    0.00000000
 H              -2.02678100   -0.19624100    0.17097300
 H              -1.18334000   -1.65712400   -0.17097300
 N               1.15052400   -0.66425600    0.00000000
 H               2.02678100   -0.19624100   -0.17097300
 H               1.18334000   -1.65712400    0.17097300
all32_cgenff q  epsilon (kJ/mol) sigma (AA) (CG2N1, NG2P1, HGP2)
 +0.64  0.46024  3.5636 # CG2N1
 -0.80  0.83680  3.2963 # NG2P1
 +0.46  0.19246  1.7961 # HGP2
 +0.46  0.19246  1.7961 # HGP2
 -0.80  0.83680  3.2963 # NG2P1
 +0.46  0.19246  1.7961 # HGP2
 +0.46  0.19246  1.7961 # HGP2
 -0.80  0.83680  3.2963 # NG2P1
 +0.46  0.19246  1.7961 # HGP2
 +0.46  0.19246  1.7961 # HGP2
```

Cl^-

```
1
Cl(-)
Cl 0.0 0.0 0.0
water_ions_tip4p   q   epsilon (kJ/mol) sigma (AA)
-1.00 0.6276 4.0447  # CLA
```

SO_4^{2-}

```
5
SO4(2-)
 S               0.00000000    0.00000000   -0.00000000
 O               0.00000000    0.00000000    1.49000000
 O              -0.00000000   -1.40478547   -0.49666667
 O              -1.21657991    0.70239274   -0.49666667
 O               1.21657991    0.70239274   -0.49666667
(JPC,98,6225) q   epsilon sigma (kJ/mol)
 +2.4  1.0455  3.55
 -1.1  1.0455  3.15
 -1.1  1.0455  3.15
```

```
 -1.1  1.0455  3.15
 -1.1  1.0455  3.15
```

Mg^{2+}

```
1
Mg(2+)
Mg 0.0 0.0 0.0
water_ions_tip4p  q   epsilon (kJ/mol) sigma (AA)
+2.00 0.06276 2.1114 # SOD
```

CH_4

```
5
CH4
 C               0.00000000   0.00000000   0.00000000
 H               0.62834000   0.62834000   0.62834000
 H              -0.62834000  -0.62834000   0.62834000
 H              -0.62834000   0.62834000  -0.62834000
 H               0.62834000  -0.62834000  -0.62834000
all36_lipid  q epsilon sigma (kJ/mol) (CTL3, HAL3)
 -0.36  0.3263  3.6348 # CTL3
 +0.09  0.1004  2.3876 # HAL3
 +0.09  0.1004  2.3876 # HAL3
 +0.09  0.1004  2.3876 # HAL3
 +0.09  0.1004  2.3876 # HAL3
```

Coronene

```
36
Coronene
 C               0.00000000   2.85411400   0.00000000
 C               0.00000000   1.42998500   0.00000000
 C               1.23840400   0.71499300   0.00000000
 C               2.47173600   1.42705700   0.00000000
 C              -2.47173600  -1.42705700   0.00000000
 C              -2.47173600   1.42705700   0.00000000
 C              -1.23840400   0.71499300   0.00000000
 C               1.23840400  -0.71499300   0.00000000
 C               0.00000000  -1.42998500   0.00000000
 C              -1.23840400  -0.71499300   0.00000000
 C               0.00000000  -2.85411400   0.00000000
 C               2.47173600  -1.42705700   0.00000000
 H               4.63700400   1.23627600   0.00000000
```

```
 H                4.63700400   -1.23627600    0.00000000
 H                1.24785600    4.63390100    0.00000000
 H                3.38914800    3.39762600    0.00000000
 H                1.24785600   -4.63390100    0.00000000
 H                3.38914800   -3.39762600    0.00000000
 H               -1.24785600    4.63390100    0.00000000
 H               -3.38914800    3.39762600    0.00000000
 H               -4.63700400    1.23627600    0.00000000
 H               -4.63700400   -1.23627600    0.00000000
 H               -1.24785600   -4.63390100    0.00000000
 H               -3.38914800   -3.39762600    0.00000000
 C                1.25031900    3.54047500    0.00000000
 C                2.44098200    2.85304500    0.00000000
 C                3.69130100    0.68743000    0.00000000
 C                3.69130100   -0.68743000    0.00000000
 C                2.44098200   -2.85304500    0.00000000
 C                1.25031900   -3.54047500    0.00000000
 C               -1.25031900   -3.54047500    0.00000000
 C               -2.44098200   -2.85304500    0.00000000
 C               -3.69130100   -0.68743000    0.00000000
 C               -3.69130100    0.68743000    0.00000000
 C               -2.44098200    2.85304500    0.00000000
 C               -1.25031900    3.54047500    0.00000000
all36_cgenff q epsilon (kJ/mol) sigma (AA)
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
0.00 0.2929 3.55005 # CG2R61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
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```
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
```

CH_3OH

```
6
CH3OH
O               0.04687300   -0.75769200    0.00000000
H              -0.87618500   -1.05160900    0.00000000
C               0.04687300    0.66094600    0.00000000
H               1.09415100    0.97510200    0.00000000
H              -0.43709600    1.08618600    0.89315300
H              -0.43709600    1.08618600   -0.89315300
all36_cgenff   q   epsilon (kJ/mol) sigma (AA)
-0.650 0.8037 3.1449 # OG311
+0.420 0.1674 0.4000 # HGP1
-0.040 0.3264 3.6527 # CG331
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
```

C_6H_6

```
12
C6H6
 C              0.00000000    1.39649000    0.00000000
 C              1.20939600    0.69824500    0.00000000
 C              1.20939600   -0.69824500    0.00000000
 C              0.00000000   -1.39649000    0.00000000
 C             -1.20939600   -0.69824500    0.00000000
```

```
 C              -1.20939600    0.69824500    0.00000000
 H               0.00000000    2.48319100    0.00000000
 H               2.15050600    1.24159500    0.00000000
 H               2.15050600   -1.24159500    0.00000000
 H               0.00000000   -2.48319100    0.00000000
 H              -2.15050600   -1.24159500    0.00000000
 H              -2.15050600    1.24159500    0.00000000
all36_cgenff q epsilon (kJ/mol) sigma (AA)
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
-0.115 0.2929 3.55005 # CG2R61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
+0.115 0.1255 2.42003 # HGR61
```

CO_2

```
3
CO2
C               0.00000000   0.00000000   0.00000000
O               0.00000000   0.00000000   1.16912100
O               0.00000000   0.00000000  -1.16912100
all36_cgenff  q   epsilon (kJ/mol) sigma (AA)
+0.60   0.2427 2.7849   # CG2O7
-0.30   0.6904 3.0148   # OG2D5
-0.30   0.6904 3.0148   # OG2D5
```

C_6H_{12}

```
18
cyclohexane
 C              -1.27062300    0.73359500    0.22925100
 C               0.00000000    1.46718900   -0.22925100
 C               1.27062300    0.73359500    0.22925100
 C               1.27062300   -0.73359500   -0.22925100
 C               0.00000000   -1.46718900    0.22925100
 C              -1.27062300   -0.73359500   -0.22925100
 H               2.16378000    1.24925900   -0.14673000
```

```
 H               0.00000000   1.53559300  -1.32756800
 H               0.00000000   2.49851800   0.14673000
 H              -1.32986200   0.76779600   1.32756800
 H              -2.16378000   1.24925900  -0.14673000
 H               1.32986200  -0.76779600  -1.32756800
 H               2.16378000  -1.24925900   0.14673000
 H               0.00000000  -2.49851800  -0.14673000
 H               0.00000000  -1.53559300   1.32756800
 H              -1.32986200  -0.76779600  -1.32756800
 H              -2.16378000  -1.24925900   0.14673000
 H               1.32986200   0.76779600   1.32756800
all36_cgenff   q   epsilon (kJ/mol) sigma (AA)
-0.180 0.3264 3.6527 # CG331
-0.180 0.3264 3.6527 # CG331
-0.180 0.3264 3.6527 # CG331
-0.180 0.3264 3.6527 # CG331
-0.180 0.3264 3.6527 # CG331
-0.180 0.3264 3.6527 # CG331
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
+0.090 0.1004 2.3876 # HGA3
```