Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Developing accurate molecular mechanics force fields for conjugated molecular systems

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This supporting information contains the force fields optimized as described in the main paper in the format suitable as direct CHARMM style input for NAMD package [J. *Comp. Chem.* **2005,** *26*, 1781-1802]. For each of the 4 molecules considered we report a "Topology" and a "Parameter" text file. Comments are included for clarification where necessary. The definition of atom type is given in Figures 1, 5, 6, 8 of the manuscript.

1. DPP force field parameters

Topology

```
MASS   1  TC1  12.01100
MASS   2  TC2  12.01100
MASS   3  TC3  12.01100
MASS   4  TN1  14.00700
MASS   5  TO1  15.99940
MASS   6  TH0   1.00800
MASS   7  THN   1.00800

RESI LIG         0.000
GROUP            ! CHARGE
ATOM C1    TC2   0.199
ATOM C2    TC1  -0.048
ATOM C3    TC1  -0.048
ATOM C4    TC3   0.545
ATOM C5    TC3   0.545
ATOM C6    TC2   0.199
ATOM N1    TN1  -0.577
ATOM N2    TN1  -0.577
ATOM O1    TO1  -0.567
ATOM O2    TO1  -0.567
ATOM H1    TH0   0.099
ATOM H2    TH0   0.099
ATOM H3    THN   0.349
ATOM H4    THN   0.349
BOND C1   H1
BOND C1   C2
BOND C1   N2
BOND C2   C5
BOND C2   C3
BOND C3   C6
```

BOND C3 C4
BOND C4 N2
BOND C4 O2
BOND C5 O1
BOND C5 N1
BOND C6 N1
BOND C6 H2
BOND N1 H3
BOND N2 H4

Parameters

BONDs
!
!V(bond) = Kb(b - b0)**2
! b0: A
!
!atom type Kb b0
TC2 TH0 417.464 1.08479
TC1 TC2 497.299 1.36559
TC2 TN1 370.198 1.36848
TC1 TC3 284.281 1.46818
TC1 TC1 315.603 1.46055
TC3 TN1 187.424 1.42808
TC3 TO1 695.901 1.21586
THN TN1 528.533 1.01283

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!
!atom types Ktheta Theta0
!
TC2 TN1 THN 32.7552 110.611
TC2 TN1 TC3 99.2878 106.824
TC1 TC1 TC2 71.5491 97.8672
TC2 TC1 TC3 25.8204 109.812
TC1 TC3 TN1 75.8123 118.318
TC1 TC3 TO1 42.5578 161.498
TC1 TC1 TC3 85.7704 101.731
TC1 TC2 TN1 78.5709 109.891
TC1 TC2 TH0 24.9797 137.467
TC3 TN1 THN 36.3281 110.746
TH0 TC2 TN1 35.7191 124.586
TN1 TC3 TO1 76.5397 140.004

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types Kchi n delta
TC2 TN1 TC3 TC1 3.10314 2 180
TC2 TN1 TC3 TO1 2.54922 2 180

```
TC2  TC1  TC3  TO1  0.319137  2  180
TC2  TC1  TC3  TN1  0.64949  2  180
TC2  TC1  TC1  TC2  4.10166  2  180
TC2  TC1  TC1  TC3  5.70044  2  180
TC1  TC3  TN1  THN  1.35102  2  180
TC1  TC1  TC2  TN1  14.533  2  180
TC1  TC1  TC2  TH0  4.79933  2  180
TC1  TC1  TC3  TN1  9.88997  2  180
TC1  TC1  TC3  TO1  1.49564  2  180
TC1  TC2  TN1  TC3  6.70496  2  180
TC1  TC2  TN1  THN  3.13263  2  180
TC3  TN1  TC2  TH0  1.56721  2  180
TC3  TC1  TC1  TC3  7.52617  2  180
TC3  TC1  TC2  TN1  2.67995  2  180
TC3  TC1  TC2  TH0  1.0909  2  180
TO1  TC3  TN1  THN  1.34065  2  180
TH0  TC2  TN1  THN  0.567993  2  180

NONBONDED
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - !2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   !eps,1-4       Rmin/2,1-4
!
!the 1-4 scaling factor is 0.5
TC1  0.0  -0.07   2.00  0.0  -0.035   1.00
TC2  0.0  -0.07   2.00  0.0  -0.035   1.00
TC3  0.0  -0.105  2.10  0.0  -0.0525  1.05
TN1  0.0  -0.17   1.82  0.0  -0.085   0.91
TO1  0.0  -0.21   1.66  0.0  -0.015   0.83
TH0  0.0  -0.03   1.36  0.0  -0.015   0.68
THN  0.0   0      0     0.0   0       0
```

2. DCV-SN5 force field parameters

Topology

```
MASS   1 TS1  32.06000
MASS   2 TS2  32.06000
MASS   3 TS3  32.06000
MASS   4 TC1  12.01100
MASS   5 TC2  12.01100
MASS   6 TC3  12.01100
MASS   7 TC4  12.01100
MASS   8 TC5  12.01100
MASS   9 TC6  12.01100
MASS  10 TC7  12.01100
MASS  11 TC8  12.01100
MASS  12 TN1  14.00700
MASS  13 TN2  14.00700
MASS  14 TH1  1.008000
MASS  15 TH2  1.008000
MASS  16 TH3  1.008000

RESI LIG          0.000
```

```
GROUP           !charge
ATOM S1     TS1   0.080
ATOM S2     TS2   0.029
ATOM S3     TS2   0.029
ATOM C1     TC1  -0.168
ATOM C2     TC1   0.194
ATOM C3     TC2   0.054
ATOM C4     TC4  -0.151
ATOM C5     TC1  -0.167
ATOM C6     TC2   0.055
ATOM C7     TC2  -0.116
ATOM C8     TC5   0.083
ATOM C9     TC3  -0.070
ATOM C10    TC6  -0.231
ATOM C11    TC7   0.464
ATOM C12    TC7   0.389
ATOM C13    TC1   0.193
ATOM C14    TC2  -0.116
ATOM C15    TC3  -0.070
ATOM C16    TC5   0.082
ATOM C17    TC7   0.464
ATOM C18    TC4  -0.151
ATOM C19    TC6  -0.231
ATOM C20    TC7   0.389
ATOM C21    TC8   0.364
ATOM C22    TC8   0.178
ATOM N1     TN1  -0.136
ATOM N2     TN1  -0.135
ATOM N3     TN2  -0.448
ATOM N4     TN2  -0.459
ATOM N5     TN2  -0.459
ATOM N6     TN2  -0.448
ATOM H1     TH1   0.102
ATOM H2     TH2   0.153
ATOM H3     TH2   0.153
ATOM H4     TH1   0.102
ATOM H5     TH3  -0.000167
ATOM H6     TH3  -0.000167
ATOM H7     TH3  -0.000167
ATOM H8     TH3  -0.000167
ATOM H9     TH3  -0.000167
ATOM H10    TH3  -0.000167

BOND H7   C21
BOND H10  C22
BOND C21  H5
BOND C21  N2
BOND C21  H6
BOND N5   C11
BOND C11  C10
BOND N6   C12
BOND C12  C10
BOND C10  C8
BOND C8   H1
BOND C8   C4
BOND S2   C4
BOND S2   C2
BOND C4   C9
BOND C9   C7
BOND C9   H2
```

BOND C2 C7
BOND C2 C1
BOND C7 N1
BOND N1 C6
BOND N1 C22
BOND C1 C6
BOND C1 S1
BOND C6 C3
BOND S1 C5
BOND C3 C5
BOND C3 N2
BOND C5 C13
BOND H3 C15
BOND N2 C14
BOND C14 C13
BOND C14 C15
BOND C13 S3
BOND C15 C18
BOND C18 S3
BOND C18 C16
BOND H4 C16
BOND C16 C19
BOND H8 C22
BOND C19 C20
BOND C19 C17
BOND C20 N3
BOND C17 N4
BOND C22 H9

Parameters

BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb b0
TC1 TS1 224.615 1.75983
TC4 TS2 176.728 1.76622
TC1 TS2 232.414 1.74496
TC1 TC2 368.499 1.41454
TC1 TC1 405.219 1.39889
TC2 TN1 354.177 1.38777
TC3 TC4 431.495 1.38702
TC2 TC2 323.37 1.40606
TC5 TH1 381.647 1.08662
TC4 TC5 364.115 1.39766
TC2 TC3 413.581 1.39431
TC3 TH2 394.265 1.08454
TC5 TC6 488.292 1.36018
TC6 TC7 366.499 1.43769
TC7 TN2 1351.92 1.16677
TC8 TH3 368.169 1.09659
TC8 TN1 297.682 1.44694

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2

!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!
!atom types Ktheta Theta0 Kub S0
TC1 TC1 TS1 31.7676 126.39
TC2 TC1 TS1 47.4843 107.75
TC3 TC4 TS2 60.9772 112.8
TC1 TC1 TS2 31.9917 126.908
TC2 TC1 TS2 50.5453 106.409
TC5 TC4 TS2 39.5982 115.748
TC1 TC2 TC2 62.4797 109.582
TC1 TS1 TC1 132.534 89.7307
TC1 TC2 TN1 71.36 111.432
TC1 TC1 TC2 65.0759 103.054
TC2 TN1 TC2 97.0388 108.348
TC4 TC3 TH2 31.1449 123.609
TC2 TC3 TC4 77.1903 111.497
TC1 TS2 TC4 136.637 90.7595
TC2 TN1 TC8 44.9065 113.677
TC2 TC2 TN1 30.0028 119.151
TC2 TC3 TH2 27.1007 129.984
TC3 TC4 TC5 32.673 121.082
TC3 TC2 TN1 40.7723 127.1
TC1 TC2 TC3 48.5252 109.171
TC4 TC5 TC6 47.9589 123.977
TC6 TC5 TH1 30.0306 122.557
TC5 TC6 TC7 45.2637 124.811
TC7 TC6 TC7 41.9202 130.469
TC4 TC5 TH1 35.6697 120.985
TC6 TC7 TN2 28.7751 180.229
TH3 TC8 TN1 55.3581 106.534
TH3 TC8 TH3 37.8774 104.933

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types Kchi n delta
TS1 TC1 TC2 TC2 -0.0422196 2 180
! Note: as a result of unconstrained optimization
! some of the barriers are negative. However as they
! minimize the objective function and they yield the correct
! equilibrium structure no attempt has been made to constrain the
! optimization to allow only for positive values of the barriers.
TS1 TC1 TC2 TN1 3.63918 2 180
TS1 TC1 TC1 TC2 2.9836 2 180
TS1 TC1 TC1 TS2 0.350206 2 180
TS2 TC4 TC5 TC6 2.39079 2 180
TS2 TC4 TC5 TH1 2.55571 2 180
TS2 TC4 TC3 TC2 6.06218 2 180
TS2 TC4 TC3 TH2 4.49626 2 180
TS2 TC1 TC2 TC3 0.742171 2 180
TS2 TC1 TC2 TN1 4.13913 2 180
TS2 TC1 TC1 TC2 3.15349 2 180
TC1 TC2 TN1 TC2 11.2497 2 180

```
TC1  TC2  TN1  TC8  2.27189  2  180
TC1  TC2  TC2  TC1  11.007  2  180
TC1  TC2  TC2  TN1  2.2599  2  180
TC1  TC1  TS2  TC4  1.82118  2  180
TC1  TC1  TC2  TC3  1.99541  2  180
TC1  TC1  TC2  TN1  -3.7535  2  180
TC1  TS1  TC1  TC2  8.85275  2  180
TC1  TS1  TC1  TC1  0.910099  2  180
TC1  TC2  TC3  TC4  8.7376  2  180
TC1  TC2  TC3  TH2  1.99403  2  180
TC1  TC1  TC2  TC2  2.55825  2  180
TC1  TS2  TC4  TC5  1.34991  2  180
TC1  TS2  TC4  TC3  5.07937  2  180
TC2  TN1  TC8  TH3  0.25441  3  -1.39723
TC2  TN1  TC2  TC3  1.5887  2  180
TC2  TC2  TN1  TC2  2.2869  2  180
TC2  TC2  TN1  TC8  0.982143  2  180
TC2  TC1  TC1  TC2  23.1518  2  180
TC4  TC3  TC2  TN1  1.85504  2  180
TC4  TC5  TC6  TC7  4.29107  2  180
TC4  TS2  TC1  TC2  11.1712  2  180
TC2  TC3  TC4  TC5  4.0153  2  180
TC5  TC6  TC7  TN2  0  2  180
TC5  TC4  TC3  TH2  2.00934  2  180
TC3  TC2  TN1  TC8  1.40286  2  180
TC3  TC4  TC5  TC6  1.6609  2  180
TC3  TC4  TC5  TH1  1.69211  2  180
TC7  TC6  TC7  TN2  0  2  180
TC7  TC6  TC5  TH1  4.86382  2  180
TN1  TC2  TC3  TH2  0.449405  2  180
TN1  TC2  TC2  TN1  0.297761  2  180

NONBONDED
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - !2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   !eps,1-4       Rmin/2,1-4
TS1  0.0  -0.450  2.00  0.0  -0.450  2.00
TS2  0.0  -0.450  2.00  0.0  -0.450  2.00
TS3  0.0  -0.450  2.00  0.0  -0.450  2.00
TC1  0.0  -0.050  2.10  0.0  -0.050  2.10
TC2  0.0  -0.050  2.10  0.0  -0.050  2.10
TC3  0.0  -0.050  2.10  0.0  -0.050  2.10
TC4  0.0  -0.050  2.10  0.0  -0.050  2.10
TC5  0.0  -0.068  2.10  0.0  -0.068  2.10
TC6  0.0  -0.068  2.10  0.0  -0.068  2.10
TC7  0.0  -0.180  1.87  0.0  -0.180  1.87
TC8  0.0  -0.180  1.87  0.0  -0.180  1.87
TN1  0.0  -0.200  1.85  0.0  -0.200  1.85
TN2  0.0  -0.180  1.79  0.0  -0.180  1.79
TH1  0.0  -0.031  1.15  0.0  -0.031  1.15
TH2  0.0  -0.030  1.36  0.0  -0.030  1.36
TH3  0.0  -0.024  1.34  0.0  -0.024  1.34
```

3. TT-DPP force field parameters

Topology

```
MASS   1  TC1  12.01100
MASS   2  TC2  12.01100
MASS   3  TC3  12.01100
MASS   4  TN1  14.00700
MASS   5  TO1  15.99940
MASS   6  TH0   1.00800
MASS   7  THN   1.00800
MASS   8  TC4  12.01100
MASS   9  TC5  12.01100
MASS   10 TC6  12.01100
MASS   11 TS1  32.06000
MASS   12 TH1  1.00800
MASS   13 TC7  12.01100
MASS   14 TC8  12.01100
MASS   15 TS2  32.06000
MASS   16 TH2   1.00800

RESI  LIG    0.000000
GROUP           !charge
ATOM  C1    TC2    0.331
ATOM  C2    TC1   -0.293
ATOM  C3    TC1   -0.296
ATOM  C4    TC3    0.628
ATOM  C5    TC3    0.627
ATOM  C6    TC2    0.320
ATOM  C7    TC4   -0.076
ATOM  C8    TC5   -0.211
ATOM  C9    TC6    0.114
ATOM  C10   TC6    0.073
ATOM  C11   TC5   -0.193
ATOM  C12   TC4    0.029
ATOM  C13   TC7    0.088
ATOM  C14   TC8   -0.097
ATOM  C15   TC8   -0.247
ATOM  C16   TC7    0.197
ATOM  S1    TS1   -0.028
ATOM  S2    TS1   -0.134
ATOM  S3    TS2   -0.108
ATOM  N1    TN1   -0.321
ATOM  N2    TN1   -0.316
ATOM  O1    TO1   -0.512
ATOM  O2    TO1   -0.511
ATOM  H1    THN    0.07075
ATOM  H2    THN    0.07075
ATOM  H3    TH1    0.204
ATOM  H4    TH1    0.188
ATOM  H5    TH2    0.133
ATOM  H6    TH2    0.128
ATOM  H7    TH0    0.07075
ATOM  H8    TH0    0.07075
BOND C1   C2
BOND C1   H8
BOND C1   N1
BOND C2   C5
BOND C2   C3
```

BOND C3 C6
BOND C3 C4
BOND C4 N1
BOND C4 O1
BOND C5 O2
BOND C5 N2
BOND C6 N2
BOND C6 C7
BOND C7 C8
BOND C7 S1
BOND C8 H3
BOND C8 C9
BOND C9 S2
BOND C9 C10
BOND C10 C11
BOND C10 S1
BOND C11 C12
BOND C11 H4
BOND C12 S2
BOND C12 C13
BOND C13 C14
BOND C13 S3
BOND C14 H5
BOND C14 C15
BOND C15 H6
BOND C15 C16
BOND C16 H7
BOND C16 S3
BOND H1 N1
BOND H2 N2

Parameters

BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb b0
TC1 TC2 462.428 1.38376
TC2 TH0 408.126 1.08566
TC2 TN1 365.66 1.40591
TC1 TC3 307.142 1.4532
TC1 TC1 341.975 1.43538
TC3 TN1 258.892 1.43731
TC3 TO1 886.222 1.22342
THN TN1 519.648 1.01316
TC4 TC5 436.509 1.37214
TC4 TS1 191.683 1.76643
TC5 TH1 392.521 1.08593
TC5 TC6 415.234 1.40202
TC6 TS1 233.715 1.77597
TC6 TC6 390.622 1.41989
TC7 TC8 493.72 1.37181
TC7 TS2 222.187 1.77177
TC8 TH2 406.366 1.08631
TC8 TC8 399.442 1.40561

```
TC7  TH0  419.988  1.08384
TC2  TC4  397.84  1.42593
TC4  TC7  370.55  1.44347

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!
!atom types     Ktheta    Theta0
TC2  TN1  THN  32.9237  111.121
TC2  TN1  TC3  108.483  106.5
TC1  TC1  TC2  72.6315  98.834
TC2  TC1  TC3  29.7981  121.557
TC1  TC3  TN1  53.9075  115.105
TC1  TC3  TO1  45.2576  161.291
TC1  TC1  TC3  86.2002  96.5999
TC1  TC2  TN1  78.8412  114.618
TC1  TC2  TH0  27.5459  142.424
TC3  TN1  THN  36.4292  108.802
TN1  TC3  TO1  79.8939  140.655
TH0  TC2  TN1  38.8457  130.099
TC4  TS1  TC6  134.281  92.1637
TC4  TC5  TC6  67.1088  105.489
TC4  TC5  TH1  28.5958  123.195
TC5  TC6  TC6  63.534  107.465
TC5  TC6  TS1  32.4342  124.245
TC5  TC4  TS1  61.1379  114.127
TC6  TC6  TS1  59.2837  111.839
TC6  TC5  TH1  31.3249  126.581
TC7  TS2  TC7  134.544  92.9507
TC8  TC8  TC7  75.101  106.522
TC7  TC8  TH2  27.194  127.513
TC8  TC8  TH2  34.5566  127.935
TC8  TC7  TS2  64.6152  108.671
TC8  TC7  TH0  25.4598  122.76
TS2  TC7  TH0  30.3333  116.251
TC1  TC2  TC4  38.6123  144.882
TC2  TC4  TS1  43.9721  129.805
TC2  TC4  TC5  42.2152  137.832
TC4  TC2  TN1  55.589  135.146
TC5  TC4  TC7  40.3289  134.938
TC4  TC7  TS2  40.4437  133.306
TC4  TC7  TC8  40.0968  128.561
TC7  TC4  TS1  45.0858  135.8

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!---flexible dihedral
TC2  TN1  TC3  TC1  13.0417  2  180
TC2  TN1  TC3  TO1  1.85497  2  180
```

```
TC2  TC1  TC3  TO1  0.040975  2  180
TC2  TC1  TC3  TN1  2.00381  2  180
TC2  TC1  TC1  TC2  1.20238  2  180
TC2  TC1  TC1  TC3  14.8586  2  180
TC1  TC3  TN1  THN  2.3407  2  180
TC1  TC1  TC2  TN1  8.52045  2  180
TC1  TC1  TC3  TN1  0.847911  2  180
TC1  TC1  TC3  TO1  2.74125  2  180
TC1  TC2  TN1  TC3  5.0478  2  180
TC1  TC2  TN1  THN  2.74687  2  180
TC1  TC1  TC2  TH0  3.43317  2  180
TC3  TN1  TC2  TH0  1.67092  2  180
TC3  TC1  TC1  TC3  9.52619  2  180
TC3  TC1  TC2  TN1  0.940196  2  180
TC3  TC1  TC2  TH0  0.755843  2  180
TO1  TC3  TN1  THN  1.59168  2  180
TH0  TC2  TN1  THN  0.537781  2  180
TC4  TS1  TC6  TC6  20.9015  2  180
TC4  TS1  TC6  TC5  -0.218884  2  180
TC4  TC5  TC6  TS1  1.97818  2  180
TC4  TC5  TC6  TC6  14.2749  2  180
TC5  TC6  TC6  TC5  6.22734  2  180
TC5  TC6  TC6  TS1  -4.26608  2  180
TC5  TC4  TS1  TC6  -0.92275  2  180
TC6  TC6  TC5  TH1  2.38607  2  180
TC6  TC5  TC4  TS1  9.20688  2  180
TS1  TC6  TC6  TS1  6.27352  2  180
TS1  TC6  TC5  TH1  0.883429  2  180
TS1  TC4  TC5  TH1  4.53256  2  180
TC8  TC7  TS2  TC7  14.4311  2  180
TC7  TC8  TC8  TC7  14.0441  2  180
TC8  TC8  TC7  TS2  0.470613  2  180
TC7  TC8  TC8  TH2  0.7393  2  180
TC8  TC8  TC7  TH0  4.48206  2  180
TS2  TC7  TC8  TH2  4.83507  2  180
TH2  TC8  TC8  TH2  1.04619  2  180
TH2  TC8  TC7  TH0  1.9927  2  180
TH0  TC7  TS2  TC7  1.97718  2  180
TC1  TC1  TC2  TC4  4.41276  2  180
TC3  TC1  TC2  TC4  1.18358  2  180
TC3  TN1  TC2  TC4  0.730651  2  180
TC4  TC2  TN1  THN  0.0220463  2  180
TC2  TC4  TC5  TH1  1.07054  2  180
TC2  TC4  TC5  TC6  2.90508  2  180
TC2  TC4  TS1  TC6  1.02878  2  180
TC6  TS1  TC4  TC7  0.958873  2  180
TC6  TC5  TC4  TC7  0.322077  2  180
TC7  TC4  TC5  TH1  1.84835  2  180
TC4  TC7  TC8  TH2  2.8056  2  180
TC4  TC7  TC8  TC8  4.50669  2  180
TC4  TC7  TS2  TC7  -0.531892  2  180
!---C1-C2-C4-C5
dihedral  TC1  TC2  TC4  TC5  0.2813      1
dihedral  TC1  TC2  TC4  TC5  7.9350      2
dihedral  TC1  TC2  TC4  TC5 -0.4550      3
dihedral  TC1  TC2  TC4  TC5 -0.4514      4
dihedral  TC1  TC2  TC4  TS1  0          0
dihedral  TC5  TC4  TC2  TN1  0          0
dihedral  TS1  TC4  TC2  TN1  0          0
!---C5-C4-C7-C8
```

```
dihedral  TC5  TC4  TC7  TC8 -1.4080      1
dihedral  TC5  TC4  TC7  TC8  4.5750      2
dihedral  TC5  TC4  TC7  TC8 -0.1908      3
dihedral  TC5  TC4  TC7  TC8 -0.4583      4
!---
dihedral  TC5  TC4  TC7  TS2  0          0
dihedral  TC8  TC7  TC4  TS1  0          0
dihedral  TS1  TC4  TC7  TS2  0          0

NONBONDED
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - !2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   !eps,1-4       Rmin/2,1-4
TC1  0.0  -0.070   2.00  0.0   -0.0350   1.00
TC2  0.0  -0.070   2.00  0.0   -0.0350   1.00
TC3  0.0  -0.105   2.10  0.0   -0.0525   1.05
TN1  0.0  -0.170   1.82  0.0   -0.0850   0.91
TO1  0.0  -0.210   1.66  0.0   -0.0150   0.83
THN  0.0  -0       0     0.0   -0        0
TC4  0.0  -0.070   2.00  0.0   -0.0350   1.00
TC5  0.0  -0.070   2.00  0.0   -0.0350   1.00
TC6  0.0  -0.070   2.00  0.0   -0.0350   1.00
TS1  0.0  -0.250   2.00  0.0   -0.1250   1.00
TH1  0.0  -0.030   1.36  0.0   -0.0150   0.68
TC7  0.0  -0.070   2.00  0.0   -0.0350   1.00
TC8  0.0  -0.070   2.00  0.0   -0.0350   1.00
TS2  0.0  -0.250   2.00  0.0   -0.1250   1.00
TH2  0.0  -0.030   1.36  0.0   -0.0150   0.68
TH0  0.0  -0.030   1.36  0.0   -0.0150   0.68
```

4. DBV force field parameters (CHARMM style)

Topology

```
MASS   244 DBVTN01  14.00700
MASS   245 DBVTN02  14.00700
MASS   246 DBVTN03  14.00700
MASS   247 DBVTN04  14.00700
MASS   248 DBVTC01  12.01100
MASS   249 DBVTC02  12.01100
MASS   250 DBVTC03  12.01100
MASS   251 DBVTC04  12.01100
MASS   252 DBVTC05  12.01100
MASS   253 DBVTC06  12.01100
MASS   254 DBVTC07  12.01100
MASS   255 DBVTC08  12.01100
MASS   256 DBVTC09  12.01100
MASS   257 DBVTC10  12.01100
MASS   258 DBVTC11  12.01100
MASS   259 DBVTC12  12.01100
MASS   260 DBVTC13  12.01100
MASS   261 DBVTC14  12.01100
MASS   262 DBVTC15  12.01100
MASS   263 DBVC321  12.01100
MASS   264 DBVC2O2  12.01100
```

```
MASS   265 DBVTO01  15.99900
MASS   266 DBVO2D1  15.99900
MASS   267 DBVO311  15.99900
MASS   268 DBVTH01  1.008000
MASS   269 DBVTH02  1.008000
MASS   270 DBVTH03  1.008000
MASS   271 DBVTH04  1.008000
MASS   272 DBVTH05  1.008000
MASS   273 DBVTH06  1.008000
MASS   274 DBVHGA2  1.008000
MASS   275 DBVHGP1  1.008000

RESI  DBV   0.000000
GROUP atom type      charges
ATOM N01D DBVTN03  -0.583732
ATOM C01D DBVTC03   0.718919
ATOM C02D DBVTC01  -0.174674
ATOM C03D DBVTC02   0.085870
ATOM C04D DBVTC04   0.179120
ATOM C05D DBVTC13   0.017959
ATOM C06D DBVTC15  -0.300772
ATOM O01D DBVTO01  -0.588453
ATOM C07D DBVTC05  -0.239748
ATOM C08D DBVTC14  -0.131542
ATOM N02D DBVTN02  -0.454160
ATOM C09D DBVTC06   0.192956
ATOM C10D DBVTC07  -0.051512
ATOM C11D DBVTC07  -0.314178
ATOM C12D DBVTC06   0.218896
ATOM C13D DBVTC05  -0.223128
ATOM C14D DBVTC12   0.025193
ATOM C15D DBVC321   0.389772
ATOM C16D DBVC321  -0.205699
ATOM C17D DBVC2O2   0.812602
ATOM O02D DBVO2D1  -0.627020
ATOM O03D DBVO311  -0.670431
ATOM C18D DBVTC10   0.000639
ATOM N03D DBVTN01  -0.615805
ATOM C19D DBVTC04   0.256269
ATOM C20D DBVTC08  -0.215143
ATOM C21D DBVTC08  -0.012020
ATOM C22D DBVTC09   0.310537
ATOM C23D DBVTC12  -0.184231
ATOM C24D DBVC321   0.162618
ATOM C25D DBVC321  -0.026651
ATOM C26D DBVC2O2   0.779233
ATOM O04D DBVO2D1  -0.624256
ATOM O05D DBVO311  -0.683230
ATOM N04D DBVTN04  -0.838752
ATOM C27D DBVTC11   0.532437
ATOM C28D DBVTC01  -0.181345
ATOM C29D DBVTC02  -0.069188
ATOM C30D DBVTC03   0.786950
ATOM C31D DBVTC12   0.062221
ATOM C32D DBVTC14  -0.109923
ATOM C33D DBVTC15  -0.364920
ATOM O06D DBVTO01  -0.624420
ATOM H01D DBVTH06   0.338015
ATOM H02D DBVTH01   0.013873
ATOM H03D DBVTH01   0.030853
```

```
ATOM H04D DBVTH01   0.030861
ATOM H05D DBVTH02   0.152762
ATOM H06D DBVTH02   0.147096
ATOM H07D DBVTH04   0.126873
ATOM H08D DBVTH02   0.132241
ATOM H09D DBVTH05   0.361156
ATOM H10D DBVTH04   0.219764
ATOM H11D DBVTH01   0.018498
ATOM H12D DBVTH01   0.008430
ATOM H13D DBVTH01  -0.001096
ATOM H14D DBVHGA2  -0.042698
ATOM H15D DBVHGA2  -0.084127
ATOM H16D DBVHGA2   0.083462
ATOM H17D DBVHGA2   0.057769
ATOM H18D DBVHGP1   0.453554
ATOM H19D DBVTH03   0.004438
ATOM H20D DBVTH03  -0.000224
ATOM H21D DBVTH01   0.042799
ATOM H22D DBVTH01   0.118778
ATOM H23D DBVTH01   0.049510
ATOM H24D DBVHGA2  -0.004689
ATOM H25D DBVHGA2  -0.021749
ATOM H26D DBVHGA2   0.037126
ATOM H27D DBVHGA2   0.019158
ATOM H28D DBVHGP1   0.458582
ATOM H29D DBVTH06   0.384122
ATOM H30D DBVTH03  -0.061016
ATOM H31D DBVTH01   0.018576
ATOM H32D DBVTH01   0.011978
ATOM H33D DBVTH01   0.001383
ATOM H34D DBVTH02   0.126951
ATOM H35D DBVTH02   0.202014
ATOM H36D DBVTH02   0.147716
BOND C01D N01D
BOND C04D N01D
BOND H01D N01D
BOND C02D C01D
BOND C01D O01D
BOND C02D C03D
BOND C02D C05D
BOND C03D C04D
BOND C08D C03D
BOND C07D C04D
BOND C05D H02D
BOND C05D H03D
BOND C05D H04D
BOND C08D C06D
BOND C06D H05D
BOND C06D H06D
BOND C07D C09D
BOND C07D H07D
BOND C08D H08D
BOND C09D N02D
BOND C12D N02D
BOND H09D N02D
BOND C09D C10D
BOND C10D C11D
BOND C10D C14D
BOND C11D C12D
BOND C11D C15D
```

BOND C13D C12D
BOND C13D C19D
BOND C13D H10D
BOND C14D H11D
BOND C14D H12D
BOND C14D H13D
BOND C15D C16D
BOND C15D H14D
BOND C15D H15D
BOND C17D C16D
BOND C16D H16D
BOND C16D H17D
BOND C17D O02D
BOND C17D O03D
BOND H18D O03D
BOND C22D C18D
BOND C18D C27D
BOND C18D H19D
BOND C18D H20D
BOND C19D N03D
BOND C22D N03D
BOND C19D C20D
BOND C20D C21D
BOND C20D C24D
BOND C21D C22D
BOND C21D C23D
BOND C23D H21D
BOND C23D H22D
BOND C23D H23D
BOND C24D C25D
BOND C24D H24D
BOND C24D H25D
BOND C26D C25D
BOND C25D H26D
BOND C25D H27D
BOND C26D O04D
BOND C26D O05D
BOND H28D O05D
BOND C27D N04D
BOND C30D N04D
BOND H29D N04D
BOND C28D C27D
BOND C27D H30D
BOND C28D C29D
BOND C28D C31D
BOND C29D C30D
BOND C29D C32D
BOND C30D O06D
BOND C31D H31D
BOND C31D H32D
BOND C31D H33D
BOND C32D C33D
BOND C32D H34D
BOND C33D H35D
BOND C33D H36D
IMPR C17D C16D O02D O03D
IMPR C26D C25D O04D O05D

Parameters

```
BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
DBVTC03  DBVTN03  345.725  1.41232
DBVTC03  DBVTO01  847.729  1.23164
DBVTC01  DBVTC03  234.289  1.47262
DBVTC01  DBVTC02  440.926  1.35985
DBVTC01  DBVTC18  454.801  1.34006
DBVTC01  DBVTC13  275.398  1.47574
DBVTC02  DBVTC04  209.5  1.45218
DBVTC04  DBVTN03  369.511  1.40969
DBVTC13  DBVTH01  340.576  1.09602
DBVTC15  DBVTH02  389.597  1.08481
DBVTC04  DBVTC05  465.707  1.36449
DBVTC17  DBVTC16  451.662  1.36215
DBVTC05  DBVTC06  255.926  1.40409
DBVTC16  DBVTC06  275.157  1.4038
DBVTC05  DBVTH04  363.398  1.09119
DBVTC16  DBVTH04  414.187  1.09214
DBVTC02  DBVTC14  274.541  1.42248
DBVTC18  DBVTC14  282.044  1.405
DBVTC14  DBVTC15  620.679  1.33577
DBVTC14  DBVTH02  383.363  1.08992
DBVTC06  DBVTN02  403.783  1.37147
DBVTC06  DBVTC07  258.778  1.38403
DBVTC07  DBVTC07  326.092  1.40869
DBVTC07  DBVTC12  274.655  1.49729
DBVC321  DBVTC07  244.149  1.47744
DBVTC12  DBVTH01  314.878  1.09757
DBVC321  DBVC321  230.41  1.54475
DBVC321  DBVHGA2  322.001  1.09654
DBVC2O2  DBVC321  205.582  1.56848
DBVC2O2  DBVO2D1  750  1.22
DBVC2O2  DBVO311  230  1.4
DBVTC10  DBVTC11  154.42  1.48052
DBVTC10  DBVTH03  350.476  1.09544
DBVTC17  DBVTN01  316.237  1.4075
DBVTC17  DBVTC08  259.011  1.47415
DBVTC08  DBVTC08  484.273  1.34951
DBVC321  DBVTC08  217.434  1.46106
DBVTC08  DBVTC09  275.671  1.4394
DBVTC08  DBVTC12  300.017  1.48788
DBVTC09  DBVTC10  246.167  1.47658
DBVTC09  DBVTN01  527.432  1.3124
DBVTC11  DBVTN04  283.172  1.45175
DBVTC11  DBVTH03  329.942  1.10364
DBVTC01  DBVTC11  202.948  1.50658
DBVTC01  DBVTC12  600.202  1.45953
DBVTC18  DBVTC03  193.861  1.46276
DBVTC03  DBVTN04  439.917  1.39671
DBVTH06  DBVTN03  533.029  1.01041
DBVTH05  DBVTN02  412.703  1.0145
DBVHGP1  DBVO311  545  0.96
```

```
DBVTH06  DBVTN04  452.506  1.01952

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!
!atom types     Ktheta    Theta0
DBVTC05  DBVTC04  DBVTN03  56.9663  135.075
DBVTC02  DBVTC04  DBVTN03  71.6942  109.321
DBVTN03  DBVTC03  DBVTO01  83.6574  144.081
DBVTC01  DBVTC03  DBVTN03  59.5321  118.575
DBVTC03  DBVTC01  DBVTC13  42.5618  122.017
DBVTC02  DBVTC01  DBVTC03  77.6048  108.632
DBVTC03  DBVTN03  DBVTH06  36.682  115.121
DBVTC03  DBVTN03  DBVTC04  88.121  104.04
DBVTC01  DBVTC13  DBVTH01  42.3268  107.515
DBVTC01  DBVTC02  DBVTC14  44.2434  123.716
DBVTC01  DBVTC18  DBVTC14  38.8387  117.638
DBVTC01  DBVTC02  DBVTC04  82.6551  113.47
DBVTC01  DBVTC03  DBVTO01  45.7026  153.573
DBVTC02  DBVTC14  DBVTH02  35.4987  121.493
DBVTC18  DBVTC14  DBVTH02  35.088  120.885
DBVTC02  DBVTC14  DBVTC15  45.2858  125.062
DBVTC18  DBVTC14  DBVTC15  42.9597  120.279
DBVTC02  DBVTC04  DBVTC05  27.9423  115.09
DBVTC02  DBVTC01  DBVTC13  44.6834  123.971
DBVTC04  DBVTC05  DBVTH04  37.3272  119.829
DBVTC17  DBVTC16  DBVTH04  34.3461  124.313
DBVTC04  DBVTC05  DBVTC06  40.3259  131.921
DBVTC17  DBVTC16  DBVTC06  48.7466  131.129
DBVTC04  DBVTC02  DBVTC14  27.1764  116.809
DBVTC04  DBVTN03  DBVTH06  33.2986  112.899
DBVTC15  DBVTC14  DBVTH02  33.4038  127.183
DBVTC16  DBVTC06  DBVTC07  25.1173  101.866
DBVTC05  DBVTC06  DBVTC07  34.5616  130.965
DBVTC05  DBVTC06  DBVTN02  45.7496  119.845
DBVTC16  DBVTC06  DBVTN02  58.6695  124.119
DBVTC14  DBVTC15  DBVTH02  36.9603  122.76
DBVTC07  DBVTC06  DBVTN02  78.2882  108.667
DBVTC06  DBVTC07  DBVTC12  42.5268  121.142
DBVTC06  DBVTC07  DBVTC07  87.8062  111.976
DBVTC06  DBVTN02  DBVTH05  34.8733  108.805
DBVTC06  DBVTN02  DBVTC06  77.574  103.319
DBVTC06  DBVTC05  DBVTH04  33.5471  116.761
DBVTC06  DBVTC16  DBVTH04  31.5335  120.969
DBVTC07  DBVTC12  DBVTH01  44.3337  107.034
DBVC321  DBVTC07  DBVTC07  45.6275  121.123
DBVHGA2  DBVC321  DBVTC07  43.9081  109.656
DBVC321  DBVC321  DBVTC07  50.8  109.119
DBVTC07  DBVTC07  DBVTC12  32.9371  125.366
DBVC321  DBVTC07  DBVTC06  36.6388  100.711
DBVTC16  DBVTC17  DBVTC08  35.4027  124.329
DBVTC16  DBVTC17  DBVTN01  41.4499  124.655
DBVC321  DBVC321  DBVHGA2  26.5  110.1
DBVC2O2  DBVC321  DBVC321  52  108
DBVC321  DBVC2O2  DBVO311  55  110.5
DBVC321  DBVC2O2  DBVO2D1  70  125
```

DBVC2O2 DBVO311 DBVHGP1 55 115
DBVC2O2 DBVC321 DBVHGA2 33 109.5
DBVO2D1 DBVC2O2 DBVO311 50 123
DBVTC10 DBVTC11 DBVTH03 35.0933 102.66
DBVTC01 DBVTC11 DBVTC10 43.3532 105.118
DBVTC10 DBVTC11 DBVTN04 62.5371 107.085
DBVTC08 DBVTC09 DBVTC10 43.7164 119.95
DBVTC10 DBVTC09 DBVTN01 45.0304 134.619
DBVTC08 DBVTC09 DBVTN01 91.1912 113.652
DBVTC08 DBVTC17 DBVTN01 95.5814 109.737
DBVC321 DBVTC08 DBVTC17 37.5008 129.858
DBVTC17 DBVTC08 DBVTC08 71.41 104.614
DBVTC17 DBVTN01 DBVTC09 105.322 101.535
DBVHGA2 DBVC321 DBVTC08 44.11 107.912
DBVC321 DBVC321 DBVTC08 64.5401 110.695
DBVTC08 DBVTC08 DBVTC12 42.4562 122.198
DBVTC08 DBVTC08 DBVTC09 62.6181 103.427
DBVTC08 DBVTC12 DBVTH01 49.5578 106.143
DBVC321 DBVTC08 DBVTC08 51.1856 117.491
DBVTC09 DBVTC08 DBVTC12 38.2748 120.631
DBVTC09 DBVTC10 DBVTH03 38.7813 108.007
DBVTC09 DBVTC10 DBVTC11 48.2673 104.641
DBVTN04 DBVTC03 DBVTO01 87.8105 145.36
DBVTC18 DBVTC03 DBVTN04 54.5223 125.364
DBVTH03 DBVTC11 DBVTN04 51.9943 105.806
DBVTC01 DBVTC11 DBVTN04 96.7902 98.1747
DBVTC11 DBVTC01 DBVTC12 43.1125 131.421
DBVTC18 DBVTC01 DBVTC11 63.8423 112.08
DBVTC11 DBVTN04 DBVTH06 30.6421 104.15
DBVTC03 DBVTN04 DBVTC11 76.4826 103.684
DBVTC11 DBVTC10 DBVTH03 39.2563 106.51
DBVTC01 DBVTC12 DBVTH01 46.2739 108.605
DBVTC01 DBVTC18 DBVTC03 88.3219 105.779
DBVTC01 DBVTC11 DBVTH03 37.2692 103.641
DBVTC18 DBVTC03 DBVTO01 50.9505 149.849
DBVTC18 DBVTC01 DBVTC12 44.2373 132.13
DBVTC03 DBVTC18 DBVTC14 32.2641 104.141
DBVTC03 DBVTN04 DBVTH06 41.8896 113.418
DBVTH01 DBVTC13 DBVTH01 37.5682 105.232
DBVTH02 DBVTC15 DBVTH02 23.2317 122.647
DBVTH01 DBVTC12 DBVTH01 39.646 102.308
DBVHGA2 DBVC321 DBVHGA2 35.5234 106.93
DBVTH03 DBVTC10 DBVTH03 35.7938 109.05

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types Kchi n delta
DBVTN03 DBVTC04 DBVTC02 DBVTC01 -19.7238 2 180
DBVTN03 DBVTC04 DBVTC02 DBVTC14 4.36735 2 123.848
DBVTN03 DBVTC04 DBVTC05 DBVTC06 3.62498 2 178.268
DBVTN03 DBVTC04 DBVTC05 DBVTH04 6.9772 2 172.248
DBVTN03 DBVTC03 DBVTC01 DBVTC02 -2.93453 2 180
DBVTN03 DBVTC03 DBVTC01 DBVTC13 3.80405 2 180
DBVTC03 DBVTC01 DBVTC02 DBVTC04 30.0337 2 180

DBVTC03 DBVTC01 DBVTC02 DBVTC14 6.46987 2 180
DBVTC03 DBVTC01 DBVTC13 DBVTH01 0.0265139 3 26.3294
DBVTC03 DBVTN03 DBVTC04 DBVTC02 23.8501 2 171.469
DBVTC03 DBVTN03 DBVTC04 DBVTC05 2.54525 2 203.129
DBVTC01 DBVTC02 DBVTC04 DBVTC05 1.73714 2 159.87
DBVTC04 DBVTC02 DBVTC14 DBVTC15 0.976226 2 173.067
DBVTC01 DBVTC02 DBVTC14 DBVTC15 0.715736 2 197.18
DBVTC01 DBVTC18 DBVTC14 DBVTC15 0.265964 2 175.219
DBVTC01 DBVTC02 DBVTC14 DBVTH02 1.02669 2 150.547
DBVTC01 DBVTC18 DBVTC14 DBVTH02 0.76808 2 200.258
DBVTC01 DBVTC03 DBVTN03 DBVTC04 2.00293 2 52.5094
DBVTC01 DBVTC03 DBVTN03 DBVTH06 2.83239 2 202.165
DBVTC02 DBVTC14 DBVTC15 DBVTH02 4.79507 2 180
DBVTC18 DBVTC14 DBVTC15 DBVTH02 5.39753 2 180
DBVTC02 DBVTC04 DBVTN03 DBVTH06 1.82638 2 149.674
DBVTC02 DBVTC04 DBVTC05 DBVTC06 4.658 2 180
DBVTC02 DBVTC04 DBVTC05 DBVTH04 2.96319 2 180
DBVTC02 DBVTC01 DBVTC03 DBVTO01 0.592848 2 180
DBVTC02 DBVTC01 DBVTC13 DBVTH01 -0.086657 3 -26.229
DBVTC04 DBVTC05 DBVTC06 DBVTN02 3.60644 2 220.224
DBVTC17 DBVTC16 DBVTC06 DBVTN02 2.556 2 229.299
DBVTC04 DBVTC05 DBVTC06 DBVTC07 -0.900395 2 140.921
DBVTC17 DBVTC16 DBVTC06 DBVTC07 1.17956 2 149.261
DBVTC04 DBVTC02 DBVTC01 DBVTC13 5.90175 2 180
DBVTC04 DBVTC02 DBVTC14 DBVTH02 1.20718 2 186.557
DBVTC04 DBVTN03 DBVTC03 DBVTO01 4.66209 2 181.896
DBVTC13 DBVTC01 DBVTC03 DBVTO01 1.57589 2 180
DBVTC13 DBVTC01 DBVTC02 DBVTC14 3.20166 2 180
DBVTO01 DBVTC03 DBVTN03 DBVTH06 1.11463 2 171.008
DBVTC05 DBVTC06 DBVTN02 DBVTC06 7.26468 2 180
DBVTC16 DBVTC06 DBVTN02 DBVTC06 5.75384 2 180
DBVTC05 DBVTC06 DBVTN02 DBVTH05 2.97875 2 169.106
DBVTC16 DBVTC06 DBVTN02 DBVTH05 2.04184 2 172.554
DBVTC05 DBVTC06 DBVTC07 DBVTC07 2.38744 2 180
DBVTC16 DBVTC06 DBVTC07 DBVTC07 1.09828 2 180
DBVTC05 DBVTC06 DBVTC07 DBVTC12 1.50918 2 180
DBVTC05 DBVTC04 DBVTN03 DBVTH06 0.918345 2 -87.6742
DBVTC05 DBVTC04 DBVTC02 DBVTC14 4.14048 2 246.963
DBVTN02 DBVTC06 DBVTC07 DBVTC07 11.4039 2 180
DBVTN02 DBVTC06 DBVTC07 DBVC321 2.87276 2 180
DBVTN02 DBVTC06 DBVTC05 DBVTH04 1.59464 2 180
DBVTN02 DBVTC06 DBVTC16 DBVTH04 3.6182 2 180
DBVTN02 DBVTC06 DBVTC07 DBVTC12 5.77505 2 200.793
DBVTC06 DBVTC07 DBVTC07 DBVTC06 0.568221 2 180
DBVTC06 DBVTC07 DBVTC07 DBVC321 5.49041 2 180
DBVTC06 DBVTC07 DBVTC12 DBVTH01 0.320305 3 483.233
DBVTC06 DBVTN02 DBVTC06 DBVTC07 7.27348 2 180
DBVTC07 DBVTC07 DBVC321 DBVC321 3.19867 3 140.542
DBVTC07 DBVTC07 DBVC321 DBVHGA2 0.751077 3 50.3226
DBVTC07 DBVTC06 DBVTC05 DBVTH04 1.52891 2 177.076
DBVTC07 DBVTC06 DBVTC16 DBVTH04 2.10275 2 220.366
DBVTC07 DBVTC06 DBVTN02 DBVTH05 2.92506 2 186.511
DBVTC07 DBVC321 DBVC321 DBVC2O2 0.195 3 0
DBVTC07 DBVC321 DBVC321 DBVHGA2 0.195 3 0
DBVTC07 DBVTC07 DBVTC12 DBVTH01 -0.17068 3 -1.01558
DBVTC06 DBVTC16 DBVTC17 DBVTN01 3.28649 2 180
DBVTC06 DBVTC16 DBVTC17 DBVTC08 4.55264 2 180
DBVTC06 DBVTC07 DBVTC07 DBVTC12 4.51194 2 224.737
DBVTC06 DBVTC07 DBVC321 DBVC321 5.12656 3 -41.4933
DBVTC06 DBVTC07 DBVC321 DBVHGA2 0.927607 3 -126.157

DBVTC16 DBVTC17 DBVTN01 DBVTC09 2.38619 2 180
DBVTC16 DBVTC17 DBVTC08 DBVTC08 0.773602 2 180
DBVTC16 DBVTC17 DBVTC08 DBVC321 0.269602 2 180
DBVTC16 DBVTC06 DBVTC07 DBVC321 2.94333 2 180
DBVTC12 DBVTC07 DBVTC07 DBVC321 1.82264 2 180
DBVC321 DBVC321 DBVC2O2 DBVO2D1 0.05 3 0
DBVC321 DBVC321 DBVC2O2 DBVO311 0.53 2 180
DBVC321 DBVC2O2 DBVO311 DBVHGP1 2.05 2 180
DBVC2O2 DBVC321 DBVC321 DBVHGA2 0.195 3 0
DBVO2D1 DBVC2O2 DBVC321 DBVHGA2 0 3 0
DBVO2D1 DBVC2O2 DBVO311 DBVHGP1 2.05 2 180
DBVO311 DBVC2O2 DBVC321 DBVHGA2 0 3 180
DBVTC10 DBVTC11 DBVTN04 DBVTC03 1.43853 3 -247.668
DBVTC10 DBVTC11 DBVTN04 DBVTH06 0.350316 3 -4.15766
DBVTC10 DBVTC11 DBVTC01 DBVTC18 -1.795 3 -68.401
DBVTC10 DBVTC11 DBVTC01 DBVTC12 0.698846 3 -55.4296
DBVTC10 DBVTC09 DBVTN01 DBVTC17 6.64298 2 180
DBVTC10 DBVTC09 DBVTC08 DBVTC08 -0.0883436 2 180
DBVTC10 DBVTC09 DBVTC08 DBVTC12 3.24772 2 180
DBVTN01 DBVTC09 DBVTC10 DBVTC11 1.03824 3 -176.642
DBVTN01 DBVTC09 DBVTC10 DBVTH03 0.24855 3 -20.8917
DBVTN01 DBVTC09 DBVTC08 DBVTC08 5.27333 2 180
DBVTN01 DBVTC09 DBVTC08 DBVTC12 4.41929 2 180
DBVTN01 DBVTC17 DBVTC16 DBVTH04 5.06546 2 180
DBVTN01 DBVTC17 DBVTC08 DBVTC08 -1.99961 2 180
DBVTN01 DBVTC17 DBVTC08 DBVC321 2.65494 2 180
DBVTC17 DBVTC08 DBVTC08 DBVTC09 19.0142 2 180
DBVTC17 DBVTC08 DBVTC08 DBVTC12 4.9139 2 180
DBVTC17 DBVTC08 DBVC321 DBVC321 3.77536 3 -115.472
DBVTC17 DBVTC08 DBVC321 DBVHGA2 0.846632 3 18.9507
DBVTC17 DBVTN01 DBVTC09 DBVTC08 7.73293 2 180
DBVTC08 DBVC321 DBVC321 DBVC2O2 0.195 3 0
DBVTC08 DBVC321 DBVC321 DBVHGA2 0.195 3 0
DBVTC08 DBVTC08 DBVTC12 DBVTH01 0.197789 3 261.855
DBVTC08 DBVTC17 DBVTC16 DBVTH04 3.5316 2 180
DBVTC08 DBVTC17 DBVTN01 DBVTC09 16.9094 2 180
DBVTC08 DBVTC09 DBVTC10 DBVTC11 2.08916 3 57.8861
DBVTC08 DBVTC09 DBVTC10 DBVTH03 0.795633 3 51.0688
DBVTC08 DBVTC08 DBVC321 DBVC321 4.25414 3 71.786
DBVTC08 DBVTC08 DBVC321 DBVHGA2 0.667872 3 140.149
DBVTC09 DBVTC08 DBVTC08 DBVC321 4.42144 2 180
DBVTC09 DBVTC08 DBVTC12 DBVTH01 0.120725 3 22.3857
DBVTC09 DBVTC10 DBVTC11 DBVTN04 2.48384 3 8.96658
DBVTC09 DBVTC10 DBVTC11 DBVTC01 -4.26999 3 -77.1944
DBVTC09 DBVTC10 DBVTC11 DBVTH03 0.468432 3 47.3634
DBVTC12 DBVTC08 DBVTC08 DBVC321 1.85824 2 180
DBVTN04 DBVTC03 DBVTC18 DBVTC01 0.372138 2 180
DBVTN04 DBVTC03 DBVTC18 DBVTC14 1.02539 2 180
DBVTN04 DBVTC11 DBVTC10 DBVTH03 -0.595391 3 -89.765
DBVTN04 DBVTC11 DBVTC01 DBVTC18 3.28538 3 -118.928
DBVTN04 DBVTC11 DBVTC01 DBVTC12 1.53613 3 128.3
DBVTC11 DBVTC01 DBVTC18 DBVTC03 13.6535 2 180
DBVTC11 DBVTC01 DBVTC18 DBVTC14 8.02488 2 180
DBVTC11 DBVTC01 DBVTC12 DBVTH01 0.223909 3 -1.14578
DBVTC11 DBVTN04 DBVTC03 DBVTC18 6.63711 2 180
DBVTC11 DBVTN04 DBVTC03 DBVTO01 6.21054 2 191.852
DBVTC01 DBVTC18 DBVTC03 DBVTO01 0.883499 2 267.929
DBVTC01 DBVTC11 DBVTC10 DBVTH03 1.13395 3 -37.9283
DBVTC01 DBVTC11 DBVTN04 DBVTC03 2.08849 3 -154
DBVTC01 DBVTC11 DBVTN04 DBVTH06 0.279066 3 -32.8653

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DBVTC18  DBVTC03  DBVTN04  DBVTH06  3.62673  2  186.57
DBVTC18  DBVTC01  DBVTC11  DBVTH03  1.52792  3  70.7487
DBVTC18  DBVTC01  DBVTC12  DBVTH01  0.100756  3  -213.411
DBVTC03  DBVTC18  DBVTC01  DBVTC12  8.92411  2  180
DBVTC03  DBVTC18  DBVTC14  DBVTC15  1.49456  2  181.554
DBVTC03  DBVTC18  DBVTC14  DBVTH02  0.760186  2  159.592
DBVTC03  DBVTN04  DBVTC11  DBVTH03  1.3352  3  -121.713
DBVTC12  DBVTC01  DBVTC11  DBVTH03  -0.23958  3  -34.9148
DBVTC12  DBVTC01  DBVTC18  DBVTC14  3.90534  2  180
DBVTC14  DBVTC18  DBVTC03  DBVTO01  1.40851  2  180
DBVTO01  DBVTC03  DBVTN04  DBVTH06  1.76067  2  192.413
DBVTH02  DBVTC15  DBVTC14  DBVTH02  5.26304  2  180
DBVHGA2  DBVC321  DBVC321  DBVHGA2  0.22  3  0
DBVTH03  DBVTC10  DBVTC11  DBVTH03  0.224431  3  63.9842
DBVTH06  DBVTN04  DBVTC11  DBVTH03  0.347083  3  -10.0499

IMPROPER
!
!V(improper) = Kpsi(psi - psi0)**2
!
!Kpsi: kcal/mole/rad**2
!psi0: degrees
!note that the second column of numbers (0) is !ignored
!
!atom types          Kpsi                   psi0
DBVC2O2  DBVC321  DBVO2D1  DBVO311  65  0  0


NONBONDED
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - !2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   !eps,1-4       Rmin/2,1-4
DBVTN03  0.0  -0.2     1.8500  0.0  -0.2     1.8500
DBVTC03  0.0  -0.02    1.2000  0.0  -0.02    1.2000
DBVTC01  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC02  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC18  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC04  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC17  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC13  0.0  -0.078   2.0500  0.0  -0.078   2.0500
DBVTC15  0.0  -0.064   2.0800  0.0  -0.064   2.0800
DBVTO01  0.0  -0.12    1.7000  0.0  -0.12    1.7000
DBVTC05  0.0  -0.068   2.0900  0.0  -0.068   2.0900
DBVTC16  0.0  -0.068   2.0900  0.0  -0.068   2.0900
DBVTC14  0.0  -0.068   2.0900  0.0  -0.068   2.0900
DBVTN02  0.0  -0.2     1.8500  0.0  -0.2     1.8500
DBVTC06  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC07  0.0  -0.05    2.1000  0.0  -0.05    2.1000
DBVTC12  0.0  -0.078   2.0500  0.0  -0.078   2.0500
DBVC321  0.0  -0.056   2.0100  0.0  -0.056   2.0100
DBVC2O2  0.0  -0.098   1.7000  0.0  -0.098   1.7000
DBVO2D1  0.0  -0.12    1.7000  0.0  -0.12    1.7000
DBVO311  0.0  -0.1921  1.7650  0.0  -0.1921  1.7650
DBVTC10  0.0  -0.056   2.0100  0.0  -0.056   2.0100
DBVTN01  0.0  -0.2     1.8500  0.0  -0.2     1.8500
DBVTC08  0.0  -0.05    2.1000  0.0  -0.05    2.1000
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DBVTC09	0.0	-0.02	2.2000	0.0	-0.02	2.2000
DBVTN04	0.0	-0.2	1.8500	0.0	-0.2	1.8500
DBVTC11	0.0	-0.036	2.0100	0.0	-0.036	2.0100
DBVTH06	0.0	-0.046	0.2245	0.0	-0.046	0.2245
DBVTH01	0.0	-0.024	1.3400	0.0	-0.024	1.3400
DBVTH02	0.0	-0.026	1.2600	0.0	-0.026	1.2600
DBVTH04	0.0	-0.031	1.2500	0.0	-0.031	1.2500
DBVTH05	0.0	-0.046	0.2245	0.0	-0.046	0.2245
DBVHGA2	0.0	-0.035	1.3400	0.0	-0.035	1.3400
DBVHGP1	0.0	-0.046	0.2245	0.0	-0.046	0.2245
DBVTH03	0.0	-0.035	1.3400	0.0	-0.035	1.3400