Supplementary Material

Evaluation of the Effect of Nickel Clusters on the Formation of Incipient Soot Particles from Polycyclic Aromatic Hydrocarbons through ReaxFF Molecular Dynamics Simulations

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1. Additional figures

The mechanism of PAH binding through physical and chemical nucleation has been observed to be similar for the different types of PAHs studied in this work. Each case is repeated three times with three different initial trajectories. The trends observed in different trajectories lead to similar conclusions, the difference being the initiation time and the size of the cluster. Some additional figures have been included here for further clarification.

1.1 Physical Nucleation

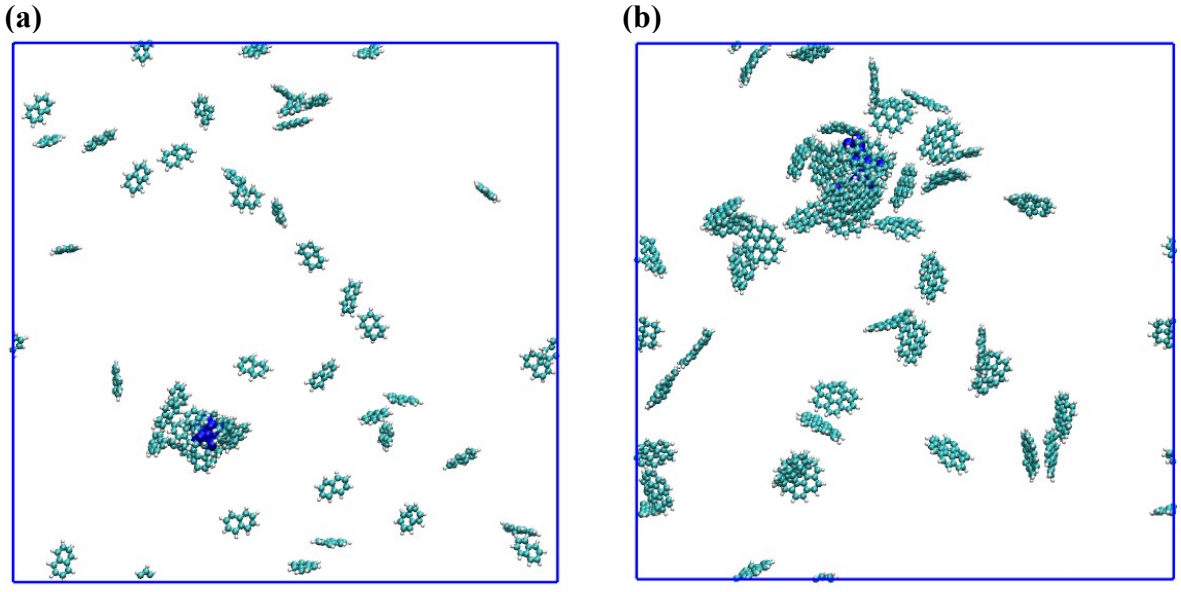

Figure S1: Snapshots demonstrating physical nucleation of soot particles obtained at the end (2000 ps) of ReaxFF-MD simulations for systems containing 50 (a) naphthalene molecules and Ni_{13} cluster

at 800 K, and (b) coronene molecules and Ni_{13} cluster at 1200 K. Cyan, white and blue spheres represent carbon, hydrogen and nickel atoms, respectively.

1.2 Chemical Nucleation

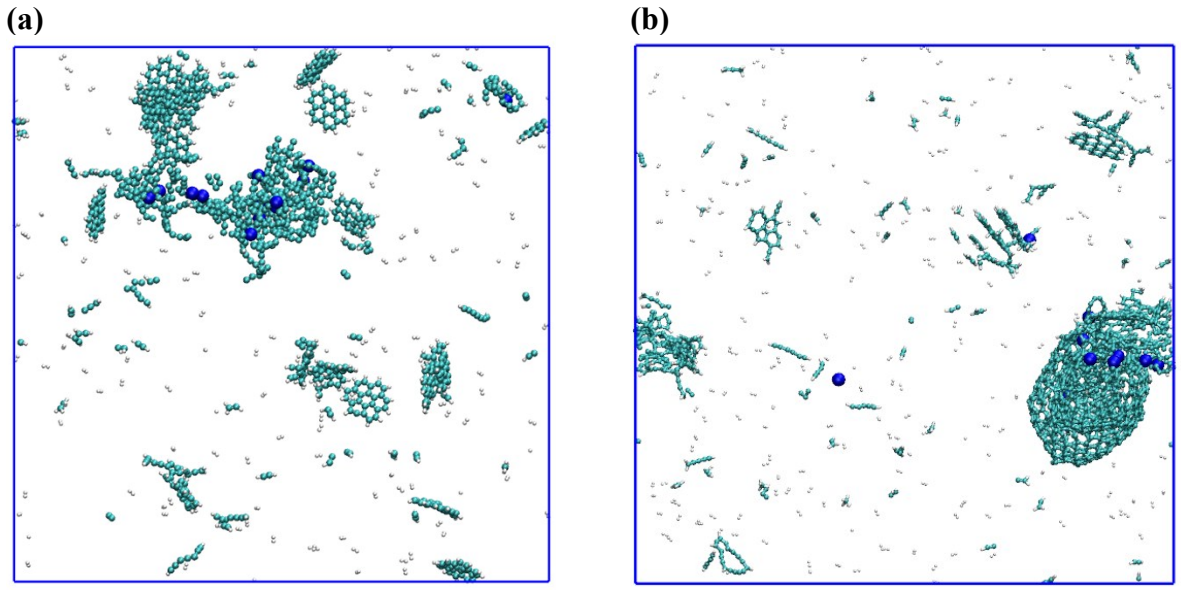

Figure S2: Snapshots demonstrating chemical nucleation of soot particles obtained at the end (2000ps) of ReaxFF-MD simulations for systems containing 50 (a) coronene molecules and Ni_{13} cluster at 2500 K, and (b) ovalene molecules and Ni_{13} cluster at 2500 K. Cyan, white and blue spheres represent carbon, hydrogen and nickel atoms, respectively.

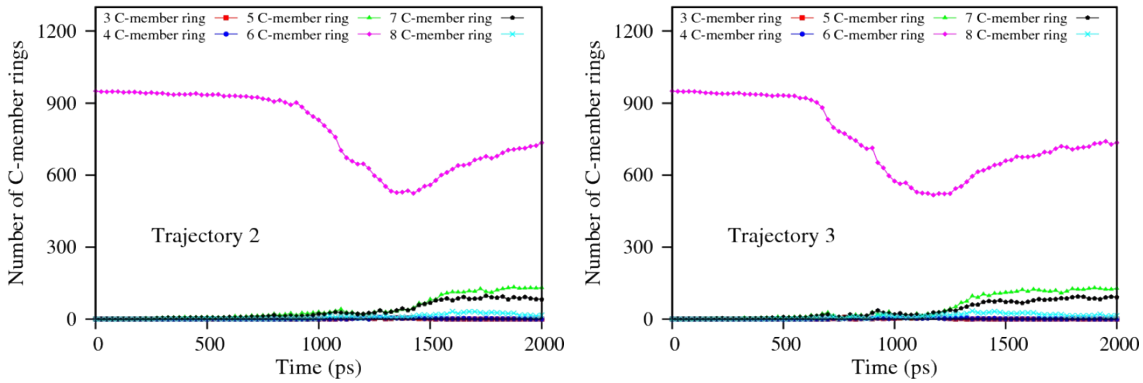

Figure S6: Ring count statistics during the soot nucleation from circumcoronene monomers as a function of simulation time at 2500 K for two additional simulations with different initial trajectories.

2. Mueller et al. Ni/C/H/O force field parameters

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Reactive MD-force field: Jan28 2014  Ni/C/H/O/vacancy + Ni/COx
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```
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
   26.5405 !Valency angle conjugation parameter
    1.7224 !Triple bond stabilisation parameter
    6.8702 !Triple bond stabilisation parameter
   70.0000 !C2-correction
    1.0588 !Undercoordination parameter
    4.6000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
  -70.5044 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.1000 !Cutoff for bond order (*100)
    2.1365 !Valency angle conjugation parameter
    0.6991 !Overcoordination parameter
   50.0000 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    2.6962 !Valency angle conjugation parameter
 10    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
            alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
            cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
            ov/un;val1;n.u.;val3,vval4
 C    1.3674   4.0000  12.0000   2.0453   0.1444   0.8485   1.1706
4.0000
      9.0000   1.5000   4.0000  30.0000  79.5548   4.8446   7.0000
0.0000
      1.1168   0.0000 181.0000  14.2732  24.4406   6.7313   0.8563
0.0000
     -4.1021   5.0000   1.0564   4.0000   2.9663   0.0000   0.0000
0.0000
```

```
 H    0.8930   1.0000   1.0080   1.3550   0.0930   0.8203  -0.1000
1.0000
      8.2230  33.2894   1.0000   0.0000 121.1250   3.7248   9.6093
1.0000
     -0.1000   0.0000  61.6606   3.0408   2.4197   0.0003   1.0698
0.0000
    -19.4571   4.2733   1.0338   1.0000   2.8793   0.0000   0.0000
0.0000
 O    1.2450   2.0000  15.9990   2.3890   0.1000   1.0898   1.0548
6.0000
      9.7300  13.8449   4.0000  37.5000 116.0768   8.5000   8.3122
2.0000
      0.9049   0.4056  59.0626   3.5027   0.7640   0.0021   0.9745
0.0000
     -3.5500   2.9000   1.0493   4.0000   2.9225   0.0000   0.0000
0.0000
 Fe   1.9029   3.0000  55.8450   2.0990   0.1181   0.4744  -1.6836
3.0000
     10.8548   2.6084   3.0000   0.0000  18.3725   1.7785   8.6281
0.0000
     -1.2000   0.0000 102.1000  25.3430  10.1260   0.7590   0.8563
0.0000
    -16.0573   2.6997   1.0338   6.0000   2.5791   0.0000   0.0000
0.0000
 Al   2.4443   3.0000  26.9820   2.0089   0.2161   0.5675  -1.6836
3.0000
     11.8538  16.3962   3.0000   0.0076  16.5151  -0.2451   6.3319
0.0000
     -1.0000   0.0000  67.5458 137.9671   0.2042   0.0000   0.8563
0.0000
    -14.9162   3.0000   1.0338   3.0000   2.5791   0.0000   0.0000
0.0000
 Ni   1.8244   2.0000  58.6900   1.8442   0.1840   0.8105   0.1000
2.0000
     12.3227   3.8387   2.0000   0.0000   0.0000   0.0100   6.1195
0.0000
     -1.0000   0.0000 103.2000  50.6786   0.6762   0.0981   0.8563
0.0000
    -19.6282   3.6035   1.0338   8.0000   2.5791   0.0000   0.0000
0.0000
 Cu   1.9202   2.0000  63.5460   1.9221   0.2826   1.0000   0.1000
1.0000
     10.9889 100.0000   1.0000   0.0000   0.0000   2.7875   6.0000
0.0000
     -1.0000   0.0000  80.7000  34.9555   0.4988   0.0000   0.8563
0.0000
     -5.1872   3.1491   1.0000   4.0000   2.5791   0.0000   0.0000
0.0000
 S    1.8328   2.0000  32.0600   1.8815   0.3236   0.7530   1.6468
6.0000
      9.0000   4.9055   4.0000  30.0000 112.1416   6.5745   9.0000
2.0000
```

```
      1.0000   3.4994  65.0000  12.0000  22.1978  15.3230   0.9745
0.0000
    -15.7363   2.8802   1.0338   6.2998   2.8793   0.0000   0.0000
0.0000
 Cr   1.8834   3.0000  51.9962   2.3133   0.2205   0.4744  -1.6836
6.0000
     10.2460   3.2000   3.0000   0.0000  18.3190   1.4000   9.0000
0.0000
     -1.2000   0.0000 102.1000  25.3430  10.1260   0.7590   0.8563
0.0000
     -4.1000   2.6997   1.0338   6.0000   2.5791   0.0000   0.0000
0.0000
 X   -0.1000   2.0000   1.0080   2.0000   0.0000   0.0100  -0.1000
6.0000
     10.0000   2.5000   4.0000   0.0000   0.0000   5.00009999.9999
0.0000
     -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745
0.0000
    -11.0000   2.7466   1.0338   2.0000   2.8793   0.0000   0.0000
0.0000
 35      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                        pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
  1  1  80.8865 107.9944  52.0636   0.5218  -0.3636   1.0000  34.9876
0.7769
         6.1244  -0.1693   8.0804   1.0000  -0.0586   8.1850   1.0000
0.0000
  1  2 180.6309   0.0000   0.0000  -0.4794   0.0000   1.0000   6.0000
0.6281
        12.2202   1.0000   0.0000   1.0000  -0.0670   6.8158   0.0000
0.0000
  2  2 153.3934   0.0000   0.0000  -0.4600   0.0000   1.0000   6.0000
0.7300
         6.2500   1.0000   0.0000   1.0000  -0.0790   6.0552   0.0000
0.0000
  1  3 163.3110  83.9973  54.4316  -0.5220  -0.3123   1.0000  10.2503
1.0000
         0.3553  -0.3757   7.0000   1.0000  -0.1331   4.6021   0.0000
0.0000
  2  3 160.0000   0.0000   0.0000  -0.5725   0.0000   1.0000   6.0000
0.5626
         1.1150   1.0000   0.0000   0.0000  -0.0920   4.2790   0.0000
0.0000
  3  3 142.2858 145.0000  50.8293   0.2506  -0.1000   1.0000  29.7503
0.6051
         0.3451  -0.1055   9.0000   1.0000  -0.1225   5.5000   1.0000
0.0000
  1  4   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000
0.5000
         0.2350  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000
0.0000
  2  4   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000
0.5000
```

```
          0.2350  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000
0.0000
  3  4  67.5128   0.0000   0.0000   0.1301  -0.3000   0.0000  36.0000
0.0852
          1.0000  -0.3500  15.0000   1.0000  -0.0629   7.1208   0.0000
0.0000
  4  4  41.4611   0.0000   0.0000   0.2931  -0.2000   0.0000  16.0000
0.2682
          0.6294  -0.2000  15.0000   1.0000  -0.0512   6.8013   0.0000
0.0000
  1  5   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000
0.5000
          0.2350  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000
0.0000
  2  5   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000
0.5000
          0.2350  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000
0.0000
  3  5 175.2517   0.0000   0.0000  -0.8707  -0.3000   0.0000  36.0000
0.0100
          0.9278  -0.3500  25.0000   1.0000  -0.1183   4.6533   0.0000
0.0000
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0.2822
          2.2322  -0.4197  14.3085   1.0000  -0.2524   7.2814   0.0000
0.0000
  5  5  65.7742   0.0000   0.0000  -0.4111  -0.3000   0.0000  16.0000
0.2955
          2.8637  -0.4197  14.3085   1.0000  -0.1993   4.8757   0.0000
0.0000
  1  6  72.3357  14.1215   0.0000   0.2743  -0.2000   1.0000  16.0000
0.0100
          3.0781  -0.0871  13.4739   1.0000  -0.1539   4.5484   1.0000
0.0000
  2  6 101.5086   0.0000   0.0000  -0.4746   0.0000   1.0000   6.0000
0.1422
          0.1863   1.0000   0.0000   1.0000  -0.0963   5.5382   0.0000
0.0000
  3  6  86.9034   0.0000   0.0000   0.3377  -0.2000   1.0000  16.0000
0.0715
          2.5302  -0.2500  15.0000   1.0000  -0.1923   4.8493   1.0000
0.0000
  4  6  77.1297   0.0000   0.0000  -0.0431  -0.2000   0.0000  16.0000
0.2063
          4.3648  -0.2000  15.0000   1.0000  -0.2542   5.5181   0.0000
0.0000
  5  6  62.3744   0.0000   0.0000  -0.0066  -0.2000   0.0000  16.0000
0.2283
         10.9966  -0.2000  15.0000   1.0000  -0.1072   4.0000   0.0000
0.0000
  6  6  90.1410   0.0000   0.0000  -0.3857  -0.2000   0.0000  16.0000
0.3225
```

```
         1.0927  -0.2000  15.0000   1.0000  -0.1027   4.6972   0.0000
0.0000
  2  7   0.0000   0.0000   0.0000   0.2000  -0.1418   1.0000  13.1260
0.5000
         0.5000  -0.2000  20.0000   1.0000  -0.1000   9.0000   0.0000
0.0000
  3  7  81.4346   0.0000   0.0000  -0.1594  -0.3000   1.0000  36.0000
0.0025
         0.2904  -0.2500  12.0000   1.0000  -0.0742   9.3638   0.0000
0.0000
  7  7  73.6263   0.0000   0.0000   0.0209  -0.2000   0.0000  16.0000
0.3414
         0.4703  -0.2000  15.0000   1.0000  -0.1319   5.9254   0.0000
0.0000
  1  8 192.1462  90.5383  55.2528  -0.5652  -0.5211   1.0000  18.9617
0.1958
         2.0000  -0.1016  13.8750   1.0000  -0.1579   5.5813   1.0000
0.0000
  2  8 188.3744   0.0000   0.0000  -0.6562   0.0000   1.0000   6.0000
0.3870
        11.8360   1.0000   0.0000   1.0000  -0.0762   5.0961   1.0000
0.0000
  3  8 107.2917 202.9813  40.0000   0.4728  -0.2406   1.0000  22.1005
0.0500
         0.6528  -0.3341   7.9877   1.0000  -0.0909   6.9512   1.0000
0.0000
  4  8  75.5280   0.0000   0.0000  -0.4815  -0.3390   0.0000  16.0000
0.1769
         0.2800  -0.1838  15.0000   1.0000  -0.0758   6.3424   0.0000
0.0000
  5  8 123.2631   0.0000   0.0000  -0.4814  -0.3000   0.0000  16.0000
0.1762
         4.6653  -0.4197  14.3085   1.0000  -0.1984   5.8018   0.0000
0.0000
  6  8  90.8688   0.0000   0.0000   0.4233  -0.2000   0.0000  16.0000
0.1000
         0.1604  -0.2500  25.0000   1.0000  -0.1028   5.0666   0.0000
0.0000
  8  8  86.8868  69.1367   0.0000  -0.9993  -0.4781   1.0000  17.8574
0.0999
         0.2799  -0.1677   8.2557   1.0000  -0.1131   6.1440   1.0000
0.0000
  2  9   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000
0.5000
         0.3000  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000
0.0000
  3  9 103.1988  13.4351   0.0000   0.3247  -0.2172   1.0000  36.0000
0.0100
         1.9519  -0.2293   9.6056   1.0000  -0.2000   5.7127   1.0000
0.0000
  8  9 103.3203   0.0000   0.0000   0.6642  -0.3891   1.0000  36.0000
0.0100
```

```
         0.1888  -0.2339  12.1279   1.0000  -0.1335   5.8332   1.0000
0.0000
  9  9  46.2167   0.0000   0.0000   1.0000  -0.3000   0.0000  16.0000
0.0145
         0.3576  -0.3000  16.0000   1.0000  -0.1252   5.5224   0.0000
0.0000
 26    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
  1  2   0.1200   1.3861   9.8561   1.1254  -1.0000  -1.0000
  1  3   0.1347   1.8343   9.7934   1.3139   1.1498   1.1039
  2  3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
  1  4   0.1500   1.9000  10.0000  -1.0000  -1.0000  -1.0000
  2  4   0.0600   1.7000  11.0000  -1.0000  -1.0000  -1.0000
  3  4   0.1000   1.8000   9.1989   1.7050  -1.0000  -1.0000
  1  5   0.1500   1.9000  10.0000  -1.0000  -1.0000  -1.0000
  2  5   0.0600   1.7000  11.0000  -1.0000  -1.0000  -1.0000
  3  5   0.3745   1.8179   9.7359   1.4165  -1.0000  -1.0000
  4  5   0.3463   1.9794  10.3688   2.4727  -1.0000  -1.0000
  1  6   0.1239   1.7447  10.2595   1.5317   1.3505  -1.0000
  2  6   0.0328   1.6857  11.0718   1.2071  -1.0000  -1.0000
  3  6   0.0514   1.7820  12.8150   1.4000  -1.0000  -1.0000
  4  6   0.2667   1.9808  11.4966   2.0682  -1.0000  -1.0000
  5  6   0.2647   1.8590  11.5886   1.5854  -1.0000  -1.0000
  2  7   0.0300   1.5200  12.5000   0.1000  -1.0000  -1.0000
  3  7   0.0348   1.7637  12.3562   1.7228  -1.0000  -1.0000
  1  8   0.3314   1.7976  10.5605   1.6918   1.4000  -1.0000
  2  8   0.1020   1.7528   9.6276   1.3714  -1.0000  -1.0000
  3  8   0.2832   1.8196  10.2295   1.4502   1.4557  -1.0000
  4  8   0.0854   1.7474  12.7924   1.9838  -1.0000  -1.0000
  5  8   0.3159   1.7365  12.1526   2.2610  -1.0000  -1.0000
  6  8   0.1917   1.6885  12.3915   1.7659  -1.0000  -1.0000
  2  9   0.1000   1.5000  11.0000  -1.0000  -1.0000  -1.0000
  3  9   0.0783   1.7000  10.3076   1.7000   1.7000  -1.0000
  8  9   0.2335   2.0105   9.9500   1.7651  -1.0000  -1.0000
125    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
  1  1  1  74.9085  44.7514   0.9144   0.0000   0.0050   0.3556
2.5715
  1  1  2  68.0294  13.4722   5.5819   0.0000   0.6849   0.0000
1.0031
  2  1  2  68.4575  22.1235   1.2937   0.0000   3.0000   0.0000
1.5009
  1  1  3  15.7798   9.0805   4.0304   0.0000   1.8785  70.0000
1.1737
  2  1  3  65.0000  13.4505   1.8249   0.0000   1.5646   0.0000
1.2173
  3  1  3  74.7266  45.0000   1.8020 -16.7178   2.6091   0.1000
2.3556
  1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000
1.0400
  1  2  1   0.0000   7.5000   5.0000   0.0000   0.0000   0.0000
1.0400
  1  2  3   0.0000  45.0000   3.0000   0.0000   1.0000   0.0000
1.0400
```

```
  2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000
1.0400
  2  2  3   0.0000   8.5744   3.0000   0.0000   0.0000   0.0000
1.0421
  3  2  3   0.0000  15.0000   2.8900   0.0000   0.0000   0.0000
2.8774
  1  3  1  76.7840  44.2266   0.9343   0.0000   1.3483   0.0000
1.8301
  1  3  3  63.9120  17.1680   0.8751   0.0000   0.0693  50.9415
3.0000
  1  3  2  79.6413  28.6488   0.3789   0.0000   1.6776   0.0000
1.0010
  2  3  2  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000
1.5800
  2  3  3  79.5453  45.0000   2.1630   0.0000   3.0000   0.0000
1.2391
  3  3  3  80.7324  30.4554   0.9953   0.0000   1.6310  50.0000
1.0783
  4  3  4  63.0740  14.8127   2.9929   0.0000   0.7552   0.0000
1.3634
  1  3  4  60.0000  10.0000   1.0000   0.0000   1.0000   0.0000
1.0500
  2  3  4  63.4137   5.0000   0.6231   0.0000   1.4521   0.0000
1.0460
  3  3  4  73.6721  32.6330   1.7223   0.0000   1.0221   0.0000
1.4351
  3  4  3  76.5431   0.0583   0.0500   0.0000   0.4968   0.0000
2.2792
  3  4  4  69.4895   5.7742   8.0001   0.0000   1.7794   0.0000
2.7889
  1  3  5  90.0000   5.0000   3.0000   0.0000   1.0000   0.0000
1.1000
  2  3  5  90.0000  11.1212   4.3379   0.0000   3.0000   0.0000
3.0000
  3  3  5  43.6280  11.0750   6.6200   0.0000   3.0000   0.0000
1.0100
  5  3  5  64.5513  10.5987   1.0471   0.0000   3.0000   0.0000
1.6045
  3  5  3  84.7469   7.3926   2.9453   0.0000   0.1000   0.0000
1.2535
  3  5  5  27.4957  14.3276   0.2771   0.0000   2.3158   0.0000
2.2134
  3  7  3  96.2265   4.5610  12.0000   0.0000   0.3211   0.0000
1.5204
  7  3  7 100.0000  10.1065   6.0000   0.0000   1.0000   0.0000
3.6601
  2  3  7  55.0417   3.5032   3.9979   0.0000   1.5171   0.0000
1.0400
  3  3  7  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000
1.2500
  3  7  7  66.7783  14.3146   0.7911   0.0000   1.0000   0.0000
1.2333
```

```
  8  5  8  92.5166   8.8772   2.9319   0.0000   0.2516   0.0000
1.0620
  5  8  5  73.8915  23.2173   2.0851   0.0000   0.0100   0.0000
2.6540
  5  5  8  69.3869   3.0494   3.0000   0.0000   0.6079   0.0000
1.0000
  5  8  8  30.9172  16.7973   1.5917   0.0000   0.9584   0.0000
2.1273
  2  8  5  83.4937  25.0000   1.0000   0.5000   0.5409   0.0000
1.1378
  5  2  8   0.0000  10.0000   1.0000   0.5000   0.2500   0.0000
1.5000
  8  8  8  84.2345  15.5790   3.7715   0.0000   1.3066   0.0000
1.6270
  1  6  1  86.9687  17.4560   0.6761   0.0000   1.3985   0.0000
1.0000
  1  1  6  81.6643  16.7896   0.9911   0.0000   0.0100   0.0000
1.2853
  6  1  6  91.9774  25.3393   3.6465   0.0000   0.0100   0.0000
3.0000
  1  6  6  28.2735   4.0839   0.8183   0.0000   0.8382   0.0000
1.8508
  2  6  2  85.1733  30.0000   1.5231   0.0000   3.0000   0.0000
3.2533
  2  2  6   0.0000   8.0096   0.3378   0.0000   0.6843   0.0000
4.0000
  6  2  6   0.0000  29.9951   5.6363   0.0000   1.2512   0.0000
2.0120
  2  6  6  42.3753   1.9810   6.2947   0.0000   0.5297   0.0000
4.0000
  2  6  6 180.0000 -30.0000  12.8298   0.0000   1.3351   0.0000
1.1937
  3  3  6  90.0000  37.7567   4.4033   0.0000   1.1448   0.0000
1.0000
  6  3  6  88.1216  15.8581   2.7094   0.0000   0.6326   0.0000
1.1340
  3  6  3  33.8130  15.1818   4.0000   0.0000   0.0354   0.0000
1.3198
  3  6  6  19.7429   2.9501   3.6277   0.0000   0.0732   0.0000
1.7069
  2  1  6  90.0000  37.8850   0.4107   0.0000   2.7596   0.0000
1.0000
  1  2  6   0.0000   0.1000   0.9742   0.0000   0.8492   0.0000
3.8603
  1  6  2 100.0000  45.0000   0.7043   0.0000   0.6704   0.0000
1.0000
  1  3  6  63.5380  29.3917   1.6142   0.0000   1.6844   0.0000
1.0470
  3  1  6  58.5735  27.3130   1.4647   0.0000   1.2802   0.0000
1.0000
  1  6  3  60.0910  28.8774   1.8703   0.0000   1.0116   0.0000
1.0796
```

```
  2  3  6  30.2285  16.5089   2.5143   0.5000   1.0129   0.0000
1.5363
  3  2  6   0.0000   7.1233   1.9895   0.5000   0.3233   0.0000
1.1000
  8  6  8   0.2000   6.6443   1.2359   0.0000   0.0156   0.0000
1.1250
  6  8  6 107.2989  23.4838   0.7435   0.0000   0.2609   0.0000
1.3395
  6  6  8  18.7110  13.5233   0.1006   0.0000   0.0747   0.0000
1.3658
  6  8  8  54.9369  16.5560   6.0000   0.0000   0.2213   0.0000
1.5255
  2  8  6  83.4937  16.7605   0.8242   0.5000   0.5409   0.0000
1.1378
  6  2  8   0.0000  10.0000   1.0000   0.5000   0.2500   0.0000
1.5000
  2  8  2  90.0601  42.2756   0.5302   0.0000   0.3707   0.0000
1.0071
  2  8  8  66.1035   8.0885   1.0424   0.0000   0.7355   0.0000
3.0000
  3  5  8  19.4072  10.4590   2.8285   0.0000   1.0074   0.0000
2.3949
  3  8  5  83.6415  19.7500   2.9247   0.0000   1.9437   0.0000
1.0348
  5  3  8  89.6617  15.3276   2.7567   0.0000   1.6031   0.0000
1.0781
  5  3  6  95.3249  30.0000   0.6664   0.0000   2.0000   0.0000
1.0000
  3  5  6   4.7439   7.2911   1.8650   0.0000   1.5814   0.0000
1.4132
  3  6  5  39.4301  10.2218   1.3968   0.0000   1.8777   0.0000
1.6288
  1  1  8  71.4462  27.2223   6.7228   0.0000   0.0050   0.0000
2.6454
  1  8  1  92.6710  15.6798   3.1104   0.0000   0.3458   0.0000
2.3207
  2  1  8  43.6595  11.8933   0.5449   0.0000   0.0050   0.0000
1.9326
  1  8  2  99.1897  14.1666   2.5588   0.0000   0.3542   0.0000
2.5990
  1  8  8  89.3910   5.0000   7.0000   0.0000   1.0050   0.0000
1.5000
  3  8  3  83.5231  37.5859   0.9881  -0.0100   1.4725   0.0000
1.0641
  1  8  3  79.9791  29.5117   7.0000   0.0000   0.0050   0.0000
1.2255
  1  3  8  83.1032  23.4174   0.7741   0.0000   1.2168   0.0000
2.7365
  3  3  8  60.2631  30.0701   2.1707   0.0000   1.3323   0.0000
1.0192
  3  8  8  55.9402  38.2990   3.6930   0.0000   2.2673   0.0000
1.0000
```

```
  2  3  8  35.9099  19.1501   1.9918   0.0000   0.9342   0.0000
2.7883
  1  2  8   0.0000   0.2500   6.0000   0.0000   0.0000   0.0000
1.0400
  3  2  8   0.0000   1.0000   6.0000   0.0000   0.0000   0.0000
1.0400
  8  2  8   0.0000   7.5000   2.0000   0.0000   0.0000   0.0000
1.0400
  8  4  8   0.2000   7.5083   1.3736   0.0000   0.0412   0.0000
1.8149
  4  8  4 100.0000   9.2519   0.7752   0.0000   0.1221   0.0000
2.2142
  4  4  8  33.4003  16.6274   0.1076   0.0000   0.0825   0.0000
1.0000
  4  8  8  77.0475   7.4569   4.9579   0.0000   0.7548   0.0000
2.3345
  2  8  4  84.8837  16.4865   0.8240   0.5000   0.5428   0.0000
1.1398
  4  2  8   0.0000  10.0000   1.0000   0.5000   0.2500   0.0000
1.5000
  3  4  8  29.3282   8.1452   2.8121   0.0000   0.2287   0.0000
1.9412
  4  3  8   4.8461   5.5458   2.9681   0.0000   1.0491   0.0000
1.4836
  3  8  4  89.9073   7.0973   1.3919   0.0000   0.8210   0.0000
2.9921
  3  9  3  72.0610   9.9276   3.7068   0.0000   2.0407   0.0000
1.4632
  9  3  9  53.2083  34.6712  10.0000   0.0000   1.4829   0.0000
1.9159
  3  3  9  71.6698  44.3637   8.2088   0.0000   1.1760   0.0000
1.5367
  3  9  9  56.4467  26.7016   0.3699   0.0000   1.7359   0.0000
1.9750
  2  3  9   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000
1.0500
  1  3  9   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000
1.0500
  8  9  8  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000
1.0000
  9  8  9  87.9918  25.0000   3.0000   0.0000   0.5523   0.0000
1.6121
  8  8  9  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000
1.0000
  8  9  9  53.1529  19.1953   0.3597   0.0000   0.2000   0.0000
1.6208
  2  8  9   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000
1.0500
  1  8  9   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000
1.0500
  5  8  6 105.0000  35.0000   2.2077   0.0000   0.5911   0.0000
2.7573
```

```
  6  5  8  72.2779  29.1869   0.2831   0.0000   0.9971   0.0000
1.2000
  5  6  8  45.7012  27.4289   0.2324   0.0000   1.1218   0.0000
1.7540
  4  3  5  29.4269  22.0505   1.8191   0.0000   3.0000   0.0000
2.5264
  3  4  5  89.9909   0.0139   1.2646   0.0000   2.7433   0.0000
2.9105
  3  5  4  28.1272  10.3178   3.0000   0.0000   1.6706   0.0000
1.9396
  4  3  6  56.8615   9.2273   1.7526   0.0000   0.9612   0.0000
1.1817
  3  6  4  35.0000   4.5000   3.0000   0.0000   1.3000   0.0000
2.3000
  3  4  6  70.0000   4.5000   3.0000   0.0000   1.3000   0.0000
2.3000
  8  3  8  76.3546  40.0000   3.3161   0.0005   1.9473   0.0000
1.0000
  4  8  5  62.8042  12.1651   0.8881   0.0000   0.1000   0.0000
3.0000
  5  4  8  64.5399   0.0100   0.0100   0.0000   0.5378   0.0000
2.9111
  4  5  8  13.6043   4.1825   2.6350   0.0000   0.7360   0.0000
3.0000
 44    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
  1  1  1  1   2.1207  26.8713   0.5160  -9.0000  -2.8394   0.0000
0.0000
  1  1  1  2   1.4658  44.1251   0.4411  -5.3120  -2.1894   0.0000
0.0000
  2  1  1  2   1.4787  40.5128   0.4396  -5.2756  -3.0000   0.0000
0.0000
  1  1  1  3   0.9963  17.2365   0.1491  -2.5000  -1.0000   0.0000
0.0000
  2  1  1  3   1.5159  28.6602   0.7169  -7.5489  -3.0000   0.0000
0.0000
  3  1  1  3  -0.2000  23.6540  -1.0000  -5.9155  -1.1552   0.0000
0.0000
  1  1  3  1   1.8231  46.5696  -1.0000  -3.0536  -3.0000   0.0000
0.0000
  1  1  3  2   1.4836  80.0000   0.0363  -4.7349  -1.0000   0.0000
0.0000
  2  1  3  1   0.5983  49.5033   0.7210  -3.4046  -1.6880   0.0000
0.0000
  2  1  3  2  -0.2000  76.3511   1.0000  -4.0709  -1.0000   0.0000
0.0000
  1  1  3  3  -0.2000   5.0000  -1.0000  -3.6523  -2.9000   0.0000
0.0000
  2  1  3  3   2.5000  80.0000   1.0000  -2.6071  -3.0000   0.0000
0.0000
  3  1  3  1  -0.2000  80.0000  -1.0000  -3.6863  -3.0000   0.0000
0.0000
```

```
  3  1  3  2   2.5000  38.8954  -0.8368  -4.6681  -2.9000   0.0000
0.0000
  3  1  3  3  -0.2000  78.1766   0.0250  -2.8895  -3.0000   0.0000
0.0000
  1  3  3  1   2.5000   0.1000   1.0000  -2.6905  -2.7573   0.0000
0.0000
  1  3  3  2   0.5241  69.2788  -1.0000  -4.4539  -2.8081   0.0000
0.0000
  2  3  3  2   2.5000   0.1000  -0.4869  -2.8372  -1.0000   0.0000
0.0000
  1  3  3  3   2.5000   0.1000   1.0000  -3.4298  -1.0000   0.0000
0.0000
  2  3  3  3  -0.2000   0.1000  -1.0000  -3.5698  -1.0000   0.0000
0.0000
  3  3  3  3  -0.2000   0.1000   1.0000  -3.8409  -1.0000   0.0000
0.0000
  0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000
0.0000
  0  1  1  0   0.0000  50.0000   0.3000  -4.0000  -2.0000   0.0000
0.0000
  0  3  3  0   0.5511  25.4150   1.1330  -5.1903  -1.0000   0.0000
0.0000
  2  3  7  3  -1.5000   6.8333  -0.1978  -1.4683   0.0000   0.0000
0.0000
  0  2  8  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  8  8  8  8   2.4661  71.9719   0.0100  -8.0000  -2.0449   0.0000
0.0000
  2  8  8  2   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000
0.0000
  2  3  8  3   2.5000   2.5000   0.2237 -10.0000   0.0000   0.0000
0.0000
  0  1  8  0   0.5000  50.0000   0.5000 -10.0000   0.0000   0.0000
0.0000
  0  3  8  0   0.5000  50.0000   0.5000  -8.0000   0.0000   0.0000
0.0000
  3  8  8  8   0.2500  90.0000   0.5000  -6.0000   0.0000   0.0000
0.0000
  3  8  8  3   0.2500  90.0000   0.5000  -6.0000   0.0000   0.0000
0.0000
  1  8  8  1   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000
0.0000
  1  8  8  2   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000
0.0000
  2  8  8  2   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000
0.0000
  1  1  1  6   0.0000   7.7112   0.4000  -6.0000   0.0000   0.0000
0.0000
```

```
  6  1  1  6   0.0000  23.4625   2.2056  -4.0000   0.0000   0.0000
0.0000
  2  1  1  6   0.0000  29.9163   0.6973  -4.0000   0.0000   0.0000
0.0000
  2  1  6  1   0.0000   0.0100   0.0100  -6.0000   0.0000   0.0000
0.0000
  1  1  6  1   0.0000   0.7817   0.0100  -5.9539   0.0000   0.0000
0.0000
  1  1  6  2   0.0000   6.0983   0.0100  -5.9539   0.0000   0.0000
0.0000
  4    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
  3  2  3   2.1200  -3.5800   1.4500  19.5000
  3  2  8   2.5000  -1.0000   1.4500  19.5000
  8  2  3   2.5000  -1.0000   1.4500  19.5000
  8  2  8   2.5000  -2.0000   1.4500  19.5000
```