Dynamic simulation of liquid molecular nanoclusters. Structure, stability and quantification of internal (pseudo)symmetries

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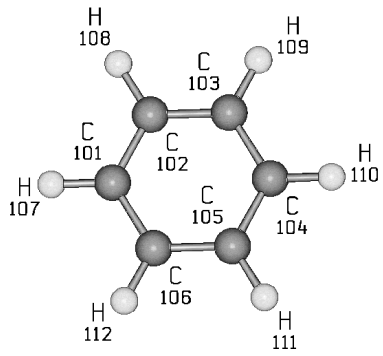
Electronic Supporting Information

S1. Force Field parameters

See the Users' Manual for full details (http://www.angelogavezzotti.it/Public/main2.htm).

S1.1 Benzene

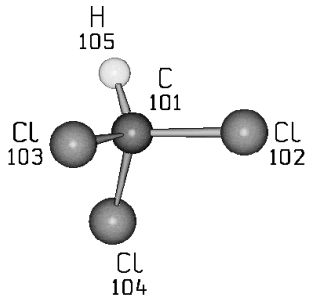
```
 #BENZNE99  Molecular dynamics force field file
 12
  1   0.00000   1.02600  -0.93778  12   -0.2878
  2   0.00000  -0.29915  -1.35743  12   -0.2878
  3   0.00000  -1.32514  -0.41965  12   -0.2878
  4   0.00000  -1.02599   0.93779  12   -0.2878
  5  -0.00000   0.29915   1.35743  12   -0.2878
  6   0.00000   1.32514   0.41964  12   -0.2878
  7   0.00000   1.82317  -1.66642   2    0.2878
  8   0.00000  -0.53158  -2.41212   2    0.2878
  9   0.00000  -2.35475  -0.74570   2    0.2878
 10   0.00000  -1.82317   1.66642   2    0.2878
 11  -0.00000   0.53158   2.41212   2    0.2878
 12   0.00000   2.35475   0.74570   2    0.2878
  0  nslav-u
  0  ncore-v
  0  nslav-v
 83.3    0.0 volu-u,volu-v
12  nstr-u
  1    2   1.390  4500.0
  1    6   1.390  4500.0
  2    3   1.390  4500.0
  3    4   1.390  4500.0
  5    6   1.390  4500.0
  4    5   1.390  4500.0
  1    7   1.080  3500.0
  2    8   1.080  3500.0
  3    9   1.080  3500.0
  4   10   1.080  3500.0
  5   11   1.080  3500.0
  6   12   1.080  3500.0
  0  nstr-v
 18  nbend-u
  1    2    3  120.00   450.0
  2    3    4  120.00   450.0
  3    4    5  120.00   450.0
  4    5    6  120.00   450.0
  5    6    1  120.00   450.0
  6    1    2  120.00   450.0
  1    2    8  120.00   450.0
  1    6   12  120.00   450.0
  2    1    7  120.00   450.0
  2    3    9  120.00   450.0
  3    2    8  120.00   450.0
  3    4   10  120.00   450.0
  4    3    9  120.00   450.0
  4    5   11  120.00   450.0
  5    4   10  120.00   450.0
  5    6   12  120.00   450.0
  6    1    7  120.00   450.0
  6    5   11  120.00   450.0
  0  nbend-v
 12  ntors-u
1  2  3  4   100.0  -1.0 1.0
2  3  4  5   100.0  -1.0 1.0
3  4  5  6   100.0  -1.0 1.0
4  5  6  1   100.0  -1.0 1.0
5  6  1  2   100.0  -1.0 1.0
6  1  2  3   100.0  -1.0 1.0
1  2  6  7   200.0  -1.0 1.0  improper
```



```
  2  3  1  8   200.0  -1.0 1.0
  3  4  2  9   200.0  -1.0 1.0
  4  5  3 10   200.0  -1.0 1.0
  5  6  4 11   200.0  -1.0 1.0
  6  1  5 12   200.0  -1.0 1.0
    0  ntors-v
    0  nlist-u
    0  nlist-v
   0.410   235.0   650.0   77000.0
    0  nintra
```

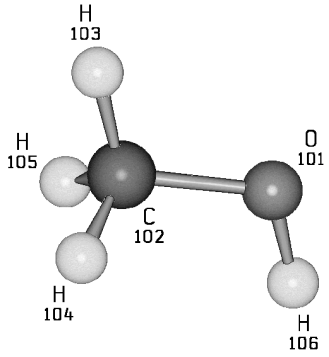
S1.2 Chloroform

```
   #chcl3  Molecular dynamics force field file
    5
    1   0.53198  -0.01997   0.00000  13    0.5127
    2  -0.07328   1.64971  -0.00001  42   -0.2610
    3  -0.07639  -0.82117  -1.46360  42   -0.2610
    4  -0.07639  -0.82116   1.46360  42   -0.2610
    5   1.61198  -0.02129  -0.00000   3    0.2703
    0  nslav-u
    0  ncore-v
    0  nslav-v
   71.3    0.0 volu-u,volu-v
   4  nstr-u
    1    2   1.776  2500.0
    1    3   1.776  2500.0
    1    4   1.776  2500.0
    1    5   1.080  2500.0
    0  nstr-v
    6  nbend-u
    2    1    3  109.47   450.0
    2    1    4  109.47   450.0
    2    1    5  109.47   450.0
    3    1    4  109.47   450.0
    3    1    5  109.47   450.0
    4    1    5  109.47   450.0
    0  nbend-v
    0  ntors-u
    0  ntors-v
    0  nlist-u
    0  nlist-v
   0.410   235.0   650.0   77000.0
    0  nintra
```



S1.3 Methanol

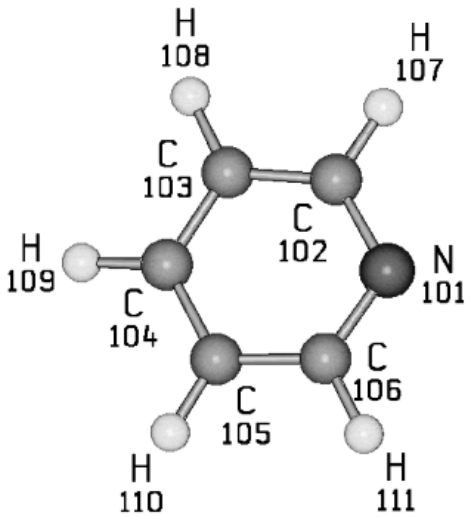
```
#METHOL99  methanol  molecular dynamics force field file
    6
    1   0.00000   1.42500   0.00000     29   -1.4250
    2   0.00000   0.00000   0.00000     13   -0.2236
    3   1.01161  -0.37822   0.00000      3    0.2864
    4  -0.50580  -0.37822  -0.87608      3    0.2826
    5  -0.50581  -0.37822   0.87608      3    0.2826
    6  -0.91620   1.75847   0.00000      5    0.7970
    0  nslav-u
    0  ncore-v
    0  nslav-v
   35.9    0.0 volu-u,volu-v
    5  nstr-u
    1    2   1.425  3200.0
    2    3   1.080  3000.0
    2    4   1.080  3000.0
```



```
    2    5   1.080  3000.0
    1    6   1.000  2500.0
    0  nstr-v
    7  nbend-u
    2  1  6  110.00   400.0
    1  2  3  110.50   450.0
    1  2  4  110.50   450.0
    1  2  5  110.50   450.0
    3  2  4  108.42   350.0
    3  2  5  108.42   350.0
    4  2  5  108.42   350.0
    0  nbend-v
    1  ntors-u
  6  1  2  3  2.5  1.0   3.0
    0  ntors-v
    0  nlist-u
    0  nlist-v
   0.410   235.0   650.0   77000.0
    0  nintra
```

S1.4 Pyridine

```
#pyri     pyridine Molecular dynamics force field file
   11
    1   0.00728  -0.03103  -1.39217  18   -0.8290
    2  -0.00725   1.12280  -0.70182  12    0.1054
    3   0.00955   1.19684   0.66470  12   -0.3177
    4  -0.01042   0.03053   1.38902  12   -0.1537
    5   0.00809  -1.16960   0.71918  12   -0.3197
    6  -0.00579  -1.14911  -0.65389  12    0.1081
    7  -0.03378   2.04725  -1.25955   2    0.2700
    8   0.03795   2.15422   1.16371   2    0.2929
    9  -0.04020   0.05574   2.46831   2    0.2812
   10   0.03292  -2.10475   1.25888   2    0.2933
   11  -0.02873  -2.09613  -1.17256   2    0.2692
    0  nslav-u
    0  ncore-v
    0  nslav-v
   79.3    0.0 volu-u,volu-v
   11  nstr-u
    1    2   1.345  4500.0
    1    6   1.340  4500.0
    2    3   1.369  4500.0
    2    7   1.080  3500.0
    3    4   1.373  4500.0
    3    8   1.080  3500.0
    4    5   1.375  4500.0
    4    9   1.080  3500.0
    5    6   1.373  4500.0
    5   10   1.080  3500.0
    6   11   1.080  3500.0
    0  nstr-v
   16  nbend-u
    1    2    3  123.98   450.0
    1    2    7  118.01   450.0
    1    6    5  124.28   450.0
    1    6   11  117.86   450.0
    2    1    6  115.66   450.0
    2    3    4  118.72   450.0
    2    3    8  120.64   450.0
    3    2    7  118.01   450.0
    3    4    5  118.97   450.0
    3    4    9  120.51   450.0
    4    3    8  120.64   450.0
    4    5    6  118.30   450.0
    4    5   10  120.85   450.0
    5    4    9  120.51   450.0
```



```
   5     6    11   117.86    450.0
   6     5    10   120.85    450.0
   0   nbend-v
  11   ntors-u
1   2   3   4    100.0   -1.0 1.0
2   3   4   5    100.0   -1.0 1.0
3   4   5   6    100.0   -1.0 1.0
4   5   6   1    100.0   -1.0 1.0
5   6   1   2    100.0   -1.0 1.0
6   1   2   3    100.0   -1.0 1.0
2   3   1   7    200.0   -1.0 1.0   improper
3   4   2   8    200.0   -1.0 1.0
4   5   3   9    200.0   -1.0 1.0
5   6   4 10    200.0   -1.0 1.0
6   1   5 11    200.0   -1.0 1.0
   0   ntors-v
   0   nlist-u
   0   nlist-v
 0.410    235.0    650.0    77000.0
   0   nintra
```

S2. Simulation outcomes

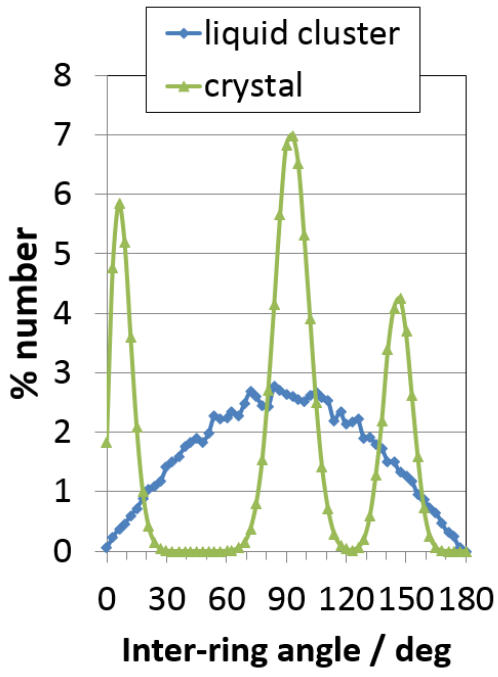


Figure S1. Distribution of angles between the normal to the ring in benzene molecular pairs. Blue: liquid nanocluster of 475 molecules. Green: crystalline benzene.

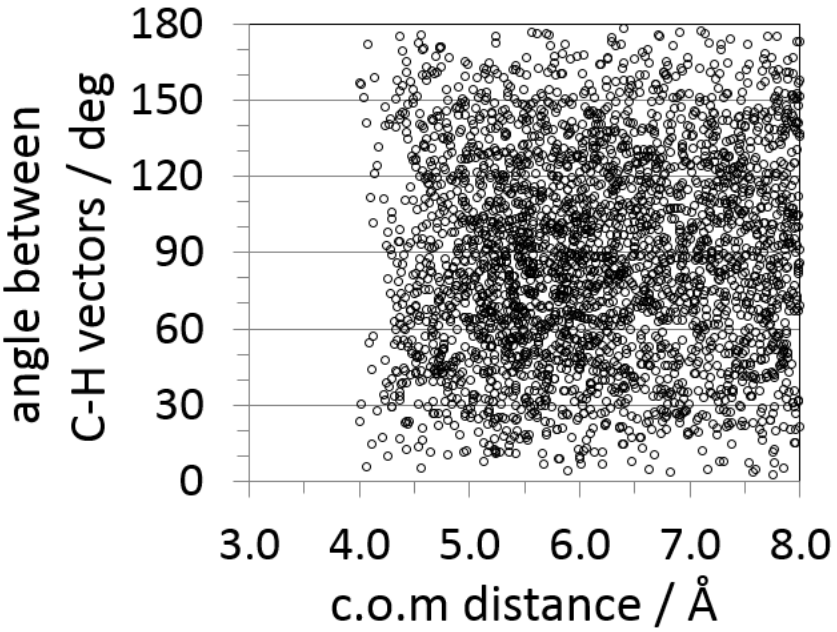


Figure S2. Distribution of angles between molecular C–H vectors in a liquid chloroform cluster consisting of 514 molecules, corresponding to the last frame of the MD simulation.

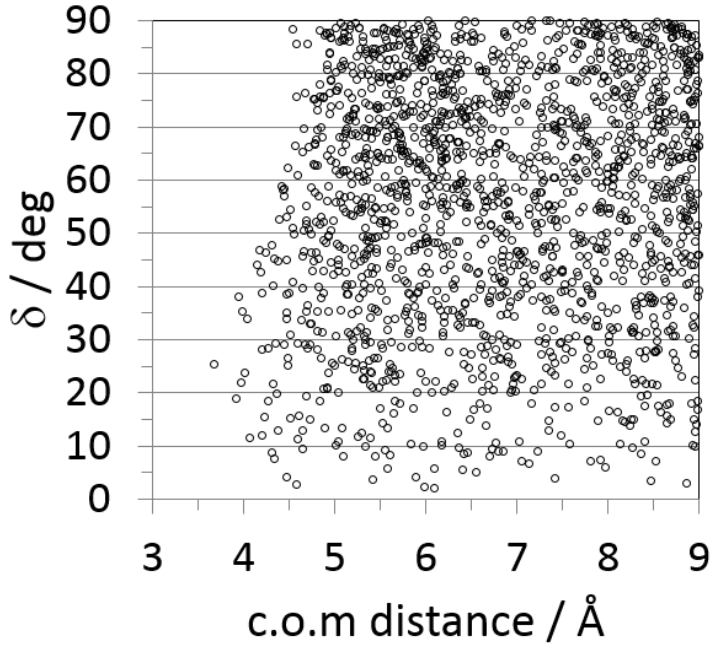


Figure S3. As Figure 1 in the main text, for bulk liquid benzene.

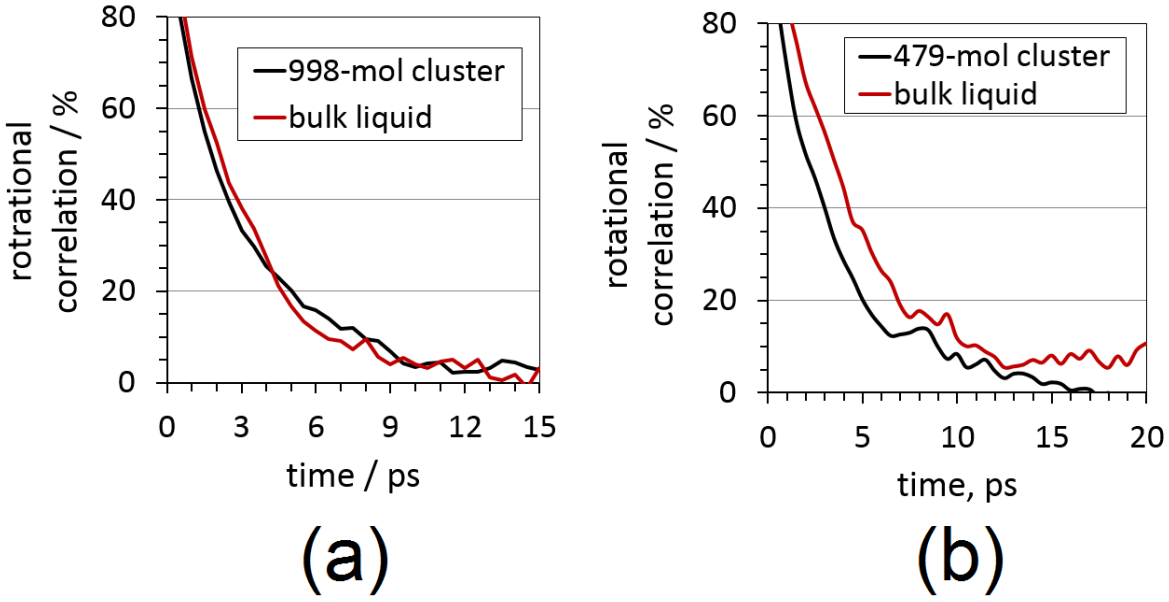


Figure S4. Comparison of cluster and bulk rotational correlation. (a) Chloroform. (b) Benzene. See also Figure 2 in the main text

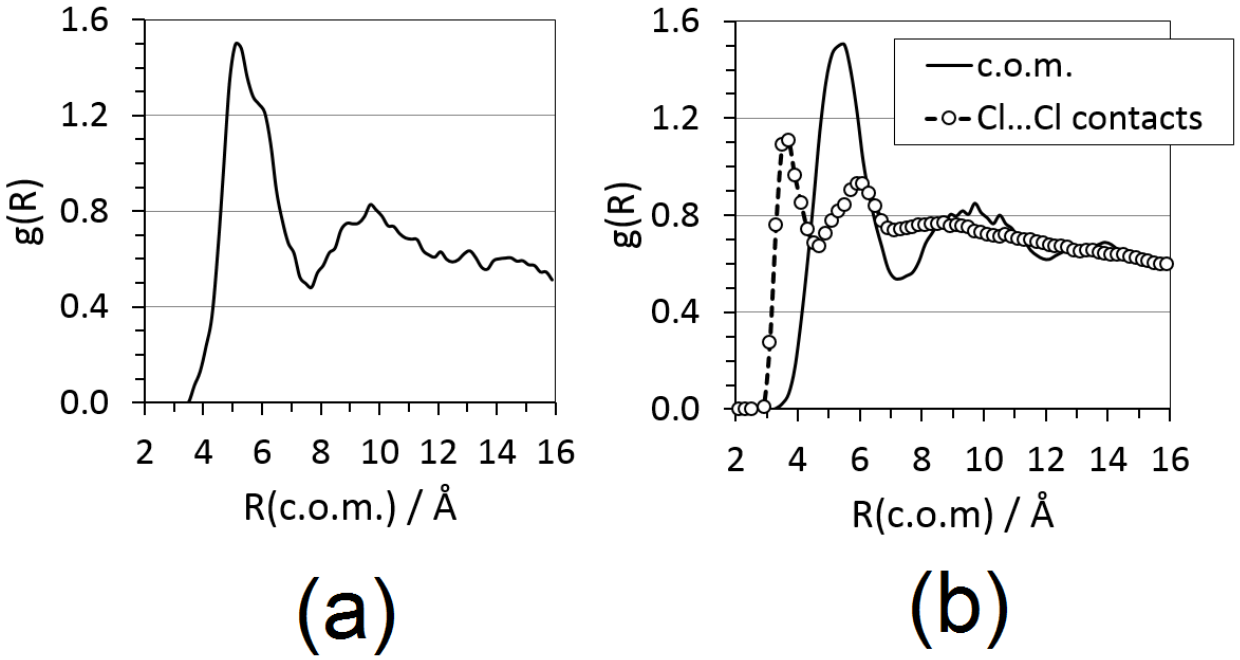


Figure S5. Center-of-mass radial distribution curves on the last frame of the MD simulation of liquid clusters. (a) Benzene, after 50 ksteps. (b) Chloroform, after 50 ksteps. Blank dots refer to the g(R) distribution of individual Cl···Cl contacts.

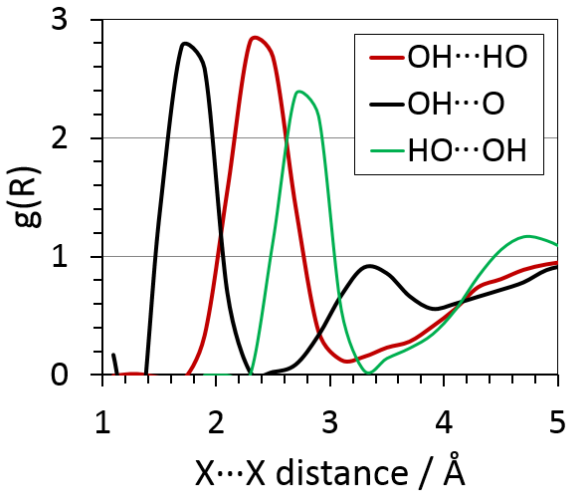


Figure S6. Radial distribution functions for the hydrogen bonding in the final frame of the MD simulation of a methanol cluster.