Supplementary Material (ESI) for New Journal of Chemistry

Efficient computer modeling of organic materials. The atom-atom, Coulomb-London-Pauli (AA-CLP) model for intermolecular electrostatic-polarization, dispersion and repulsion energies

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Details of Monte Carlo procedures

NOTE: full manual for the computer package with detailed theory, instructions for use and worked examples can be obtained from the author at his email address angelo.gavezzotti@unimi.it

Molecular structures
(as used in present paper)

Each molecular entity in the Monte Carlo computational box consists of a number of "core" atoms (≥ 3) and a number of "slave" atoms (≥ 0). The coordinates of core atoms are given explicitly in Cartesian form, the position of slave atom *X* can be specified according to various geometrical procedures: a) from three previously determined atoms A,B and C, on the chain *A-B-C-X*, by specifying the *C-X* distance, *R*, the *BCX* bond angle, α, and the *ABCX* torsion angle, τ;
b) from four known atoms in a pyramidal configuration, *X-A(BCD)*, by specifying the *XA* bond distance, *R*, with three equal *XAY* angles; c) from three known atoms, *ABC*, by specifying the *BX* distance, *R*, with equal *ABX* and *XBC* angles; d) for CX_2 groups, as in c), but specifying the C-X distance, *R*, and the XCX bond angle, α; e) for CX_3 groups (typically, X=H for a methyl group), as in a), specifying the C-X distance, the X*CB* bond angle, and one torsion angle τ, with the three X-atoms at τ, τ+120°, τ+240°. The geometry of core-atoms fragments are unchanged during the simulation, while the *R*, α and τ values described above maybe either constant or variable parameters. In practice, only torsional degrees of freedom are usually allowed (see below). The user manual, available upon request from the author at his e-mail address, contains full documentation.

In summary, for each of the molecules in the computational box, the following procedure applies: 1) starting from core atoms, Cartesian coordinates are calculated for slave atoms using current values for intramolecular parameters; 2) a chirality index is applied to produce the desired enantiomer, if necessary; 3) the molecular object in its current conformation and chirality is then positioned into the computational box by its rigid-body translation vector and rigid-body rotation by three Euler angles.

Virial pressure control
(as used in preliminary simulations in present paper)

For isotropic box dimensions change in a rectangular box, a weak-coupling algorithm similar to those used in molecular dynamics simulations can also be used. The algorithm involves the equipartition kinetic energy, E_{kin}, the virial, *W*, calculated from derivatives of the potentials, and the current pressure, *P*, to estimate a variation factor μ for box periodicity such that $a' = \mu a$, $b' = \mu b$, $c' = \mu c$:

$$E_{kin} = 1/2\ k_B\ N_{dof}\ T\ ; \qquad P = 2/(3V)\ (E_{kin} - W)$$
$$V° = a\ b\ c; \quad V' = \mu^3\ V°; \qquad \mu = (1 + DV/V°)^{1/3}$$

The number of degrees of freedom N_{dof} is determined in principle as the sum of rigid-body parameters of all molecules, plus internal degrees of freedom when present, *i.e.* N_{dof} = *N*(molecules) [6 + *N*(internal)] – 6 + 1. The last two addends are the degrees of freedom of the whole box, and the box volume change d.o.f., respectively. The temperature is taken equal to the MC-Metropolis temperature parameter (see below), in absence of an actual estimate of the molecular velocities. Then if P° is the target pressure one gets:

$$\Delta P = P° - P; \quad \mu = [1 - (P° - P)\beta]^{1/3}$$

where $\beta = (1/V°)\,\Delta V/\Delta P$ is the compressibility. As an order of magnitude, $\beta(\text{water}) = 5 \cdot 10^{-10}$ m^2 N^{-1}, but this number is to be considered as an adjustable parameter in the range down to $3 \cdot 10^{-11}$.

The molecular virial is calculated as follows, if one recalls that in the atom-atom scheme interatomic forces project like the interatomic distance vectors and that derivatives *wrt* distances between molecular centers are equivalent to derivatives *wrt* interatomic distances. Let *M* and *N* be two different molecules with atom *i* on the former and atom *j* in the latter:

$$E(M,N) = \Sigma_{i,M;j,N}\, E_{ij}$$
$$F(M,N) = -dE_{MN}/dR_{MN} = -\Sigma\, dE_{ij}/dR_{MN} = -\Sigma\, dE_{ij}/dR_{ij} = \Sigma\, F_{ij}$$
$$F_{ij} = -dE_{ij}/R_{ij}$$
$$F_x = |F|\, R_x/R\ ; \quad F_x(M,N) = \Sigma\, F_{ij,x}\ , \text{ etc. for } y, z$$
$$W(M,N) = -1/2\ \boldsymbol{F}(M,N) \bullet \boldsymbol{R}(M,N) =$$
$$= -1/2\ [F_x(M,N)R_x + F_y(M,N)R_y + F_z(M,N)R_z]$$
$$W_{TOT} = \Sigma_{M,N} W(M,N)$$

The current value of the virial is calculated to obtain in turn the current pressure, the correction factor μ, and the new box periodicities.

Asymmetry indices (order parameters) and symmetry bias
(prepared for future use with crystal structure simulations)

Although not used in the present paper, asymmetry indices (order parameters) have been designed to provide a quantitative measure of the deviation of a given configuration from perfect symmetry. If MC moves are accepted subject to a decrease in asymmetry indices, this symmetry bias helps simulating a transition from an isotropic structure like a liquid to a more anisotropic structure, ideally simulation a path to crystallization.

Asymmetry indices between pairs of identical molecules are calculated as follows. Let N_{atoms} be the number of atoms in each molecule, and N_{mol} the number of molecules in the box. Consider molecule *k* and each of its $N_{mol} - 1$ neighbors in the box, denoted by index *m*. The coordinates of all atoms in the two molecules *k* and *m* are referred to a common origin, namely the inertial coordinate system of the molecular pair. Six indicators are computed, quantifying the average sign relationship between coordinates of atoms *i* of molecule *k* with corresponding atoms *i* of molecule *m*:

$$s_1 = 1/N_{atoms} \textstyle\sum_i\ (x_{ki} + x_{mi})$$
$$s_2 = 1/N_{atoms} \textstyle\sum_i\ (x_{ki} - x_{mi})$$
$$s_3 = 1/N_{atoms} \textstyle\sum_i\ (y_{ki} + y_{mi})$$
$$s_4 = 1/N_{atoms} \textstyle\sum_i\ (y_{ki} - y_{mi})$$
$$s_5 = 1/N_{atoms} \textstyle\sum_i\ (z_{ki} + z_{mi})$$
$$s_6 = 1/N_{atoms} \textstyle\sum_i\ (z_{ki} - z_{mi})$$

Indices *b, d, e* are zero (no sign inversions) for perfect translational symmetry; indices *a, c, e* are zero (three sign inversions) for a perfect inversion-center symmetry; combinations *b, c, e*, or *a, c, f*, or *a, d, e* are zero (two sign inversions) for a perfect twofold axis or screw axis symmetry; combinations *a, d, f*, or *b, d, e*, or *b, c, f* are zero (one sign inversion) for a perfect mirror plane (glide plane) symmetry. These indicators are intuitive and computationally cheap, hence suitable for extensive simulation runs. They are however sensitive to molecular shape (e.g. an asymmetry index can decrease through an intramolecular change from an elongated to a globular conformation), and do not account for molecular point-group symmetry, i.e. the indices may be ambiguous when the latter is present.

For an imperfect symmetry, each of the above eight combinations will differ from zero by some amount. Let Dt, Di, Ds and Dm be four threshold limits in Å per atom, and wt, wi, ws and wm four disposable weighting parameters. The asymmetry is measured by the following indices

for translation: Ft = wt (s2+s4+s6)/(3 Dt)
for inversion: Fi = wi (s1+s3+s5)/(3 Di)
for twofold axis: Fs1 = ws (s2+s3+s5)/(3 Ds)
or Fs2 = ws (s1+s3+s6)/(3 Ds)
or Fs3 = ws (s1+s4+s5)/(3 Ds)
for a mirror plane: Fm1 = wm (s1+s4+s6)/(3 Dm)
or Fm2 = wm (s2+s4+s5)/(3 Dm)

or Fm3 = wm (s2+s3+s6)/(3 Dm)

Each *k*-*m* pair is assigned the smallest of the F's, Fmin(k,m). When a zero weight is assigned, the corresponding symmetry type is not considered, e.g. ws = wm = 0 for a check of translation and inversion symmetry only, etc.

The total asymmetry index for the *k*-th molecule in the box is the average over all *k*-*m* pairs, and the overall index for the whole box is the average over all molecules:

$$S_k = 1 / (N_{mol} - 1) \Sigma_m \text{Fmin(k,m)}$$
$$S_{all} = 1 / N_{mol} \ \Sigma_k S_k$$

The decrease in S_{all} is the top-priority discriminator when the MC run includes a symmetry bias.

When no symmetry bias is applied, each MC move is accepted according to the usual Metropolis criterion: calling ΔE the energy change, each move is accepted if $\Delta E < 0$ or, when $\Delta E > 0$, it is accepted only if $\exp(-\Delta E/RT) > r$, where r is a random number between 0 and 1. Setting $T = 0$ is then equivalent to forced energy decrease (optimization). When the symmetry bias applies, symmetry control precedes the energy check: irrespective of the change in energy, an MC move is accepted if S_{all} decreases or increases below a threshold value. The threshold is a measure of the tightness of the symmetry bias: if it is set at a very small number (e.g. 10^{-7}), only symmetry-enhancing moves have a chance of being accepted. Using a higher threshold gives the system more Monte Carlo 'time' to relax while the symmetrization proceeds. Moves that pass this preliminary symmetry test are then subjected to the usual Metropolis algorithm for acceptance.

Radial density functions

Consider a pair of atomic species (atom-atom RDF), or pairs of molecular centers (center of mass RDF). N_i is the number of distances in a spherical distance bin of volume V_i, N is the total number of distance points and V is the total volume of the distance sphere. The radial density function *g(R)* is:

$$g(R_i) = (N_i/V_i) / (N/V)$$

N/V is the total number density of distances, corresponding to uniform and random distribution. g(R) is thus normalized and $g(R_i) > 1$ indicates a significantly high frequency of distances at R_i. RDF's are smoothed according to a numerical recipe (Allen & Tildesley, Molecular simulation of liquids, Section 6.5.4).

Translational (diffusion) and rotational correlation

The diffusion coefficient *D* and rotational correlation function τ(rot) are estimated as follows. The standard time-dependent formulations are:

$$\tau(t) = [\Sigma_k \mathbf{u}_k(t) \cdot \mathbf{u}_k(0)] / N_{mol}$$
$$D = (1/6) < |\mathbf{r}(t+Dt) - \mathbf{r}(t)|^2 > / \Delta t$$

where **u**(t) is an orientation vector within the molecule, and **r**(t) is the position of a specified atom or of the center of coordinates at time *t*. The number of MC moves takes here the place of time, and an approximate scaling, with an estimate of the time equivalent of a MC move, results in 1Mmove approximately equal to 2 ps. The correlation functions are dimensionless numbers between 1 (complete correlation) and 0 (no correlation), and are averaged over all molecules in the box. They can be compared with experimentally determined correlation times, i.e. the time for the liquid to completely lose rotational memory. The *D* functions are averaged over the molecules within a radius of usually 30 Å from the overall center of the box.

Debye scattering profile

The scattering profile of a given simulation frame containing N_{mol} molecules can be calculated by the Debye equation

$$I(\theta) = N_{mol} \Sigma f_k f_n (\sin kR_{kn})/(kR_{kn})$$

where *I* is the scattered intensity, θ is the scattering angle, and the summation runs on all pairs of atoms at distance R_{kn}. The *f*'s are the atomic scattering factors, and $k = 4\pi \sin\theta/\lambda$. For a crystalline system simulated in a computational box, the scattering profile should ideally be identical to the powder diffraction pattern, except that the limited size of the computational box introduces a large truncation error and a broadening of the peaks.

Table S1. Average point charges for the atomic species considered in the CLP intermolecular energy scheme. First row: MP2 calculation, second row: rescaled EHT. Data are for the molecules comprised in the structural database of Figure 1.

atom type	q(min)	q(max)	average	
hydrogen				
aromatic (C)-H	0.085 0.101	0.233 0.135	0.137 0.119	Mulliken MP2/631G** EHT*0.41
aliphatic CH, CH_2, CH_3	0.074 0.103	0.238 0.160	0.130 0.122	
(R-O)H			0.34 0.27	
(COO-)H acid	0.349 0.269	0.410 0.277	0.360 0.274	
(CON)-H amide	0.270 0.199	0.310 0.204	0.294 0.201	
carbon				
carbonyl C=(O)	0.324 0.321	0.811 0.569	0.544 0.488	
≡C-				
sp^2 C	-0.209 -0.184	-0.001 0.159	-0.119 -0.093	
sp^3 C	-0.429 -0.371	0.040 0.348	-0.238 -0.232	
nitrogen				
aromatic N			-0.403 -0.587	
-C≡N			-0.321 -0.412	
nitro N			0.412 0.623	
amide N			-0.640 -0.329	
oxygen				
-O-			-0.517 -0.321	
(C=)O	-0.559 -0.527	-0.349 -0.442	-0.439 -0.482	
alcohol O(-H)			-0.60 -0.44	
Chlorine			0.075 -0.077	

Table S2. Molecular models used in Monte Carlo simulations for the present paper: Cartesian orthogonal coordinates, species indicator, and original non-rescaled Extended Huckel charges. NOTE: the EHT charges are to be multiplied by Fq = 0.41.

```
#acetic acid
   1  -1.49000   0.00000   0.00000   1  13   -0.8891
   2   0.00000   0.00000   0.00000   1  10   1.3434
   3   0.52680  -1.21140   0.00000   1  28   -0.9725
   4   0.69050   1.00090   0.00000   1  27   -1.1710
   5  -1.84998   1.01824   0.00000   1   3   0.3358
   6  -1.84998  -0.50912  -0.88182   1   3   0.3358
   7  -1.84998  -0.50912   0.88182   1   3   0.3358
   8   1.51250  -1.04286   0.00000   1   6   0.6819
#acetone
   1   1.21000   0.00000   0.00000   1  27   -1.00
   2   0.00000   0.00000   0.00000   1  10    1.00
   3  -0.76740   1.27720   0.00000   1  13   -0.90
   4  -0.76740  -1.27720   0.00000   1  13   -0.90
   5  -0.19690   2.03990  -0.50910   1   3    0.3
   6  -1.70870   1.13160  -0.50910   1   3    0.3
   7  -0.95280   1.58580   1.01820   1   3    0.3
   8  -0.51640  -1.84800  -0.88180   1   3    0.3
   9  -1.82560  -1.06130   0.00000   1   3    0.3
  10  -0.51640  -1.84800   0.88180   1   3    0.3
#acetonitrile
   1   0.00000   0.00000   0.00000   1  13   -0.7536
   2   1.46170   0.00000   0.00000   1  12    0.7602
   3   2.61840   0.00000   0.00000   1  19   -1.0798
   4  -0.36490   1.03210   0.00000   1   1    0.3577
   5  -0.36490  -0.51600   0.89380   1   1    0.3577
   6  -0.36490  -0.51600  -0.89380   1   1    0.3577
#benzene
   1   0.00000   0.00000  -1.40000   1  12   -0.2895
   2   0.00000   1.21240  -0.70000   1  12   -0.2895
   3   0.00000   1.21240   0.70000   1  12   -0.2895
   4   0.00000   0.00000   1.40000   1  12   -0.2895
   5   0.00000  -1.21240   0.70000   1  12   -0.2895
   6   0.00000  -1.21240  -0.70000   1  12   -0.2895
   7   0.00000   0.00000  -2.48000   1   2    0.2895
   8   0.00000   2.14770  -1.24000   1   2    0.2895
   9   0.00000   2.14770   1.24000   1   2    0.2895
  10   0.00000   0.00000   2.48000   1   2    0.2895
  11   0.00000  -2.14770   1.24000   1   2    0.2895
  12   0.00000  -2.14770  -1.24000   1   2    0.2895
#ccl4
   1   0.00000   0.00000   0.00000   1  13    1.0470
   2   1.77500   0.00000   0.00000   1  42   -0.2618
   3  -0.59170   1.67350   0.00000   1  42   -0.2618
   4  -0.59170  -0.83670   1.44930   1  42   -0.2618
   5  -0.59170  -0.83670  -1.44930   1  42   -0.2618
#chcl3
   1   0.00000   0.00000   0.00000   1  13    0.5127
   2   1.77600   0.00000   0.00000   1  42   -0.261
   3  -0.54590  -0.84500   1.46360   1  42   -0.261
   4  -0.54590  -0.84500  -1.46360   1  42   -0.261
   5  -0.36930   1.01490   0.00000   1   3    0.2703
#dimethylformamide
   1  -0.74680   1.24290   0.00000   1  13   -0.6416
   2  -0.74680  -1.24290   0.00000   1  13   -0.6414
   3   1.32000   0.00000   0.00000   1  12    0.6842
   4   0.00000   0.00000   0.00000   1  17   -0.1791
   5   2.02550  -1.00760   0.00000   1  27   -1.2317
   6  -1.36910   1.28890  -0.88150   1   3    0.2925
   7  -0.05940   2.07590  -0.00070   1   3    0.2894
   8  -1.36810   1.28960   0.88220   1   3    0.2925
   9  -1.36860  -1.28920  -0.88180   1   3    0.2932
  10  -0.05940  -2.07590   0.00000   1   3    0.2903
  11  -1.36860  -1.28920   0.88180   1   3    0.2932
  12   1.81870   0.95800   0.00000   1   2    0.2585

#ethyl alcohol
   1  -1.53000   0.00000   0.00000   1  13   -0.90
   2  -1.89000   1.01820   0.00000   1   3    0.30
   3  -1.89000  -0.50910   0.88180   1   3    0.30
   4  -1.89000  -0.50910  -0.88180   1   3    0.30
   5   0.00000   0.00000   0.00000   1  13    0.11
```

```
   6   0.36650   0.50440   0.88180   1   3    0.27
   7   0.36550   0.50440  -0.88180   1   3    0.27
   8   0.44190  -1.36000   0.00000   1  29   -1.40
   9   1.44190  -1.36000   0.00000   1   5    0.75
#formamide from formam02
   1   0.00000   0.00000   0.00000   1  21   -0.8088
   2  -1.31700   0.00000   0.00000   1  10    0.7809
   3  -2.02823  -1.01570   0.00000   1  27   -1.2157
   4  -1.75628   0.98663   0.00000   1   2    0.2624
   5   0.50000   0.86603   0.00000   1   8    0.4896
   6   0.50000  -0.86603   0.00000   1   8    0.4916
#n-hexane
   1  -0.76000   0.00000   0.00000   1  13   -0.5635
   2   0.76000   0.00000   0.00000   1  13   -0.5635
   3   1.35391  -1.39917   0.00000   1  13   -0.5525
   4   2.87391  -1.39917   0.00000   1  13   -0.8983
   5  -1.35391   1.39917   0.00000   1  13   -0.5525
   6  -2.87391   1.39917   0.00000   1  13   -0.8983
   7  -1.10190  -0.51656  -0.88468   1   3    0.2819
   8  -1.10190  -0.51656   0.88468   1   3    0.2819
   9   1.10190   0.51656   0.88468   1   3    0.2819
  10   1.10190   0.51656  -0.88468   1   3    0.2819
  11   1.01201  -1.91573  -0.88468   1   3    0.2825
  12   1.01200  -1.91573   0.88468   1   3    0.2825
  13   3.24329  -2.41404   0.00000   1   3    0.2953
  14   3.24329  -0.89174  -0.87890   1   3    0.2952
  15   3.24329  -0.89174   0.87891   1   3    0.2952
  16  -1.01201   1.91573   0.88468   1   3    0.2825
  17  -1.01201   1.91573  -0.88469   1   3    0.2825
  18  -3.24329   2.41404   0.00000   1   3    0.2953
  19  -3.24329   0.89173  -0.87890   1   3    0.2952
  20  -3.24329   0.89174   0.87890   1   3    0.2952
#methyl acetate
   1  -0.50960  -1.40010   0.00000   1  13   -0.8893
   2   0.00000   0.00000   0.00000   1  12    1.3381
   3   1.98560   1.30320   0.00000   1  13   -0.4173
   4  -0.65360   1.00640   0.00000   1  27   -1.1412
   5   1.35000   0.00000   0.00000   1  23   -0.7584
   6  -1.11110  -1.56420  -0.88180   1   3    0.3492
   7   0.32410  -2.08660   0.00000   1   3    0.3084
   8  -1.11110  -1.56420   0.88180   1   3    0.3492
   9   1.68580   1.84990  -0.88180   1   3    0.2873
  10   3.05860   1.18040   0.00000   1   3    0.2866
  11   1.68580   1.84990   0.88180   1   3    0.2873
#methyl ether from ABEWAG
   1   0.00000   0.55000  -0.00140   1  23   -0.8682
   2   0.00000  -0.25120   1.16580   1  13   -0.4100
   3   0.00000  -0.25210  -1.16440   1  13   -0.4097
   4   0.88410  -0.87130   1.17670   1   3    0.2807
   5  -0.00460   0.38460   2.03880   1   3    0.2831
   6  -0.87950  -0.87790   1.17220   1   3    0.2807
   7   0.87980  -0.87850  -1.16970   1   3    0.2803
   8   0.00410   0.38180  -2.03890   1   3    0.2828
   9  -0.88390  -0.87270  -1.17380   1   3    0.2803
#methyl alcohol
   1   0.00000   0.00000   0.00000   1  29   -1.45
   2  -1.41500   0.00000   0.00000   1  13   -0.19
   3  -1.77500   1.01820   0.00000   1   3    0.28
   4  -1.77500  -0.50910   0.88180   1   3    0.28
   5  -1.77500  -0.50910  -0.88180   1   3    0.28
   6   0.33330  -0.94280   0.00000   1   5    0.75
#pyridine
   1   0.00000   0.00080  -1.39880   1  18   -0.8204
   2   0.00020  -1.14420  -0.69340   1  12    0.1038
   3  -0.00020  -1.19730   0.70040   1  12   -0.3235
   4   0.00010  -0.00090   1.41560   1  12   -0.1626
   5   0.00000   1.19630   0.70250   1  12   -0.3235
   6  -0.00020   1.14530  -0.69220   1  12    0.1039
   7   0.00070  -2.07690  -1.23780   1   2    0.2726
   8  -0.00070  -2.14670   1.21530   1   2    0.2956
   9   0.00040  -0.00180   2.49560   1   2    0.2857
  10   0.00010   2.14490   1.21890   1   2    0.2956
  11  -0.00050   2.07870  -1.23550   1   2    0.2727
#water
   1   0.00000   0.00000   0.00000   1  24   -1.3217
   2   0.75695   0.58588   0.00000   1   9    0.6609
   3  -0.75695   0.58588   0.00000   1   9    0.6609
```

Table S2 (continued): "Topology" files: for each entry:
Cartesian orthogonal coordinates and original non-rescaled EHT charges of core atoms
NOTE: charges must be multiplied by Fq = 0.41
For non-rigid molecules:
Codes for the generation of slave atoms (see text)
Torsional energy functions:
a) fi(zero), 1/2Kbarrier and n for Etors= 1/2K * (1.0-cos n(fi-fizero))
b) polynomial coefficients for Etors = a*fi**4 + b*fi**3 + c*fi**2 + d*fi + e

acetic acid

```
     4   ncoreu
   1  -1.4900   0.0000   0.0000   13 -0.8891
   2   0.0000   0.0000   0.0000   10  1.3434
   3   0.5268  -1.2114   0.0000   28 -0.9725
   4   0.6905   1.0009   0.0000   27 -1.1710
     2   ncardu
 5  6  7  1  2  4   3  0.3358    methyl H's
 8 -1  0  3  2  1   6  0.6819    acid H
2  ntors-u
8  3  2  1  0.0 0.0  0  1.0030e-6 -3.5870e-4 3.3570e-2 -0.46754 34.80  H-O-C-C
5  1  2  4  0.0 1.0  3  0.0   0.0   0.0   0.0   0.0    methyl  rot
```

acetone

```
     4   ncoreu
   1   1.21000   0.00000   0.00000    27   -1.0000
   2   0.00000   0.00000   0.00000    10    1.0000
   3  -0.76740   1.27720   0.00000    13   -0.9000
   4  -0.76740  -1.27720   0.00000    13   -0.9000
     2   ncardu
 5  6  7  3  2  1   3  0.3000    methyl H's
 8  9 10  4  2  1   3  0.3000    methyl H's
2  ntors-u
5  3  2  1  0.0 4.0  3  0.0   0.0   0.0   0.0   0.0   methyl rot
8  4  2  1  0.0 4.0  3  0.0   0.0   0.0   0.0   0.0
```

acetonitrile

```
          6  ncoreu
   1   0.00000   0.00000   0.00000     13   -0.7536
   2   1.46170   0.00000   0.00000     12    0.6602
   3   2.61840   0.00000   0.00000     19   -0.9798
   4  -0.36490   1.03210   0.00000      3    0.3577
   5  -0.36490  -0.51600   0.89380      3    0.3577
   6  -0.36490  -0.51600  -0.89380      3    0.3577
```

benzene

```
         12
   1   0.0000   0.0000  -1.4000   12 -0.2895
   2   0.0000   1.2124  -0.7000   12 -0.2895
   3   0.0000   1.2124   0.7000   12 -0.2895
   4   0.0000   0.0000   1.4000   12 -0.2895
   5   0.0000  -1.2124   0.7000   12 -0.2895
   6   0.0000  -1.2124  -0.7000   12 -0.2895
   7   0.0000   0.0000  -2.4800    2  0.2895
   8   0.0000   2.1477  -1.2400    2  0.2895
   9   0.0000   2.1477   1.2400    2  0.2895
  10   0.0000   0.0000   2.4800    2  0.2895
  11   0.0000  -2.1477   1.2400    2  0.2895
  12   0.0000  -2.1477  -1.2400    2  0.2895
```

#chcl3

```
          5
   1   0.0000   0.0000   0.0000   13  0.5127
   2   1.7760   0.0000   0.0000   42 -0.2610
   3  -0.5459  -0.8450   1.4636   42 -0.2610
   4  -0.5459  -0.8450  -1.4636   42 -0.2610
   5  -0.3693   1.0149   0.0000    3  0.2703
```

#ccl4

```
          5
   1   0.0000   0.0000   0.0000   13  1.0470
   2   1.7750   0.0000   0.0000   42 -0.2618
   3  -0.5917   1.6735   0.0000   42 -0.2618
   4  -0.5917  -0.8367   1.4493   42 -0.2618
   5  -0.5917  -0.8367  -1.4493   42 -0.2618
```

dimethylformamide

```
     4
   1  -0.74680   1.24290   0.00000    13   -0.6416
   2  -0.74680  -1.24290   0.00000    13   -0.6414
   3   1.32000   0.00000   0.00000    10    0.6842
   4   0.00000   0.00000   0.00000    17   -0.1791
     4   ncardu
 5 -1  0  3  4  2  27 -1.2317     Oxygen
 6  7  8  1  4  3   3  0.29185    methyl H's
 9 10 11  2  4  3   3  0.29185    methyl H's
12  0  0  3  4  5   2  0.2585     H(CO)
3  ntors-u
5  3  4  2  0.0 0.0  0   0.   0.   0.02663   0.06668  -0.07363   O-C-N-C
6  1  4  3  0.0 5.0  3   0.   0.   0.   0.   0.    methyl rot
9  2  4  3  0.0 2.5  3   0.   0.   0.   0.   0.    methyl rot
```

ethanol

```
     3   ncoreu
   1  -1.53000  0.0000   0.0000   13 -0.9000
   2   0.00000  0.0000   0.0000   13  0.1100
   3   0.44190 -1.3600   0.0000   29 -1.4000
     3   ncardu
 4  5  6  1  2  3   3  0.3000  0.  methyl H's
 7  8  0  2  1  3   3  0.2700  0.  methylene H's
 9 -1  0  3  2  1   5  0.7500  0.  alcohol H
2  ntors-u
4  1  2  3  60. 7.0  3   0.   0.   0.   0.   0.   methyl rot
9  3  2  1  0.0 0.0  0  -7.9641e-9 -4.5212e-6 1.7043e-3 -0.17234 10.672   H-O-C-C
```

formamide

```
     4   ncoreu
   1   0.00000   0.00000   0.00000     21   -0.8088
   2  -1.31700   0.00000   0.00000     10    0.7809
   3  -2.02823  -1.01570   0.00000     27   -1.2157
   4  -1.75628   0.98663   0.00000      2    0.2624
     2   ncardu
 5 -1  0  1  2  4   8  0.4896   amide H
 6 -1  0  1  2  3   8  0.4916   amide H
2  ntors-u
5  1  2  4  0.0 0.0  0  0.00000  0.00140 -0.01280  0.08030  0.00000    H-N-C-O (out-of-plane NH2)
6  1  2  3  0.0 0.0  0  0.0      0.00140 -0.01280  0.0803   0.00000    H-N-C-O
```

n-hexane

```
    3   ncoreu
   1   -0.76000   0.00000   0.0000   13   -0.5640   0
   2    0.76000   0.00000   0.0000   13   -0.5640   0
   3    1.35391  -1.39917   0.0000   13   -0.5640   0
     9   ncardu
 4 -1  0  3  2  1  13 -0.9000 0.   C
 5 -1  0  1  2  3  13 -0.5640 0.   C
 6 -1  0  5  1  2  13 -0.9000 0.   C
 7  8  0  1  5  2   3  0.2820 0.   methylene H's
 9 10  0  2  1  3   3  0.2820 0.
11 12  0  3  2  4   3  0.2820 0.
16 17  0  5  6  1   3  0.2820 0.
13 14 15  4  3  2   3  0.3000 0.   methyl H's
18 19 20  6  5  1   3  0.3000 0.
5       ntors-u
13  4  3  2   60.  7.0  3      0.  0.  0.  0.  0.   methyl rotr
 4  3  2  1    0.  0.0  0  0.4793E-06 -0.2371E-03 0.3922E-01 -0.2484E+01 0.5566E+02
                                                              C-C-C-C
 3  2  1  5    0.  0.0  0  0.4793E-06 -0.2371E-03 0.3922E-01 -0.2484E+01 0.5566E+02
 2  1  5  6    0.  0.0  0  0.4793E-06 -0.2371E-03 0.3922E-01 -0.2484E+01 0.5566E+02
18  6  5  1   60.  7.0  3      0.  0.  0.  0.  0.   methyl rot
 37   nlistu list of intramolecular nonbonded contacts
 7 13  7 14  7 15
 8 13  8 14  8 15
 9 18  9 19  9 20
10 18 10 19 10 20
11 16 11 17 11 18 11 19 11 20
12 16 12 17 12 18 12 19 12 20
13 16 13 17 13 18 13 19 13 20
14 16 14 17 14 18 14 19 14 20
15 16 15 17 15 18 15 19 15 20
```

methyl acetate

```
      4
 1  -0.50961  -1.40014   0.00000   13  -0.8875
 2   0.00000   0.00000   0.00000   10   1.3385
 3  -0.65357   1.00640   0.00000   27  -1.1391
 4   1.35000   0.00000   0.00000   28  -0.7610
     3   ncardu
 5 -1  0  4  2  1  13 -0.4173
 6  7  8  1  2  4   3  0.33506
 9 10 11  5  4  2   3  0.28706
3  ntors-u
1  2  4  5  0.0 0.0  0   0.   0.   0.0076   -3.0300  298.00   C-C-O-C
6  1  2  3  0.0 1.0  3   0.   0.   0.   0.   0.   H-C-C-O
9  5  4  2  60.0 1.6  3   0.   0.   0.   0.   0.  H-C-O-C
```

methyl ether

```
      3
   1    0.0000    0.5500   -0.0014   23   -0.8681
   2    0.0000   -0.2512    1.1658   13   -0.4100
   3    0.0000   -0.2521   -1.1644   13   -0.4100
     2   ncardu
 4  5  6  2  1  3   3  0.28135
 7  8  9  3  1  2   3  0.28135
2  ntors-u
4  2  1  3  60.0 1.6  3   0.   0.   0.   0.   0.        methyl rot
7  3  1  2  60.0 1.6  3   0.   0.   0.   0.   0.
```

methanol

```
     5   ncoreu
   1   0.0000   0.0000   0.0000   29 -1.4000
   2  -1.4150   0.0000   0.0000   13 -0.1900
   3  -1.7750   1.0182   0.0000    3  0.2800
   4  -1.7750  -0.5091   0.8818    3  0.2800
   5  -1.7750  -0.5091  -0.8818    3  0.2800
     1   ncardu
 6 -1  0  1  2  4   5  0.7500
1  ntors-u
6  1  2  4  60. 2.0  3   0.   0.   0.   0.   0.      methyl rot
```

pyridine

```
    11
   1   0.00000   0.00080  -1.39880     18   -0.8204
   2   0.00020  -1.14420  -0.69340     12    0.1038
   3  -0.00020  -1.19730   0.70040     12   -0.3235
   4   0.00010  -0.00090   1.41560     12   -0.1626
   5   0.00000   1.19630   0.70250     12   -0.3235
   6  -0.00020   1.14530  -0.69220     12    0.1039
   7   0.00070  -2.07690  -1.23780      2    0.2726
   8  -0.00070  -2.14670   1.21530      2    0.2956
   9   0.00040  -0.00180   2.49560      2    0.2857
  10   0.00010   2.14490   1.21890      2    0.2956
  11  -0.00050   2.07870  -1.23550      2    0.2727
```

Table S3. UNI parameters for E = A exp(-BR) - $CR^{(-6)}$, used for intramolecular contacts. e° and R are the well depth and equilibrium distance.

non-hydrogen bonding potential parameters

	A	B	C	e°	R
O...O	195309	3.74	1335	0.337	3.61
F...F	170916	4.22	564.8	0.29	3.20
Si...Si	972667	3.21	16540	1.46	4.00
S...S	1087673	3.52	10757	1.89	3.83
Cl..Cl	585969	3.52	5795	1.02	3.83
Ar...Ar	675524.	3.58	5409.5		
Br...Br	2017608	3.57	10786	1.38	4.074
I...I	1505374	3.11	26517	1.95	4.445

hydrogen-bonding potential parameters:

A	B	C	
18868790	7.78	1247	alcohol O acceptor, H donor
26416400	8.75	857.7	carbonyl O acceptor, acid H donor
15095080	7.78	995.8	carbonyl O acceptor, amide H donor
22325910	8.27	1033	carbonyl O acceptor, H alcohol donor
23867340	7.78	1577	N acceptor, COH donor
30190070	7.78	1992	N acceptor, NHR donor
7547602	7.37	690.4	N acceptor, NH_2 donor

Noble gases from Williams, D.E. (1972) Acta Cryst. A28, 84:

Ne...Ne	190016	4.36	454.3
Ar...Ar	675524	3.58	5409.5
Kr...Kr	2017608	3.57	10786
Xe...Xe	1505374	3.11	26517

Table S4. Data to figures 1-4: Comparison of atom-atom (AA) and PIXEL energies for molecular crystals; total, Coulombic, polarization, dispersion. repulsion (kJ/mole units). Choice of experimental crystal structures according to criteria outlined in refs. 16 and 24.

For each entry:

CSD refcode

DH(subl); PIXEL Etot, AA Etot, PIXEL Ec, AA Ec, PIXEL Ep, AA Ep, PIXEL Ed, AA Ed, PIXEL Er, AA Er

ACETAC01 ACETAC01 ACETAC01
68.0 -62.4 -61.2 -79.2 -29.7 -36.3 -29.0 -39.0 -52.1 92.2 44.7
ADIPAC08 ADIPAC08 ADIPAC08
134.0 -130.9 -130.6 -154.2 -52.4 -77.4 -55.0 -89.7 -115.9 190.5 87.8
ANISIC02 ANISIC02 ANISIC02
110.0 -105.0 -98.2 -95.9 -29.1 -44.8 -29.6 -94.9 -107.2 130.6 62.8
BENZDC01 BENZDC01 BENZDC01
110.0 -132.1 -124.6 -160.7 -55.3 -82.6 -39.6 -99.0 -131.0 210.2 96.4
CLACET01 CLACET01 CLACET01
75.0 -82.9 -68.9 -75.9 -31.7 -36.8 -20.0 -59.8 -66.8 89.6 44.7
CLBZAP02 CLBZAP02 CLBZAP02
102.0 -103.2 -89.1 -93.6 -29.4 -48.5 -22.5 -92.8 -106.0 131.6 63.9
CROTAC CROTAC CROTAC
72.0 -80.3 -73.0 -83.5 -30.2 -38.2 -26.1 -54.3 -65.4 95.6 43.8
DMBZAC01 DMBZAC01 DMBZAC01
103.0 -97.8 -94.6 -85.1 -24.7 -41.5 -28.5 -95.6 -104.0 124.4 57.7
DMOXBA01 DMOXBA01 DMOXBA01
122.0 -128.5 -126.2 -94.7 -49.4 -44.7 -34.8 -102.9 -109.8 113.8 62.8
DMXBZA01 DMXBZA01 DMXBZA01
130.0 -111.1 -111.5 -100.2 -34.3 -48.1 -36.4 -116.0 -129.2 153.2 83.5
FORMAC01 FORMAC01 FORMAC01
61.0 -55.4 -50.6 -84.1 -32.4 -40.0 -24.1 -36.0 -52.6 104.7 53.6

FUFBOX01 FUFBOX01 FUFBOX01
102.0 -108.0 -102.8 -95.5 -40.2 -48.0 -28.8 -95.0 -106.4 130.5 67.6
FUMAAC01 FUMAAC01 FUMAAC01
124.0 -124.1 -116.9 -148.8 -57.5 -63.2 -47.1 -72.5 -99.1 160.4 81.8
HEKMOZ HEKMOZ HEKMOZ
127.0 -114.1 -115.1 -94.6 -30.2 -44.6 -37.4 -111.4 -123.6 136.5 71.1
ISUQUI ISUQUI ISUQUI
123.0 -113.4 -114.5 -105.2 -33.5 -50.2 -40.3 -124.7 -135.8 166.8 90.2
ISURAP ISURAP ISURAP
116.0 -101.6 -112.0 -55.7 -30.3 -18.5 -34.1 -114.3 -114.7 86.9 62.1
MALIAC11 MALIAC11 MALIAC11
108.0 -104.0 -104.7 -105.1 -49.7 -42.7 -44.2 -66.4 -85.6 110.2 69.9
MALNAC06 MALNAC06 MALNAC06
111.0 -105.8 -117.8 -137.3 -55.4 -60.2 -53.4 -62.2 -88.0 153.9 74.1
NAPOAC01 NAPOAC01 NAPOAC01
115.0 -104.8 -102.8 -75.0 -20.3 -38.8 -23.1 -113.7 -120.2 122.6 55.8
NICOAC02 NICOAC02 NICOAC02
123.0 -102.0 -86.8 -110.4 -29.0 -62.6 -21.4 -84.2 -97.8 155.2 56.4
OXALAC04 OXALAC04 OXALAC04
95.0 -106.3 -112.4 -146.8 -55.6 -69.2 -56.3 -60.5 -91.1 170.2 85.7
PFBZAD10 PFBZAD10 PFBZAD10
91.0 -86.0 -85.8 -91.3 -34.9 -42.6 -26.0 -71.1 -90.0 119.1 60.1
SUCACB11 SUCACB11 SUCACB11
122.0 -115.9 -121.8 -139.3 -47.5 -64.8 -55.8 -78.4 -102.4 166.7 79.1
TEPHTH12 TEPHTH12 TEPHTH12
135.0 -147.8 -126.5 -178.6 -58.4 -86.2 -42.3 -106.1 -139.5 223.1 108.7
CRESOL01 CRESOL01 CRESOL01
74.0 -73.4 -76.3 -53.8 -17.7 -23.0 -22.7 -82.5 -77.9 85.9 37.0
DIMPHE12 DIMPHE12 DIMPHE12
84.0 -88.2 -99.3 -58.2 -25.2 -27.5 -27.4 -97.1 -91.3 94.6 39.6
DMEPOL10 DMEPOL10 DMEPOL10
76.0 -83.0 -90.9 -51.9 -21.2 -24.1 -25.0 -92.1 -86.5 85.1 36.8
DMPHOL11 DMPHOL11 DMPHOL11
85.0 -80.2 -79.9 -47.2 -14.4 -22.9 -27.2 -100.1 -91.9 89.9 48.6
IPMEPL IPMEPL IPMEPL
92.0 -84.0 -95.2 -64.6 -24.9 -35.7 -27.6 -86.7 -86.4 103.1 38.9
NITPOL02 NITPOL02 NITPOL02
94.0 -94.6 -84.4 -71.5 -26.5 -28.8 -34.1 -90.1 -96.9 95.8 68.2
ACANIL03 ACANIL03 ACANIL03
84.0 -94.6 -101.5 -56.0 -36.6 -21.8 -24.0 -87.4 -84.7 70.6 39.0
AMIPYR AMIPYR AMIPYR
84.0 -75.5 -65.8 -49.3 -11.5 -20.1 -11.9 -74.0 -69.6 67.9 22.4
AMPYRE AMPYRE AMPYRE
88.0 -88.4 -80.5 -59.8 -21.6 -24.5 -15.6 -76.7 -73.2 72.6 25.0
BAPLOT01 BAPLOT01 BAPLOT01
126.0 -121.5 -125.1 -93.9 -28.2 -45.5 -40.4 -105.2 -117.6 123.2 56.3
BZAMID01 BZAMID01 BZAMID01
101.0 -100.9 -93.9 -74.6 -36.0 -26.5 -21.0 -83.8 -85.5 83.9 43.8
CAPLAC CAPLAC CAPLAC
90.0 -79.3 -75.2 -59.3 -29.3 -20.3 -24.3 -69.2 -68.8 69.4 42.3
CYANAC CYANAC CYANAC
100.0 -112.7 -117.1 -89.5 -62.3 -32.3 -36.1 -61.1 -66.7 70.2 43.2
DIXTAF DIXTAF DIXTAF
87.0 -88.8 -85.9 -72.4 -32.6 -25.4 -32.9 -69.6 -69.5 78.7 44.2
FORMAM02 FORMAM02 FORMAM02
72.0 -73.0 -61.0 -80.1 -41.5 -26.2 -19.8 -39.9 -47.5 73.1 42.9
GLUTIM GLUTIM GLUTIM
94.0 -83.3 -96.2 -57.9 -35.6 -18.1 -35.8 -68.3 -72.5 60.9 42.9
IBURAM IBURAM IBURAM
86.0 -83.1 -75.8 -74.5 -37.4 -25.9 -26.3 -53.4 -56.9 70.7 39.9
IMAZOL13 IMAZOL13 IMAZOL13
82.0 -84.6 -65.4 -78.7 -25.2 -36.0 -8.3 -53.0 -56.3 83.2 19.6
JEXNAB JEXNAB JEXNAB
126.0 -126.9 -122.5 -110.5 -58.4 -38.3 -44.3 -89.1 -95.2 111.0 70.6

MALOAM MALOAM MALOAM
126.0 -143.0 -139.3 -140.1 -77.6 -47.2 -48.3 -75.3 -87.1 119.6 68.8
MEADEN01 MEADEN01 MEADEN01
121.0 -125.5 -130.4 -99.0 -21.4 -36.9 -36.3 -109.1 -113.6 119.5 36.0
MEUREA MEUREA MEUREA
96.0 -102.6 -88.3 -95.6 -45.5 -32.4 -29.7 -55.7 -61.2 81.0 43.2
MNIANL02 MNIANL02 MNIANL02
95.0 -91.3 -83.5 -50.5 -14.3 -20.4 -30.5 -93.2 -95.6 72.9 52.0
NANILI02 NANILI02 NANILI02
100.0 -98.6 -96.1 -64.2 -32.4 -20.4 -28.8 -93.7 -97.0 79.7 57.3
PYRZOL02 PYRZOL02 PYRZOL02
73.0 -75.7 -56.3 -67.5 -19.0 -28.2 -5.3 -52.8 -54.5 72.8 17.6
TNIOAN TNIOAN TNIOAN
120.0 -95.5 -136.7 -45.8 -44.4 -16.3 -57.5 -99.0 -120.7 65.7 81.1
TRAZOL03 TRAZOL03 TRAZOL03
82.0 -87.9 -70.7 -87.2 -24.4 -39.7 -13.4 -58.4 -65.3 97.4 27.4
UREAXX09 UREAXX09 UREAXX09
92.0 -107.8 -95.6 -97.9 -47.3 -32.3 -34.9 -51.0 -58.4 73.4 40.2
VAYJIO VAYJIO VAYJIO
127.0 -126.7 -126.4 -75.4 -12.6 -30.9 -47.0 -131.4 -127.7 110.9 56.0
WIFKEB WIFKEB WIFKEB
90.0 -94.6 -84.9 -78.2 -34.8 -26.4 -31.8 -75.5 -75.9 85.5 52.7
ZZZKAY01 ZZZKAY01 ZZZKAY01
79.0 -77.7 -74.2 -77.0 -40.5 -27.6 -28.0 -54.2 -59.2 81.0 48.6
ACRDIN01 ACRDIN01 ACRDIN01
93.0 -95.9 -97.9 -23.2 -5.8 -14.4 -13.2 -124.5 -113.5 66.3 29.7
AZBENC01 AZBENC01 AZBENC01
93.0 -90.0 -83.1 -26.3 -6.7 -12.5 -11.8 -103.4 -95.0 52.2 25.6
BIPYRL04 BIPYRL04 BIPYRL04
82.0 -86.8 -91.7 -31.5 -13.2 -14.5 -14.1 -114.7 -104.3 73.9 34.9
BISJIW BISJIW BISJIW
70.0 -65.4 -63.0 -41.1 -27.5 -10.2 -14.1 -45.2 -47.4 31.1 21.1
CYAPYR CYAPYR CYAPYR
73.0 -69.6 -62.7 -39.0 -18.9 -10.9 -12.3 -64.9 -65.1 45.3 28.7
DAZNAP DAZNAP DAZNAP
83.0 -89.4 -81.2 -39.2 -21.5 -14.0 -7.5 -88.0 -81.8 51.8 24.7
MALONT MALONT MALONT
79.0 -62.1 -74.9 -43.3 -40.4 -11.2 -19.3 -38.7 -41.2 31.1 21.1
NMCABZ NMCABZ NMCABZ
95.0 -94.3 -91.6 -29.3 -9.7 -13.8 -13.1 -116.2 -103.1 65.0 29.4
PHENAT02 PHENAT02 PHENAT02
95.0 -102.9 -104.4 -34.5 -10.3 -15.2 -11.9 -135.4 -122.4 82.3 35.3
PYRAZI01 PYRAZI01 PYRAZI01
56.0 -60.2 -45.0 -34.8 -9.6 -10.6 -5.2 -61.8 -59.4 47.1 24.4
QUINAZ QUINAZ QUINAZ
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TCYQME TCYQME TCYQME
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TEPNIT11 TEPNIT11 TEPNIT11
89.0 -84.2 -89.4 -46.7 -29.9 -11.2 -17.0 -73.6 -75.6 47.4 28.1
TETDAM06 TETDAM06 TETDAM06
62.0 -68.4 -60.8 -29.3 -5.5 -11.7 -13.9 -92.0 -80.0 64.7 33.8
TRIZIN01 TRIZIN01 TRIZIN01
55.0 -53.9 -59.8 -25.3 -8.1 -7.1 -19.9 -53.9 -54.0 32.4 17.4
CPTCET10 CPTCET10 CPTCET10
118.0 -125.9 -117.6 -35.0 -5.6 -15.3 -11.5 -162.4 -145.3 86.8 39.9
DCLBEN01 DCLBEN01 DCLBEN01
65.0 -68.7 -59.5 -18.6 -2.2 -6.4 -5.4 -86.0 -76.7 42.3 19.9
DCLBIP DCLBIP DCLBIP
96.0 -91.2 -82.2 -23.2 -5.8 -11.3 -8.3 -114.4 -101.7 57.6 28.7
DCLBIQ10 DCLBIQ10 DCLBIQ10
104.0 -100.5 -93.5 -26.2 -5.9 -11.7 -8.8 -128.1 -114.5 65.6 30.8
HCLBNZ11 HCLBNZ11 HCLBNZ11
90.0 -93.5 -89.6 -23.3 5.5 -12.4 -3.0 -148.3 -135.6 90.5 38.6

HCLBPH HCLBPH HCLBPH
103.0 -101.1 -103.6 -24.3 0.1 -11.7 -7.9 -149.5 -136.8 84.5 36.0
HEXCET02 HEXCET02 HEXCET02
59.0 -70.5 -66.3 -16.5 -0.3 -6.6 -5.5 -101.0 -89.8 53.6 24.5
PNCLBZ PNCLBZ PNCLBZ
87.0 -88.4 -80.1 -24.5 3.1 -11.9 -3.8 -131.8 -118.8 79.7 34.5
TCBENZ TCBENZ TCBENZ
75.0 -75.8 -67.3 -20.9 -2.1 -7.9 -4.8 -98.6 -89.2 51.6 23.9
TCHLBZ TCHLBZ TCHLBZ
73.0 -73.9 -68.1 -19.4 0.3 -8.2 -6.4 -102.4 -91.6 56.1 24.7
TCLBZN TCLBZN TCLBZN
80.0 -80.9 -74.6 -21.5 0.4 -9.4 -4.9 -114.6 -103.4 64.6 28.5
ANTCEN14 ANTCEN14 ANTCEN14
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BENZEN07 BENZEN07 BENZEN07
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BIPHEN04 BIPHEN04 BIPHEN04
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BULVAL02 BULVAL02 BULVAL02
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CYCHEX05 CYCHEX05 CYCHEX05
43.0 -41.7 -45.7 -15.1 -0.2 -7.4 -17.0 -79.8 -65.3 60.5 31.9
DBNTHR02 DBNTHR02 DBNTHR02
150.0 -153.7 -149.2 -39.5 -18.0 -18.1 -12.1 -190.2 -163.2 94.1 39.3
DITBOX DITBOX DITBOX
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DMANTR DMANTR DMANTR
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DMNAPH05 DMNAPH05 DMNAPH05
83.0 -82.4 -85.0 -22.1 -8.7 -9.9 -13.6 -108.8 -94.0 58.4 26.4
DMNPTL01 DMNPTL01 DMNPTL01
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DPANTR DPANTR DPANTR
157.0 -134.3 -133.1 -28.4 -6.3 -15.1 -14.5 -178.7 -158.5 87.8 41.2
DURENE05 DURENE05 DURENE05
73.0 -67.3 -75.2 -17.2 -7.1 -6.0 -17.7 -89.2 -76.9 45.1 21.6
FEWWEJ FEWWEJ FEWWEJ
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FLUANT FLUANT FLUANT
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FLUREN01 FLUREN01 FLUREN01
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HEPTAN02 HEPTAN02 HEPTAN02
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MANTHR03 MANTHR03 MANTHR03
102.0 -100.9 -98.6 -18.6 -2.0 -10.4 -11.8 -137.4 -119.1 65.5 29.4
NAPHTA10 NAPHTA10 NAPHTA10
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OCTANE01 OCTANE01 OCTANE01
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PERLEN04 PERLEN04 PERLEN04
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PHENAN08 PHENAN08 PHENAN08
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TOLUEN TOLUEN TOLUEN
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TRIPHE11 TRIPHE11 TRIPHE11

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DNBENZ15 DNBENZ15 DNBENZ15
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OCHTET12 OCHTET12 OCHTET12
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MLEICA MLEICA MLEICA
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PHBENZ PHBENZ PHBENZ
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PHTHAO PHTHAO PHTHAO

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DCLBQN DCLBQN DCLBQN
70.0 -71.6 -84.9 -36.0 -35.3 -11.7 -16.0 -76.8 -80.0 52.8 41.5
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FELSEU FELSEU FELSEU
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HIHHAH HIHHAH HIHHAH
110.0 -80.9 -98.2 -36.3 -31.5 -12.3 -28.1 -84.9 -90.1 52.6 46.5
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OCDBDO10 OCDBDO10 OCDBDO10
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TCBENQ01 TCBENQ01 TCBENQ01
99.0 -83.7 -117.3 -40.4 -51.5 -12.8 -11.5 -102.8 -104.0 72.2 44.9
TNPHNT TNPHNT TNPHNT
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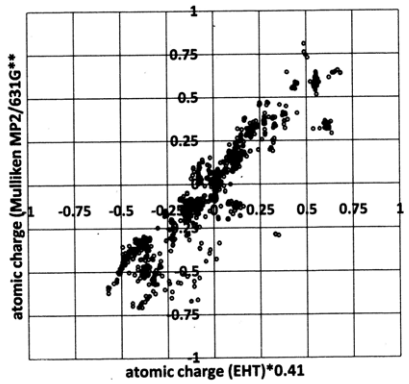

Fig. S1. Comparison of point charges (electrons) from rescaled Extended Huckel and MP2/6-31G** calculations.

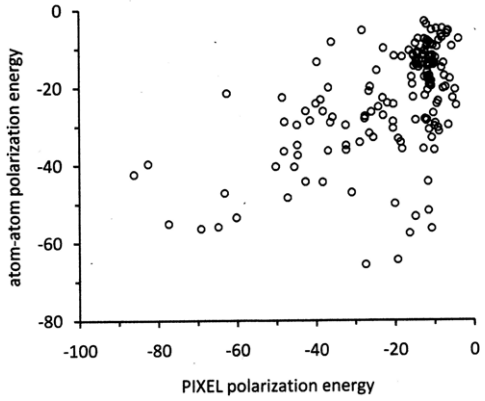

Fig. S2. Comparison of PIXEL and atom-atom polarization energies. kJ/mol units. Same sample as in Fig. 1.

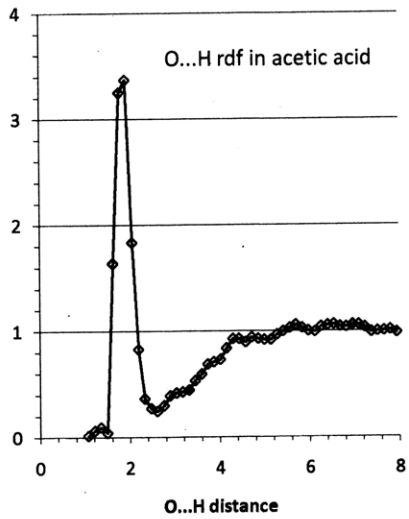

Fig. S3. Radial O...H(O) intermolecular density function from the final frame of the Monte Carlo simulation of acetic acid.

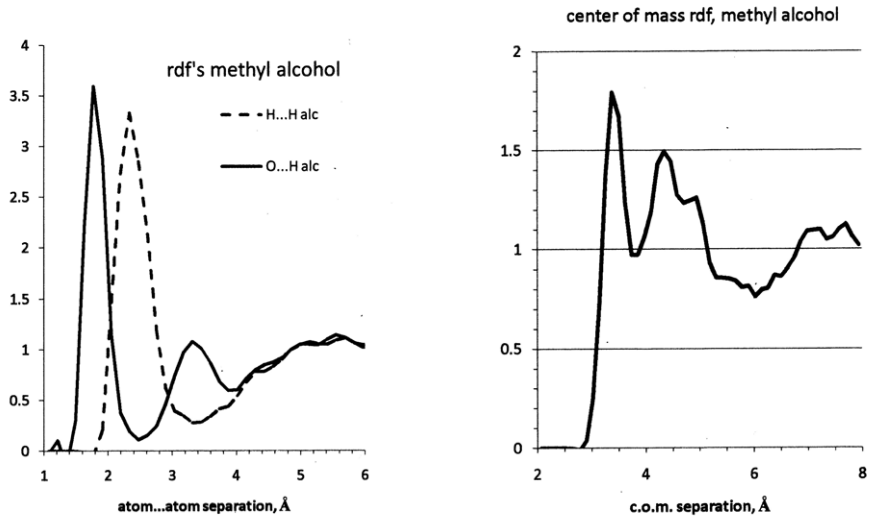

Fig. S4-S5. Intermolecular radial density functions from the final frame of the Monte Carlo simulation of methyl alcohol: left, atom-atom, right, center of mass. .

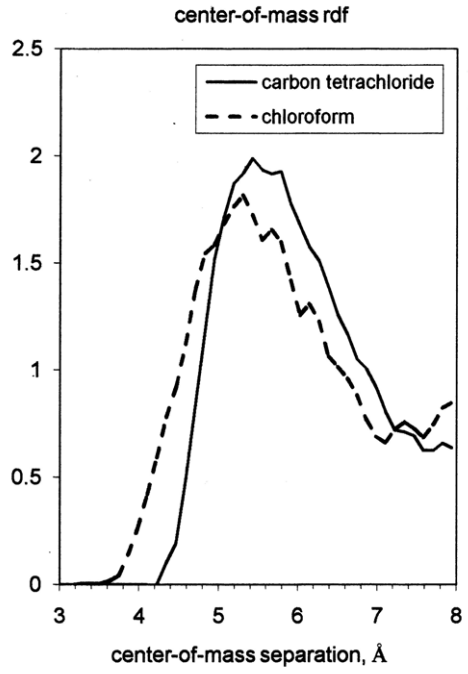

Fig. S6. Intermolecular center of mass radial density functions from the final frame of the Monte Carlo simulation of halohydrocarbons.

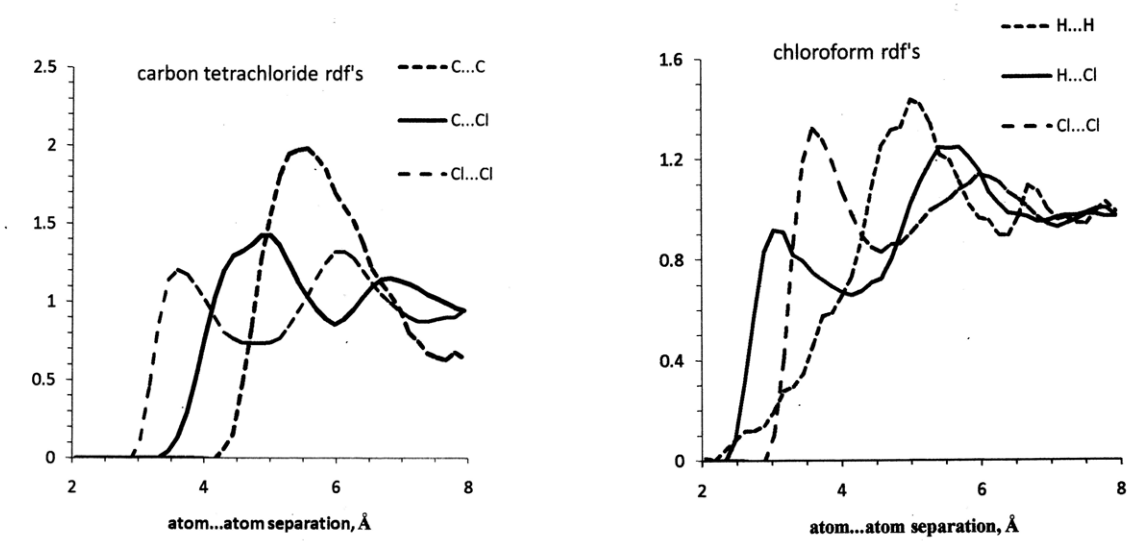

Fig. S7-S8. Intermolecular atom-atom radial density functions from the final frame of the Monte Carlo simulation of halohydrocarbons.

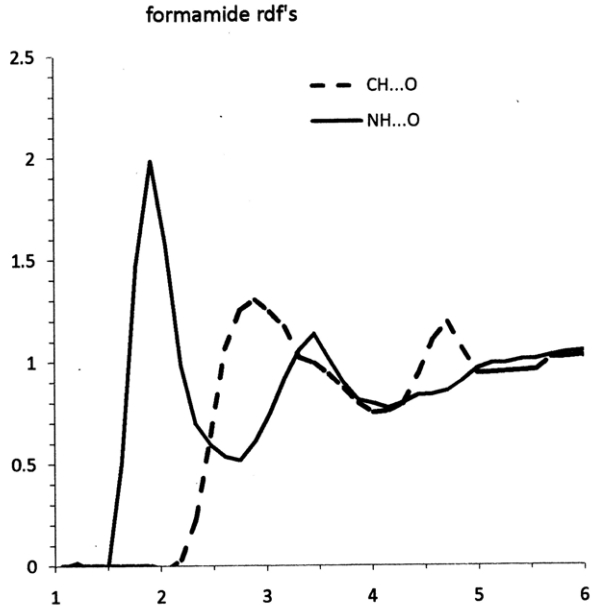

Fig. S9. Intermolecular radial density functions from the final frame of the Monte Carlo simulation of formamide.