Mining the Cambridge Database for theoretical chemistry. Mi–LJC: A new set of Lennard–Jones–Coulomb atom–atom potentials for the computer simulation of organic condensed matter

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ESI

ELECTRONIC SUPPLEMENTARY INFORMATION

INDEX

S1. Handling the SE–LE comparison.

The lattice energy LE is the difference in calculated intermolecular energy between one mole of molecules at infinite separation and one mole in the crystal (LE is stabilizing i.e. < 0). The sublimation enthalpy SE is a measure of purely intermolecular cohesion energy in the crystal when it does not include contributions from the enthalpy of any concomitant intramolecular process. A very approximate consideration of global equipartition energies for an ensemble of non–interacting particles leads to the following relationships: for vaporization enthalpy, ΔH(gas–liq) = –U(liq) +RT, for sublimation enthalpy, □H(gas–cry) = –U(cry) – 2RT or SE = –LE – 2RT (in molar quantities). In brief, the RT terms account for differences in kinetic energies between the various phases due to a change in the number of translational and rotational degrees of freedom, plus the Legendre transform molar PV = RT term that converts internal energies into enthalpies. The main assumptions are revised and commented in detail in the following.

Thermodynamic internal energy also has translational and rotational kinetic terms and vibrational terms:

$$U(tot,gas) = U(interm,gas) + E(kin,trasl) + E(kin,rot) + E(vib,intram) \quad \text{(S1)}$$

$$U(tot,liq) = U(interm,liq) + E(kin,trasl) + E(kin,rot) + E(vib,intram) \quad \text{(S2)}$$

where E(vib,intram) denotes the intramolecular vibrational energy. In the crystal, translational and rotational energies are replaced by potential end kinetic terms for translational and rotational librations (t–lib and r–lib):

$$U(tot,cry) = U(interm,cry) + E(kin,t-lib) + E(pot,t-lib) + E(kin,r-lib) + E(pot,r-lib) + E(vib,intram) \quad \text{(S3)}$$

If E(vib,intram) is the same in all aggregation states (a far–fetched assumption except for rigid molecules), it can be neglected in energy differences. U(interm,gas) is assumed as zero for vapors of a solid at room temperature (semi–ideal gas assumption). In the harmonic equipartition regime, each energy term is worth 3/2RT; then:

$$U(tot,gas) = 3RT \quad \text{(S4)}$$

$$U(tot,liq) = U(interm,liq) + 3RT \quad \text{(S5)}$$

$$U(tot,cry) = U(interm,cry) + 6RT \quad \text{(S6)}$$

Since H = U + PV, for the phase transition functions one gets at constant pressure:

Vaporization enthalpy:

$$\Delta H(gas-liq) = \Delta U(gas-liq) + P\Delta V = \Delta U(gas-liq) + PV_{gas} = \Delta U(gas-liq) + RT = U(tot,gas) - U(tot,liq) + RT = 3RT - U(interm,liq) - 3RT + RT = -U(interm.liq) + RT \quad \text{(S7)}$$

where the V_{liq}, is negligible against V_{gas}. For sublimation enthalpy (SE):

$$\Delta H(gas-cry) = \Delta U(gas-cry) + P\Delta V = \Delta U(gas-cry) + RT = U(tot,gas) - U(tot,cry) + RT = 3RT - U(interm,cry) - 6RT + RT = -U(cry) - 2RT \quad \text{(S8)}$$

$$\Rightarrow SE = -LE - 2RT \quad \text{(S9)}$$

Another way of seeing the matter is to assign a constant heat capacity of 3R to the gas and of 6R to the solid, and to perform the standard thermodynamic integration:

$$\Delta U_s(T) = \Delta U_s(0) + \int_0^T C_v dT = \Delta U_s(0) - 3R\int_0^T dT = \Delta U_s(0) - 3RT \quad \text{(S10)}$$

$$\Delta H_s = \Delta U_s + \Delta(PV) = \Delta U_s + PV = \Delta U_s + RT = \Delta U_s(0) - 2RT \quad \text{(S11)}$$

whereby the calculated LE is the sublimation internal energy at 0 K. However, the assumption of constant C_v breaks one of the basic laws of thermodynamics, namely the convergence to zero of solid heat capacities at low temperature. In general, these corrections depend on a number of heavy approximations (ideal or semi–ideal behavior, vibrational behaviour independent on the chemical environment, constant heat capacity), almost none of which apply to real organic molecules. At room temperature, the correction may introduce more inaccuracy than adhesion to physical principles; no correction is better than a bad correction.

Table S1.

Vaporization energies (VE) (kJ·mol^{-1}) and their dispersive–repulsive (E_{dr}) and Coulomb (E_C) contributions, from NPT-MD simulations of liquids, 432 molecule box, T = 298 K and P = 1 bar (weak coupling barostat).

Substance[a]	VE	E_{dr}	E_C	Functional
(a) pyridine	–39.1	–32.0	–7.2	CLP
	–32.6	–26.3	–6.3	LJC
(b) aminobenzene	–48.4	–44.1	–4.4	CLP
	–56.8	–28.7	–28.0	LJC
(c) benzaldehyde	–50.4	–36.9	–13.4	CLP
	–41.2	–34.6	–6.7	LJC
(d) methoxybenzene	–48.1	–41.6	–6.5	CLP
	–41.7	–36.6	–5.1	LJC
(e) ethanol	–35.6	–20.3	–15.3	CLP
	–46.7	–3.5	–43.1	LJC
(f) dichloroethane	–26.1	–22.3	–3.8	CLP
	–32.3	–25.2	–7.1	LJC
(g) n–pentane	–27.3	–27.1	–0.1	CLP
	–23.1	–23.1	0.0	LJC

[a] See Figure 1 in the main text

Table S2.

Cell dimensions and densities (Å, deg and g·cm–3) from NPT-MD simulations of molecular crystals (1)–(6) (Figure 1 in the main text) at P = 1 bar and variable T. Starting reference parameters, in bold, CLP with weak-coupling barostat, LJC with weak-coupling barostat and LJC with Parrinello–Rahman (PR) barostat. Computational boxes from duplication of unit cells to dimensions of at least 35 Å.

Crystal	Space group	T / K	*a*	*b*	*c*	α	β	γ	Density	Functional
(1) n–hexane	$P\bar{1}$	90	**4.131**	**4.696**	**8.539**	**83.4**	**87.3**	**75.2**	**0.900**	MC (starting)
			4.206	4.527	8.440	83.5	87.2	74.3	0.931	CLP
			4.070	4.429	8.474	83.7	87.3	74.5	0.978	LJC
			4.255	4.467	8.546	83.7	87.8	75.7	0.915	LJC (PR)
(2) Naphthalene	$P2_1/a$	298	**8.266**	**5.968**	**8.669**	**90.0**	**122.9**	**90.0**	**1.186**	MC (starting)
			7.804	5.808	8.693	90.0	120.8	90.0	1.257	CLP
			8.510	6.013	8.761	90.0	123.6	90.0	1.140	LJC
			8.368	5.982	8.502	90.0	115.7	90.6	1.110	LJC (PR)
(3) Maleic anhydride	$P2_12_12_1$	130	**7.032**	**11.020**	**5.332**	**90.0**	**90.0**	**90.0**	**1.576**	MC (starting)
			6.587	11.753	5.158	90.0	90.0	90.0	1.631	CLP
			7.030	11.503	5.249	90.0	90.0	90.0	1.535	LJC
			7.091	11.519	5.281	91.3	90.3	89.7	1.510	LJC (PR)
(4) Methylurea	$P2_12_12_1$	298	**8.477**	**6.981**	**6.923**	**90.0**	**90.0**	**90.0**	**1.201**	MC (starting)
			8.466	7.012	6.912	90.0	90.0	90.0	1.199	CLP
			7.890	7.331	6.511	90.0	90.0	90.0	1.307	LJC
			8.006	7.366	6.555	90.2	89.3	90.5	1.273	LJC (PR)
(5) p–nitrophenol	$P2_1/c$	110	**6.166**	**8.837**	**11.543**	**90.0**	**103.4**	**90.0**	**1.510**	MC (starting)
			6.914	8.466	10.432	90.0	106.7	90.0	1.580	CLP
			6.031	8.857	11.704	90.0	102.9	90.0	1.516	LJC
			6.122	8.724	11.932	89.5	105.1	89.2	1.502	LJC (PR)
(6) Trimethyltrioxane $CHCl_3$ solvate	$P2_1/c$	190	**11.579**	**13.627**	**7.941**	**90.0**	**107.0**	**90.0**	**1.394**	MC (starting)
			13.070	11.866	8.004	90.0	109.1	90.0	1.424	CLP
			12.279	12.012	8.005	90.0	107.9	90.0	1.487	LJC
			12.362	12.214	8.111	90.0	111.3	90.0	1.464	LJC (PR))

Table S3.

Lattice energies (LE, kJ·mol^{-1}) and their dispersive–repulsive (E_{dr}) and Coulomb (E_C) contributions, from NPT-MD simulations of molecular crystals. See Table S2 above for explanation of symbols. .

Crystal[a]	Space group	T / K	LE	E_{dr}	E_C	Functional
(1) n–hexane	$P\bar{1}$	90	–55.8 –51.9 –46.4	–55.74 –52.00 –46.40	–0.03 0.08 0.00	CLP LJC LJC (PR)
(2) Naphthalene	$P2_1/a$	298	–74.1 –59.3 –56.1	–66.79 –54.13 –51.81	–7.35 –5.13 –4.27	CLP LJC LJC (PR)
(3) Maleic anhydride	$P2_12_12_1$	130	–84.6 –68.3 –65.9	–46.68 –40.84 –39.28	–37.95 –27.47 –26.65	CLP LJC LJC (PR)
(4) Methylurea	$P2_12_12_1$	298	–83.5 –95.0 –91.7	–46.94 –16.69 –17.28	–36.58 –78.31 –74.44	CLP LJC LJC (PR)
(5) p–nitrophenol	$P2_1/c$	110	–101.2 –95.0 –92.9	–71.50 –55.88 –54.81	–29.66 –39.10 –38.07	CLP LJC LJC (PR)
Crystal[a]	Space group	T / K	LE(solute)	LE(solvent)	LE(solvation)	Functional
(6) Trimethyltrioxane $CHCl_3$ solvate[b]	$P2_1/c$	190	–50.6 –39.8 –39.8	–10.4 –8.9 –8.5	–56.5 –60.4 –58.7	CLP LJC LJC (PR)

[a] See Figure 1 in the main text

[b] Trimethyltrioxane part, chloroform part, and solvation part (left to right).

Table S4

Force field data for crystal structures and liquids in Molecular Dynamics. Atomic coordinates and charges, stretching functions for $Es=1/2K(R-R°)^2$, bending functions for $Eb=1/2K(\cos(t)-\cos(t°))^2$, torsional functions, K, f and n for $E(t) = K(1-f(\cosnt))$.

```
#HEXANE01
   20
    1  -0.00257   0.22174  -3.19137  13   -0.8984
    2   0.00280  -0.53915  -1.87570  13   -0.5518
    3   0.00541   0.37514  -0.66189  13   -0.5632
    4  -0.00541  -0.37514   0.66189  13   -0.5632
    5  -0.00280   0.53916   1.87570  13   -0.5518
    6   0.00257  -0.22174   3.19137  13   -0.8984
    7   0.86830   0.85839  -3.24260   3    0.2957
    8   0.01515  -0.47928  -4.01275   3    0.2957
    9  -0.89498   0.82678  -3.25368   3    0.2957
   10   0.87757  -1.17152  -1.84005   3    0.2816
   11  -0.86989  -1.17406  -1.83437   3    0.2816
   12  -0.86320   1.01541  -0.70640   3    0.2815
   13   0.88423   1.00175  -0.69984   3    0.2815
   14   0.86320  -1.01540   0.70640   3    0.2815
   15  -0.88423  -1.00174   0.69984   3    0.2815
   16  -0.87757   1.17152   1.84005   3    0.2817
   17   0.86989   1.17407   1.83437   3    0.2816
   18   0.87563  -0.85586   3.23697   3    0.2957
   19   0.02357   0.47934   4.01263   3    0.2957
   20  -0.88768  -0.82941   3.25943   3    0.2957

   19  stretching
    1    2   1.520  2146.2   C- C
    1    7   1.080  3600.0   C- H
    1    8   1.080  3600.0   C- H
    1    9   1.080  3600.0   C- H
    2    3   1.520  2151.1   C- C
    2   10   1.080  3600.0   C- H
    2   11   1.080  3600.0   C- H
    3    4   1.522  2108.7   C- C
    3   12   1.080  3600.0   C- H
    3   13   1.080  3600.0   C- H
    4    5   1.520  2151.1   C- C
    4   14   1.080  3600.0   C- H
    4   15   1.080  3600.0   C- H
    5    6   1.520  2146.2   C- C
    5   16   1.080  3600.0   C- H
    5   17   1.080  3600.0   C- H
    6   18   1.080  3600.0   C- H
    6   19   1.080  3600.0   C- H
    6   20   1.080  3600.0   C- H

   36  bending
    1    2    3  113.00   534.6   C- C- C
    1    2   10  109.50   642.5   C- C- H
    1    2   11  109.50   642.5   C- C- H
    2    1    7  109.50   642.5   C- C- H
    2    1    8  109.50   642.5   C- C- H
    2    1    9  109.50   642.5   C- C- H
    2    3    4  113.00   534.6   C- C- C
    2    3   12  109.50   642.5   C- C- H
    2    3   13  109.50   642.5   C- C- H
    3    2   10  109.50   642.5   C- C- H
    3    2   11  109.50   642.5   C- C- H
    3    4    5  113.00   534.6   C- C- C
    3    4   14  109.50   642.5   C- C- H
    3    4   15  109.50   642.5   C- C- H
    4    3   12  109.50   642.5   C- C- H
    4    3   13  109.50   642.5   C- C- H
    4    5    6  113.00   534.6   C- C- C
    4    5   16  109.50   642.5   C- C- H
    4    5   17  109.50   642.5   C- C- H
    5    4   14  109.50   642.5   C- C- H
    5    4   15  109.50   642.5   C- C- H
    5    6   18  109.50   642.5   C- C- H
    5    6   19  109.50   642.5   C- C- H
    5    6   20  109.50   642.5   C- C- H
    6    5   16  109.50   642.5   C- C- H
    6    5   17  109.50   642.5   C- C- H
    7    1    8  109.50   470.0   H- C- H
    7    1    9  109.50   470.0   H- C- H
    8    1    9  109.50   470.0   H- C- H
```

```
   10    2   11  108.00   470.0   H- C- H
   12    3   13  108.00   470.0   H- C- H
   14    4   15  108.00   470.0   H- C- H
   16    5   17  108.00   470.0   H- C- H
   18    6   19  109.50   470.0   H- C- H
   18    6   20  109.50   470.0   H- C- H
   19    6   20  109.50   470.0   H- C- H

    5  torsion
   7   1   2   3  7.50   1.0    3.0   H- C- C- C
   1   2   3   4  6.00   1.0    3.0   C- C- C- C
   2   3   4   5  6.00   1.0    3.0   C- C- C- C
   3   4   5   6  6.00   1.0    3.0   C- C- C- C
   4   5   6  18  7.50   1.0    3.0   C- C- C- H
```

```
#HOZNOB   methyltrioxane,chloroform solvate
   21  trioxane
    1  -0.12691   0.73456  -1.11331  23   -0.9197
    2  -0.10989  -1.33712  -0.08012  23   -0.9284
    3  -0.10486   0.59215   1.19698  23   -0.9194
    4   0.34204   1.34148   0.07572  13    0.6932
    5   0.34521  -0.59651  -1.21136  13    0.6942
    6   0.33810  -0.74301   1.12703  13    0.6943
    7  -0.22339  -1.50492   2.28066  13   -0.9286
    8  -0.21827   2.72887   0.17243  13   -0.9296
    9  -0.21817  -1.21549  -2.44823  13   -0.9281
   10   1.42161   1.31869   0.05450   3    0.2388
   11   1.42501  -0.57578  -1.20586   3    0.2404
   12   1.41795  -0.72750   1.11479   3    0.2367
   13   0.12787  -2.52554   2.24321   3    0.3061
   14   0.09772  -1.04739   3.20477   3    0.3066
   15  -1.30208  -1.49325   2.22896   3    0.3055
   16  -1.29607   2.68644   0.11814   3    0.3057
   17   0.07772   3.17192   1.11183   3    0.3070
   18   0.15998   3.32760  -0.64301   3    0.3064
   19   0.05224  -0.61694  -3.30560   3    0.3072
   20   0.18003  -2.21259  -2.56524   3    0.3061
   21  -1.29409  -1.26455  -2.36833   3    0.3056

    5  chcl3
    1  -0.07039   1.54371  -0.61151  42   -0.2877
    2  -0.07161  -0.24633   1.64739  42   -0.2856
    3  -0.06953  -1.29841  -1.03956  42   -0.2923
    4   0.49245   0.00240   0.00856  13    0.6209
    5   1.57230   0.00760   0.02729   3    0.2447

   21  stretching
    1    4   1.415  3755.2   O- C
    1    5   1.416  3737.8   O- C
    2    5   1.427  3492.9   O- C
    2    6   1.418  3685.4   O- C
    3    4   1.421  3625.7   O- C
    3    6   1.408  3900.3   O- C
    4    8   1.499  2577.6   C- C
    4   10   1.080  3600.0   C- H
    5    9   1.493  2702.5   C- C
    5   11   1.080  3600.0   C- H
    6    7   1.492  2728.8   C- C
    6   12   1.080  3600.0   C- H
    7   13   1.080  3600.0   C- H
    7   14   1.080  3600.0   C- H
    7   15   1.080  3600.0   C- H
    8   16   1.080  3600.0   C- H
    8   17   1.080  3600.0   C- H
    8   18   1.080  3600.0   C- H
    9   19   1.080  3600.0   C- H
    9   20   1.080  3600.0   C- H
    9   21   1.080  3600.0   C- H
    4  nstr-v
    1    4   1.754  3600.0  Cl- C
    2    4   1.751  3600.0  Cl- C
    3    4   1.763  3600.0  Cl- C
    4    5   1.080  3600.0   C- H
   39  bending
    1    4    3  109.00   475.3   O- C- O
    1    4    8  109.00   475.3   O- C- C
    1    4   10  108.00   655.0   O- C- H
    1    5    2  109.00   475.3   O- C- O
    1    5    9  109.00   475.3   O- C- C
    1    5   11  108.00   655.0   O- C- H
```

```
    2    5    9  109.00   475.3   O- C- C
    2    5   11  109.00   642.5   O- C- H
    2    6    3  110.00   493.3   O- C- O
    2    6    7  109.00   475.3   O- C- C
    2    6   12  108.00   655.0   O- C- H
    3    4    8  109.00   475.3   O- C- C
    3    4   10  109.00   642.5   O- C- H
    3    6    7  109.00   475.3   O- C- C
    3    6   12  108.00   655.0   O- C- H
    4    1    5  111.00   511.3   C- O- C
    4    3    6  111.00   511.3   C- O- C
    4    8   16  109.50   642.5   C- C- H
    4    8   17  109.50   642.5   C- C- H
    4    8   18  109.50   642.5   C- C- H
    5    2    6  111.00   511.3   C- O- C
    5    9   19  109.50   642.5   C- C- H
    5    9   20  109.50   642.5   C- C- H
    5    9   21  109.50   642.5   C- C- H
    6    7   13  109.50   642.5   C- C- H
    6    7   14  109.50   642.5   C- C- H
    6    7   15  109.50   642.5   C- C- H
    7    6   12  113.00   592.5   C- C- H
    8    4   10  113.00   592.5   C- C- H
    9    5   11  113.00   592.5   C- C- H
   13    7   14  109.50   470.0   H- C- H
   13    7   15  109.50   470.0   H- C- H
   14    7   15  109.50   470.0   H- C- H
   16    8   17  109.50   470.0   H- C- H
   16    8   18  109.50   470.0   H- C- H
   17    8   18  109.50   470.0   H- C- H
   19    9   20  109.50   470.0   H- C- H
   19    9   21  109.50   470.0   H- C- H
   20    9   21  109.50   470.0   H- C- H
    6  nbend-v
    1    4    2  111.00   500.0  Cl- C-Cl ?
    1    4    3  110.00   500.0  Cl- C-Cl
    1    4    5  109.00   642.5  Cl- C- H
    2    4    3  110.00   500.0  Cl- C-Cl
    2    4    5  108.00   655.0  Cl- C- H
    3    4    5  109.00   642.5  Cl- C- H
    9  torsion
   1  4  3  6  6.00   1.0    3.0   C- O- C- O
   4  3  6  2  6.00   1.0    3.0   C- O- C- O
   3  6  2  5  6.00   1.0    3.0   C- O- C- O
   2  5  1  4  6.00   1.0    3.0   C- O- C- O
   5  1  4  3  6.00   1.0    3.0   C- O- C- O
   1  4  3  6  6.00   1.0    3.0   C- O- C- O
   1   4   8  16  7.50   1.0    3.0   O- C- C- H
   1   5   9  19  7.50   1.0    3.0   O- C- C- H
   2   6   7  13  7.50   1.0    3.0   O- C- C- H
```

```
#MEUREA  methylurea
   11
    1   0.00434  -0.05564  -0.47598  10    1.2133
    2  -0.00657   0.02736   1.95453  13   -0.6380
    3  -0.01806   0.64533  -1.61806  21   -0.9755
    4   0.01035   0.64993   0.65834  21   -0.6511
    5   0.00121  -1.30400  -0.47945  27   -1.2843
    6   0.78152  -0.70899   2.01059   3    0.2871
    7   0.14679   0.77753   2.71621   3    0.2881
    8  -0.96075  -0.45405   2.11023   3    0.2857
    9   0.09215   0.13648  -2.47186   7    0.4947
   10   0.02762   1.64337  -1.57484   7    0.4930
   11   0.02701   1.64259   0.53844   7    0.4870

   10  stretching
    1    3   1.340  5845.9   C- N
    1    4   1.336  5949.1   C- N
    1    5   1.248  7484.0   C- O
    2    4   1.438  3532.4   C- N
    2    6   1.080  3600.0   C- H
    2    7   1.080  3600.0   C- H
    2    8   1.080  3600.0   C- H
    3    9   1.000  5300.0   N- H
    3   10   1.000  5300.0   N- H
    4   11   1.000  5300.0   N- H
   15  bending
    1    3    9  117.00   460.0   C- N- H
    1    3   10  119.00   460.0   C- N- H
    1    4    2  122.00   627.4   C- N- C
    1    4   11  115.00   460.0   C- N- H
```

```
    2    4   11  123.00   460.0   C- N- H
    3    1    4  117.00   580.9   N- C- N
    3    1    5  121.00   702.0   N- C- O
    4    1    5  122.00   702.0   N- C- O
    4    2    6  109.00   642.5   N- C- H
    4    2    7  109.00   642.5   N- C- H
    4    2    8  109.00   642.5   N- C- H
    6    2    7  109.00   470.0   H- C- H
    6    2    8  109.00   470.0   H- C- H
    7    2    8  109.00   470.0   H- C- H
    9    3   10  123.00   445.0   H- N- H
    6  torsion
   5   1   3   9  45.00   -1.0    2.0   O- C- N- H amide
   5   1   4  11  45.00   -1.0    2.0   O- C- N- H amide
   1   3   4   5 100.00   -1.0    1.0   C- N- N- O
   6   2   4   1   7.50    1.0    3.0   H- C- N- C methyl tors
   3   1   9  10 100.00   -1.0    1.0   N- C- H- H
   4   1   2  11 100.00   -1.0    1.0   N- C- C- H

 #MLEICA01 maleic anhydride
    9
    1   0.02552   0.92681   0.00431  23   -0.7536
    2   0.00300   0.10952  -1.11818  10    1.3867
    3   0.00238  -1.29766  -0.67111  12   -0.2214
    4   0.00257  -1.30367   0.66051  12   -0.2185
    5   0.00028   0.10436   1.12150  10    1.3867
    6  -0.01648   0.57192  -2.22305  27   -1.0952
    7  -0.01560   0.56736   2.22536  27   -1.0936
    8   0.00186  -2.16790  -1.31070   2    0.3046
    9   0.00409  -2.17954   1.29236   2    0.3044
    9  stretching
    1    2   1.389  4342.7   O- C
    1    5   1.388  4369.2   O- C
    2    3   1.476  3059.6   C- C
    2    6   1.198  8614.2   C- O
    3    4   1.332  6109.9   C- C
    3    8   1.080  3600.0   C- H
    4    5   1.482  2952.4   C- C
    4    9   1.080  3600.0   C- H
    5    7   1.197  8631.0   C- O
   13  bending
    1    2    3  108.00   457.2   O- C- C
    1    2    6  121.00   691.6   O- C- O
    1    5    4  108.00   457.2   O- C- C
    1    5    7  121.00   691.6   O- C- O
    2    1    5  108.00   457.2   C- O- C
    2    3    4  108.00   499.5   C- C- C
    2    3    8  126.00   430.0   C- C- H
    3    2    6  130.00   853.9   C- C- O
    3    4    5  108.00   499.5   C- C- C
    3    4    9  126.00   430.0   C- C- H
    4    3    8  126.00   430.0   C- C- H
    4    5    7  131.00   871.9   C- C- O
    5    4    9  126.00   430.0   C- C- H
    9  torsion
   5   1   2   3  50.00   -1.0    1.0   C- O- C- C
   2   1   5   4  50.00   -1.0    1.0   C- O- C- C
   1   2   3   4  50.00   -1.0    1.0   O- C- C- C
   2   1   3   6 100.00   -1.0    1.0   C- O- C- O
   2   3   4   5  50.00   -1.0    1.0   C- C- C- C
   3   2   4   8 100.00   -1.0    1.0   C- C- C- H
   3   4   5   1  50.00   -1.0    1.0   C- C- C- O
   4   3   5   9 100.00   -1.0    1.0   C- C- C- H
   5   1   4   7 100.00   -1.0    1.0   C- O- C- O
```

```
#NAPHTA13 naphthalene
   18
    1   0.00004   0.70617  -0.00009  14    0.0511
    2  -0.00023   1.39916   1.24243  12   -0.3093
    3   0.00020   1.39946  -1.24251  12   -0.3095
    4   0.00013   0.70047   2.42124  12   -0.2917
    5  -0.00006   0.70021  -2.42146  12   -0.2917
    6  -0.00004  -0.70617   0.00009  14    0.0511
    7   0.00006  -0.70021   2.42146  12   -0.2917
    8  -0.00013  -0.70047  -2.42124  12   -0.2917
    9   0.00023  -1.39916  -1.24243  12   -0.3093
   10  -0.00020  -1.39946   1.24251  12   -0.3095
   11  -0.00075   2.47905   1.25665   2    0.2886
   12   0.00049   2.47939  -1.25671   2    0.2886
   13   0.00049   1.23520   3.35956   2    0.2868
   14  -0.00022   1.23460  -3.35999   2    0.2869
```

```
  15   0.00022  -1.23460   3.35999   2    0.2869
  16  -0.00049  -1.23520  -3.35956   2    0.2868
  17   0.00075  -2.47905  -1.25665   2    0.2886
  18  -0.00049  -2.47939   1.25671   2    0.2886
  19  stretching
   1    2   1.423  4192.1   C- C
   1    3   1.423  4191.0   C- C
   1    6   1.412  4410.2   C- C
   2    4   1.370  5295.3   C- C
   2   11   1.080  3600.0   C- H
   3    5   1.371  5286.6   C- C
   3   12   1.080  3600.0   C- H
   4    7   1.401  4656.0   C- C
   4   13   1.080  3600.0   C- H
   5    8   1.401  4656.0   C- C
   5   14   1.080  3600.0   C- H
   6    9   1.423  4192.1   C- C
   6   10   1.423  4191.0   C- C
   7   10   1.371  5286.6   C- C
   7   15   1.080  3600.0   C- H
   8    9   1.370  5295.3   C- C
   8   16   1.080  3600.0   C- H
   9   17   1.080  3600.0   C- H
  10   18   1.080  3600.0   C- H
  30  bending
   1    2    4  120.00   583.8   C- C- C
   1    2   11  120.00   505.0   C- C- H
   1    3    5  120.00   583.8   C- C- C
   1    3   12  120.00   505.0   C- C- H
   1    6    9  119.00   576.7   C- C- C
   1    6   10  119.00   576.7   C- C- C
   2    1    3  122.00   597.8   C- C- C
   2    1    6  119.00   576.7   C- C- C
   2    4    7  121.00   590.8   C- C- C
   2    4   13  120.00   505.0   C- C- H
   3    1    6  119.00   576.7   C- C- C
   3    5    8  121.00   590.8   C- C- C
   3    5   14  120.00   505.0   C- C- H
   4    2   11  120.00   505.0   C- C- H
   4    7   10  121.00   590.8   C- C- C
   4    7   15  120.00   505.0   C- C- H
   5    3   12  120.00   505.0   C- C- H
   5    8    9  121.00   590.8   C- C- C
   5    8   16  120.00   505.0   C- C- H
   6    9    8  120.00   583.8   C- C- C
   6    9   17  120.00   505.0   C- C- H
   6   10    7  120.00   583.8   C- C- C
   6   10   18  120.00   505.0   C- C- H
   7    4   13  120.00   505.0   C- C- H
   7   10   18  120.00   505.0   C- C- H
   8    5   14  120.00   505.0   C- C- H
   8    9   17  120.00   505.0   C- C- H
   9    6   10  122.00   597.8   C- C- C
   9    8   16  120.00   505.0   C- C- H
  10    7   15  120.00   505.0   C- C- H
  21  torsion
   6   1   2   4  50.00   -1.0    1.0   C- C- C- C
   6   1   3   5  50.00   -1.0    1.0   C- C- C- C
   2   1   6  10  50.00   -1.0    1.0   C- C- C- C
   1   2   3   6 100.00   -1.0    1.0   C- C- C- C
   1   2   4   7  50.00   -1.0    1.0   C- C- C- C
   2   1   4  11 100.00   -1.0    1.0   C- C- C- H
   1   3   5   8  50.00   -1.0    1.0   C- C- C- C
   3   1   5  12 100.00   -1.0    1.0   C- C- C- H
   2   4   7  10  50.00   -1.0    1.0   C- C- C- C
   4   2   7  13 100.00   -1.0    1.0   C- C- C- H
   3   5   8   9  50.00   -1.0    1.0   C- C- C- C
   5   3   8  14 100.00   -1.0    1.0   C- C- C- H
   1   6   9   8  50.00   -1.0    1.0   C- C- C- C
   1   6  10   7  50.00   -1.0    1.0   C- C- C- C
   6   1   9  10 100.00   -1.0    1.0   C- C- C- C
   4   7  10   6  50.00   -1.0    1.0   C- C- C- C
   7   4  10  15 100.00   -1.0    1.0   C- C- C- H
   5   8   9   6  50.00   -1.0    1.0   C- C- C- C
   8   5   9  16 100.00   -1.0    1.0   C- C- C- H
   9   6   8  17 100.00   -1.0    1.0   C- C- C- H
  10   6   7  18 100.00   -1.0    1.0   C- C- C- H
```

```
#NITPOL03 p-nitrophenol
   15
    1   0.02946  -0.06511  -3.48537  29   -1.2281
    2   0.00996  -1.09037   2.68977  30   -0.8337
    3   0.03677   1.08737   2.70110  30   -0.8620
    4   0.00634  -0.00689   2.09485  20    1.1626
    5   0.00138   0.00264  -2.12840  12    0.7539
    6  -0.02829   1.22814  -1.42918  12   -0.3430
    7  -0.04283   1.23164  -0.03756  12   -0.2172
    8  -0.01954   0.00631   0.64288  12    0.2097
    9  -0.01716  -1.22231  -0.03470  12   -0.2201
   10  -0.01655  -1.21766  -1.42576  12   -0.3475
   11  -0.03968   2.16123  -1.97287   2    0.2975
   12  -0.07158   2.16273   0.50893   2    0.2963
   13  -0.01581  -2.15321   0.51286   2    0.2964
   14  -0.02986  -2.15165  -1.96790   2    0.2980
   15   0.32503   0.81508  -3.85675   5    0.7370
   15  stretching
    1    5   1.359  5008.5   O- C
    1   15   1.000  4250.0   O- H
    2    4   1.236  6000.0   O- N
    3    4   1.251  6000.0   O- N
    4    8   1.452  3196.5   N- C
    5    6   1.411  4433.3   C- C
    5   10   1.408  4496.7   C- C
    6    7   1.392  4844.9   C- C
    6   11   1.080  3600.0   C- H
    7    8   1.402  4632.9   C- C
    7   12   1.080  3600.0   C- H
    8    9   1.403  4605.5   C- C
    9   10   1.391  4858.2   C- C
    9   13   1.080  3600.0   C- H
   10   14   1.080  3600.0   C- H
   22  bending
    1    5    6  123.00   727.7   O- C- C
    1    5   10  117.00   619.5   O- C- C
    2    4    3  122.00   700.0   O- N- O
    2    4    8  119.00   701.0   O- N- C
    3    4    8  118.00   701.0   O- N- C
    4    8    7  120.00   608.8   N- C- C
    4    8    9  118.00   590.2   N- C- C
    5    1   15  109.00   450.0   C- O- H
    5    6    7  120.00   583.8   C- C- C
    5    6   11  120.00   505.0   C- C- H
    5   10    9  120.00   583.8   C- C- C
    5   10   14  120.00   505.0   C- C- H
    6    5   10  120.00   583.8   C- C- C
    6    7    8  119.00   576.7   C- C- C
    6    7   12  121.00   492.5   C- C- H
    7    6   11  120.00   505.0   C- C- H
    7    8    9  122.00   597.8   C- C- C
    8    7   12  121.00   492.5   C- C- H
    8    9   10  119.00   576.7   C- C- C
    8    9   13  121.00   492.5   C- C- H
    9   10   14  120.00   505.0   C- C- H
   10    9   13  121.00   492.5   C- C- H
   15  torsion
  15   1   5   6   7.00   -1.0    2.0   H- O- C- C phenol OH
   2   4   8   9  10.00   -1.0    2.0   O- N- C- C nitro group
   4   2   3   8 100.00   -1.0    1.0   N- O- O- C
  10   5   6   7  50.00   -1.0    1.0   O- C- C- C
   6   5  10   9  50.00   -1.0    1.0   O- C- C- C
   5   1   6  10 100.00   -1.0    1.0   C- O- C- C
   5   6   7   8  50.00   -1.0    1.0   C- C- C- C
   6   5   7  11 100.00   -1.0    1.0   C- C- C- H
   6   7   8   9  50.00   -1.0    1.0   C- C- C- N
   7   6   8  12 100.00   -1.0    1.0   C- C- C- H
   7   8   9  10  50.00   -1.0    1.0   N- C- C- C
   8   4   7   9 100.00   -1.0    1.0   C- N- C- C
   8   9  10   5  50.00   -1.0    1.0   C- C- C- C
   9   8  10  13 100.00   -1.0    1.0   C- C- C- H
  10   5   9  14 100.00   -1.0    1.0   C- C- C- H
```

```
benzaldehyde liquid
   14
    1   0.00000   0.23168   0.48549  12    0.0197
    2   0.00000   1.29040  -0.41518  12   -0.2284
    3   0.00000   1.03976  -1.78240  12   -0.2915
    4   0.00000  -0.26961  -2.24894  12   -0.2261
    5  -0.00000  -1.32833  -1.34827  12   -0.2912
    6  -0.00000  -1.07768   0.01894  12   -0.2285
    7   0.00000   0.49855   1.94123  10    0.6560
    8   0.00000   2.30775  -0.05269   2    0.2875
    9   0.00000   1.86237  -2.48220   2    0.2878
   10   0.00000  -0.46435  -3.31124   2    0.2874
   11  -0.00000  -2.34568  -1.71077   2    0.2878
   12   0.00000  -1.90029   0.71874   2    0.2876
   13   0.00000  -0.35124   2.80261  27   -1.1086
   14   0.00000   1.53074   2.25901   3    0.2606
   14  stretching
    1    2   1.390  4880.7   C- C
    1    6   1.390  4880.9   C- C
    1    7   1.480  2985.6   C- C
    2    3   1.390  4880.8   C- C
    2    8   1.080  3600.0   C- H
    3    4   1.390  4880.7   C- C
    3    9   1.080  3600.0   C- H
    4    5   1.390  4880.9   C- C
    4   10   1.080  3600.0   C- H
    5    6   1.390  4880.8   C- C
    5   11   1.080  3600.0   C- H
    6   12   1.080  3600.0   C- H
    7   13   1.210  8342.8   C- O
    7   14   1.080  3600.0   C- H
   21  bending
    1    2    3  120.00   583.8   C- C- C
    1    2    8  120.00   505.0   C- C- H
    1    6    5  120.00   583.8   C- C- C
    1    6   12  120.00   505.0   C- C- H
    1    7   13  125.00   763.8   C- C- O
    1    7   14  118.00   530.0   C- C- H
    2    1    6  120.00   583.8   C- C- C
    2    1    7  120.00   583.8   C- C- C
    2    3    4  120.00   583.8   C- C- C
    2    3    9  120.00   505.0   C- C- H
    3    2    8  120.00   505.0   C- C- H
    3    4    5  120.00   583.8   C- C- C
    3    4   10  120.00   505.0   C- C- H
    4    3    9  120.00   505.0   C- C- H
    4    5    6  120.00   583.8   C- C- C
    4    5   11  120.00   505.0   C- C- H
    5    4   10  120.00   505.0   C- C- H
    5    6   12  120.00   505.0   C- C- H
    6    1    7  120.00   583.8   C- C- C
    6    5   11  120.00   505.0   C- C- H
   13    7   14  117.00   542.5   O- C- H
   14  torsion
   6   1   2   3  50.00   -1.0    1.0   C- C- C- C
   2   1   6   5  50.00   -1.0    1.0   C- C- C- C
   2   1   7  13  16.00   -1.0    2.0   C- C- C- O ald.
   1   2   6   7 100.00   -1.0    1.0   C- C- C- C
   1   2   3   4  50.00   -1.0    1.0   C- C- C- C
   2   1   3   8 100.00   -1.0    1.0   C- C- C- H
   2   3   4   5  50.00   -1.0    1.0   C- C- C- C
   3   2   4   9 100.00   -1.0    1.0   C- C- C- H
   3   4   5   6  50.00   -1.0    1.0   C- C- C- C
   4   3   5  10 100.00   -1.0    1.0   C- C- C- H
   4   5   6   1  50.00   -1.0    1.0   C- C- C- C
   5   4   6  11 100.00   -1.0    1.0   C- C- C- H
   6   1   5  12 100.00   -1.0    1.0   C- C- C- H
   7   1  13  14 100.00   -1.0    1.0   C- C- O- H
```

```
aniline  liquid
   14
    1   0.00000  -0.00000   0.92675  12    0.3359
    2   0.00000   1.20378   0.23175  12   -0.3800
    3   0.00000   1.20378  -1.15825  12   -0.2824
    4   0.00000  -0.00001  -1.85325  12   -0.3584
    5  -0.00000  -1.20377  -1.15825  12   -0.2824
    6   0.00000  -1.20377   0.23175  12   -0.3800
    7   0.00000   0.00000   2.32175  17   -1.0719
    8   0.00000   2.13909   0.77175   2    0.2926
    9   0.00000   2.13909  -1.69825   2    0.2876
   10   0.00000  -0.00001  -2.93325   2    0.2877
```

```
   11  -0.00000  -2.13908  -1.69825   2    0.2876
   12   0.00000  -2.13908   0.77175   2    0.2926
   13   0.00000   0.86602   2.82175   8    0.4856
   14   0.00000  -0.86603   2.82175   8    0.4856

   14  stretching
    1    2   1.390  4880.7   C- C
    1    6   1.390  4880.9   C- C
    1    7   1.395  4550.6   C- N
    2    3   1.390  4880.8   C- C
    2    8   1.080  3600.0   C- H
    3    4   1.390  4880.7   C- C
    3    9   1.080  3600.0   C- H
    4    5   1.390  4880.9   C- C
    4   10   1.080  3600.0   C- H
    5    6   1.390  4880.8   C- C
    5   11   1.080  3600.0   C- H
    6   12   1.080  3600.0   C- H
    7   13   1.000  5300.0   N- H
    7   14   1.000  5300.0   N- H

   21  bending
    1    2    3  120.00   583.8   C- C- C
    1    2    8  120.00   505.0   C- C- H
    1    6    5  120.00   583.8   C- C- C
    1    6   12  120.00   505.0   C- C- H
    1    7   13  120.00   460.0   C- N- H
    1    7   14  120.00   460.0   C- N- H
    2    1    6  120.00   583.8   C- C- C
    2    1    7  120.00   608.8   C- C- N
    2    3    4  120.00   583.8   C- C- C
    2    3    9  120.00   505.0   C- C- H
    3    2    8  120.00   505.0   C- C- H
    3    4    5  120.00   583.8   C- C- C
    3    4   10  120.00   505.0   C- C- H
    4    3    9  120.00   505.0   C- C- H
    4    5    6  120.00   583.8   C- C- C
    4    5   11  120.00   505.0   C- C- H
    5    4   10  120.00   505.0   C- C- H
    5    6   12  120.00   505.0   C- C- H
    6    1    7  120.00   608.8   C- C- N
    6    5   11  120.00   505.0   C- C- H
   13    7   14  120.00   445.0   H- N- H

   14  torsion
   6   1   2   3  50.00   -1.0    1.0   C- C- C- C
   2   1   6   5  50.00   -1.0    1.0   C- C- C- C
   2   1   7  13  20.00   -1.0    2.0   C- C- N- H amine
   1   2   6   7 100.00   -1.0    1.0   C- C- C- N
   1   2   3   4  50.00   -1.0    1.0   C- C- C- C
   2   1   3   8 100.00   -1.0    1.0   C- C- C- H
   2   3   4   5  50.00   -1.0    1.0   C- C- C- C
   3   2   4   9 100.00   -1.0    1.0   C- C- C- H
   3   4   5   6  50.00   -1.0    1.0   C- C- C- C
   4   3   5  10 100.00   -1.0    1.0   C- C- C- H
   4   5   6   1  50.00   -1.0    1.0   C- C- C- C
   5   4   6  11 100.00   -1.0    1.0   C- C- C- H
   6   1   5  12 100.00   -1.0    1.0   C- C- C- H
   7   1  13  14 100.00   -1.0    1.0   N- C- H- H
```

```
methoxybenzene liquid
   16
    1  -0.00000   0.31045   0.46528  12    0.5237
    2   0.00000   1.30648  -0.50428  12   -0.3534
    3   0.00000   0.96483  -1.85163  12   -0.2818
    4   0.00000  -0.37285  -2.22943  12   -0.3315
    5  -0.00000  -1.36887  -1.25988  12   -0.2812
    6  -0.00000  -1.02722   0.08748  12   -0.3615
    7  -0.00000   0.64596   1.78841  23   -0.8067
    8   0.00000   2.34582  -0.21073   2    0.2970
    9   0.00000   1.73871  -2.60496   2    0.2875
   10   0.00000  -0.63831  -3.27630   2    0.2879
   11  -0.00000  -2.40821  -1.55342   2    0.2873
   12  -0.00000  -1.80111   0.84081   2    0.3023
   13  -0.00000  -0.42953   2.73087  13   -0.4209
   14  -0.00000  -0.04727   3.74096   3    0.2832
   15   0.87608  -1.04734   2.59974   3    0.2841
   16  -0.87607  -1.04734   2.59974   3    0.2841
   16  stretching
    1    2   1.390  4880.7   C- C
    1    6   1.390  4880.9   C- C
```

```
    1    7   1.365  4873.1   C- O
    2    3   1.390  4880.8   C- C
    2    8   1.080  3600.0   C- H
    3    4   1.390  4880.7   C- C
    3    9   1.080  3600.0   C- H
    4    5   1.390  4880.9   C- C
    4   10   1.080  3600.0   C- H
    5    6   1.390  4880.8   C- C
    5   11   1.080  3600.0   C- H
    6   12   1.080  3600.0   C- H
    7   13   1.430  3418.1   O- C
   13   14   1.080  3600.0   C- H
   13   15   1.080  3600.0   C- H
   13   16   1.080  3600.0   C- H
   25  bending
    1    2    3  120.00   583.8   C- C- C
    1    2    8  120.00   505.0   C- C- H
    1    6    5  120.00   583.8   C- C- C
    1    6   12  120.00   505.0   C- C- H
    1    7   13  117.00   619.5   C- O- C
    2    1    6  120.00   583.8   C- C- C
    2    1    7  120.00   673.6   C- C- O
    2    3    4  120.00   583.8   C- C- C
    2    3    9  120.00   505.0   C- C- H
    3    2    8  120.00   505.0   C- C- H
    3    4    5  120.00   583.8   C- C- C
    3    4   10  120.00   505.0   C- C- H
    4    3    9  120.00   505.0   C- C- H
    4    5    6  120.00   583.8   C- C- C
    4    5   11  120.00   505.0   C- C- H
    5    4   10  120.00   505.0   C- C- H
    5    6   12  120.00   505.0   C- C- H
    6    1    7  120.00   673.6   C- C- O
    6    5   11  120.00   505.0   C- C- H
    7   13   14  110.00   630.0   O- C- H
    7   13   15  111.00   617.5   O- C- H
    7   13   16  111.00   617.5   O- C- H
   14   13   15  108.00   470.0   H- C- H
   14   13   16  108.00   470.0   H- C- H
   15   13   16  108.00   470.0   H- C- H
   14  torsion
    6    1    2    3   50.00   -1.0    1.0   C- C- C- C
    2    1    6    5   50.00   -1.0    1.0   C- C- C- C
    1    2    6    7  100.00   -1.0    1.0   C- C- C- O
    1    2    3    4   50.00   -1.0    1.0   C- C- C- C
    2    1    3    8  100.00   -1.0    1.0   C- C- C- H
    2    3    4    5   50.00   -1.0    1.0   C- C- C- C
    3    2    4    9  100.00   -1.0    1.0   C- C- C- H
    3    4    5    6   50.00   -1.0    1.0   C- C- C- C
    4    3    5   10  100.00   -1.0    1.0   C- C- C- H
    4    5    6    1   50.00   -1.0    1.0   C- C- C- C
    5    4    6   11  100.00   -1.0    1.0   C- C- C- H
    6    1    5   12  100.00   -1.0    1.0   C- C- C- H
    6    1    7   13   2.00   -1.0    2.0   C- C- O- C
    1    7   13   14   2.50    1.0    3.0   C- O- C- H
```

```
1,2-dichloroethane liquid
    8
    1   0.00000  -0.53608  -0.52454  13   -0.2698
    2  -0.00000   0.53604   0.52454  13   -0.2698
    3   0.00000  -0.05451   2.20371  42   -0.2840
    4  -0.88468   1.13932   0.38390   3    0.2769
    5   0.88468   1.13932   0.38390   3    0.2769
    6   0.00000   0.05452  -2.20371  42   -0.2839
    7  -0.88469  -1.13937  -0.38391   3    0.2769
    8   0.88468  -1.13936  -0.38391   3    0.2769
    7  stretching
    1    2   1.500  2564.5   C- C
    1    6   1.780  2500.0   C-Cl
    1    7   1.080  3600.0   C- H
    1    8   1.080  3600.0   C- H
    2    3   1.780  2500.0   C-Cl
    2    4   1.080  3600.0   C- H
    2    5   1.080  3600.0   C- H
   12  bending
    1    2    3  115.00   601.0   C- C-Cl
    1    2    4  108.00   655.0   C- C- H
    1    2    5  108.00   655.0   C- C- H
    2    1    6  115.00   601.0   C- C-Cl
    2    1    7  108.00   655.0   C- C- H
    2    1    8  108.00   655.0   C- C- H
```

```
     3    2    4  108.00   655.0  Cl- C- H
     3    2    5  108.00   655.0  Cl- C- H
     4    2    5  110.00   470.0   H- C- H
     6    1    7  108.00   655.0  Cl- C- H
     6    1    8  108.00   655.0  Cl- C- H
     7    1    8  110.00   470.0   H- C- H
     1  torsion
    6   1   2   3  7.50   1.0    3.0  Cl- C- C-Cl
     1 intram.nonbonded
     3 6
```

```
ethanol liquid
     9
     1  -0.00000  -0.23739  -1.29910  13   -0.9094
     2   0.00000   0.54635   0.00909  13    0.0717
     3  -0.00000  -0.31271   1.14603  29   -1.3356
     4   0.00000   0.21725   1.96443   5    0.7314
     5  -0.87374   1.18024   0.04314   3    0.2680
     6   0.87374   1.18024   0.04314   3    0.2680
     7  -0.87608  -0.86566  -1.36361   3    0.2995
     8   0.00000   0.43602  -2.14345   3    0.3068
     9   0.87608  -0.86567  -1.36360   3    0.2995
     8  stretching
     1    2   1.525  2038.1   C- C
     1    7   1.080  3600.0   C- H
     1    8   1.080  3600.0   C- H
     1    9   1.080  3600.0   C- H
     2    3   1.425  3529.9   C- O
     2    5   1.080  3600.0   C- H
     2    6   1.080  3600.0   C- H
     3    4   1.000  4250.0   O- H
    13  bending
     1    2    3  112.00   529.4   C- C- O
     1    2    5  109.00   642.5   C- C- H
     1    2    6  109.00   642.5   C- C- H
     2    1    7  110.00   630.0   C- C- H
     2    1    8  110.00   630.0   C- C- H
     2    1    9  110.00   630.0   C- C- H
     2    3    4  110.00   450.0   C- O- H
     3    2    5  109.00   642.5   O- C- H
     3    2    6  109.00   642.5   O- C- H
     5    2    6  108.00   470.0   H- C- H
     7    1    8  108.00   470.0   H- C- H
     7    1    9  108.00   470.0   H- C- H
     8    1    9  108.00   470.0   H- C- H
     2  torsion
    7   1   2   3  7.50   1.0    3.0   H- C- C- O
    1   2   3   4  2.00   1.0    3.0   C- C- O- H
     3  intram.nonbonded
   4 7  4 8  4 9
```

```
n-pentane liquid
    17
     1   0.00000   0.33158   2.52857  13   -0.8988
     2   0.00000  -0.52118   1.26428  13   -0.5522
     3  -0.00000   0.33159  -0.00000  13   -0.5622
     4  -0.00000  -0.52119  -1.26428  13   -0.5522
     5  -0.00000   0.33159  -2.52856  13   -0.8988
     6  -0.87608   0.96242   2.55929   3    0.2952
     7   0.00000  -0.29557   3.40781   3    0.2950
     8   0.87608   0.96242   2.55929   3    0.2952
     9   0.87374  -1.15599   1.26428   3    0.2824
    10  -0.87374  -1.15599   1.26428   3    0.2824
    11   0.87374   0.96640   0.00000   3    0.2818
    12  -0.87374   0.96640  -0.00000   3    0.2818
    13  -0.87374  -1.15599  -1.26428   3    0.2824
    14   0.87374  -1.15599  -1.26428   3    0.2824
    15   0.87608   0.96242  -2.55928   3    0.2952
    16  -0.00000  -0.29556  -3.40781   3    0.2950
    17  -0.87607   0.96242  -2.55929   3    0.2952
    16  stretching
     1    2   1.525  2037.9   C- C
     1    6   1.080  3600.0   C- H
     1    7   1.080  3600.0   C- H
     1    8   1.080  3600.0   C- H
     2    3   1.525  2038.1   C- C
     2    9   1.080  3600.0   C- H
     2   10   1.080  3600.0   C- H
     3    4   1.525  2038.0   C- C
     3   11   1.080  3600.0   C- H
```

```
    3   12   1.080  3600.0   C- H
    4    5   1.525  2038.1   C- C
    4   13   1.080  3600.0   C- H
    4   14   1.080  3600.0   C- H
    5   15   1.080  3600.0   C- H
    5   16   1.080  3600.0   C- H
    5   17   1.080  3600.0   C- H

   30  bending
    1    2    3  112.00   527.6   C- C- C
    1    2    9  109.00   642.5   C- C- H
    1    2   10  109.00   642.5   C- C- H
    2    1    6  110.00   630.0   C- C- H
    2    1    7  111.00   617.5   C- C- H
    2    1    8  110.00   630.0   C- C- H
    2    3    4  112.00   527.6   C- C- C
    2    3   11  109.00   642.5   C- C- H
    2    3   12  109.00   642.5   C- C- H
    3    2    9  109.00   642.5   C- C- H
    3    2   10  109.00   642.5   C- C- H
    3    4    5  112.00   527.6   C- C- C
    3    4   13  109.00   642.5   C- C- H
    3    4   14  109.00   642.5   C- C- H
    4    3   11  109.00   642.5   C- C- H
    4    3   12  109.00   642.5   C- C- H
    4    5   15  111.00   617.5   C- C- H
    4    5   16  111.00   617.5   C- C- H
    4    5   17  111.00   617.5   C- C- H
    5    4   13  109.00   642.5   C- C- H
    5    4   14  109.00   642.5   C- C- H
    6    1    7  108.00   470.0   H- C- H
    6    1    8  108.00   470.0   H- C- H
    7    1    8  108.00   470.0   H- C- H
    9    2   10  108.00   470.0   H- C- H
   11    3   12  108.00   470.0   H- C- H
   13    4   14  108.00   470.0   H- C- H
   15    5   16  108.00   470.0   H- C- H
   15    5   17  108.00   470.0   H- C- H
   16    5   17  108.00   470.0   H- C- H

    4  torsion
   6   1   2   3  6.00   1.0    3.0   H- C- C- C
   1   2   3   4  6.00   1.0    3.0   C- C- C- C
   2   3   4   5  6.00   1.0    3.0   C- C- C- C
   3   4   5  15  6.00   1.0    3.0   C- C- C- H

    21  intram.nonbonded
 6 13  6 14  6 15  6 16  6 17
 7 13  7 14  7 15  7 16  7 17
 8 13  8 14  8 15  8 16  8 17
 9 15  9 16  9 17  10 15  10 16  10 17
```

```
pyridine liquid
   11
    1   0.00002   0.00155  -1.39998  18   -0.8204
    2   0.00017  -1.14382  -0.69520  12    0.1038
    3  -0.00023  -1.19767   0.69858  12   -0.3235
    4   0.00011  -0.00166   1.41442  12   -0.1626
    5   0.00006   1.19593   0.70196  12   -0.3235
    6  -0.00014   1.14567  -0.69277  12    0.1039
    7   0.00063  -2.07623  -1.24010   2    0.2726
    8  -0.00077  -2.14735   1.21297   2    0.2956
    9   0.00041  -0.00314   2.49442   2    0.2857
   10   0.00020   2.14425   1.21887   2    0.2956
   11  -0.00040   2.07937  -1.23557   2    0.2727
   11  stretching
    1    2   1.345  5736.7   N- C
    1    6   1.345  5731.9   N- C
    2    3   1.395  4779.5   C- C
    2    7   1.080  3600.0   C- H
    3    4   1.394  4799.2   C- C
    3    8   1.080  3600.0   C- H
    4    5   1.393  4807.4   C- C
    4    9   1.080  3600.0   C- H
    5    6   1.396  4762.2   C- C
    5   10   1.080  3600.0   C- H
    6   11   1.080  3600.0   C- H
   16  bending
    1    2    3  124.00   646.0   N- C- C
    1    2    7  118.00   530.0   N- C- H
    1    6    5  124.00   646.0   N- C- C
```

```
   1    6   11  118.00   530.0   N- C- H
   2    1    6  117.00   580.9   C- N- C
   2    3    4  119.00   576.7   C- C- C
   2    3    8  121.00   492.5   C- C- H
   3    2    7  118.00   530.0   C- C- H
   3    4    5  118.00   569.7   C- C- C
   3    4    9  121.00   492.5   C- C- H
   4    3    8  121.00   492.5   C- C- H
   4    5    6  119.00   576.7   C- C- C
   4    5   10  121.00   492.5   C- C- H
   5    4    9  121.00   492.5   C- C- H
   5    6   11  118.00   530.0   C- C- H
   6    5   10  121.00   492.5   C- C- H

  11  torsion
   6   1   2   3  50.00   -1.0    1.0   C- N- C- C
   2   1   6   5  50.00   -1.0    1.0   C- N- C- C
   1   2   3   4  50.00   -1.0    1.0   N- C- C- C
   2   1   3   7 100.00   -1.0    1.0   C- N- C- H
   2   3   4   5  50.00   -1.0    1.0   C- C- C- C
   3   2   4   8 100.00   -1.0    1.0   C- C- C- H
   3   4   5   6  50.00   -1.0    1.0   C- C- C- C
   4   3   5   9 100.00   -1.0    1.0   C- C- C- H
   4   5   6   1  50.00   -1.0    1.0   C- C- C- N
   5   4   6  10 100.00   -1.0    1.0   C- C- C- H
   6   1   5  11 100.00   -1.0    1.0   C- N- C- H
```

Table S5

Data for outliers in the sublimation enthalpy-lattice energy match with LJC force field. CSD refcode, sublimation enthalpy, lattice energy and deviations, number of experimental determinations of SE, and compound name. Data from Table S1 arranged by chemical class.

refco	DHs	Eljc,	%Dev	D(abs)	Nexpt	name	
FUMAAC01	136.4	119.6	12.3	16.8	2	trans-butenedioic	acids
FURDCA	122.8	109.4	11.0	13.5	1	furan-2,5-dicarboxylic	
MXCINN02	134	117.3	12.5	16.7	1	trans-4-methoxycinnamic	
AMBACO08	110	96.5	12.3	13.5	2	2-aminobenzoic	
NICOAC02	115	102.2	11.1	12.8	2	3-pyridinecarboxylic	
QQQFDJ01	122.1	135.5	-11.0	-13.4	1	9-anthracenecarboxylic	
PCPHOL01	93.2	107.9	-15.8	-14.7	1	pentachlorophenol	alcohols
UCAYED01	67.2	79.7	-18.6	-12.5	1	pentaFluorophenol	
CATCOL16	85	96.1	-13.0	-11.1	2	1,2-dihydroxybenzene	
FECCOF01	110	125.6	-14.2	-15.6	2	1,6-hexanediol	
HYQUIN08	100.4	111.2	-10.7	-10.8	6	1,4-dihydroxybenzene	
RESORA03	93	105.7	-13.6	-12.7	5	1,3-dihydroxybenzene	
PHBALD11	101	90.8	10.1	10.2	3	4-hydroxybenzaldehyde	H..O=C,no alc-alc Hbond
XAYCIJ	100	88.3	11.7	11.7	2	3-hydroxybenzaldehyde	id.
FAMDIG	112	93.6	16.4	18.4	2	5-chloro-8-hydroxyquinoline	OH...N
CLNOBE02	103	119.3	-15.9	-16.3	2	1-chloro-2,4,6-trinitrobenzene	nitro
BECJEY	90	100.1	-11.2	-10.1	4	2,3-dinitro-2,3-dimethylbutane	
DNBENZ15	85	95.1	-11.9	-10.1	3	1,3-dinitrobenzene	
MLEICA01	86.4	69.9	19.1	16.5	1	maleic anhydride	diones N-oxides
NIKVUZ	69	57.3	17.0	11.8	1	cyclobutane-1,2-dione	
INDDON	97	84.9	12.5	12.1	1	1,3-indandione	
ZZZPRC03	106	88.4	16.6	17.6	1	1-methyl-1H-indole-2,3-dione	
RAJGUG	89	70.6	20.7	18.4	2	2-methylpyridine Noxide	
VAKJUM	124	105	15.3	19	1	2,3-dimethylquinoxaline 1,4dioxide	
CAACTY	41.2	30	27.3	11.2	1	cyanoacetylene	cyano
CYNGEN	31.2	35.8	-14.6	-4.6	4	cyanogen	
MALONT	79	61.4	22.3	17.6	2	malononitrile	
BETHAZ01	71	82	-15.5	-11	1	2,1,3-benzothiadiazole	sulfa
DMSULO04	77	87.5	-13.6	-10.5	1	dimethyl sulfone	
THIOUR16	108.6	84.4	22.3	24.2	7	thiourea	
PRYLTS	96	111.6	-16.2	-15.6	1	p-tolyl propenylsulfone	
MOYGUC01	62.2	77.6	-24.8	-15.4	1	thiocamphor	
TUXFIC02	125	142.7	-14.1	-17.7	1	dibenzyl sulfone	
PHUREA02	138.2	121	12.4	17.2	1	monophenylurea	NH..O=
DIKPIP03	106.6	123.9	-16.3	-17.3	1	2,5-piperazinedione	
MODYAG01	138.2	122.1	11.6	16.1	1	4-aminophthalimide	
ACANIL06	87	98.3	-13	-11.3	2	acetanilide	
HQOXAL01	120.9	104.5	13.6	16.4	2	2-hydroxyquinoxaline	keto form NH..O=
NONMEI	93	83.4	10.4	9.6	1	8-aminoquinoline	NH..N
NICOAM06	120	104.2	13.2	15.8	2	3-pyridinecarboxamide	
FULPIM	88.4	77.3	12.5	11.1	1	2-methylimidazole	
IMAZOL13	83	71.8	13.5	11.2	4	imidazole	
ZBCNON	58	65.8	-13.4	-7.8	1	3-azabicyclo 3.2.2nonane	aza
HXMTAM23	80	89.5	-11.9	-9.5	5	1,3,5,7-tetraazatricyclo 3.3.1.13,7decane	
HEYJOK01	68	76.7	-12.8	-8.7	2	quinoxaline 1,4	
MPYRAZ02	95	78.1	17.8	16.9	1	tetramethylpyrazine	wrong DHs pyrazine 56
TROXAN	56	63.3	-12.9	-7.3	3	1,3,5-trioxane	ether Oxygen
GOCWEA	82	91.7	-11.8	-9.7	1	trans-1,3,5,7-tetraoxadecalin	
XOGJAG	53.6	63.4	-18.3	-9.8	1	trifluoromethylbenzene	
NMACRO11	105	118.5	-12.8	-13.5	1	10-methylacridin-9 10H -one	
TMOXBZ10	100	89.2	10.8	10.8	1	1,3,5-trimethoxybenzene	
TEKQIJ	100.6	113.2	-12.5	-12.6	2	2,2',5,5'-tetrachlorobiphenyl	
FELSEU	112.9	124.7	-10.5	-11.9	1	1,2,3,4-tetrachlorodibenzo-1,4 dioxin	
BEOXAZ	65	75.2	-15.6	-10.2	2	benzofurazan	unreliable Xray 1951 22%R
CLANIC06	86	73.1	15.0	12.9	2	4-chloroaniline	short CH..Cl

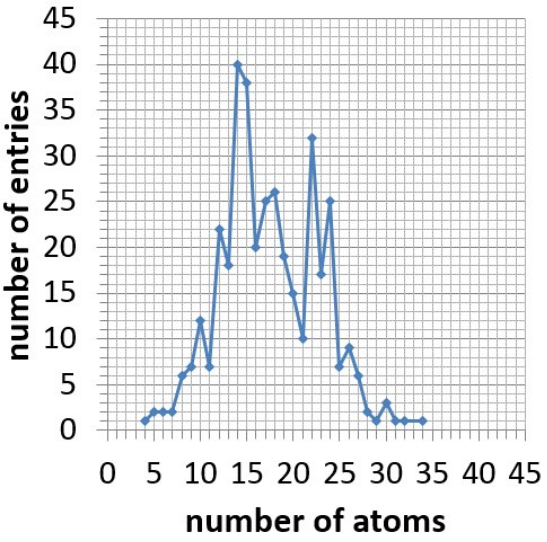

Figure S1.
Distribution of number of atoms per molecule in the 377–molecule data set.

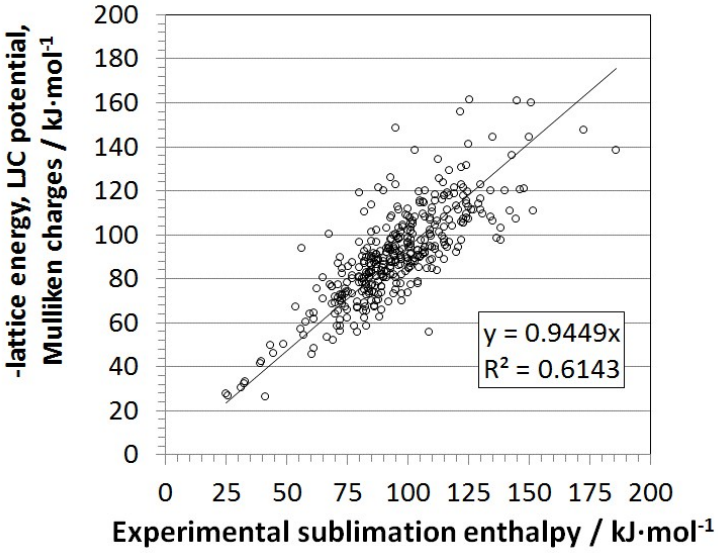

Figure S2.
Performance of the LJC potential with Mulliken charges to reproduce experimental sublimation enthalpies for the 377 crystal structures in the current dataset (see text).

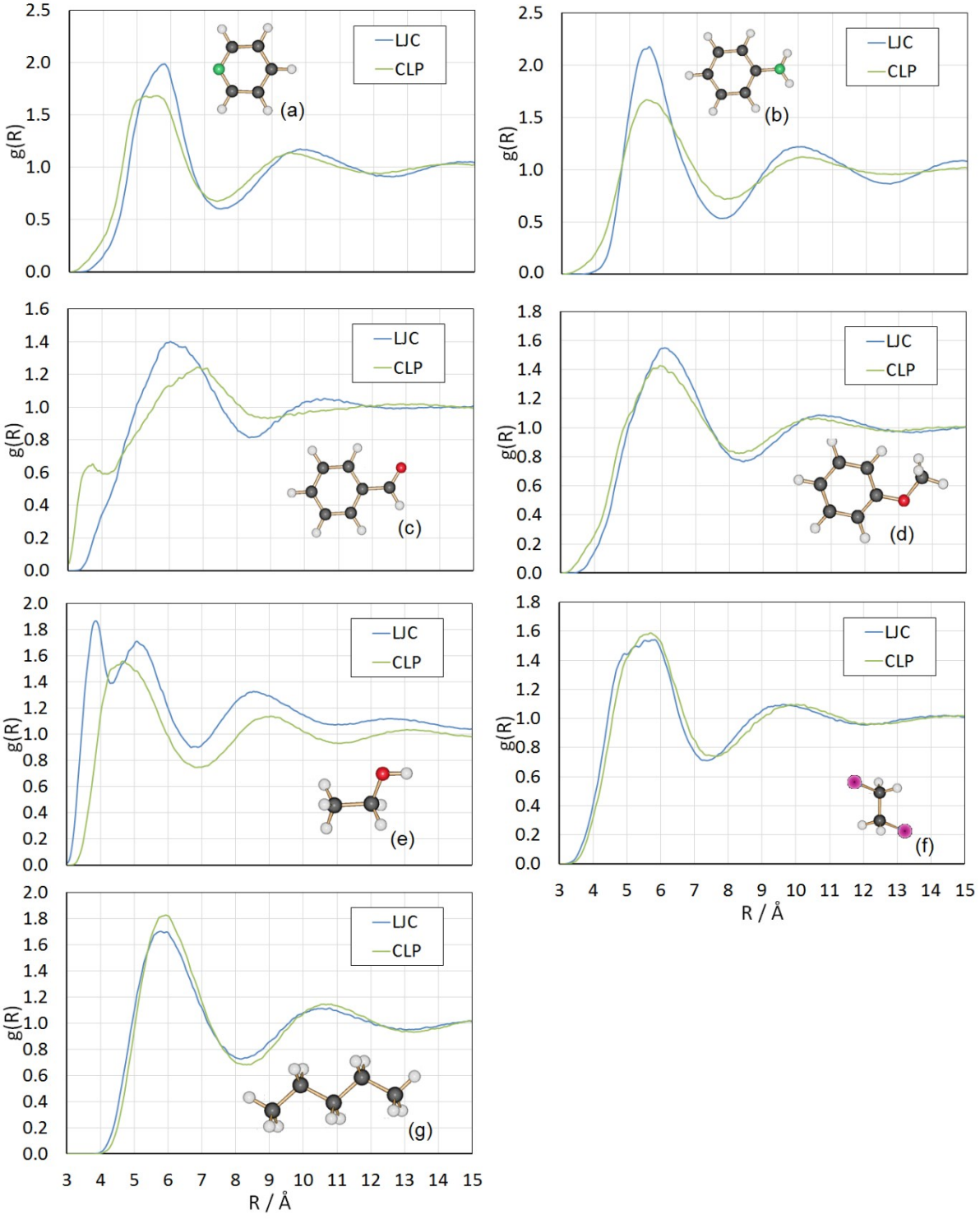

Figure S3.

Centre–of–mass radial distribution functions, $g(R)$, averaged through the last 200 ps of the simulation for liquids (a)–(g) (see main text, Figure 1). Atom code: C: black; H: white; O: red; N: green; Cl: purple. CLP (LJC) results are shown as green (blue) lines.

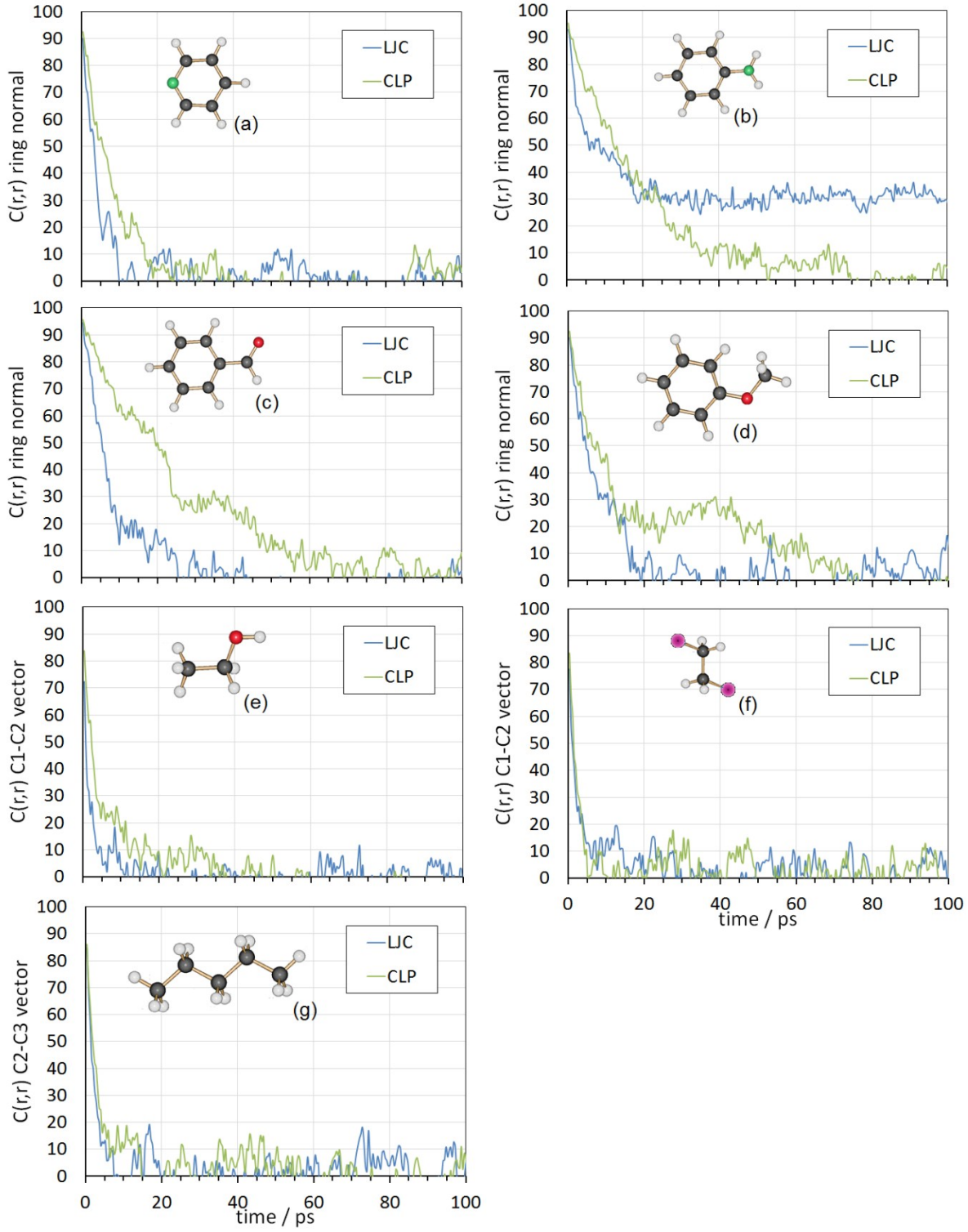

Figure S4.

Raw rotational correlation function, C(**u**) (uncorrected for smoothing) as a function of time in the first 100 ps of the trajectory for liquids. See Fig. S3 above for explanation of symbols.

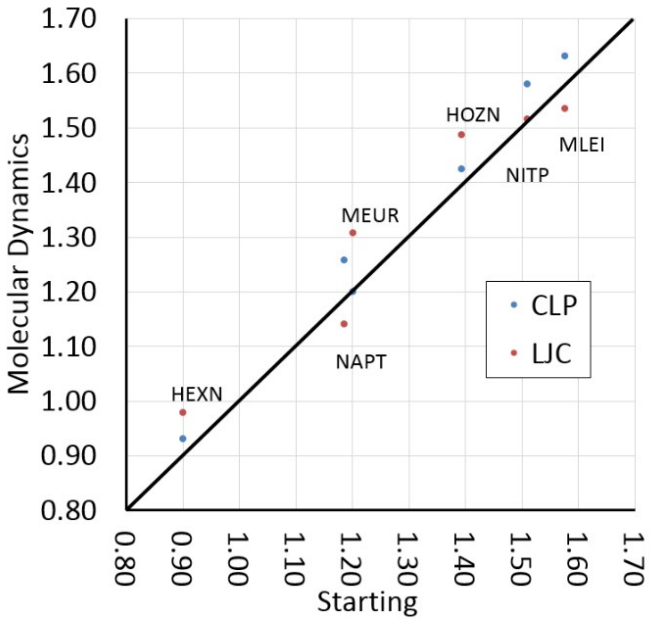

Figure S5.

Comparison between crystal densities from Molecular Dynamics simulations and experiment: HEXN: n–hexane at 90 K; NAPT: naphthalene at 298 K; MEUR: methylurea at 298 K; HOZN: trimethyltrioxane $CHCl_3$ solvate at 190 K; NITP: p–nitrophenol at 110 K; maleic anhydride at 130 K.

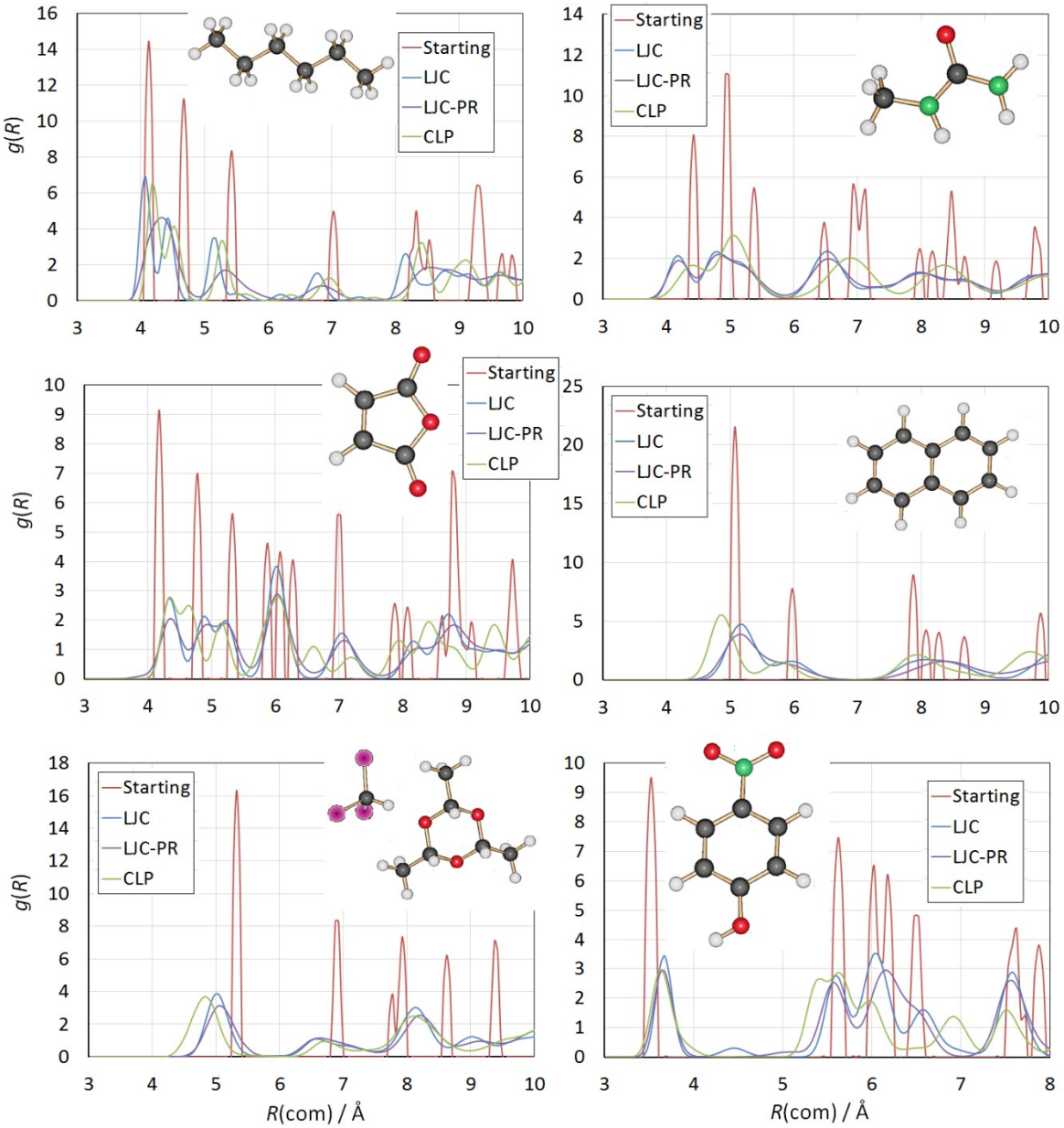

Figure S6.

Centre–of–mass radial distribution functions, $g(R)$, from MD simulation of crystals (1)–(6) (see main text, Figure 1). Red lines: starting crystal structures after short MC thermalization; CLP results, and 6-12-q with weak-coupling (LJC) or Parrinello–Rahman (LJC–PR) barostat. Atom code: C: black; H: white; O: red; N: green; Cl: purple.