Supporting Information

The DFT-ReaxFF Hybrid Reactive Dynamics Method with application to the Reductive Decomposition Reaction of the TFSI and DOL Electrolyte at a Lithium-Metal Anode Surface

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Hybrid AIMD-ReaxFF Scheme (HAIR). In order to retain a balance between accuracy and computational cost, we propose the hybrid method combining AIMD and ReaxFF procedures, As shown in Figure S1, the molecular dynamics simulations start with the AIMD (0.5 ps), followed by ReaxFF MD (5 ps), and continued alternatively. The high computational efficiency of ReaxFF makes the cost of ReaxFF only marginally higher than the AIMD. Thus, the Hair method leads to computational efficiency increased by 10-100 times compared to AIMD.

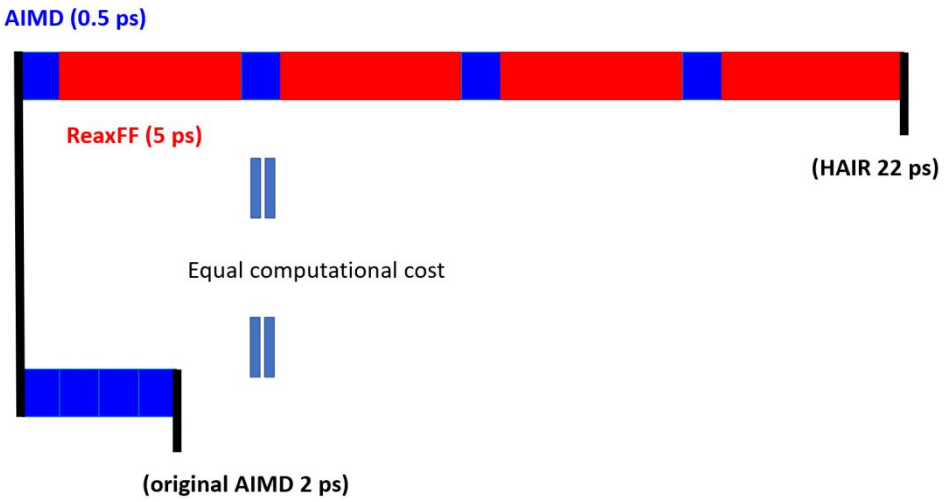


Figure S1. The schematic diagram for the HAIR method compared with AIMD.

Reactive force field parameters optimization. The ReaxFF reactive force field uses bond order-dependence to describe bond breaking. The parameters were optimized by fitting QM but including some experimental results. ReaxFF bond orders (BO_{ij}) are calculated instantaneously. They contain sigma, pi, and double-pi bonds, as in Eq. (S1).

$$BO'_{ij} = BO^{\sigma}_{ij} + BO^{\pi}_{ij} + BO^{\pi\pi}_{ij} = exp\left[p_{bo1} \cdot \left(\frac{r_{ij}}{r^{\sigma}_{o}}\right)^{p_{bo2}}\right] + exp\left[p_{bo3} \cdot \left(\frac{r_{ij}}{r^{\pi}_{o}}\right)^{p_{bo4}}\right] + exp\left[p_{bo5} \cdot \left(\frac{r_{ij}}{r^{\pi\pi}_{o}}\right)^{p_{bo6}}\right] \quad \text{Eq. (S1)}$$

During the force field optimization procedure, the error objective function was expressed as deviations between QM and ReaxFF energies and forces as in Eq. (2). Here $x_{i,QM}$ and $x_{i,\,ReaxFF}$ are the corresponding values for QM and ReaxFF results, σ_i is the weight parameter adjusted based on the accuracy in the training data.

$$Error = \sum_{i=1}^{n}\left[\frac{(x_{i,QM} - x_{i,Re\,axFF})}{\sigma_i}\right]^2 \qquad \text{Eq. (S2)}$$

Since finding the global minimum in the error function is essential to guarantee the accuracy of ReaxFF, we use Monte Carlo Simulated Annealing (MC) to optimize ReaxFF force field parameters. H-TFSI leads to a suitable description for LiTFSI-containing systems.

Model of the lithium-electrolyte system. The Li-metal anode was represented by a 6-layer (3 × 3) supercell slab, where the two bottom layers of the slab were fixed (Figure S2). Later, we used the Li (100) surface to react with the electrolyte. Li (100) was shown by Camacho-Forero to be the most stable surface among the (100), (110), and (111) surfaces calculated. [22]

To represent the electrolyte, we placed 13 DOL molecules in a periodic box with a density of 1.06 g/cm^3. To achieve the desired 1 M concentration of Li-salts in the electrolyte, we used one molecule of LiTFSI to model the Li-salt-containing system. The final simulation periodic cell was 10.5 × 10.5 × 26.5 Å, approximately.

The functional form of ReaxFF used in this work is from the work reported by Chenoweth et al. in 2008 (Ref 28). This framework is insufficient to simulate electrochemical reactions. For example, the chemical reaction in the training set, such as

$$Li\cdot + F\cdot \rightarrow LiF \qquad \text{(S3)}$$

is significantly different from the electrochemical reaction, when an electron is involved.

$$Li^{\cdot} + F^{-} \rightarrow LiF + e^{-} \quad \text{(S4)}$$

The energy difference of the above two reactions is as large as 3.48 eV, which cannot be captured in the QEq scheme. To overcome the above problem, we take advantage of AIMD to simulate the electrochemical reactions, while utilizing the efficiency of ReaxFF to simulate other processes such as diffusion. Therefore, our method uses AIMD to overcome the shortcomings of ReaxFF, while taking advantage of ReaxFF efficiency for simulations.

Using an Intel(R) Xeon(R) Gold 6226R CPU @ 2.90GHz, a 660 ps simulation of brute force AIMD simulation takes about 160 days (too long), while in the hybrid scheme this reduces to about 16 days (practical).

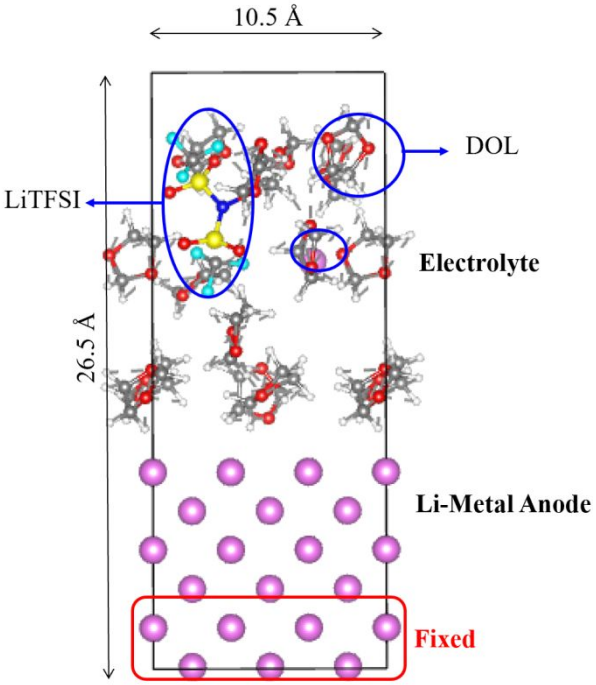


Figure S2. Model of the lithium−metal anode surface and constituents of the electrolyte (DOL and LiTFSI) used in HAIR simulations. Color code: lithium, purple; oxygen, red; carbon, gray; fluorine, cyan; sulfur, yellow, nitrogen, blue; hydrogen, white.

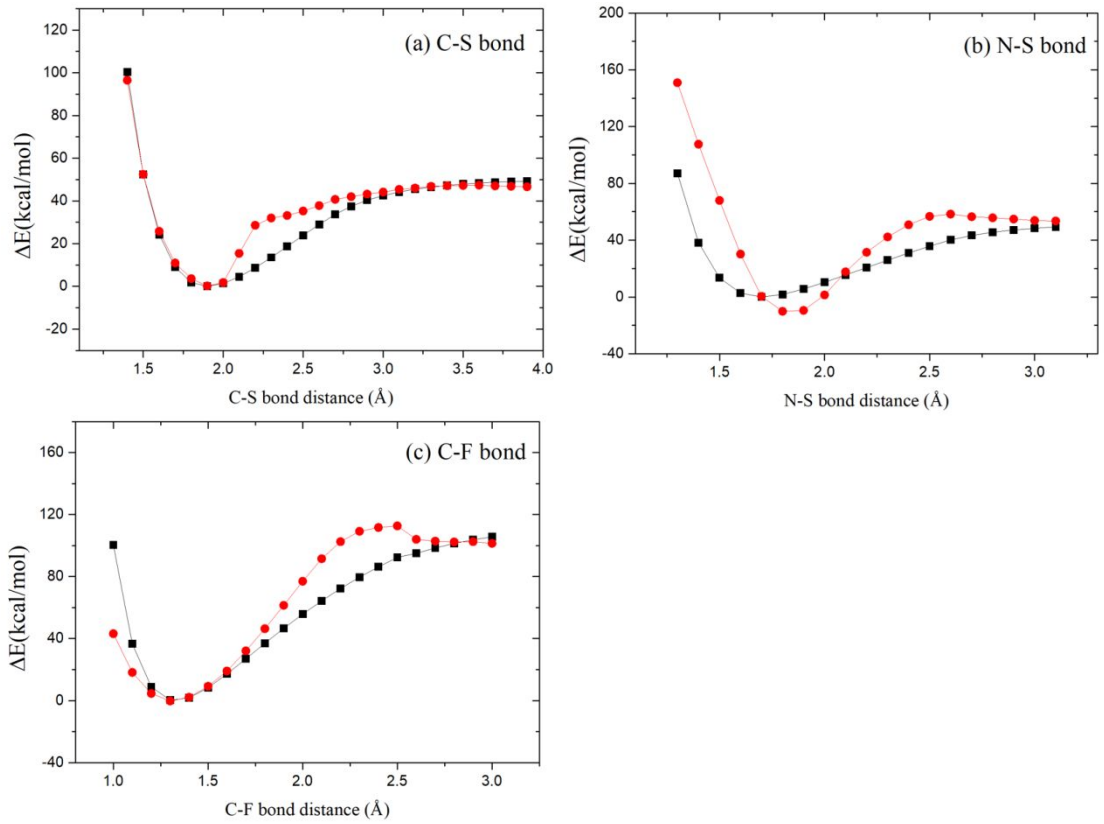


Figure S3. Bond dissociation curves for $HN(SO_2CF_3)_2$ for QM and ReaxFF. (a) C-S bond; (b) N-S bond; (c) C-F bond.

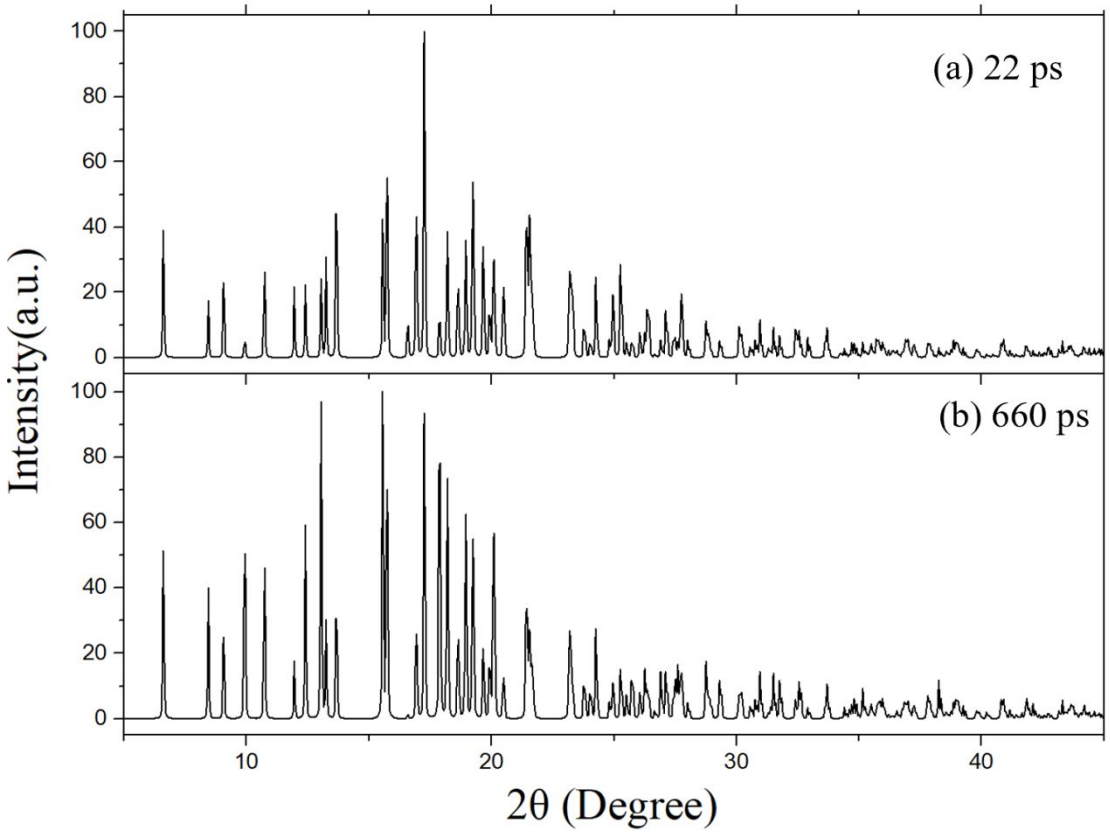
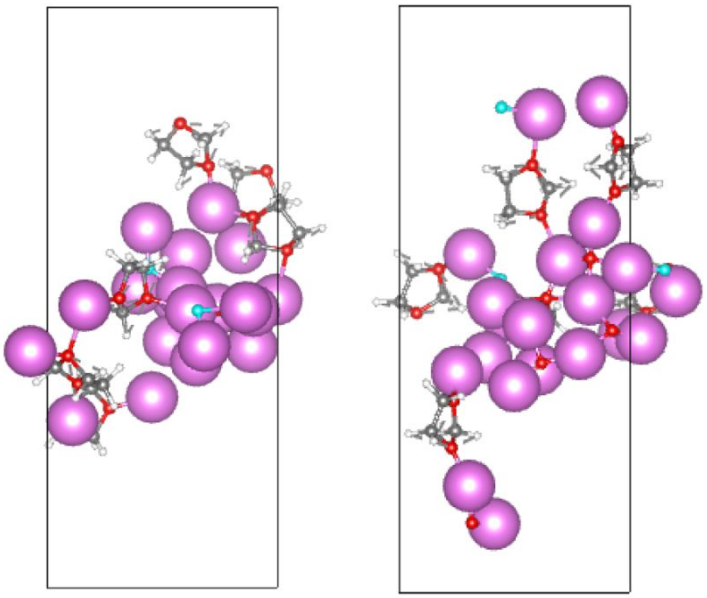


Figure S4. XRD patterns from MD simulations at 22 ps and 660 ps.



(a) 660 ps (b) 20 ns

Figure S5. The clusters obtained from HAIR simulations at (a) 660 ps. (other atoms are hidden) (b) and 20 ns. The colors are lithium in purple, oxygen in red, carbon in gray, fluorine in cyan, sulfur in yellow, nitrogen in blue, and hydrogen in white.

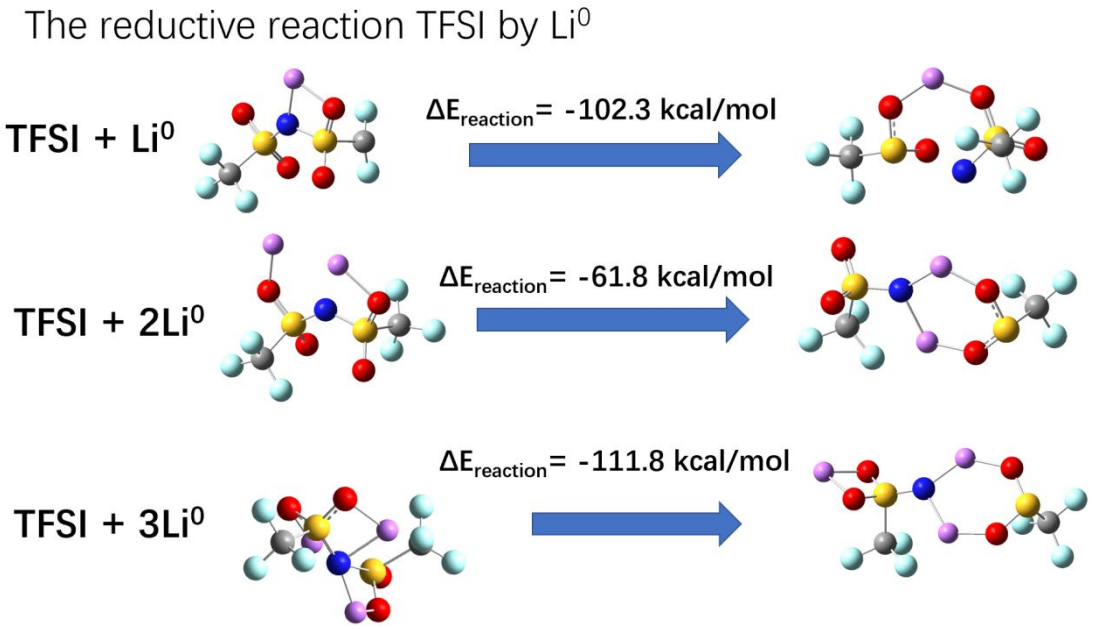


Figure S6. The reductive reaction energies by Li^0.

Reactive MD-force field: C/O/H/F/Li/S Yue liu 2020-09-22 version

39 ! Number of general parameters

50.0000 !p_boc1 Eq(4c): Overcoordination parameter

9.5469 !p_boc2 Eq(4d): Overcoordination parameter

26.5405 !p_coa2 Eq(15): Valency angle conjugation

1.5105 !p_trip4 Eq(20): Triple bond stabilisation

6.6630 !p_trip3 Eq(20): Triple bond stabilisation

70.0000 !k_c2 Eq(19): C2-correction

1.0588 !p_ovun6 Eq(12): Undercoordination

4.6000 !p_trip2 Eq(20): Triple bond stabilisation

12.1176 !p_ovun7 Eq(12): Undercoordination

13.3056 !p_ovun8 Eq(12): Undercoordination

-10.1292 !p_trip1 Eq(20): Triple bond stabilization

0.0000 !Lower Taper-radius (must be 0)

10.0000 !R_cut Eq(21): Upper Taper-radius

0.0000 !p_fe1 Eq(6a): Fe dimer correction

33.8667 !p_val6 Eq(13c): Valency undercoordination

6.0891 !p_lp1 Eq(8): Lone pair param

1.0563 !p_val9 Eq(13f): Valency angle exponent

2.0384 !p_val10 Eq(13g): Valency angle parameter

6.1431 !p_fe2 Eq(6a): Fe dimer correction

6.9290 !p_pen2 Eq(14a): Double bond/angle param

0.3989 !p_pen3 Eq(14a): Double bond/angle param

3.9954 !p_pen4 Eq(14a): Double bond/angle param

```
   0.0000 !p_fe3 Eq(6a): Fe dimer correction
   5.7796 !p_tor2 Eq(16b): Torsion/BO parameter
  10.0000 !p_tor3 Eq(16c): Torsion overcoordination
   1.9487 !p_tor4 Eq(16c): Torsion overcoordination
   0.0000 !p_elho Eq(26a): electron-hole interaction
   2.1645 !p_cot2 Eq(17b): Conjugation if tors13=0
   1.5591 !p_vdW1 Eq(23b): vdWaals shielding
   0.1000 !Cutoff for bond order (*100)
   2.1365 !p_coa4 Eq(15): Valency angle conjugation
   0.6991 !p_ovun4 Eq(11b): Over/Undercoordination
  50.0000 !p_ovun3 Eq(11b): Over/Undercoordination
   1.8512 !p_val8 Eq(13d): Valency/lone pair param
   0.0000 !X_soft Eq(25): ACKS2 softness for X_ij
   0.0000 !d Eq(23d): Scale factor in lg-dispersion
   0.0000 !p_val Eq(27): Gauss exponent for electrons
   0.0000 !1 Eq(13e): disable undecoord in val angle
   2.6962 !p_coa3 Eq(15): Valency angle conjugation
11      ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
                alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
                cov r3;Elp;Heat inc.;bo131;bo132;bo133;softcut;n.u.
                ov/un;val1;n.u.;val3,vval4
C     1.3825    4.0000   12.0000    1.9133    0.1853    0.9000    1.1359    4.0000
      9.7602    2.1346    4.0000   33.2433   79.5548    5.8678    7.0000    0.0000
      1.2104    0.0000  199.0303    8.6991   34.7289   13.3894    0.8563    0.0000
     -2.8983    2.5000    1.0564    4.0000    2.9663    1.6737    0.1421   14.0707
```

H	0.7853	1.0000	1.0080	1.5904	0.0419	1.0206	-0.1000	1.0000
	9.3557	5.0518	1.0000	0.0000	121.1250	5.3200	7.4366	1.0000
	-0.1000	0.0000	54.5000	1.9771	3.3517	0.7571	1.0698	0.0000
	-15.7683	2.1488	1.0338	1.0000	2.8793	1.2669	0.0139	12.4538
O	1.2477	2.0000	15.9990	1.9236	0.0904	1.0503	1.0863	6.0000
	10.2127	7.7719	4.0000	36.9573	116.0768	8.5000	8.9989	2.0000
	0.9088	1.0003	60.8726	20.4140	3.3754	0.2702	0.9745	0.0000
	-3.6141	2.7025	1.0493	4.0000	2.9225	1.7221	0.1670	13.9991
S	1.9186	2.0000	32.0600	1.6516	0.4937	0.7530	1.6593	6.0000
	9.0227	4.9055	4.0000	30.0000	112.1416	6.5745	9.0000	2.0000
	1.0000	3.4994	65.0000	12.0000	22.1978	15.3230	0.9745	0.0000
	-15.7363	2.8802	1.0338	6.2998	2.8793	1.8000	0.0000	14.0000
Mo	2.4695	5.6375	95.9400	1.8471	0.3413	1.0000	0.1000	6.0000
	13.1958	44.8826	4.0000	0.0000	0.0000	0.7695	6.0677	0.0000
	0.1000	0.0000	152.6300	3.4529	0.0722	3.1767	0.8563	0.0000
	-17.9815	3.1072	1.0338	8.0000	3.4590	1.0000	0.0000	0.0000
Ni	1.8201	2.0000	58.6900	1.9449	0.1880	0.8218	0.1000	2.0000
	12.1594	3.8387	2.0000	0.0000	0.0000	4.8038	7.3852	0.0000
	-1.0000	0.0000	95.6300	50.6786	0.6762	0.0981	0.8563	0.0000
	-3.7733	3.6035	1.0338	8.0000	2.5791	1.0000	0.0000	0.0000
Li	1.9814	1.0000	6.9410	1.8000	0.2939	0.9387	-0.1000	1.0000
	9.0616	1.3258	1.0000	0.0000	0.0000	-3.0000	10.0241	0.0000
	-1.0000	0.0000	37.5000	5.4409	6.9107	0.1973	0.8563	0.0000
	-2.5068	2.2989	1.0338	1.0000	2.8103	1.3000	0.2000	13.0000
B	1.5530	3.0000	10.8110	1.6512	0.1000	0.9480	1.0000	3.0000

```
      10.3025    2.3647    3.0000    0.7036   80.0000    4.0000    7.0000    0.0000
      -1.3000    0.0000  151.3700    7.6069    1.9324    1.0943    0.0000    0.0000
      -3.1611    4.0000    1.0564    3.0000    2.8413    1.0000    0.0000    0.0000
F     1.1620    1.0000   18.9984    1.5562    0.1213    0.5000   -0.1000    7.0000
      10.2712    7.5000    1.0000    9.2533    0.2000    9.0000    8.0000    0.0000
      -1.0000    3.4296   18.0000    6.9821    4.1799    1.0561    0.0000    0.0000
      -7.3000    2.6656    1.0493    4.0000    2.9225    1.0000    0.0000    0.0000
P     1.5994    3.0000   30.9738    1.7000    0.1743    1.0000    1.3000    5.0000
      9.1909   14.9482    5.0000    0.0000    0.0000    1.8000    7.0946    0.0000
      -1.0000   25.0000    1.5000    0.2187   21.4305   15.1425    0.0000    0.0000
      -3.9294    3.4831    1.0338    5.0000    2.8793    1.0000    0.0000    0.0000
N     1.6157    3.0000   14.0000    1.9376    0.1203    1.0000    1.2558    5.0000
      9.4267   26.8500    4.0000    8.6294  100.0000    7.6099    7.7500    2.0000
      1.0439    0.1000  119.9837    1.7640    2.7409    2.3814    0.9745    0.0000
      -6.5798    4.4843    1.0183    4.0000    2.8793    1.5967    0.1649   13.9888
51      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                                pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1   1 156.5953  100.0397   80.0000   -0.8157   -0.4591    1.0000   37.7369    0.4235
           0.4527   -0.1000    9.2605    1.0000   -0.0750    6.8316    1.0000    0.0000
 1   2 170.2316    0.0000    0.0000   -0.5931    0.0000    1.0000    6.0000    0.7140
           5.2267    1.0000    0.0000    1.0000   -0.0500    6.8315    0.0000    0.0000
 2   2 156.0973    0.0000    0.0000   -0.1377    0.0000    1.0000    6.0000    0.8240
           2.9907    1.0000    0.0000    1.0000   -0.0593    4.8358    0.0000    0.0000
 1   3 160.4802  105.1693   23.3059   -0.3873   -0.1613    1.0000   10.8851    1.0000
           0.5341   -0.3174    7.0303    1.0000   -0.1463    5.2913    0.0000    0.0000
```

3	3	60.1463	176.6202	51.1430	-0.2802	-0.1244	1.0000	29.6439	0.9114
		0.2441	-0.1239	7.6487	1.0000	-0.1302	6.2919	1.0000	0.0000
2	3	180.4373	0.0000	0.0000	-0.8074	0.0000	1.0000	6.0000	0.5514
		1.2490	1.0000	0.0000	1.0000	-0.0657	5.0451	0.0000	0.0000
1	4	225.4439	144.9402	56.2870	-0.2639	-0.5205	1.0000	11.1308	0.1903
		4.0223	-0.7380	25.5687	1.0000	-0.3045	4.3709	1.0000	0.0000
2	4	183.1582	0.0000	0.0000	-0.7544	0.0000	1.0000	6.0000	0.3725
		11.7366	1.0000	0.0000	1.0000	-0.0595	4.6177	0.0000	0.0000
4	4	84.3765	31.1563	0.0000	-0.8610	-0.4781	1.0000	17.8574	0.3198
		0.4942	-0.1773	8.4125	1.0000	-0.0889	6.8515	1.0000	0.0000
1	5	0.5356	0.9614	0.0000	0.3817	-0.3000	1.0000	36.0000	0.2142
		0.6116	-0.2579	6.1366	1.0000	-0.0913	6.6008	1.0000	0.0000
2	5	101.0000	0.0000	0.0000	-0.5019	-0.3000	0.0000	36.0000	0.3712
		0.0705	-0.3027	15.0243	1.0000	-0.0950	6.5090	0.0000	0.0000
3	5	108.9868	10.5806	137.5564	0.8861	-0.2172	1.0000	19.1047	1.2087
		0.9510	-0.1831	7.2198	1.0000	-0.1266	6.0906	1.0000	0.0000
4	5	82.5107	27.2572	137.6546	1.0000	-0.2304	1.0000	19.1688	0.4660
		1.0151	-0.1596	7.8950	1.0000	-0.0909	5.5509	1.0000	0.0000
5	5	51.8235	0.0000	0.0000	0.8271	-0.3000	0.0000	16.0000	0.2670
		0.2248	-0.3000	16.0000	1.0000	-0.1908	7.3978	0.0000	0.0000
3	4	145.3431	237.5033	0.0000	0.1826	-0.2406	1.0000	22.1005	0.0500
		0.6769	-0.2612	8.4442	1.0000	-0.1154	6.2859	1.0000	0.0000
1	6	83.5810	9.0383	0.0000	0.2531	-0.2000	1.0000	16.0000	0.0529
		1.4085	-0.1113	13.3900	1.0000	-0.1436	4.5683	1.0000	0.0000
2	6	114.7566	0.0000	0.0000	-0.8939	0.0000	1.0000	6.0000	0.1256

		0.1054	1.0000	0.0000	1.0000	-0.1196	5.0815	0.0000	0.0000
3	6	105.3618	0.0000	0.0000	-0.0456	-0.2000	1.0000	16.0000	0.1870
		0.7193	-0.2500	15.0000	1.0000	-0.0880	5.7169	1.0000	0.0000
6	6	91.2220	0.0000	0.0000	-0.2538	-0.2000	0.0000	16.0000	0.2688
		1.4651	-0.2000	15.0000	1.0000	-0.1435	4.3908	0.0000	0.0000
5	6	56.5379	0.0000	0.0000	-0.3241	-0.2000	0.0000	16.0000	0.1607
		2.6232	-0.2000	15.0000	1.0000	-0.1790	4.4051	0.0000	0.0000
4	6	79.7256	0.0000	0.0000	0.3100	-0.2000	0.0000	16.0000	0.1466
		0.7435	-0.2500	25.0000	1.0000	-0.0929	5.3027	0.0000	0.0000
1	7	61.3690	-0.0200	0.0000	0.2609	-0.5000	0.0000	35.0000	0.4256
		0.8408	-0.2500	11.9965	1.0000	-0.0888	9.4023	0.0000	0.0000
2	7	59.2034	0.0000	0.0000	0.1240	0.0000	0.0000	6.0000	0.4000
		1.0000	0.0000	12.0000	1.0000	-0.0565	4.9575	0.0000	0.0000
3	7	70.6356	-0.0200	0.0000	0.0250	0.3000	0.0000	6.0000	0.4553
		0.8513	-0.2500	11.9965	1.0000	-0.0980	9.4453	0.0000	0.0000
4	7	63.3690	0.0000	0.0000	0.1253	-0.5000	0.0000	25.0000	0.3678
		0.3008	-0.2500	20.0000	1.0000	-0.1504	5.6465	0.0000	0.0000
7	7	34.3154	0.0000	0.0000	0.5995	0.3000	0.0000	26.0000	0.5445
		0.5752	0.0000	12.0000	1.0000	-0.1382	4.5000	0.0000	0.0000
1	8	180.3526	50.0000	0.0000	-0.1860	-0.4591	1.0000	37.7369	0.2590
		0.2807	-0.2047	10.2887	1.0000	-0.0641	5.9561	1.0000	0.0000
2	8	165.3660	0.0000	0.0000	-0.2658	-0.3000	1.0000	25.0000	0.3019
		6.1522	0.0000	0.0000	1.0000	-0.0933	5.4815	1.0000	0.0000
3	8	236.5417	65.2243	0.0000	-0.4987	-0.2500	1.0000	25.0000	1.0000
		0.9994	-0.2342	17.4842	1.0000	-0.1262	5.8863	1.0000	0.0000

4	8	0.0000	0.0000	0.0000	0.9000	-0.2500	1.0000	25.0000	0.5201
		1.0000	-0.1488	10.0786	1.0000	-0.1647	6.3839	1.0000	0.0000
8	8	85.8601	0.0000	0.0000	1.0000	-0.2500	1.0000	25.0000	0.7894
		0.8860	-0.2000	25.0000	1.0000	-0.0820	8.6292	1.0000	0.0000
1	9	185.5818	0.0000	0.0000	-0.6890	-0.5000	1.0000	35.0000	0.9001
		4.7476	-0.2500	15.0000	1.0000	-0.1113	4.1292	1.0000	0.0000
2	9	267.6768	0.0000	0.0000	-0.5583	-0.2000	0.0000	16.0000	0.3499
		9.9251	-0.2000	15.0000	1.0000	-0.0794	6.1403	0.0000	0.0000
3	9	162.9300	0.0000	0.0000	-0.4700	-0.5000	1.0000	45.0000	0.5600
		1.4200	-0.2500	15.0000	1.0000	-0.0400	5.5700	1.0000	0.0000
4	9	203.2300	0.0000	0.0000	-0.2500	-0.5000	1.0000	45.0000	0.4600
		1.0200	-0.2500	15.0000	1.0000	-0.2000	4.3000	1.0000	0.0000
7	9	82.6470	0.0000	0.0000	-1.1768	-0.5000	0.0000	45.0000	0.5079
		1.2920	-0.2500	15.0000	1.0000	-0.0880	5.1154	0.0000	0.0000
8	9	150.6978	0.0000	0.0000	0.1373	-0.1418	1.0000	13.1260	0.3916
		0.2867	-0.1310	10.7257	1.0000	-0.1182	6.8737	1.0000	0.0000
9	9	80.0731	0.0000	0.0000	0.9476	-0.3500	1.0000	25.0000	1.1955
		0.2638	-0.2500	15.0000	1.0000	-0.1442	5.2741	1.0000	0.0000
1	10	0.0000	0.0000	0.0000	0.2500	-0.5000	1.0000	45.0000	0.6000
		0.4000	-0.2500	15.0000	1.0000	-0.1000	10.0000	1.0000	0.0000
2	10	0.0000	0.0000	0.0000	0.2500	-0.5000	1.0000	45.0000	0.6000
		0.4000	-0.2500	15.0000	1.0000	-0.1000	10.0000	1.0000	0.0000
3	10	0.0000	0.0000	0.0000	0.2500	-0.5000	1.0000	45.0000	0.6000
		0.4000	-0.2500	15.0000	1.0000	-0.1000	10.0000	1.0000	0.0000
7	10	0.0000	0.0000	0.0000	0.2500	-0.5000	1.0000	45.0000	0.6000

```
          0.4000   -0.2500   15.0000    1.0000   -0.1000   10.0000    1.0000    0.0000
 9 10 153.5200    0.0000    0.0000    0.3010   -0.5000    1.0000   50.0000    0.1025
          0.4150   -0.5000   15.0000    1.0000   -0.0723    5.3872    1.0000    0.0000
10 10    0.0000    0.0000    0.0000    0.2500   -0.5000    1.0000   45.0000    0.6000
          0.4000   -0.2500   15.0000    1.0000   -0.1000   10.0000    1.0000    0.0000
 1 11 175.7446 131.3190 132.3859   -0.5827   -0.2709    1.0000   29.9009    0.8400
          1.9511   -0.2103    7.4487    1.0000   -0.1150    5.8717    1.0000    0.0000
 2 11 161.1063    0.0000    0.0000   -0.1387    0.0000    1.0000    6.0000    0.7276
          0.6127    1.0000    0.0000    1.0000   -0.0395    7.2218    0.0000    0.0000
 3 11   86.0536 180.5864   40.0000    1.0000   -0.4462    1.0000   34.9336    0.2000
          0.8154   -0.2175    7.0255    1.0000   -0.1937    5.2140    1.0000    0.0000
 4 11 123.8328 158.4019   10.6453    0.5925   -0.2136    1.0000   42.7701    0.3161
          1.2547   -0.3819    5.6392    1.0000   -0.1836    4.4561    1.0000    0.0000
 7 11   70.3690    0.0000    0.0000   -0.2559   -0.5000    0.0000   25.0000    0.3574
          1.3920   -0.2500   20.0000    1.0000   -0.0880    9.4453    0.0000    0.0000
 9 11    0.0000    0.0000    0.0000    0.2500   -0.5000    1.0000   45.0000    0.6000
          0.4000   -0.2500   15.0000    1.0000   -0.1000   10.0000    1.0000    0.0000
11 11 134.6492   66.2329 149.2707   -0.7228   -0.1000    1.0000   19.0850    1.0000
          0.6060   -0.2050    9.7308    1.0000   -0.1791    5.8008    1.0000    0.0000
36       ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2    0.1219    1.4000    9.8442    1.1203   -1.0000   -1.0000
 2  3    0.0344    1.6800   10.3247    0.9013   -1.0000   -1.0000
 1  3    0.1131    1.8523    9.8442    1.2775    1.1342    1.0621
 1  4    0.3482    1.8429   10.5150    1.8199    1.1925   -0.9360
 2  4    0.1017    1.7755    9.6088    1.3696   -1.0000   -1.0000
```

1	5	0.1495	2.0794	12.2376	0.0100	1.4060	-1.0000
2	5	0.1361	1.5875	11.9875	1.4900	-1.0000	-1.0000
3	5	0.2011	2.0377	10.4646	1.6025	1.4785	1.6595
4	5	0.2161	1.8729	9.9069	2.0896	1.6848	-1.0000
3	4	0.1869	2.0146	11.0000	1.5197	1.3888	-1.0000
1	6	0.0800	1.7085	10.0895	1.5504	1.4005	-1.0000
2	6	0.0366	1.7306	11.1019	1.2270	-1.0000	-1.0000
3	6	0.0500	1.8000	11.6139	1.4652	-1.0000	-1.0000
4	6	0.1664	1.7078	11.8610	1.7692	-1.0000	-1.0000
5	6	0.3188	2.0391	11.1208	2.3703	-1.0000	-1.0000
1	7	0.0876	2.3874	11.0445	1.6854	1.0000	1.0000
2	7	0.1149	1.4658	11.0886	1.3337	-1.0000	-1.0000
3	7	0.3476	1.6208	10.5680	1.5144	1.0000	1.0000
4	7	0.1576	2.3196	10.8298	1.8159	-1.0000	-1.0000
1	8	0.0956	1.7010	11.7436	1.3003	1.1889	-1.0000
2	8	0.0472	1.4236	11.8887	1.1333	-1.0000	-1.0000
3	8	0.0907	2.3192	9.8579	1.3103	1.2629	-1.0000
4	8	0.1000	2.0000	10.0000	-1.0000	-1.0000	-1.0000
1	9	0.0501	1.6854	11.0421	1.2644	-1.0000	-1.0000
2	9	0.0695	1.8063	9.8138	1.0303	-1.0000	-1.0000
3	9	0.1055	1.7390	10.2770	1.2126	-1.0000	-1.0000
4	9	0.3035	1.7000	9.7770	1.6126	-1.0000	-1.0000
7	9	0.1076	1.8923	9.8011	1.5644	-1.0000	-1.0000
8	9	0.0830	1.7419	10.8641	1.3592	-1.0000	-1.0000
9	10	0.1211	1.7575	9.6653	1.3555	-1.0000	-1.0000

1 11 0.1398 1.9263 10.1847 1.4778 1.1446 1.1216

2 11 0.0480 2.3000 9.0050 1.0156 -1.0000 -1.0000

3 11 0.0942 1.9531 10.3265 1.3018 1.0984 1.0125

4 11 0.2460 1.8345 10.0270 1.6073 1.4576 1.0220

7 11 0.1676 1.9765 10.3296 1.5844 -1.0000 -1.0000

8 11 0.1208 1.7469 9.8490 1.3889 -1.0000 -1.0000

137 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2

1 1 1 67.2326 22.0695 1.6286 0.0000 1.7959 15.4141 1.8089

1 1 2 65.2527 14.3185 6.2977 0.0000 0.5645 0.0000 1.1530

2 1 2 70.0840 25.3540 3.4508 0.0000 0.0050 0.0000 3.0000

1 2 2 0.0000 0.0000 6.0000 0.0000 0.0000 0.0000 1.0400

1 2 1 0.0000 3.4110 7.7350 0.0000 0.0000 0.0000 1.0400

2 2 2 0.0000 27.9213 5.8635 0.0000 0.0000 0.0000 1.0400

1 1 3 49.5561 7.3771 4.9568 0.0000 0.7533 15.9906 1.0010

3 1 3 77.1171 39.8746 2.5403 -24.3902 1.7740 -42.9758 2.1240

2 1 3 65.0000 14.2057 4.8649 0.0000 0.3504 0.0000 1.7185

1 3 1 74.3994 44.7500 0.7982 0.0000 3.0000 0.0000 1.0528

1 3 3 77.9854 36.6201 2.0201 0.0000 0.7434 67.0264 3.0000

3 3 3 80.7324 30.4554 0.9953 0.0000 1.6310 50.0000 1.0783

1 3 2 71.5018 21.7062 0.4735 0.0000 0.5186 0.0000 1.1793

2 3 3 84.9468 23.3540 1.5057 0.0000 2.6374 0.0000 1.3023

2 3 2 77.0645 10.4737 1.2895 0.0000 0.9924 0.0000 1.1043

1 2 3 0.0000 25.0000 3.0000 0.0000 1.0000 0.0000 1.0400

3 2 3 0.0000 0.0148 6.0000 0.0000 0.0000 0.0000 1.0400

2 2 3 0.0000 9.7025 6.0000 0.0000 0.0000 0.0000 1.0400

3	5	3	80.0647	49.0226	1.1861	0.7271	0.1000	0.0000	1.5321
1	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	1	4	66.9986	31.4422	4.7773	0.1463	0.0050	0.0000	2.4042
1	4	1	5.0000	5.0000	7.0000	0.1463	1.4754	0.0000	2.8158
2	1	4	30.9196	11.3010	0.5535	0.0000	0.0050	0.0000	1.9267
1	4	2	100.0000	14.2598	4.2424	0.0000	0.0050	0.0000	3.0000
1	4	4	92.3921	5.2669	6.7198	0.1463	0.0050	0.0000	2.9982
2	4	2	92.1229	42.8350	0.6163	0.0000	1.0235	0.0000	1.0010
2	4	4	70.9476	9.9024	0.6923	0.0000	0.2031	0.0000	2.9811
5	3	5	16.5418	38.3796	0.5347	0.0000	0.1000	0.0000	2.3535
3	3	5	34.0844	11.5602	1.5428	0.0000	0.4319	0.0000	1.0500
3	5	5	6.0985	0.0302	0.1000	0.0000	0.6142	0.0000	1.7575
2	3	5	88.3222	7.1767	2.4747	0.0000	0.6219	0.0000	3.1507
1	3	5	76.5850	8.7797	0.8099	0.0000	2.5889	0.0000	1.0500
4	5	4	66.1778	17.0744	4.2862	0.0984	1.4056	0.0000	1.7545
5	4	5	35.4696	10.5159	5.6990	0.0000	3.9985	0.0000	1.3642
4	4	5	90.0000	32.0246	1.1683	0.0000	3.9500	0.0000	1.3617
4	5	5	41.9144	0.5409	7.1700	0.0000	3.4295	0.0000	3.2326
2	4	5	90.0000	20.3126	0.7222	0.0000	0.6873	0.0000	2.2146
4	4	4	70.3671	5.7180	7.0000	0.0000	0.3683	0.0000	2.4869
2	5	5	57.6230	6.3083	5.0722	0.0000	0.6873	0.0000	1.5510
2	5	4	54.6337	8.6317	6.9912	0.0000	1.6873	0.0000	2.8674
2	5	2	76.2482	11.2841	7.6230	0.0000	0.9375	0.0000	1.0586
3	4	3	73.1328	40.1854	1.2970	-1.0365	0.0101	0.0000	1.0010
1	4	3	78.7291	29.2617	6.9375	0.0000	0.0197	0.0000	1.2505

1	3	4	83.3532	22.9357	0.8136	0.0000	1.1543	0.0000	2.6844
3	3	4	70.2283	45.0000	6.1591	0.0000	2.7147	0.0000	1.0010
2	3	4	45.6742	13.4413	1.5725	0.0000	0.7737	0.0000	2.6616
4	2	4	0.0000	7.5000	2.0000	0.0000	0.0000	0.0000	1.0400
4	2	5	0.0000	7.5000	2.0000	0.0000	0.0000	0.0000	1.0400
5	2	5	0.0000	7.5000	2.0000	0.0000	0.0000	0.0000	1.0400
1	6	1	62.5000	16.6806	0.7981	0.0000	0.9630	0.0000	1.0711
1	1	6	87.6241	12.6504	1.8145	0.0000	0.6154	0.0000	1.5298
6	1	6	100.0000	40.4895	1.6455	0.0000	0.0100	0.0000	1.7667
1	6	6	5.0994	3.1824	0.7016	0.0000	0.7465	0.0000	2.2665
3	6	3	28.9047	27.3847	2.5790	0.0000	0.1078	0.0000	2.4145
3	3	6	90.0000	39.1857	4.8200	0.0000	0.9067	0.0000	1.9533
6	3	6	51.5671	2.9451	0.6657	0.0000	1.6341	0.0000	1.9057
3	6	6	56.7026	3.2665	4.3063	0.0000	0.6729	0.0000	2.7490
2	6	2	106.3969	30.0000	0.9614	0.0000	1.9664	0.0000	2.2693
2	2	6	0.0000	26.3327	4.6867	0.0000	0.8177	0.0000	1.0404
6	2	6	0.0000	60.0000	1.8471	0.0000	0.6331	0.0000	1.8931
2	6	6	30.3748	1.0000	4.8528	0.0000	0.1019	0.0000	3.1660
2	6	6	180.0000	-27.2489	8.3752	0.0000	0.8112	0.0000	1.0004
1	6	2	97.5742	10.9373	2.5200	0.0000	1.8558	0.0000	1.0000
1	2	6	0.0000	0.2811	1.1741	0.0000	0.9136	0.0000	3.8138
2	1	6	84.0006	45.0000	0.6271	0.0000	3.0000	0.0000	1.0000
2	3	6	28.4774	12.0885	3.2396	0.5000	0.0778	0.0000	1.6733
1	6	3	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
1	3	6	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500

3	1	6	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
3	2	6	0.0000	1.0000	1.3402	0.5000	0.0500	0.0000	1.5379
3	5	4	75.0000	25.0000	2.0000	0.0984	1.0000	0.0000	1.5000
4	3	5	35.0000	12.5000	1.5000	0.0000	0.5000	0.0000	1.0500
3	4	5	90.0000	30.0000	1.2500	0.0000	3.0000	0.0000	1.3000
3	4	4	70.0000	45.0000	3.0000	0.0000	2.0000	0.0000	1.1000
2	5	3	70.0000	12.0000	4.0000	0.0000	1.0000	0.0000	1.2500
3	2	5	0.0000	15.0000	2.0000	0.0000	0.0000	0.0000	1.0500
4	6	4	2.7962	7.1073	0.5589	0.0000	0.0554	0.0000	1.1473
6	4	6	92.9945	26.8345	0.9189	0.0000	0.0100	0.0000	1.4683
4	6	6	48.7356	9.9227	0.1206	0.0000	0.0893	0.0000	1.1108
4	4	6	64.5223	7.2562	5.2298	0.0000	0.5459	0.0000	1.0400
2	4	6	83.4937	16.7605	0.8242	0.5000	0.5409	0.0000	1.1378
4	2	6	0.0000	10.0000	1.0000	0.5000	0.2500	0.0000	1.5000
5	4	6	61.8263	20.8696	0.2450	0.0000	0.7429	0.0000	1.0400
4	5	6	60.0000	1.0000	1.0000	0.0000	1.0000	0.0000	1.2500
4	6	5	60.0000	1.0000	1.0000	0.0000	1.0000	0.0000	1.2500
4	1	9	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
5	3	6	44.9106	2.7940	0.5834	0.0000	0.9597	0.0000	1.3151
3	5	6	60.0000	1.0000	1.0000	0.0000	1.0000	0.0000	1.2500
3	6	5	60.0000	1.0000	1.0000	0.0000	1.0000	0.0000	1.2500
2	8	2	50.0000	26.9005	1.7315	0.0000	0.1848	0.0000	1.0400
2	8	8	55.2500	36.5272	6.0000	0.0000	0.4281	0.0000	2.1149
2	2	8	0.0000	10.4651	0.1000	0.0000	0.0000	0.0000	3.0000
2	3	8	75.9746	10.9523	0.8687	0.0000	1.8256	0.0000	2.9875

2	8	3	65.0000	40.0000	6.0000	0.0000	0.1000	0.0000	3.0000
3	8	3	50.4947	12.1095	3.5926	0.0000	3.0000	35.0000	1.0400
8	3	8	90.0000	40.0000	4.7885	0.0000	2.7146	0.0000	1.0400
3	2	8	52.0162	2.5267	0.3146	0.0000	2.2070	0.0000	2.9111
3	3	8	90.0000	27.7492	6.0000	0.0000	0.1870	0.0000	1.0400
8	2	8	0.5000	3.4405	0.9580	0.0000	0.8031	0.0000	1.0000
8	8	8	60.9386	12.9033	7.8607	0.0000	1.7515	0.0000	2.2405
3	8	8	70.7224	5.3644	3.4424	0.0000	0.8219	0.0000	2.8000
1	1	8	30.0491	23.9749	3.2341	0.0000	1.0000	0.0000	1.0000
1	8	1	80.6555	40.0000	5.6273	0.0000	1.0000	0.0000	3.7089
1	8	8	70.5217	39.3118	7.9958	0.0000	1.0000	0.0000	1.0000
8	1	8	47.0626	4.5590	5.6859	0.0000	1.0000	0.0000	1.4685
1	8	3	75.0000	30.0000	2.0000	0.0000	1.0000	0.0000	2.0000
1	8	2	65.0000	35.0000	4.0000	0.0000	0.5000	0.0000	2.0000
1	1	9	75.1647	40.0000	7.6174	0.0000	2.9750	0.0000	3.2465
9	1	9	76.5153	40.0000	6.1232	0.0000	3.0000	0.0000	1.0000
2	1	9	85.4658	0.0100	1.9807	0.0000	1.4400	0.0000	2.9068
3	1	9	70.0000	35.0000	2.0000	0.0000	1.0000	0.0000	1.2500
9	8	9	65.0386	28.8263	2.2480	0.0000	1.1021	0.0000	1.0400
8	9	9	70.0000	28.7353	1.2918	0.0000	1.0913	0.0000	1.0400
8	8	9	70.0000	25.0000	2.5000	0.0000	1.0000	0.0000	1.0400
9	10	9	92.7358	25.0000	2.5000	0.0000	1.1355	0.0000	1.1514
1	1	11	61.6894	9.9742	3.5920	0.0000	5.0000	50.0000	2.2098
3	1	11	67.5853	29.6915	1.8611	0.0000	3.0000	0.0000	1.5926
11	1	11	53.0437	35.9280	1.7824	0.0000	5.0000	0.0000	4.0000

```
 2    1 11    66.9313    25.8025     3.5718     0.0000     0.0600     0.0000     1.0946
 1    3 11    71.7246    38.5022     1.1738     0.0000     1.6310     0.0000     1.2782
 3    3 11    83.0764    35.5413     1.4072     0.0000     1.6310     0.0000     1.1439
11    3 11    79.3317    40.0000     2.3424     0.0000     1.6310     0.0000     1.0061
 2    3 11    81.0695    40.0000     2.0285     0.0000     0.1218     0.0000     1.4477
 1 11    1    68.9764    14.3404     1.9702     0.0000     1.3606     0.0000     1.0000
 1 11    3    76.1086    35.0355     1.0724     0.0000     1.6777     0.0000     1.6071
 1 11 11    81.8917    25.7475     0.7287     0.0000     2.0100     0.0000     1.9350
 3 11    3    80.1274    24.7547     1.7946   -10.0963     1.6777     0.0000     3.2815
 3 11 11    83.6527    36.3627     1.0967    -0.9193     1.6777     0.0000     1.0000
11 11 11    90.0000    44.3028     1.6659     0.0000     0.7529     0.0000     1.2398
 1 11    2    76.9847    29.2262     0.9407     0.0000     0.0300     0.0000     2.6196
 2 11    3    85.4080    40.0000     1.7549     0.0000     0.0222     0.0000     1.0774
 2 11 11    83.5658    40.0000     1.3540     0.0000     0.0222     0.0000     2.6397
 2 11    2    58.0387     1.1862     3.9770     0.0000     0.0222     0.0000     1.0000
 3    4 11    81.4437    30.6060     4.3693     0.5372     3.2454    -0.4915     0.9818
 1    4 11    79.9876    41.3429     7.3989    -2.1973     2.7027     9.0051     1.0305
 4 11    4    52.1338    40.7611     5.4069    -0.4228     2.9699    -1.8296     1.2543
11    2 11     0.0000     0.0019     6.0000     0.0000     0.0000     0.0000     1.0400
65        ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1    1    1    1   -0.2500    11.5822     0.1879    -4.7057    -2.2047     0.0000     0.0000
 1    1    1    2   -0.2500    31.2596     0.1709    -4.6391    -1.9002     0.0000     0.0000
 2    1    1    2   -0.1770    30.0252     0.4340    -5.0019    -2.0697     0.0000     0.0000
 1    1    1    3   -0.7098    22.2951     0.0060    -2.5000    -2.1688     0.0000     0.0000
 2    1    1    3   -0.3568    22.6472     0.6045    -4.0088    -1.0000     0.0000     0.0000
```

3	1	1	3	-0.0528	6.8150	0.7498	-5.0913	-1.0000	0.0000	0.0000
1	1	3	1	2.0007	25.5641	-0.0608	-2.6456	-1.1766	0.0000	0.0000
1	1	3	2	-1.1953	42.1545	-1.0000	-8.0821	-1.0000	0.0000	0.0000
2	1	3	1	-0.9284	34.3952	0.7285	-2.5440	-2.4641	0.0000	0.0000
2	1	3	2	-2.5000	79.6980	1.0000	-3.5697	-2.7501	0.0000	0.0000
1	1	3	3	-0.0179	5.0603	-0.1894	-2.5000	-2.0399	0.0000	0.0000
2	1	3	3	-0.5583	80.0000	1.0000	-4.4000	-3.0000	0.0000	0.0000
3	1	3	1	-2.5000	76.0427	-0.0141	-3.7586	-2.9000	0.0000	0.0000
3	1	3	2	0.0345	78.9586	-0.6810	-4.1777	-3.0000	0.0000	0.0000
3	1	3	3	-2.5000	66.3525	0.3986	-3.0293	-3.0000	0.0000	0.0000
1	3	3	1	2.5000	-0.5332	1.0000	-3.5096	-2.9000	0.0000	0.0000
1	3	3	2	-2.5000	3.3219	0.7180	-5.2021	-2.9330	0.0000	0.0000
2	3	3	2	2.2500	-6.2288	1.0000	-2.6189	-1.0000	0.0000	0.0000
1	3	3	3	0.0531	-17.3983	1.0000	-2.5000	-2.1584	0.0000	0.0000
2	3	3	3	0.4723	-12.4144	-1.0000	-2.5000	-1.0000	0.0000	0.0000
3	3	3	3	-2.5000	-25.0000	1.0000	-2.5000	-1.0000	0.0000	0.0000
0	1	2	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0	2	2	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0	2	3	0	0.0000	0.1000	0.0200	-2.5415	0.0000	0.0000	0.0000
0	1	1	0	0.0000	50.0000	0.3000	-4.0000	-2.0000	0.0000	0.0000
0	3	3	0	0.5511	25.4150	1.1330	-5.1903	-1.0000	0.0000	0.0000
0	1	4	0	-0.2500	80.0000	1.0000	-3.0140	-2.4381	0.0000	0.0000
0	2	4	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	4	4	4	1.8235	-11.0688	-0.4137	-2.7875	0.0000	0.0000	0.0000
2	1	3	5	2.1344	29.9850	0.3398	-3.1459	-2.1000	0.0000	0.0000

1	1	3	5	0.4573	10.0000	1.0000	-7.3632	-2.1000	0.0000	0.0000
2	3	5	3	0.3709	10.0000	0.9625	-9.0000	-1.0000	0.0000	0.0000
2	3	4	3	2.5000	2.5000	0.2237	-10.0000	0.0000	0.0000	0.0000
0	3	4	0	0.5000	50.0000	0.5000	-10.0000	0.0000	0.0000	0.0000
3	4	4	4	0.2500	90.0000	0.5000	-6.0000	0.0000	0.0000	0.0000
3	4	4	3	0.2500	90.0000	0.5000	-6.0000	0.0000	0.0000	0.0000
1	4	4	1	0.0000	50.0000	0.0000	-8.0000	0.0000	0.0000	0.0000
1	4	4	2	0.0000	50.0000	0.0000	-8.0000	0.0000	0.0000	0.0000
2	4	4	2	0.0000	50.0000	0.0000	-8.0000	0.0000	0.0000	0.0000
1	1	1	6	0.0000	5.0000	0.4000	-6.0000	0.0000	0.0000	0.0000
6	1	1	6	0.0000	44.3024	0.4000	-4.0000	0.0000	0.0000	0.0000
2	1	1	6	0.0000	21.7038	0.0100	-4.0000	0.0000	0.0000	0.0000
2	1	6	1	0.0000	5.2500	0.0100	-6.0000	0.0000	0.0000	0.0000
1	1	6	1	0.0000	5.1676	0.0100	-5.9539	0.0000	0.0000	0.0000
1	1	6	2	0.0000	5.1676	0.0100	-5.9539	0.0000	0.0000	0.0000
6	3	3	6	0.0509	30.0000	0.5000	-4.0000	0.0000	0.0000	0.0000
0	8	8	0	0.0000	42.3911	-0.3192	-4.3105	0.0000	0.0000	0.0000
0	3	8	0	-2.0000	48.7726	-0.5000	-2.5000	0.0000	0.0000	0.0000
8	3	3	8	2.0000	75.0000	0.3000	-5.0000	0.0000	0.0000	0.0000
0	1	8	0	0.0000	30.0000	-0.1000	-5.0000	0.0000	0.0000	0.0000
1	1	1	8	0.0000	2.0000	0.0000	-6.0000	0.0000	0.0000	0.0000
8	1	1	8	0.0000	2.0000	0.0000	-6.0000	0.0000	0.0000	0.0000
1	1	1	9	0.0000	20.0000	-0.2000	-4.0648	-2.0000	0.0000	0.0000
2	1	1	9	0.0000	20.0000	1.0000	-5.0000	-2.0000	0.0000	0.0000
9	1	1	9	0.0000	36.7385	0.6148	-5.0000	-2.0000	0.0000	0.0000

```
 0   1   9   0     0.0000   50.0000    0.5000   -6.0000    0.0000    0.0000    0.0000
 0   9   9   0     0.0000    1.0000    0.1000   -6.0000    0.0000    0.0000    0.0000
 0   1  11   0    -0.5473   25.3808    0.9931   -4.3407   -3.0000    0.0000    0.0000
 0   2  11   0     0.0000    0.1000    0.0200   -2.5415    0.0000    0.0000    0.0000
 0   3  11   0     2.0000   71.9948   -0.8805   -6.1274   -2.7831    0.0000    0.0000
 0  11  11   0     2.0000   90.0000   -0.7837   -9.0000   -2.0000    0.0000    0.0000
11   1  11  11    -2.0000   90.0000   -0.0279   -7.5866   -0.1000    0.0000    0.0000
 9   1   1  11     0.0000   46.2320    0.4578   -2.5000   -0.1000    0.0000    0.0000
 3   1  11   1     0.0000   90.0000   -0.2000   -2.5000   -2.0000    0.0000    0.0000
 3   1   1   9    -1.0000    5.0000   -0.2000   -2.6902   -1.9240    0.0000    0.0000
 7       ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3   2   3     1.9682   -4.4628    1.7976    3.0000
 3   2   4     2.5000   -1.0000    1.7976    3.0000
 4   2   3     2.5000   -1.0000    1.7976    3.0000
 4   2   4     1.5000   -2.0000    1.7976    3.0000
 3   2  11     2.0000   -2.5000    1.7976    3.0000
11   2   3     2.0000   -2.5000    1.7976    3.0000
11   2  11     2.0000   -2.5000    1.7976    3.0000
```