Supporting Information

Effects of High and Low Salt Concentration in Electrolytes at Lithium−Metal Anode Surfaces using DFT-ReaxFF Hybrid Molecular Dynamics Method

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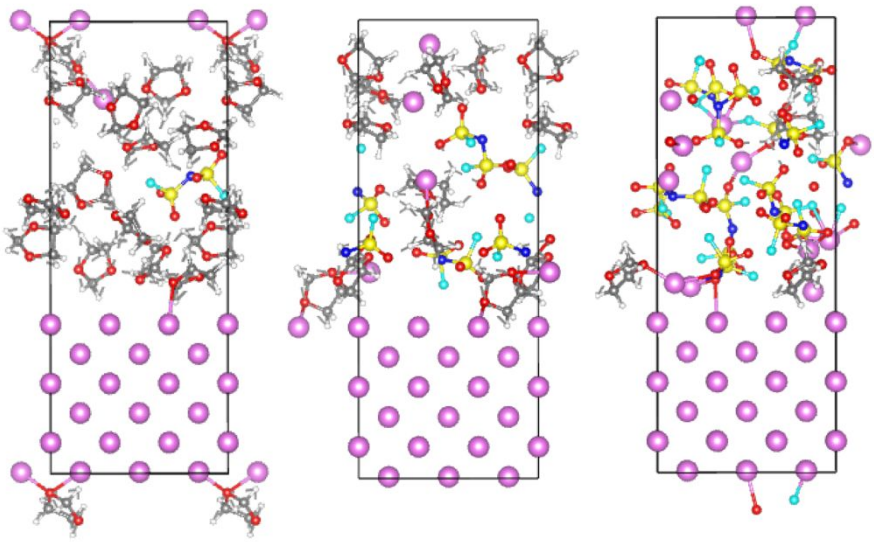
Force field optimization: To provide a training set of QM data to train the ReaxFF for LiTFSI, we use the B3LYP hybrid flavor of density functional method with the 6-311+G(d,p) basis set. All QM calculations were conducted using Jaguar 8.8. During the force field optimization procedure, the error objective function was expressed as deviations between QM and ReaxFF energies and forces as in Eq. (1). 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.

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

Model of the lithium-electrolyte system: The Li-metal anode was represented by a 6-layer (3 × 3) supercell slab, where two of the bottom layers of the slab were fixed (Figure S1) with the most stable Li (100) surface. To achieve the desired concentrations of Li-salts in the electrolyte, we used 1, 4 and 10 molecules LiFSI dissolved in DOL solvents to represent 1M, 4M and 10M LiFSI/DOL electrolyte systems. The final simulation periodic cell was 10.5 × 10.5 × 26.5 Å, approximately.



(a) 1M LiFSI/DOL (b) 4M LiFSI/DOL (c) 10M LiFSI/DOL

Figure S1. Model of the lithium−metal anode surface and electrolyte for 1M, 4M and 10M LiFSI/DOL electrolyte systems. Color code: lithium, purple; oxygen, red; carbon, gray; fluorine, cyan; sulfur, yellow, nitrogen, blue; hydrogen, white.

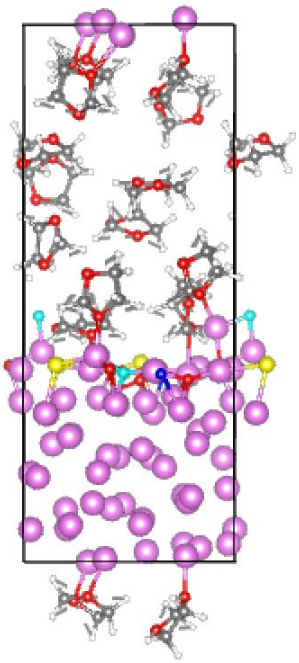


Figure S2. Snapshots from AIMD simulation after 3.5 ps for (a) 1M LiFSI/DOL. Color code as shown in Figure S1.

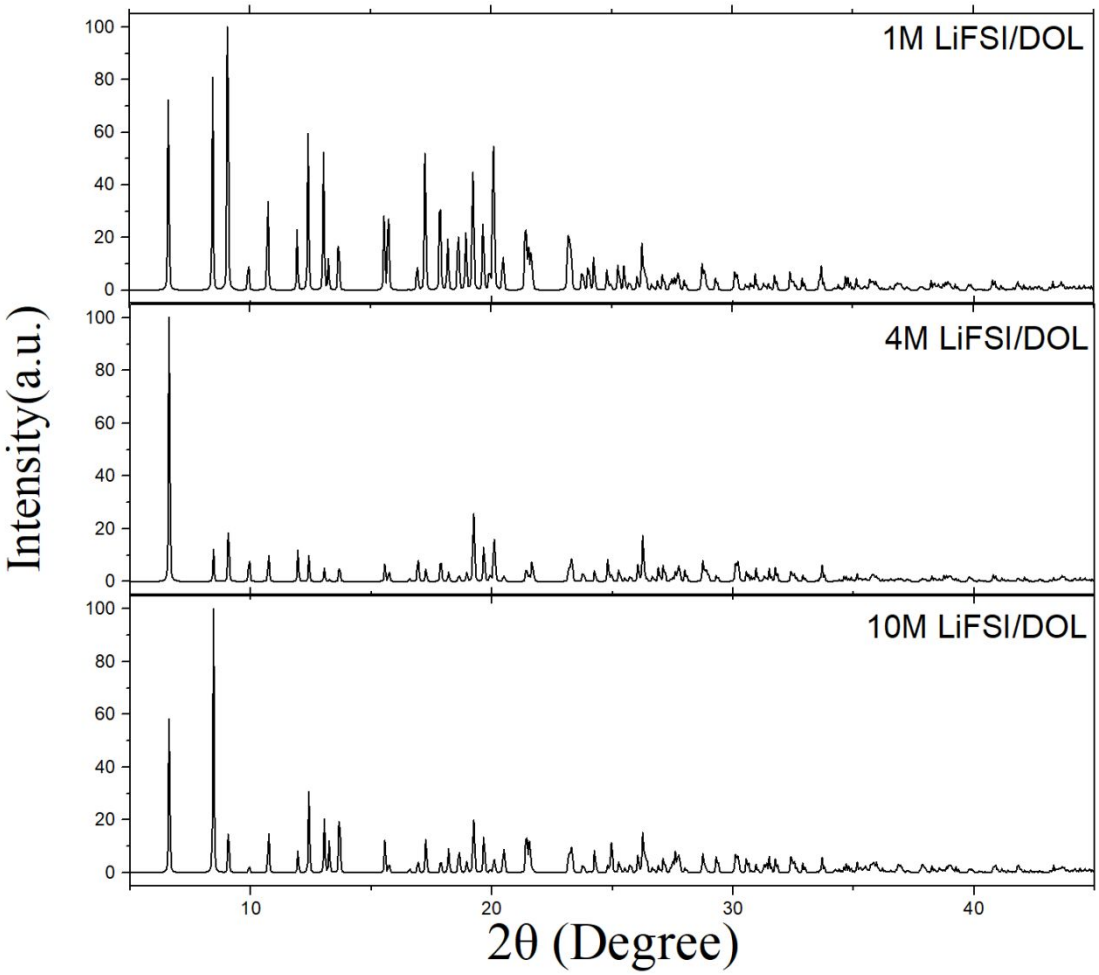


Figure S3. XRD patterns from MD simulations for 1 M LiFSI/DOL, 4 M LiFSI/DOL, and 10 M LiFSI/DOL systems after long-time simulations (more than 1 ns).

Table S1. The bond distances and angles predicted by QM and ReaxFF methods.

Molecule	Bond/angle	QM (B3lyp/6-311+G**)	ReaxFF
	N1-S2	1.679	1.676
FSIH	S3=O6	1.430	1.515
	S3=O7	1.430	1.513
	S3-F10	1.612	1.679
	S2-F9	1.612	1.631
	S3-N1-S2	128.2	127.7
	O4=S2=O5	125.8	123.1
	O4=S2-F9	106.4	112.4
	N1-S2=O4	105.5	100.8
	N1-S2	1.676	1.732
	N1-S3	1.763	1.768
FSIH-F	S2=O4	1.436	1.503
	S2-F9	1.609	1.654
	S3=O6	1.464	1.508
	S3-N1-S2	127.2	127.7
	N1-S2=O4	106.4	101.7
	N1-S2=O5	110.7	102.2
	N1-S2=F9	98.6	106.5
	N1-S3=O7	102.3	100.9
	N1-S2	1.645	1.655
	S2=O3	1.431	1.438
$HNSO_2F$	S2-F6	1.632	1.639
	N1-S2=O3	108.6	108.5
	N1-S2-F6	102.3	102.3
	O3=S2=O4	123.4	123.3
	O3=S2=F6	106.0	105.9
	S1=O2	1.461	1.517
SO_2F	S1-F4	1.657	1.629
	O3=S1=O2	126.0	122.9
	O2=S1-F4	112.7	106.0

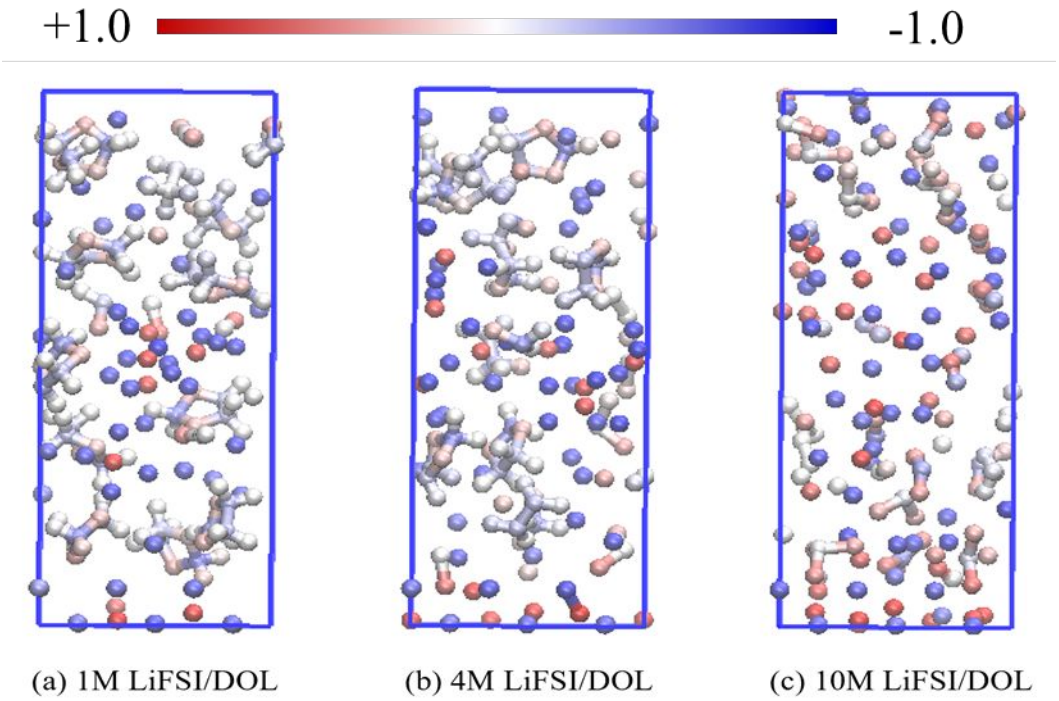


Figure S4. The charge distribution of (a) 1M, (b) 4M and (c) 10 M LiFSI/DOL after 1.015 ns HAIR simulation by using electronegativity equalization method (EEM) in ReaxFF.

Force field paramaters:

```
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
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-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.
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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	268.0938	0.0000	0.0000	-0.3519	-0.2000	0.0000	16.0000	0.3499
		12.4802	-0.2000	15.0000	1.0000	-0.0794	4.0105	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	251.1235	0.0000	0.0000	-0.5153	0.0000	1.0000	6.0000	0.3725
		9.4369	1.0000	0.0000	1.0000	-0.0595	7.3071	0.0009	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 11 120.9234 163.0723     8.0909    0.8263   -0.1762    1.0000   38.8347    0.3161
          2.2691   -0.3344   11.3015    1.0000   -0.1176    5.1163    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 11 223.3300      0.0000    0.0000   -0.5700   -0.5000    1.0000   45.0000    0.4600
          1.2200   -0.2500   15.0000    1.0000   -0.0600    5.1800    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	0.0814	1.7391	9.9396	1.1557	-0.7890	-0.8569
3	9	0.1055	1.7390	10.2770	1.2126	-1.0000	-1.0000
4	9	0.1847	1.8609	10.4814	1.6457	-0.7563	-0.9312
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	0.2138	1.5077	9.8197	1.6430	1.5853	0.9993
7	11	0.1676	1.9765	10.3296	1.5844	-1.0000	-1.0000
9	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	67.3348	36.5492	0.2772	-2.2112	0.3639	-1.8564	0.9182
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
3	4	9	68.1313	38.0466	3.6065	-4.5089	-0.2510	7.0204	1.1707
9	4	11	81.7441	32.1342	3.6919	-2.4231	0.0151	-2.0195	1.2858
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
```