

Supplementary Information

for

Theoretical-computational modelling of CD
spectra of aqueous monosaccharides by means of
Molecular Dynamics simulations and Perturbed
Matrix Method

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Outline.

- S1. Cartesian coordinates, energies and transition moments for PMM-calculations
- S2. Composition of the essential eigenvectors of the covariance matrix
- S3. Location of the Representative Conformations on the Essential plane
- S4. Spectra of the GG and GT rotamers for Alpha and Beta D-glucose
- S5. Eigenvalues of the D-Galactose covariance matrix

S1. Geometries, energies and transition moments for PMM-calculations

The geometries are reported in Angstrom (the first column refers to the atomic number)

The expectation values of the electric dipoles (i,i) are reported in Debye

The transition electric dipoles (i,j) are reported in atomic units

The transition magnetic dipoles (i,j) are reported in atomic units

Ground energy is reported in atomic units

Vertical Excitation energies are reported in eV

D-glucose

Structure A-alpha

Number of atoms : 24

1	-3.80346	-0.68433	0.79396
8	-3.50506	-0.69963	-0.12594
6	-2.59574	0.36188	-0.34719
1	-2.564	0.50143	-1.43175
1	-2.93506	1.29625	0.11314
6	-1.19016	0.05228	0.1451
1	-1.20951	-0.11967	1.23134
6	-0.21995	1.19278	-0.14365
1	-0.27262	1.42733	-1.22137
8	-0.633	2.3102	0.61987
1	0.02668	3.01195	0.5041
6	1.21199	0.79848	0.20164
1	1.2836	0.64004	1.28185
8	2.10196	1.87169	-0.07037
1	2.09256	2.06748	-1.02048
6	1.58616	-0.48143	-0.54171
1	1.57241	-0.29145	-1.62167
8	2.88469	-0.94457	-0.25672
1	3.01402	-0.94757	0.70389
6	0.54548	-1.5705	-0.256291

8	-0.75864	-1.12553	-0.53622
1	0.6976	-2.43087	-0.9136
8	0.69072	-1.95525	1.09587
1	-0.17422	-2.24687	1.42133

Electric dipoles

0	0	-0.937200010	1.54579997	0.578000009		
0	1	5.92000000E-02	-0.103000000	0.118000001		
0	2	0.153300002	-3.88000011E-02	0.125699997		
0	3	0.129600003	-0.116099998	1.72000006E-02		
0	4	1.09999999E-02	7.93000013E-02	0.147300005		
0	5	-3.46000008E-02	0.146300003	-0.195700005		
0	6	0.224399999	-8.11000019E-02	-5.93000017E-02		
0	7	-0.103699997	0.184000000	0.330199987		
0	8	-0.111100003	-0.195800006	2.58000009E-02		
0	9	-0.102799997	-0.246299997	-4.47999984E-02		
0	10	9.99999978E-03	0.224800006	-7.50999972E-02		
0	11	0.0841	-0.1190	-0.0458	0.0233	0.0046
0	12	-0.0628	0.1214	0.0803	0.0251	0.0050
0	13	0.0633	0.1510	-0.3376	0.1408	0.0282
0	14	0.0412	-0.0736	0.1123	0.0197	0.0040
0	15	-0.1458	-0.0670	-0.1461	0.0471	0.0096
0	16	-0.0026	0.1412	-0.0400	0.0216	0.0044
	1	1	-1.68400002	-2.85770011	3.44510007	
	2	2	1.65849996	1.52479994	-2.67980003	
	3	3	0.548799992	4.08729982	-4.53459978	
	4	4	-2.37109995	-4.42729998	5.74720001	
	5	5	-0.382600009	2.21860003	-0.981199980	
	6	6	-2.12400007	-2.45860004	3.56110001	
	7	7	-1.10769999	0.981500030	0.250299990	
	8	8	2.17050004	4.28299999	-3.70919991	
	9	9	-1.53219998	1.41020000	0.200499997	
	10	10	-2.09340000	-1.34010005	2.01440001	
11	11	1.8278	5.4269	-0.1257		
12	12	-0.9134	-0.4147	-1.1480		
13	13	-1.5668	-0.4194	3.6157		
14	14	-1.3355	0.0461	1.4263		
15	15	0.3037	0.2385	-0.2648		
16	16	-2.0189	0.8425	0.7661		

Magnetic moments

1	0.335900009	-4.50999998E-02	1.89999994E-02
2	-0.283800006	-0.437299997	-0.587800026
3	-9.71999988E-02	-0.107699998	-0.524999976
4	0.121100001	-0.294400007	-0.214599997
5	0.133900002	6.80999979E-02	-0.144199997
6	-0.314399987	4.54999991E-02	0.674799979
7	-0.484200001	7.37000033E-02	-0.619000018
8	-0.856899977	-2.03000009E-02	0.396400005
9	-0.135499999	-0.373100013	7.25999996E-02
10	-0.137300000	8.85000005E-02	6.97000027E-02
11	-0.0488	-0.1443	0.2430
12	0.3288	-0.3707	0.4956
13	0.2104	0.0329	-0.3305

14	-0.2191	-0.0972	-0.1637
15	-0.0186	0.3791	-0.0576
16	0.2563	-0.2248	0.4416

Ground energy
-686.914978

Vertical Excitation energies

6.69320011
6.76429987
6.96530008
7.15619993
7.31160021
7.43769979
7.63290024
7.65189981
7.70480013
7.92070007
8.0128
8.1414
8.1726
8.2402
8.2766
8.3475

Structure B-alpha

Number of atoms 24

1	-4.01394	-1.04232	-0.49575
8	-3.47016	-0.63667	0.18965
6	-2.59778	0.32913	-0.38461
1	-2.62737	0.29248	-1.4799
1	-2.89391	1.33049	-0.05808
6	-1.18207	0.05892	0.07828
1	-1.21146	-0.12809	1.16158
6	-0.22239	1.22336	-0.19933
1	-0.24232	1.46954	-1.26758
8	-0.64181	2.40231	0.45793
1	-0.52633	2.30186	1.41517
6	1.20074	0.81342	0.19986
1	1.2058	0.62069	1.28181
8	2.13857	1.84799	-0.00174
1	2.5463	1.76127	-0.87572
6	1.58698	-0.4755	-0.52805
1	1.58874	-0.28868	-1.60898
8	2.88874	-0.92037	-0.224
1	2.99357	-0.94877	0.73958
6	0.54768	-1.56668	-0.26484
8	-0.74192	-1.12225	-0.59846
1	0.73014	-2.43393	-0.90649
8	0.65072	-1.92172	1.09485
1	-0.14128	-2.42468	1.34067

Electric dipoles

0	0	-1.50790000	-1.48640001	-0.849600017
0	1	-0.215599999	0.125799999	2.21999995E-02

0	2	-8.79999995E-02	-3.99000011E-02	1.84000004E-02
0	3	0.110699996	-6.47000000E-02	0.146100000
0	4	-5.79000004E-02	1.83000006E-02	-2.50000004E-02
0	5	-1.09999999E-02	4.56000008E-02	0.289000005
0	6	1.42000001E-02	-0.254599988	6.40000030E-02
0	7	-0.120499998	-0.111400001	7.29999989E-02
0	8	5.55999987E-02	-7.28999972E-02	-0.100199997
0	9	4.08999994E-02	0.235100001	0.205300003
0	10	4.63000014E-02	-8.30999985E-02	3.59000005E-02
0	11	-0.0317	-0.2965	0.1478
0	12	0.0399	0.0848	-0.0488
0	13	-0.0250	-0.0758	0.1062
0	14	-0.0847	0.0783	0.2332
0	15	0.3103	-0.0501	-0.0431
0	16	-0.1453	0.3641	-0.1056
	1	1	4.07969999	0.908599973
	2	2	-1.65489995	-3.31060004
	3	3	-5.65630007	-2.62249994
	4	4	-2.75270009	1.47090006
	5	5	-1.28810000	-2.44090009
	6	6	-1.54200006	-2.96000000E-02
	7	7	-2.02710009	-1.75820005
	8	8	7.01000020E-02	3.89619994
	9	9	-1.44360006	-3.72539997
	10	10	-2.11089993	1.24839997
11	11	-1.8993	0.6614	0.5506
12	12	5.6871	-0.2600	1.3221
13	13	-2.6187	-0.9086	-0.8635
14	14	-0.7052	-0.7120	0.5859
15	15	-2.2486	-0.7730	-3.1810
16	16	-1.4871	-2.5930	1.2248

Magnetic moments

1	0.183300003	-4.60000010E-03	0.654999971
2	-3.84000018E-02	0.328700006	-0.160500005
3	-1.00999996E-02	0.407499999	0.185900003
4	-0.132699996	0.184499994	0.734899998
5	0.189600006	-0.259700000	2.49999994E-03
6	-0.278499991	0.139599994	7.78999999E-02
7	-0.215900004	9.89999995E-03	-0.899900019
8	0.668299973	-4.47999984E-02	3.84999998E-02
9	-0.257299989	-8.00000038E-03	2.03000009E-02
10	-0.411900014	-7.00000003E-02	-1.83000006E-02
11	-0.4018	-0.3612	0.3345
12	-0.0916	-0.1752	0.0980
13	0.0896	0.0061	0.0937
14	0.0070	0.2742	-0.2740
15	-0.0861	-0.2237	0.5213
16	0.0806	0.0800	0.2118

Ground energy

-686.913208

Excitation energies

6.72840023

6.83020020
 7.02829981
 7.06829977
 7.28310013
 7.38749981
 7.52530003
 7.68779993
 7.78020000
 7.87589979
 7.8858
 7.9871
 8.1295
 8.1473
 8.2316
 8.3065

Structure C-alpha

Number of atom: 24

1	-3.14896	-1.35098	-0.75953
8	-3.45166	-0.6781	-0.13282
6	-2.60073	0.44226	-0.26129
1	-2.56953	0.79173	-1.30296
1	-3.02209	1.23979	0.35245
6	-1.18664	0.12432	0.20357
1	-1.19307	-0.09463	1.27985
6	-0.18803	1.23037	-0.11646
1	-0.27906	1.50135	-1.17279
8	-0.49571	2.42547	0.5959
1	-0.32798	2.28375	1.54105
6	1.25591	0.80529	0.14341
1	1.42317	0.69184	1.22546
8	2.14702	1.75617	-0.40423
1	2.05481	2.58668	0.08468
6	1.55771	-0.5298	-0.51955
1	1.55385	-0.37069	-1.60779
8	2.8334	-0.94893	-0.08582
1	2.96419	-1.88495	-0.29434
6	0.47033	-1.56459	-0.21165
8	-0.80735	-1.05866	-0.51846
1	0.57682	-2.43759	-0.86869
8	0.5701	-1.94585	1.13506
1	-0.24992	-2.40417	1.37741

Electric dipoles

0	0	-0.589399993	-1.64110005	0.337700009
0	1	-1.54999997E-02	8.51000026E-02	7.40000000E-03
0	2	-0.100000001	3.75000015E-02	-1.85000002E-02
0	3	-0.217999995	8.34000036E-02	-0.105200000
0	4	7.06999972E-02	-0.176899999	0.141399994
0	5	0.241500005	4.47999984E-02	-0.143199995
0	6	6.94999993E-02	0.155200005	0.180099994
0	7	9.74000022E-02	0.216299996	-0.202999994
0	8	-1.66999996E-02	7.24999979E-02	0.396699995

0	9	7.49999983E-03	0.130500004	0.154200003		
0	10	-8.89999978E-03	-0.173999995	-1.24000004E-02		
0	11	0.0503	-0.1141	-0.1633	0.0422	0.0082
0	12	0.0216	0.0561	-0.0618	0.0074	0.0015
0	13	-0.0286	0.1315	0.0483	0.0204	0.0041
0	14	0.1495	-0.1135	-0.2699	0.1081	0.0215
0	15	-0.1825	0.0940	0.0196	0.0425	0.0086
0	16	-0.0221	-0.2781	0.2207	0.1265	0.0256
	1	1	-1.36960006	-5.54379988	-4.78889990	
	2	2	-2.90420008	4.73280001	2.68700004	
	3	3	0.801500022	2.68659997	2.08629990	
	4	4	2.21530008	3.16149998	-1.75870001	
	5	5	-1.04939997	-3.90050006	-2.15969992	
	6	6	1.88720000	-3.07000000E-02	1.29400003	
	7	7	-0.657000005	-1.40840006	-0.983699977	
	8	8	-1.27139997	3.10000009E-03	-3.63369989	
	9	9	-1.94430006	1.69309998	0.669900000	
	10	10	-0.210099995	-0.219099998	0.274399996	
11	11	-1.8222	0.3580	0.9934		
12	12	-0.9045	-3.0999	-3.5985		
13	13	0.7624	-2.0270	-1.3049		
14	14	-2.0858	-1.8855	0.5922		
15	15	5.3702	1.9463	-0.2296		
16	16	0.1317	1.6093	0.9862		

Magnetic moments

1	0.106600001	-0.370000005	0.128600001
2	0.310600013	0.416999996	0.410699993
3	-0.330599993	0.445499986	0.355599999
4	-3.04000005E-02	0.150500000	5.27999997E-02
5	-0.172199994	-2.19999999E-02	0.657700002
6	0.471899986	-0.141700000	0.324200004
7	0.180000007	3.57999988E-02	0.180000007
8	-0.448900014	-0.160300002	-3.95999998E-02
9	-1.72000006E-02	0.445499986	0.225099996
10	-6.94999993E-02	0.290100008	7.55999982E-02
11	-0.3414	-0.5560	0.2965
12	0.5719	-0.1556	-0.2448
13	-0.3802	0.4980	0.1997
14	-0.0917	0.1238	0.0885
15	0.2921	0.3815	-0.0576
16	0.0072	-0.0622	0.0276

Ground energy

-686.914062

Excitation energies

6.62169981
6.81050014
7.03739977
7.20149994
7.25939989
7.54680014
7.61579990
7.70030022

7.85920000
 7.88560009
 7.9077
 8.0372
 8.0996
 8.1300
 8.2291
 8.2686

Structure D-alpha

Number of atomd: 24

1	-4.3575	-0.44373	-0.24175
8	-3.45034	-0.69071	-0.01838
6	-2.57973	0.37225	-0.36829
1	-2.54622	0.50205	-1.45978
1	-2.89023	1.31645	0.09446
6	-1.19071	0.03674	0.12719
1	-1.23305	-0.1784	1.20133
6	-0.21397	1.19316	-0.12763
1	-0.26717	1.45769	-1.19389
8	-0.62197	2.34707	0.60522
1	0.0395	2.57285	1.27504
6	1.21103	0.78046	0.19686
1	1.31205	0.60871	1.27694
8	2.17005	1.76831	-0.18711
1	1.72708	2.58653	-0.45437
6	1.55839	-0.51093	-0.53119
1	1.48694	-0.32529	-1.61228
8	2.84613	-0.97126	-0.19762
1	3.47485	-0.26412	-0.41002
6	0.52546	-1.58204	-0.19571
8	-0.74985	-1.12134	-0.578
1	0.70288	-2.47719	-0.79744
8	0.5943	-1.86895	1.174
1	0.38142	-2.79837	1.32951

Electric dipoles

0	0	-0.865000010	1.73490000	-0.853299975		
0	1	3.89999989E-03	3.68999988E-02	0.118000001		
0	2	6.12000003E-02	-9.00000036E-02	0.135800004		
0	3	-5.44999987E-02	-2.00999994E-02	0.118600003		
0	4	5.00000007E-02	0.161899999	0.121399999		
0	5	7.82999992E-02	-0.117299996	3.64000015E-02		
0	6	-0.105200000	3.33000012E-02	-3.20999995E-02		
0	7	-0.247400001	2.47000009E-02	-9.20000020E-03		
0	8	4.60000010E-03	-1.84000004E-02	-0.316300005		
0	9	-0.162799999	-0.119800001	0.176699996		
0	10	1.96000002E-02	5.53999990E-02	0.229000002		
0	11	0.1329	-0.0995	0.3232	0.1321	0.0258
0	12	-0.0032	-0.1971	-0.2498	0.1013	0.0199
0	13	-0.0162	-0.1276	0.2716	0.0903	0.0178
0	14	-0.1047	-0.0996	0.1709	0.0501	0.0100
0	15	-0.2021	-0.0943	0.2591	0.1169	0.0235

0	16	0.0825	-0.0494	-0.1475	0.0310	0.0063
	1	1	5.96059990	0.484699994	0.634100020	
	2	2	-3.01929998	-4.56850004	-1.55170000	
	3	3	-4.44000006	-1.71519995	-0.831600010	
	4	4	-2.21269989	0.906300008	0.133900002	
	5	5	-2.41790009	5.34119987	0.750199974	
	6	6	-1.40020001	1.07319999	-1.00660002	
	7	7	-0.415499985	8.52770042	-2.47900009	
	8	8	0.808600008	-2.75939989	-0.574899971	
	9	9	6.29449987	-7.89999962E-03	0.661000013	
	10	10	1.28400004	1.23549998	-2.00029993	
11	11	-0.8846	-0.0528	0.7072		
12	12	-3.4524	-2.7081	-2.6006		
13	13	-2.9906	-1.9849	0.4471		
14	14	-6.6475	-4.7816	-4.0475		
15	15	-2.8149	3.9473	0.6003		
16	16	-3.3277	5.4574	-1.6607		

Magnetic moments

1	0.298400015	-0.576499999	0.346399993
2	-0.694800019	0.106399998	-0.213799998
3	-8.37000012E-02	0.282700002	-0.351599991
4	4.17999998E-02	0.385800004	-0.166999996
5	0.235200003	-0.581200004	-0.184200004
6	3.28000002E-02	-0.426699996	0.236399993
7	6.92000017E-02	0.325800002	0.321000010
8	3.13999988E-02	-0.545700014	3.42000015E-02
9	-0.291399986	0.331499994	-0.603299975
10	-0.306699991	0.322299987	-0.180000007
11	0.1023	-0.1205	0.2647
12	-0.0315	0.2897	-0.2990
13	-0.2106	-0.5472	-0.2614
14	0.3603	-0.3068	-0.1255
15	0.1144	-0.0132	0.0575
16	0.2787	0.0717	0.0623

Ground energy

-686.912048

Excitation energy

6.60580015
6.79740000
7.06059980
7.27920008
7.37309980
7.48579979
7.57060003
7.75719976
7.82789993
7.94430017
7.9815
8.0079
8.0493
8.1862
8.2158

8.2628

Structure E-alpha

Number of atoms: 24

1	3.0975	0.83995	-0.32794
8	3.48538	-0.03114	-0.13828
6	2.50246	-0.86652	0.43546
1	2.76535	-1.90037	0.19594
1	2.49892	-0.76821	1.53206
6	1.09247	-0.58381	-0.07451
1	1.05126	-0.76614	-1.15509
6	0.6083	0.83812	0.19797
1	0.70185	1.03547	1.27894
8	1.4166	1.75464	-0.5222
1	0.96874	2.61681	-0.51158
6	-0.85401	0.99602	-0.20469
1	-0.94866	0.86356	-1.28591
8	-1.25423	2.34194	0.05015
1	-1.66883	2.41531	0.92203
6	-1.71045	-0.05369	0.49174
1	-1.6563	0.09322	1.58121
8	-3.05306	-0.03981	0.05049
1	-3.59727	0.49926	0.63823
6	-1.12295	-1.44337	0.21559
8	0.23013	-1.49456	0.61268
1	-1.62813	-2.19334	0.83167
8	-1.28291	-1.71006	-1.14627
1	-1.01467	-2.62419	-1.32156

Electric dipoles

0	0	-3.58360004	0.235200003	3.08489990	
0	1	-1.20999999E-02	-0.170000002	8.16999972E-02	
0	2	-7.68000036E-02	-9.47000012E-02	-0.108900003	
0	3	8.87999982E-02	5.62999994E-02	5.68000004E-02	
0	4	0.151299998	7.94000030E-02	0.205500007	
0	5	7.24000037E-02	-0.139300004	5.92000000E-02	
0	6	-5.00999987E-02	-1.61000006E-02	0.160899997	
0	7	1.65999997E-02	1.13000004E-02	9.13999975E-02	
0	8	-0.108300000	0.112099998	0.247899994	
0	9	-0.274599999	-7.85000026E-02	-4.99999989E-03	
0	10	-0.146699995	-0.102200001	-5.33000007E-02	
0	11	-0.0969	-0.0630	0.3581	
0	12	0.0801	-0.1490	0.0375	
0	13	-0.1436	-0.2226	0.0926	
0	14	0.0903	0.0746	0.1253	
0	15	-0.0306	0.0411	-0.1202	
0	16	0.0555	-0.0100	0.0014	
	1	1	1.43850005	-3.24099994	-1.83910000
	2	2	1.47440004	-2.84739995	-1.45350003
	3	3	-2.02679992	-4.14150000	1.37979996
	4	4	-2.27430010	5.95489979	2.88479996
	5	5	-2.15980005	-3.76239991	1.20980000
	6	6	9.44340038	-3.41240001	-1.33560002

7	7	1.78520000	5.96099997	3.15490007
8	8	0.467799991	-0.366800010	-0.128600001
9	9	-1.11660004	-1.13810003	1.00160003
10	10	-0.173099995	1.55390000	-2.30000005E-03
11	11	4.2199	0.2617	1.0464
12	12	-1.3481	1.8788	3.0193
13	13	-0.3294	-1.7056	-0.2396
14	14	-0.2759	0.9669	-0.2261
15	15	-0.2903	-1.4227	-0.1269
16	16	1.5326	0.7414	1.2596

Magnetic moments

1	0.108599998	-0.315200001	-0.227400005
2	0.182699993	0.243399993	-0.588699996
3	-0.309700012	0.455799997	-0.182500005
4	-7.72999972E-02	0.131500006	-0.318500012
5	-0.535200000	0.131799996	0.194999993
6	-7.80000016E-02	0.474099994	-0.159600005
7	0.203500003	0.243100002	-0.247400001
8	0.320600003	0.446000010	0.363400012
9	0.254799992	-0.516900003	-0.301099986
10	-0.316700011	1.18000004E-02	-0.250200003
11	0.0993	0.4600	0.0597
12	-0.1306	0.2516	0.0425
13	-0.2767	-0.1520	-0.5021
14	0.0327	0.3211	0.0581
15	0.0635	0.0086	0.4691
16	-0.3639	0.0082	0.1538

Ground energy

-686.916565

Excitation energies

6.39370012
 6.79099989
 7.10580015
 7.30039978
 7.38059998
 7.49919987
 7.59200001
 7.61269999
 7.71509981
 7.76999998
 7.8000
 7.9052
 7.9928
 8.0773
 8.1230
 8.2354

Structure F-alpha

Number of atoms : 24

1	-3.18635	0.87255	0.00315
8	-3.47059	-0.04599	0.12666
6	-2.4975	-0.91225	-0.40955

1	-2.76508	-1.92523	-0.10123
1	-2.50486	-0.88609	-1.5111
6	-1.07819	-0.60906	0.06861
1	-1.0133	-0.83453	1.13983
6	-0.62094	0.83752	-0.14149
1	-0.73752	1.06105	-1.21814
8	-1.43333	1.72466	0.60935
1	-1.21051	2.6282	0.3374
6	0.85306	1.02168	0.21407
1	0.98169	0.93033	1.29519
8	1.25585	2.35185	-0.10028
1	1.36809	2.43603	-1.05984
6	1.713	-0.03046	-0.48062
1	1.67205	0.13169	-1.56825
8	3.04973	-0.00341	-0.0203
1	3.62378	0.40402	-0.68042
6	1.13285	-1.42651	-0.22581
8	-0.20791	-1.47503	-0.65621
1	1.66137	-2.16394	-0.83576
8	1.2554	-1.71469	1.13815
1	1.50379	-2.63864	1.26892

Electric dipoles

0	0	3.29229999	-3.88999991E-02	-4.03560019		
0	1	-2.52999999E-02	0.103000000	8.87999982E-02		
0	2	3.24999988E-02	0.167999998	4.10000002E-03		
0	3	-0.232500002	6.67999983E-02	-2.64999997E-02		
0	4	0.112700000	0.164499998	1.11999996E-02		
0	5	3.80000006E-03	2.58000009E-02	-0.188099995		
0	6	0.230299994	-0.224600002	3.53000015E-02		
0	7	7.24999979E-02	0.118900001	0.149900004		
0	8	0.294099987	8.22999999E-02	-0.255800009		
0	9	-0.118299998	0.155300006	3.10999993E-02		
0	10	-1.46000003E-02	1.65999997E-02	4.39000018E-02		
0	11	0.2314	-0.0908	0.1681	0.0900	0.0172
0	12	-0.0439	0.0359	-0.0601	0.0068	0.0013
0	13	-0.0299	0.1054	-0.3104	0.1084	0.0210
0	14	0.1404	0.1245	0.2055	0.0775	0.0152
0	15	0.0278	-0.1661	-0.2172	0.0755	0.0149
0	16	0.0756	-0.0979	0.0429	0.0171	0.0034
	1	1	-0.672599971	-2.99119997	1.46500003	
	2	2	0.883700013	-4.47310019	0.322800010	
	3	3	2.35630012	-4.66750002	-0.777400017	
	4	4	1.20630002	-2.97839999	-0.510299981	
	5	5	0.753700018	5.42589998	-2.97219992	
	6	6	1.87950003	-4.40089989	0.458099991	
	7	7	-2.00200009	3.53340006	-2.25370002	
	8	8	-1.98559999	-0.352400005	-0.824000001	
	9	9	-1.03279996	0.908200026	-1.45930004	
	10	10	0.150999993	3.01869988	-3.31769991	
11	11	-2.0892	-0.6333	-1.0829		
12	12	0.4341	0.7993	-2.5828		
13	13	-1.2531	1.4122	-1.4468		

14	14	-1.2899	-0.9838	-0.3641
15	15	-1.3867	0.4054	-1.6513
16	16	-0.3609	-2.6547	-0.1448

Magnetic moments

1	0.196999997	0.353399992	-0.153300002
2	-2.65999995E-02	-0.307900012	-0.383500010
3	0.342599988	0.325700015	-0.427300006
4	-0.218700007	-0.113499999	0.577099979
5	7.95999989E-02	7.60000013E-03	8.59000012E-02
6	0.439799994	-0.305000007	0.680999994
7	0.137700006	-0.465499997	-0.551199973
8	6.23000003E-02	0.457899988	-0.247700006
9	0.166099995	0.137199998	-0.100100003
10	0.182999998	8.03999975E-02	0.140900001
11	-0.0376	-0.2687	0.1196
12	-0.1950	0.1822	-0.2335
13	-0.1124	0.0317	-0.0104
14	-0.4148	-0.0159	0.0679
15	-0.4225	0.4701	-0.0761
16	0.3530	0.0312	-0.1010

Ground energy

-686.912170

Excitation energy

6.33839989
6.64239979
6.89659977
7.16510010
7.27829981
7.37559986
7.44759989
7.51889992
7.63420010
7.71939993
7.7913
7.8220
7.9221
8.0096
8.0450
8.1568

Structure G-alpha

Number of atoms: 24

1	-3.4746	0.73465	-0.25684
8	-3.45899	-0.11145	0.21349
6	-2.47284	-0.94687	-0.36507
1	-2.68798	-1.96631	-0.03833
1	-2.52549	-0.92643	-1.46185
6	-1.05625	-0.57837	0.07307
1	-0.96773	-0.76496	1.15404
6	-0.64943	0.87462	-0.20681
1	-0.74908	1.0794	-1.28123
8	-1.48457	1.80987	0.4546

1	-1.89098	1.39214	1.22938
6	0.81597	1.0731	0.19639
1	0.88438	0.94639	1.28521
8	1.25825	2.38538	-0.07832
1	1.82767	2.38666	-0.86061
6	1.69325	0.02093	-0.48715
1	1.68701	0.21794	-1.56705
8	3.04611	0.1191	-0.09771
1	3.12558	-0.26917	0.78844
6	1.15031	-1.39665	-0.29031
8	-0.19781	-1.47482	-0.6286
1	1.66429	-2.08499	-0.96681
8	1.3565	-1.79951	1.05545
1	2.06492	-2.45446	1.10359

Electric dipoles

0	0	1.72950006	-3.22770000	-0.978699982		
0	1	-0.203700006	-2.80000009E-02	-0.103100002		
0	2	0.159899995	-0.143999994	-0.143299997		
0	3	8.30999985E-02	5.27999997E-02	0.316500008		
0	4	4.52999994E-02	0.179600000	-0.159199998		
0	5	-0.233500004	0.249300003	-6.03000000E-02		
0	6	0.166600004	0.171499997	6.78000003E-02		
0	7	0.224500000	-2.72000004E-02	-4.58000004E-02		
0	8	-4.98999991E-02	7.19999969E-02	6.09999988E-03		
0	9	1.53999999E-02	-6.99999975E-04	0.100800000		
0	10	9.82000008E-02	1.76999997E-02	-6.67999983E-02		
0	11	-0.0875	0.0078	0.1240	0.0231	0.0045
0	12	0.3148	0.1491	0.1125	0.1340	0.0262
0	13	0.0368	0.2578	0.2726	0.1421	0.0284
0	14	0.0087	0.1207	0.1688	0.0431	0.0086
0	15	0.0842	0.3533	-0.2982	0.2208	0.0445
0	16	0.0311	-0.1258	-0.1147	0.0299	0.0061
	1	1	5.28230000	-4.64440012	-1.25440001	
	2	2	-2.87140012	2.47280002	-2.81480002	
	3	3	-2.08990002	-3.90680003	3.75029993	
	4	4	-1.21169996	-0.293500006	-1.82400000	
	5	5	-2.79480004	2.45840001	0.186800003	
	6	6	-2.88150001	0.460099995	-9.48999971E-02	
	7	7	0.184000000	-1.08990002	0.580200016	
	8	8	3.72989988	-4.08269978	1.25849998	
	9	9	-0.709200025	-2.45239997	1.24129999	
	10	10	-9.30000003E-03	-0.383300006	-2.34859991	
11	11	3.4263	-2.4035	-3.0387	Tot=	5.1721
12	12	2.6380	-0.3815	-1.5272	Tot=	3.0719
13	13	2.8893	-0.1995	-0.0857	Tot=	2.8975
14	14	-0.0622	0.4467	-0.4042	Tot=	0.6057
15	15	0.8602	-1.0197	2.5304	Tot=	2.8606
16	16	-0.5762	-1.2728	2.8810	Tot=	3.2019

Magnetic moment

1	3.99999990E-04	0.762899995	-0.488999993
2	9.36999992E-02	-0.205300003	0.294400007
3	-0.265399992	4.76000011E-02	0.494899988

4	-2.67999992E-02	8.25999975E-02	0.256700009
5	6.93000033E-02	-3.50000011E-03	-0.214699998
6	0.644500017	6.71000034E-02	-0.765600026
7	-1.00000005E-03	0.185699999	-0.301299989
8	9.10999998E-02	-0.213799998	-0.192399994
9	-0.290600002	-4.89999987E-02	-3.02000009E-02
10	-0.345400006	0.324600011	-0.185699999
11	-0.1996	-0.1748	-0.3405
12	-0.2165	-0.1814	0.4792
13	-0.1544	-0.1977	0.1645
14	-0.1916	0.0544	-0.1134
15	-0.1819	0.2069	-0.3250
16	-0.4788	0.5269	-0.2067

Ground energy

-686.908936

Excitation energies

6.71420002

6.83790016

6.93120003

7.08479977

7.26609993

7.42189980

7.46799994

7.54969978

7.67500019

7.88180017

7.9106

7.9850

8.1596

8.1837

8.2197

8.2599

Structure H-alpha

Number of atoms: 24

1	-4.11961	0.27249	-0.57445
8	-3.43274	0.05574	0.06972
6	-2.45555	-0.78616	-0.54201
1	-2.73227	-1.83928	-0.41897
1	-2.36649	-0.57551	-1.61474
6	-1.10439	-0.54403	0.11839
1	-1.18516	-0.69329	1.20185
6	-0.59478	0.88826	-0.11559
1	-0.7728	1.17493	-1.16621
8	-1.25527	1.76653	0.77043
1	-2.19412	1.79408	0.52772
6	0.90023	0.99504	0.17677
1	1.03845	0.87364	1.25529
8	1.43393	2.27214	-0.11361
1	1.40039	2.43184	-1.06927
6	1.65466	-0.10713	-0.56049
1	1.47169	-0.01284	-1.64086

8	3.05004	-0.04142	-0.37755
1	3.25141	0.54011	0.36986
6	1.1072	-1.47332	-0.15319
8	-0.26699	-1.54252	-0.47217
1	1.57273	-2.27179	-0.73863
8	1.33374	-1.66317	1.22027
1	0.6899	-2.30875	1.54856

Electric dipoles

0	0	-3.79780006	-1.36199999	-2.83240008		
0	1	0.115199998	0.185100004	5.02000004E-02		
0	2	-2.51000002E-02	1.99999996E-02	-0.122400001		
0	3	0.179700002	-0.101999998	-3.18000019E-02		
0	4	8.83999988E-02	-0.151800007	0.103100002		
0	5	-1.59000009E-02	0.109899998	-1.35000004E-02		
0	6	3.59999994E-03	8.78999978E-02	-0.354200006		
0	7	-1.26999998E-02	5.49999997E-03	-7.20999986E-02		
0	8	1.09999999E-02	0.121799998	8.65999982E-02		
0	9	5.11000007E-02	-0.180800006	-2.51000002E-02		
0	10	-0.122800000	-4.05000001E-02	0.106399998		
0	11	-0.0290	-0.2398	-0.1330	0.0760	0.0146
0	12	0.0388	-0.1830	0.0096	0.0351	0.0068
0	13	0.1057	0.2395	0.0399	0.0701	0.0137
0	14	-0.2117	0.2019	0.0321	0.0866	0.0171
0	15	-0.0135	0.0721	-0.0154	0.0056	0.0011
0	16	-0.0175	0.4209	-0.0718	0.1826	0.0369
	1	1	2.65330005	-2.77390003	0.934300005	
	2	2	-0.148599997	-4.23229980	2.01220012	
	3	3	-1.91410005	-3.89619994	1.72800004	
	4	4	-2.80749989	3.58410001	-4.95620012	
	5	5	-3.88989997	-3.60249996	-1.06480002	
	6	6	-3.77060008	-2.24020004	-0.656099975	
	7	7	-0.518800020	0.768999994	-1.93990004	
	8	8	-3.04080009	1.43040001	-1.82299995	
	9	9	2.05539989	-1.91009998	-0.475600004	
	10	10	-0.496499985	-1.59340000	-0.939700007	
11	11	-3.6080	-1.3731	-0.2397	Tot=	3.8679
12	12	3.6290	0.6710	-1.1149	Tot=	3.8553
13	13	-0.3797	4.5867	-4.9134	Tot=	6.7323
14	14	-3.3302	-0.2530	0.0727	Tot=	3.3406
15	15	-0.9201	2.1514	-2.1538	Tot=	3.1802
16	16	0.2729	1.6530	-1.4715	Tot=	2.2298

Magnetic moments

1	0.335999995	-6.78000003E-02	0.716600001
2	-0.277200013	-9.45999995E-02	-0.128800005
3	5.93999997E-02	0.305599988	0.617100000
4	4.34999987E-02	-0.281500012	-0.626500010
5	0.289099991	-0.282400012	-0.350499988
6	-0.213799998	-0.213799998	7.60000013E-03
7	0.412699997	0.220799997	-5.66999987E-02
8	-0.548600018	9.10999998E-02	0.165700004
9	-0.232800007	-0.229200006	8.06000009E-02
10	-0.462500006	-0.361299992	-0.506399989

11	0.3370	-0.0655	0.2026
12	0.0100	0.3814	0.0046
13	0.3161	0.3854	0.3071
14	0.0839	0.1610	0.0537
15	0.0185	-0.2448	0.0191
16	-0.0608	0.3117	0.4323

Energy ground

-686.912109

Excitation energy

6.66590023

6.95709991

7.01370001

7.04230022

7.25120020

7.33300018

7.56610012

7.61250019

7.71820021

7.79879999

7.8311

7.9417

8.0016

8.0732

8.1998

8.2393

Structure I-alpha

Number of atoms: 24

1	-2.32995	-0.89257	-1.58911
8	-2.97086	-0.30868	-1.15419
6	-2.67738	-0.32141	0.23042
1	-3.16245	0.55138	0.67212
1	-3.08242	-1.22853	0.70002
6	-1.18357	-0.26307	0.50112
1	-1.00178	-0.3782	1.57616
6	-0.53106	1.03264	0.02117
1	-0.78764	1.19823	-1.0347
8	-1.03087	2.09141	0.81303
1	-0.44382	2.85153	0.67521
6	0.9798	0.91896	0.15664
1	1.23715	0.79603	1.2148
8	1.55229	2.12826	-0.34228
1	2.32739	2.35486	0.18862
6	1.48076	-0.28835	-0.62034
1	1.201	-0.17184	-1.67508
8	2.88045	-0.45309	-0.49652
1	3.31278	0.04074	-1.20613
6	0.77386	-1.53922	-0.10404
8	-0.62533	-1.37532	-0.21657
1	1.00947	-2.4046	-0.73032
8	1.16625	-1.74777	1.22137
1	0.8904	-2.63283	1.49989

Electric dipoles

0	0	3.06620002	-0.981700003	0.136700004	
0	1	7.69999996E-02	0.105700001	-4.01999988E-02	
0	2	3.37000005E-02	0.208000004	0.201100007	
0	3	0.201299995	5.97999990E-02	3.53999995E-02	
0	4	-0.247199997	9.10000037E-03	-4.19999985E-03	
0	5	0.228000000	-0.206499994	5.70000000E-02	
0	6	-1.04000000E-02	-0.117200002	7.85999969E-02	
0	7	-0.266400009	-0.235300004	0.129800007	
0	8	5.53000011E-02	-0.170499995	7.59999976E-02	
0	9	8.26999992E-02	-0.257900000	0.166600004	
0	10	-4.08000015E-02	-0.104900002	0.101899996	
0	11	0.0153	0.0292	-0.1363	0.0197 0.0039
0	12	0.0454	-0.0841	-0.0458	0.0112 0.0022
0	13	-0.0015	0.0818	0.0397	0.0083 0.0016
0	14	0.0941	-0.0667	-0.4298	0.1981 0.0397
0	15	0.0152	-0.0009	0.1137	0.0132 0.0026
0	16	0.1158	0.0066	-0.4654	0.2301 0.0468
	1	-2.44650006	-4.40740013	1.35609996	
	2	-2.43999995E-02	-2.17829990	1.99689996	
	3	1.85350001	1.92279994	3.66479993	
	4	2.62000002E-02	-2.98650002	-0.852699995	
	5	1.82760000	3.63229990	-1.57459998	
	6	2.26430011	-0.485100001	-0.616800010	
	7	2.46000004	4.65170002	-3.07870007	
	8	2.63070011	2.38459992	-2.48160005	
	9	2.20289993	7.44080019	-0.136199996	
	10	-6.25409985	-5.03009987	1.38999999	
11	11	-0.7238	-0.8604	-1.4984 Tot=	1.8733
12	12	0.3655	1.1233	-0.0536 Tot=	1.1825
13	13	-3.0533	0.3192	1.9236 Tot=	3.6228
14	14	0.8276	-1.6717	2.5488 Tot=	3.1584
15	15	-7.0035	-7.2021	1.5173 Tot=	10.1598
16	16	2.5373	4.1377	-1.7290 Tot=	5.1525

Magnetic moments

1	0.339899987	0.279599994	-0.124899998
2	-0.393700004	3.72000001E-02	-0.473300010
3	-0.484200001	0.252900004	0.277500004
4	0.181299999	0.244499996	-0.687099993
5	0.105099998	-0.359600008	-9.29000005E-02
6	-0.416700006	5.16000018E-02	-0.620500028
7	0.500299990	-0.135399997	6.49999976E-02
8	1.57999992E-02	-0.670000017	3.81999984E-02
9	0.437400013	-0.208399996	-0.247899994
10	-0.210899994	-0.370400012	0.179499999
11	0.3706	0.2117	0.2085
12	0.0539	-0.3313	0.0115
13	0.0836	0.0078	-0.3541
14	0.4182	-0.3416	0.5442
15	-0.2055	-0.1683	-0.1494
16	0.6797	-0.0937	0.0563

Energy ground

-686.923096
Excitation energy
6.56209993
6.96950006
7.12620020
7.25600004
7.33290005
7.60230017
7.65969992
7.75500011
7.86969995
7.93230009
8.0088
8.0386
8.0856
8.1867
8.1999
8.3049

Structure L-alpha
Number of atoms 24

1	-2.40745	0.02159	-1.60495
8	-3.12281	-0.28364	-1.03278
6	-2.64584	-0.51667	0.28181
1	-3.13469	0.18836	0.96296
1	-2.92862	-1.53534	0.56778
6	-1.14465	-0.38099	0.46438
1	-0.92426	-0.52171	1.52997
6	-0.56506	0.96014	0.01719
1	-0.79487	1.13678	-1.04433
8	-1.15133	1.97372	0.81245
1	-0.90629	2.8333	0.44024
6	0.95778	0.95652	0.1624
1	1.20222	0.81347	1.22352
8	1.49591	2.18924	-0.29841
1	1.59587	2.79819	0.44499
6	1.54592	-0.19103	-0.64941
1	1.31672	-0.03612	-1.70818
8	2.94577	-0.30768	-0.56807
1	3.23557	-0.09511	0.33054
6	0.87335	-1.49474	-0.19997
8	-0.52846	-1.42105	-0.30363
1	1.16715	-2.31854	-0.85585
8	1.28822	-1.73248	1.12432
1	1.03126	-2.62915	1.38389

Electric moments

0	0	1.46659994	0.537199974	2.46210003
0	1	-4.30999994E-02	0.136399999	8.47999975E-02
0	2	-3.22000012E-02	0.246600002	3.46999988E-02
0	3	8.32000002E-02	3.70999984E-02	-2.74999999E-02
0	4	3.44000012E-02	-8.79999995E-02	0.169000000
0	5	-0.241999999	-2.47000009E-02	-3.00999992E-02

0	6	0.182600006	-9.04999971E-02	-1.81000009E-02		
0	7	6.65000007E-02	-0.210600004	-0.233799994		
0	8	-0.141000003	0.186399996	-0.171800002		
0	9	0.212899998	4.08000015E-02	0.248199999		
0	10	-5.99999987E-02	-0.253199995	1.39999995E-03		
0	11	-0.1897	-0.1787	-0.0653	0.0722	0.0139
0	12	0.2578	-0.1708	-0.0815	0.1023	0.0200
0	13	-0.0510	-0.0043	-0.0855	0.0099	0.0020
0	14	-0.0770	-0.1413	0.0987	0.0356	0.0071
0	15	0.0474	0.0267	-0.1323	0.0205	0.0041
0	16	0.0079	-0.1371	0.0601	0.0225	0.0045
	1	1	-0.375699997	-5.38600016	3.92000005E-02	
	2	2	-0.502099991	-2.02649999	6.52839994	
	3	3	-1.94700003	-1.22230005	-2.05290008	
	4	4	1.36689997	4.30429983	1.06289995	
	5	5	1.01979995	-2.89949989	2.20499992	
	6	6	0.763400018	0.490599990	0.718500018	
	7	7	1.80149996	0.451099992	2.06019998	
	8	8	1.80920005	-3.37960005	0.798500001	
	9	9	1.02419996	-1.51329994	2.34010005	
	10	10	-2.24379992	-1.40540004	-0.960900009	
11	11	-1.8194	0.4361	0.0553	Tot=	1.8717
12	12	0.6744	6.5079	1.0896	Tot=	6.6329
13	13	-0.2704	-2.9645	0.6525	Tot=	3.0475
14	14	-0.9991	3.2824	-0.4308	Tot=	3.4580
15	15	-3.3212	3.9599	-0.7607	Tot=	5.2240
16	16	1.1629	-0.8826	2.7225	Tot=	3.0892

Magnetic moments

1	-0.143000007	-0.356500000	-0.216000006
2	-0.568000019	-0.171900004	0.414999992
3	5.53000011E-02	-0.133000001	-0.631099999
4	-1.15000000E-02	5.07000014E-02	-0.520900011
5	0.263999999	0.117399998	-0.595600009
6	4.17999998E-02	-0.145699993	0.645500004
7	-0.404399991	-0.108099997	-0.273600012
8	0.219799995	0.257400006	-0.228200004
9	-0.395999998	-0.166700006	0.152899995
10	0.186199993	0.250299990	0.451099992
11	0.3550	0.1020	-0.2018
12	0.0672	-0.4116	-0.1535
13	-0.4389	-0.0909	0.1115
14	-0.2133	-0.2452	0.3722
15	-0.3994	0.0340	0.2179
16	-0.2167	-0.0535	0.2699

Energy ground

-686.913330

Excitation energies

6.57690001
6.94899988
6.96210003
7.19589996
7.27479982

7.56930017
7.63219976
7.68889999
7.71780014
7.78030014
7.8342
7.9866
8.0835
8.1410
8.2154
8.2411

Structure M-alpha

Number of atoms: 24

1	-3.78739	0.62761	-0.25619
8	-3.42335	-0.06962	0.30358
6	-2.4935	-0.84955	-0.4408
1	-2.71488	-1.90665	-0.26824
1	-2.57928	-0.65653	-1.51645
6	-1.07516	-0.56622	0.03245
1	-1.04411	-0.74819	1.11739
6	-0.58221	0.85716	-0.23946
1	-0.6319	1.05715	-1.31709
8	-1.37465	1.86004	0.38556
1	-1.86648	1.46679	1.12336
6	0.8756	1.00686	0.1932
1	0.94047	0.86075	1.28271
8	1.37641	2.28025	-0.16103
1	0.89876	2.94141	0.36271
6	1.71522	-0.05177	-0.51035
1	1.64491	0.11408	-1.59103
8	3.08501	-0.02247	-0.18597
1	3.2123	0.42939	0.65951
6	1.12607	-1.43605	-0.21761
8	-0.22681	-1.50027	-0.6246
1	1.63988	-2.19598	-0.81144
8	1.26639	-1.6869	1.15655
1	1.26768	-2.64048	1.31747

Electric moments

0	0	-1.88409996	-1.37179995	0.977800012		
0	1	0.178599998	0.104300000	0.121699996		
0	2	0.192499995	2.74999999E-02	-1.86999999E-02		
0	3	-7.58000016E-02	3.70000005E-02	-2.29000002E-02		
0	4	-1.78999994E-02	-0.175500005	0.261500001		
0	5	-0.142000005	4.50999998E-02	-0.242699996		
0	6	6.44999966E-02	0.209099993	9.80000012E-03		
0	7	0.207300007	7.90999979E-02	-7.94999972E-02		
0	8	-0.107600003	-0.252499998	-0.215900004		
0	9	-0.171499997	0.241500005	0.108999997		
0	10	0.143399999	4.85000014E-02	0.234099999		
0	11	-0.0112	-0.0027	0.0347	0.0013	0.0003
0	12	0.2618	0.1733	-0.1454	0.1197	0.0236

0	13	0.0906	-0.1296	0.0838	0.0320	0.0064
0	14	0.1718	-0.0074	-0.1253	0.0453	0.0091
0	15	0.0816	0.1056	0.2082	0.0611	0.0124
0	16	-0.0183	-0.1730	-0.1965	0.0689	0.0140
	1	1	1.67700005	-4.14160013	-0.181199998	
	2	2	-0.837700009	-4.27409983	2.52999999E-02	
	3	3	-4.08230019	4.32550001	-1.88240004	
	4	4	-3.27390003	-1.15470004	-1.24000001	
	5	5	-1.36059999	-2.76830006	0.543399990	
	6	6	4.17999998E-02	-1.06019998	0.648100019	
	7	7	-3.30590010	4.52159977	-0.452399999	
	8	8	2.56809998	-1.77419996	0.388200015	
	9	9	3.15000005E-02	3.06719995	1.67530000	
	10	10	-0.123000003	0.911099970	1.91989994	
11	11	-2.3999	5.2599	0.3867	Tot=	5.7944
12	12	-2.7788	-2.3033	-0.1884	Tot=	3.6142
13	13	-1.9654	-1.5954	0.3540	Tot=	2.5561
14	14	-1.8195	0.1083	0.5064	Tot=	1.8917
15	15	-0.9968	1.5128	1.6602	Tot=	2.4573
16	16	-1.1351	0.1047	0.5572	Tot=	1.2688

Magnetic moments

1	0.119199999	-0.602100015	0.522300005
2	-0.104699999	9.66000035E-02	0.611699998
3	-0.161500007	0.115300000	0.649699986
4	3.13000008E-02	0.110799998	3.39000002E-02
5	0.415399998	2.29000002E-02	-0.475499988
6	-0.279100001	-0.189700007	-0.101499997
7	5.86000010E-02	-7.85000026E-02	-0.293399990
8	0.278400004	0.248300001	-1.59999996E-03
9	1.99999995E-04	0.284599990	0.119800001
10	9.22999978E-02	-0.391600013	-0.277700007
11	0.7761	0.0803	0.2098
12	-0.1558	-0.2922	0.4017
13	-0.4319	-0.0342	-0.0033
14	0.1279	0.4046	-0.2445
15	-0.0087	-0.1954	0.3618
16	0.2406	-0.3447	-0.2354

Ground energy

-686.917175

Excitation energies

6.61560011
6.92729998
7.07070017
7.23689985
7.40959978
7.54110003
7.56780005
7.66060019
7.76859999
7.82390022
8.0036
8.0351

8.1169
8.1836
8.2559
8.2704

Structure A-beta

Number of atoms: 24

1	4.1559	-1.15107	0.02443
8	3.43629	-0.76438	-0.48976
6	2.63646	0.06426	0.34187
1	2.99379	1.09931	0.30314
1	2.6476	-0.28075	1.38328
6	1.2114	0.0204	-0.16474
1	1.24486	0.03605	-1.26443
6	0.36906	1.2003	0.32366
1	0.33857	1.19404	1.42415
8	0.93582	2.41011	-0.1374
1	0.2235	3.06722	-0.1886
6	-1.04045	1.02356	-0.21186
1	-0.99565	1.08096	-1.31055
8	-1.83071	2.09364	0.28074
1	-2.67971	2.07639	-0.18619
6	-1.61693	-0.331	0.16721
1	-1.74014	-0.36721	1.25858
8	-2.87292	-0.45875	-0.48562
1	-3.55331	-0.72562	0.14433
6	-0.66686	-1.45841	-0.24887
8	0.61649	-1.19264	0.28552
1	-0.62601	-1.53753	-1.34241
8	-1.07453	-2.70204	0.21254
1	-1.04889	-2.69391	1.18257

Electric moments

0	0	-1.96259999	0.797900021	2.72530007		
0	1	-3.19999992E-03	-9.40999985E-02	0.116599999		
0	2	-0.140900001	-0.104400001	1.03000002E-02		
0	3	0.119199999	2.84000002E-02	-0.309199989		
0	4	-8.52999985E-02	0.128199995	4.28000018E-02		
0	5	0.100199997	0.195099995	0.115900002		
0	6	0.200100005	-7.02000037E-02	0.330700010		
0	7	3.46000008E-02	-6.04999997E-02	3.07000000E-02		
0	8	-9.61999968E-02	8.07000026E-02	0.174199998		
0	9	-0.128199995	0.168500006	6.31999969E-02		
0	10	5.88000007E-02	-3.48000005E-02	-0.159600005		
0	11	0.1064	0.0764	-0.0901	0.0253	0.0050
0	12	0.0683	0.0855	-0.3522	0.1360	0.0269
0	13	0.1399	0.0213	-0.1651	0.0473	0.0094
0	14	-0.0114	0.0194	0.0931	0.0092	0.0018
0	15	-0.0436	-0.2018	-0.0641	0.0467	0.0094
0	16	-0.0571	0.0945	-0.0326	0.0133	0.0027
	1	1	4.94110012	2.17589998	-1.62759995	
	2	2	-8.05329990	2.89919996	-0.316700011	
	3	3	1.39900005	-1.39129996	2.36800003	

4	4	0.393599987	-2.13459992	1.25100005
5	5	2.14520001	-2.25219989	3.15129995
6	6	0.819400012	2.25670004	0.671500027
7	7	0.102200001	3.68390012	1.84700000
8	8	3.35990000	1.28489995	0.156100005
9	9	-4.45330000	2.00329995	-0.953499973
10	10	-2.45560002	-1.80890000	1.06770003
11 11	2.7616	2.2590	-0.6619 Tot=	3.6287
12 12	1.9541	1.7881	0.7825 Tot=	2.7619
13 13	5.0497	1.5275	0.8854 Tot=	5.3494
14 14	-1.1996	0.3961	0.9234 Tot=	1.5649
15 15	2.3083	-3.3504	0.4567 Tot=	4.0941
16 16	2.4514	0.5345	1.6985 Tot=	3.0298

Magnetic moments

1	0.467700005	0.187500000	-0.140300006
2	0.279799998	4.99999989E-03	0.648199975
3	6.44999966E-02	-2.40000002E-02	-0.169499993
4	0.792699993	-5.09999990E-02	0.522099972
5	5.05000018E-02	0.379099995	0.736899972
6	-0.258700013	-9.09999982E-02	-0.493900001
7	6.97000027E-02	0.101700000	-0.365900010
8	-0.151199996	-8.33000019E-02	0.246999994
9	-0.131400004	-0.187999994	-1.72000006E-02
10	0.323500007	-0.110399999	-2.55999994E-02
11	0.2092	-0.1475	-0.2744
12	0.2254	-0.0518	0.2642
13	0.1634	0.0792	0.1799
14	-0.2771	0.0252	0.2505
15	0.2088	0.0507	0.7211
16	-0.1264	0.0309	0.4103

Ground energy

-686.916870

Excitation energies

6.52860022
6.69379997
6.99090004
7.35790014
7.42530012
7.55189991
7.66109991
7.79750013
7.91200018
7.94110012
8.0263
8.0770
8.0962
8.1075
8.2388
8.3137

Structure B-beta

Number of atoms: 24

1	-2.88814	-1.61132	0.44563
8	-3.45228	-0.91317	0.08193
6	-2.63094	0.15194	-0.36038
1	-3.09578	1.09294	-0.05812
1	-2.55851	0.12561	-1.45702
6	-1.23303	0.08129	0.22055
1	-1.30672	0.08627	1.32147
6	-0.35558	1.26686	-0.19431
1	-0.3779	1.36353	-1.28852
8	-0.89128	2.42557	0.41989
1	-0.77147	3.18554	-0.16438
6	1.08804	1.04491	0.2341
1	1.13691	1.08797	1.33283
8	1.88485	2.07499	-0.31741
1	2.80743	1.77665	-0.2877
6	1.54989	-0.32711	-0.23154
1	1.51349	-0.3758	-1.32672
8	2.88167	-0.53894	0.2287
1	3.42225	-0.88853	-0.49145
6	0.61095	-1.40552	0.29905
8	-0.67651	-1.16179	-0.20009
1	0.60162	-1.38945	1.40283
8	0.96654	-2.67211	-0.16977
1	1.63684	-3.04401	0.42025

Electric moments

0	0	4.30749989	-6.01999983E-02	-0.347299993		
0	1	5.05999997E-02	-5.88999987E-02	4.14000005E-02		
0	2	0.185200006	2.30999999E-02	4.78000008E-02		
0	3	-9.08999965E-02	-1.92000009E-02	-6.21999986E-02		
0	4	-2.29000002E-02	-1.84000004E-02	-0.251599997		
0	5	1.75999999E-02	0.222200006	0.345200002		
0	6	-0.161899999	-0.220100001	0.185800001		
0	7	9.96999964E-02	1.04999999E-02	-9.18999985E-02		
0	8	2.41000000E-02	0.106500000	-0.249200001		
0	9	0.185800001	-7.53000006E-02	2.00999994E-02		
0	10	-0.105800003	1.42000001E-02	-4.14999984E-02		
0	11	-0.0262	-0.0323	0.3309	0.1112	0.0218
0	12	-0.0180	-0.0341	0.0252	0.0021	0.0004
0	13	-0.0304	0.2526	-0.2522	0.1283	0.0255
0	14	-0.0133	-0.0298	-0.0840	0.0081	0.0016
0	15	-0.1960	-0.0366	-0.1408	0.0596	0.0119
0	16	0.0758	0.1291	-0.0734	0.0278	0.0056
	1	1	-2.88689995	2.22650003	1.78999996	
	2	2	3.22239995	2.73110008	-2.44140005	
	3	3	4.30310011	-2.84089994	1.06309998	
	4	4	3.59999990	2.25169992	-2.41720009	
	5	5	-0.894999981	8.96999985E-02	0.493499994	
	6	6	2.12680006	1.50940001	-1.47730005	
	7	7	3.48180008	1.61020005	1.21280003	
	8	8	2.69799995	-5.76090002	4.43639994	
	9	9	-1.14639997	0.532999992	2.73620009	
	10	10	2.15000010	-1.83570004	1.61280000	

11	11	1.8868	1.6274	-3.1638	Tot=	4.0272
12	12	-14.7072	2.5612	1.0698	Tot=	14.9668
13	13	0.2300	0.6880	-2.1686	Tot=	2.2867
14	14	-0.3708	-2.1189	-1.8544	Tot=	2.8401
15	15	0.9531	1.5450	0.7251	Tot=	1.9547
16	16	-2.1025	0.3644	1.0337	Tot=	2.3710

Magnetic moments

1	-0.435200006	0.217500001	0.158199996
2	-0.195700005	-3.09999995E-02	-0.145699993
3	-0.155100003	0.590799987	-0.777100027
4	-0.484600008	0.518299997	8.30999985E-02
5	-0.298400015	0.198300004	-0.172999993
6	0.423099995	0.250699997	0.551800013
7	0.373899996	-0.234599993	0.251300007
8	0.242200002	0.191900000	9.21000019E-02
9	-0.454800010	0.248400003	-0.115500003
10	8.07000026E-02	-0.178299993	-0.469099998
11	-0.1118	0.0806	0.6719
12	0.0144	-0.0487	-0.0079
13	0.0890	-0.0291	-0.1948
14	-0.1567	0.0815	-0.1092
15	0.2654	-0.0942	0.2881
16	-0.2906	-0.3396	-0.6574

Ground energy

-686.914551

Excitation energies

6.53100014
6.87729979
7.02899981
7.09740019
7.25600004
7.52710009
7.66669989
7.68160009
7.77610016
7.85680008
7.9844
8.0571
8.1145
8.1306
8.1624
8.2327

Structure C-beta

Numer of atoms: 24

1	4.1763	-1.03844	0.22508
8	3.41699	-0.823	-0.33073
6	2.63894	0.18581	0.29118
1	3.02377	1.18448	0.0544
1	2.62561	0.05829	1.38182
6	1.21895	0.07847	-0.21991
1	1.24139	0.07074	-1.32061

6	0.33639	1.22618	0.26987
1	0.34438	1.2304	1.37058
8	0.83526	2.45216	-0.22671
1	0.19169	3.13927	0.00773
6	-1.08569	0.98821	-0.21139
1	-1.09157	1.04762	-1.30786
8	-1.91198	2.02261	0.32437
1	-2.53548	2.31921	-0.35155
6	-1.59823	-0.38631	0.19873
1	-1.65457	-0.43291	1.29656
8	-2.86592	-0.636	-0.37963
1	-3.55456	-0.28151	0.19837
6	-0.60853	-1.45996	-0.26645
8	0.66723	-1.13914	0.2622
1	-0.56458	-1.49646	-1.36269
8	-0.94442	-2.73583	0.14476
1	-1.19076	-2.72147	1.08183

Electric moments

0	0	-1.81369996	2.95009995	2.43729997		
0	1	-9.65000018E-02	2.85999998E-02	-5.49999997E-03		
0	2	-0.130199999	-8.87999982E-02	4.14000005E-02		
0	3	2.41999999E-02	0.145999998	-0.211199999		
0	4	0.151999995	-3.46000008E-02	-7.78999999E-02		
0	5	0.162900001	0.177399993	0.227300003		
0	6	0.149700001	-7.66000003E-02	-4.08000015E-02		
0	7	0.204099998	-4.80000004E-02	0.275999993		
0	8	-5.29000014E-02	-0.183100000	-4.00000019E-03		
0	9	5.11999987E-02	8.11000019E-02	-0.183100000		
0	10	3.04000005E-02	8.38999972E-02	-5.99000007E-02		
0	11	-0.0320	-0.0373	0.0559	0.0055	0.0011
0	12	-0.0834	0.1452	-0.1490	0.0503	0.0099
0	13	0.0460	0.1224	-0.0205	0.0175	0.0035
0	14	-0.1127	-0.0106	0.1306	0.0299	0.0059
0	15	0.1379	0.1649	-0.3577	0.1742	0.0351
0	16	-0.0644	-0.0214	-0.1976	0.0436	0.0089
	1	1	4.32100010	-0.469799995	2.46309996	
	2	2	-8.05459976	4.06780005	-0.714699984	
	3	3	2.42219996	2.31419992	5.27999997E-02	
	4	4	0.925599992	-0.711099982	0.890200019	
	5	5	1.51810002	1.81540000	0.209700003	
	6	6	7.01070023	-2.99040008	2.39199996	
	7	7	1.44579995	3.83769989	-1.96019995	
	8	8	0.424100012	2.23930001	1.97189999	
	9	9	-1.13820004	3.82540011	4.45009995	
	10	10	-7.89669991	7.94999972E-02	-1.82009995	
11	11	2.4198	0.4318	-0.2619	Tot=	2.4720
12	12	4.8117	1.9321	1.1962	Tot=	5.3213
13	13	9.1492	-5.8787	3.9386	Tot=	11.5664
14	14	-3.1334	1.2481	0.8569	Tot=	3.4800
15	15	1.4394	0.4709	2.6302	Tot=	3.0350
16	16	-6.4290	4.7403	1.2308	Tot=	8.0819

Magnetic monents

1	-0.424299985	0.242599994	0.104300000
2	0.322299987	0.167799994	0.613399982
3	-3.33000012E-02	-0.129099995	0.235799998
4	-0.555800021	-2.96000000E-02	2.08999999E-02
5	0.171200007	0.402500004	0.863499999
6	-2.08000001E-02	-1.31000001E-02	0.161100000
7	-3.42000015E-02	-0.204099998	-0.443599999
8	0.259900004	-0.225400001	-0.701399982
9	0.263900012	0.152600005	6.44999966E-02
10	2.45999992E-02	-8.34999979E-02	-0.159899995
11	-0.2729	-0.4646	-0.5456
12	-0.0703	0.1457	0.4022
13	-0.1349	0.0352	-0.3939
14	0.2468	-0.2602	-0.3225
15	0.3238	-0.1936	-0.0832
16	0.1785	0.4825	0.1209

Ground energy

-686.914185

Excitation energy

6.53910017

6.63290024

6.90450001

7.17360020

7.35270023

7.44619989

7.58419991

7.60260010

7.74289989

7.86730003

7.9736

8.0091

8.0862

8.1158

8.2232

8.2976

Structure D-beta

Number of atoms : 24

1	-3.33438	-1.00951	1.09992
8	-3.4963	-0.89882	0.15264
6	-2.63072	0.08983	-0.37359
1	-3.02905	1.09529	-0.19068
1	-2.59949	-0.07883	-1.45333
6	-1.21489	0.02445	0.17532
1	-1.2625	0.00151	1.28443
6	-0.38365	1.24938	-0.23864
1	-0.43964	1.37547	-1.32466
8	-0.90929	2.44625	0.30443
1	-1.03143	2.34355	1.26068
6	1.08233	1.06299	0.14927
1	1.16343	1.19619	1.23982
8	1.85109	2.04126	-0.52012

1	2.57219	2.33345	0.05202
6	1.61677	-0.32877	-0.17204
1	1.7389	-0.39868	-1.2636
8	2.86786	-0.43297	0.4881
1	3.44484	-1.05184	0.02166
6	0.65997	-1.43103	0.27638
8	-0.61672	-1.17192	-0.28196
1	0.59483	-1.47176	1.37168
8	1.05922	-2.69401	-0.13563
1	1.35643	-2.65429	-1.05778

Electric moments

0	0	2.57489991	0.460000008	1.63269997		
0	1	-0.162900001	2.22999994E-02	0.136199996		
0	2	8.38000029E-02	8.13999996E-02	0.119900003		
0	3	1.48999998E-02	0.150800005	-8.48999992E-02		
0	4	0.153600007	-0.104000002	-0.235400006		
0	5	-4.16000001E-02	4.58000004E-02	-0.283300012		
0	6	-4.34000008E-02	-0.135700002	7.60000013E-03		
0	7	0.163299993	5.27000017E-02	0.300799996		
0	8	-9.95000005E-02	-8.00999999E-02	-5.93999997E-02		
0	9	-0.231800005	-0.100599997	3.83000001E-02		
0	10	0.208800003	-9.45999995E-02	-7.50999972E-02		
0	11	0.0365	0.2131	0.0185	0.0471	0.0090
0	12	0.0078	-0.0934	0.1102	0.0209	0.0041
0	13	0.0078	0.1085	0.0233	0.0124	0.0025
0	14	0.1059	0.0458	-0.0900	0.0214	0.0043
0	15	-0.0988	-0.0420	0.0145	0.0117	0.0023
0	16	0.0188	-0.0354	0.2657	0.0722	0.0145
	1	1	2.06890011	0.218400002	-2.51519990	
	2	2	-1.85230005	3.39809990	3.44160008	
	3	3	2.87949991	7.40000010E-02	-3.05240011	
	4	4	0.134499997	-3.40109992	-2.90450001	
	5	5	3.74900007	0.637700021	-2.58929992	
	6	6	0.130199999	1.99290001	2.16599989	
	7	7	-2.75889993	4.99639988	5.38049984	
	8	8	-1.33819997	1.22950006	4.01809978	
	9	9	-0.543500006	0.576300025	1.00769997	
	10	10	-0.773299992	0.201199993	1.97479999	
11	11	-1.2443	1.5187	1.1798	Tot=	2.2906
12	12	3.6391	-1.8365	-0.0313	Tot=	4.0764
13	13	1.4537	-1.9835	1.1390	Tot=	2.7102
14	14	-0.0184	-0.3761	1.0750	Tot=	1.1391
15	15	0.0510	-2.2825	-0.8569	Tot=	2.4385
16	16	0.4197	-0.2732	0.4721	Tot=	0.6882

Magnetic moments

1	0.289400011	0.247299999	8.29999987E-03
2	0.127399996	-0.338600010	-0.245199993
3	0.303900003	-0.273699999	0.583899975
4	0.321099997	-3.86999995E-02	0.145099998
5	5.99000007E-02	-0.108199999	-0.656700015
6	0.494700015	-9.29000005E-02	0.797599971
7	0.290899992	-6.92000017E-02	0.311600000

8	-0.154300004	-2.30000005E-03	0.478500009
9	0.290800005	0.271699995	0.136000007
10	0.210999995	9.97999981E-02	-0.576399982
11	0.0298	0.1955	0.0399
12	0.2863	0.4854	-0.2370
13	0.2312	-0.5288	0.1965
14	0.0157	0.1236	0.2496
15	-0.1261	-0.2080	-0.2459
16	0.2951	-0.3088	-0.0602

Ground energy

-686.907166

Excitation energies

6.58300018

6.65199995

6.81669998

6.98579979

7.22030020

7.39890003

7.47700024

7.60249996

7.77330017

7.80410004

7.8409

7.9048

8.0827

8.1024

8.1537

8.2044

Structure E-beta

Number of atoms: 24

1	-3.62984	-0.18827	0.98552
8	-3.57219	-0.33685	0.03128
6	-2.42786	-1.09932	-0.27505
1	-2.37134	-1.13648	-1.36605
1	-2.51971	-2.13171	0.09039
6	-1.11482	-0.53357	0.26712
1	-1.14262	-0.50287	1.36968
6	-0.72969	0.84905	-0.25371
1	-0.79193	0.8368	-1.35332
8	-1.61148	1.81477	0.27923
1	-1.2135	2.6856	0.11763
6	0.69892	1.19094	0.17132
1	0.70573	1.30162	1.26319
8	1.03126	2.47737	-0.33804
1	1.62503	2.40097	-1.09765
6	1.70013	0.10376	-0.18876
1	1.80761	0.02528	-1.28016
8	2.94585	0.37041	0.43066
1	3.63331	0.51636	-0.22966
6	1.18036	-1.24516	0.29645
8	-0.13447	-1.47161	-0.17302

1	1.18044	-1.26834	1.39936
8	1.99594	-2.23344	-0.23225
1	1.63519	-3.0985	0.01399

Electric moments

0	0	2.22210002	-0.983099997	-0.283399999	
0	1	4.96999994E-02	-0.157299995	-0.104699999	
0	2	9.70000029E-02	2.64999997E-02	9.60000046E-03	
0	3	-9.65000018E-02	2.62000002E-02	-0.113600001	
0	4	7.15999976E-02	-5.88999987E-02	-0.157299995	
0	5	-6.36999980E-02	-0.118000001	-0.204400003	
0	6	0.183300003	0.128900006	-0.221100003	
0	7	5.88999987E-02	-3.68999988E-02	0.493000001	
0	8	2.86999997E-02	-0.272700012	0.242500007	
0	9	-9.10999998E-02	-7.84000009E-02	-8.56000036E-02	
0	10	-5.29000014E-02	9.84999985E-02	-1.86000001E-02	
0	11	-0.0376	0.2330	-0.0494	0.0581 0.0112
0	12	0.1409	0.0706	0.0829	0.0317 0.0062
0	13	-0.1977	-0.0753	0.1618	0.0709 0.0139
0	14	0.0665	-0.1550	0.1212	0.0431 0.0086
0	15	0.0958	-0.0810	-0.0860	0.0231 0.0046
0	16	0.0443	0.1313	-0.0513	0.0218 0.0044
	1	1	-3.58150005	-3.86910009	4.42329979
	2	2	3.29600000	-1.12769997	-3.05870008
	3	3	-2.22320008	-2.52789998	2.13280010
	4	4	1.49170005	6.15430021	-3.73289990
	5	5	1.50650001	-4.38819981	0.573300004
	6	6	-0.926599979	0.360300004	-1.35790002
	7	7	0.660700023	0.956700027	-0.978200018
	8	8	-1.66380000	0.797900021	0.872399986
	9	9	-1.39880002	-0.150000006	2.74810004
	10	10	0.766399980	0.307000011	0.636500001
11	11	2.1289	-1.7725	0.1382 Tot=	2.7736
12	12	-6.4505	-2.3404	1.8775 Tot=	7.1141
13	13	-1.3081	-0.5543	0.9327 Tot=	1.6995
14	14	1.6247	2.7046	2.3539 Tot=	3.9364
15	15	1.6909	-2.2586	-1.4355 Tot=	3.1656
16	16	0.4065	-0.1278	0.1414 Tot=	0.4490

Magnetic moments

1	-0.175899997	-0.158999994	0.372000009
2	0.396400005	-0.237200007	0.349299997
3	7.66000003E-02	-0.208000004	-0.469099998
4	0.563799977	-7.00000003E-02	-0.264099985
5	0.720600009	0.164399996	-0.148499995
6	5.29000014E-02	0.417299986	0.403100014
7	0.220599994	0.183899999	0.478599995
8	0.262899995	6.27999976E-02	-5.77000007E-02
9	6.00000005E-03	-0.388399988	0.247600004
10	3.18000019E-02	-1.68999992E-02	-0.769599974
11	0.0474	0.1469	-0.0158
12	-0.4949	0.0617	0.1281
13	-0.3848	-0.1636	-0.1010
14	-0.1383	0.1944	-0.1352

15	-0.2460	-0.0568	0.1370
16	0.1262	-0.0778	-0.1211

Ground energy

-686.908813

Excitation energy

6.55070019

6.72760010

6.76469994

7.06669998

7.29640007

7.53039980

7.56400013

7.67180014

7.79330015

7.82000017

7.8548

7.9584

8.0275

8.1047

8.1324

8.1751

Structure F-beta

Number of atoms: 24

1	-4.25725	-0.57146	0.11458
8	-3.37425	-0.38107	0.45782
6	-2.39813	-1.15295	-0.24027
1	-2.52686	-1.06328	-1.32583
1	-2.45506	-2.2103	0.04051
6	-1.04434	-0.60653	0.17564
1	-1.03608	-0.59077	1.28086
6	-0.72461	0.79884	-0.34437
1	-0.64736	0.74393	-1.4381
8	-1.70733	1.77613	-0.04801
1	-2.36154	1.40669	0.56682
6	0.6341	1.24402	0.19215
1	0.56054	1.34619	1.28946
8	1.02864	2.46576	-0.38876
1	0.48267	3.17086	-0.01103
6	1.67982	0.18958	-0.15314
1	1.8437	0.19845	-1.23412
8	2.95381	0.44257	0.4181
1	2.87022	0.5067	1.38221
6	1.21626	-1.21927	0.23476
8	-0.05532	-1.50408	-0.28996
1	1.17512	-1.30776	1.33966
8	2.05741	-2.18903	-0.30384
1	2.94962	-2.03348	0.04349

Electric moments

0	0	-2.83209991	-0.828800023	3.02839994
0	1	6.53000027E-02	-5.18000014E-02	0.226199999
0	2	3.62000018E-02	7.15999976E-02	9.73000005E-02

0	3	7.77999982E-02	8.47999975E-02	-9.43000019E-02		
0	4	-7.06000030E-02	0.101499997	0.100900002		
0	5	-7.76000023E-02	-8.20000023E-02	0.212699994		
0	6	-5.22000007E-02	4.61999997E-02	0.157900006		
0	7	7.98000023E-02	-7.31000006E-02	0.176400006		
0	8	-8.91000032E-02	-0.165199995	-0.335999995		
0	9	-0.210099995	9.51000005E-02	0.261299998		
0	10	-1.72000006E-02	-2.70000007E-03	0.102600001		
0	11	0.0805	0.1977	-0.1610	0.0715	0.0139
0	12	-0.0569	-0.2952	0.0548	0.0934	0.0183
0	13	0.2430	0.0847	0.2983	0.1552	0.0306
0	14	0.1391	0.0406	0.2838	0.1015	0.0203
0	15	-0.1087	-0.1274	-0.0159	0.0283	0.0057
0	16	-0.0627	0.1005	-0.1409	0.0339	0.0069
	1	1	-6.70389986	-0.749499977	-2.75390005	
	2	2	0.589600027	-2.29229999	0.894599974	
	3	3	-0.680199981	-0.574699998	0.992299974	
	4	4	-2.34870005	0.238000005	0.178900003	
	5	5	-5.18629980	-0.233500004	0.524900019	
	6	6	4.60000010E-03	0.799799979	9.70000029E-03	
	7	7	5.00920010	-1.03120005	2.44600010	
	8	8	3.02519989	3.72000001E-02	0.739000022	
	9	9	-4.97770023	2.09969997	0.112999998	
	10	10	-1.05060005	2.08240008	3.02270007	
11	11	-1.0384	-0.5755	2.8007	Tot=	3.0419
12	12	-1.6833	1.0547	2.5453	Tot=	3.2287
13	13	-3.6109	-1.0654	-0.8406	Tot=	3.8575
14	14	-1.1535	-2.2737	2.0241	Tot=	3.2553
15	15	-1.6123	-0.3142	3.4917	Tot=	3.8588
16	16	2.2958	-1.9154	2.0072	Tot=	3.6011

Magnetic moments

1	-0.273400009	4.38000001E-02	0.209600002
2	8.08999985E-02	-0.225600004	0.507300019
3	0.216499999	0.550499976	0.409999996
4	4.16000001E-02	-0.107500002	-0.388999999
5	0.392300010	0.214499995	0.252000004
6	0.218500003	0.438699991	-0.217399999
7	-0.323799998	-0.134000003	0.290499985
8	0.656199992	0.150500000	-3.06000002E-02
9	0.443399996	0.290300012	-0.363499999
10	0.462599993	-0.308800012	-0.613799989
11	0.0343	-0.3151	0.3152
12	0.0657	-0.0001	0.1363
13	-0.3586	-0.4668	0.1282
14	0.2426	0.4268	0.5301
15	0.2522	-0.1302	-0.0760
16	0.1107	-0.1954	0.0936

Ground energy

-686.911133

Excitation energy

6.55649996

6.68820000

6.87039995
 7.11369991
 7.24590015
 7.32929993
 7.40040016
 7.50339985
 7.69670010
 7.74779987
 7.9574
 7.9941
 8.0378
 8.1635
 8.1969
 8.2712

Structure G-beta

Numer of atoms 24

1	-3.27138	0.5061	0.01696
8	-3.50779	-0.42642	0.14681
6	-2.38733	-1.24123	-0.12019
1	-2.32691	-1.48393	-1.19163
1	-2.52316	-2.17842	0.42449
6	-1.04761	-0.62643	0.28906
1	-1.01128	-0.54837	1.38859
6	-0.7643	0.76007	-0.29893
1	-0.76499	0.6899	-1.39565
8	-1.76465	1.67622	0.12255
1	-1.46364	2.57432	-0.08289
6	0.618	1.21294	0.17002
1	0.58386	1.28404	1.27019
8	0.9498	2.48426	-0.37241
1	0.76987	3.1843	0.26833
6	1.66735	0.18464	-0.22398
1	1.76593	0.15149	-1.31235
8	2.96009	0.48612	0.27085
1	2.89942	0.80353	1.18424
6	1.24626	-1.21298	0.25316
8	-0.05199	-1.52325	-0.17188
1	1.29418	-1.25257	1.35907
8	2.0587	-2.19414	-0.30984
1	2.90059	-2.21471	0.16711

Electric moments

0	0	2.23090005	3.47189999	3.14569998
0	1	3.59999994E-03	5.79000004E-02	0.272799999
0	2	-0.162900001	0.104699999	-6.37999997E-02
0	3	-9.79000032E-02	3.04000005E-02	-0.144099995
0	4	-4.19000015E-02	8.10000021E-03	2.43999995E-02
0	5	0.140499994	0.102600001	0.223900005
0	6	-0.175300002	-0.142000005	0.203700006
0	7	-0.125400007	0.146599993	-0.139500007
0	8	-3.04000005E-02	0.199699998	0.245800003
0	9	-0.160099998	-6.71999976E-02	-0.300700009

0	10	-0.141000003	8.91000032E-02	1.35000004E-02	
0	11	0.0480	0.0196	-0.1619	0.0289 0.0056
0	12	0.0818	-0.1468	0.1146	0.0414 0.0080
0	13	0.2644	0.0087	0.0638	0.0740 0.0146
0	14	0.0586	-0.2050	-0.2839	0.1261 0.0250
0	15	-0.0203	0.0935	0.1320	0.0266 0.0053
0	16	-0.0171	-0.1395	0.3208	0.1227 0.0247
	1	1	-0.282599986	-0.489399999	-2.06900001
	2	2	1.16869998	-2.26690006	-0.117399998
	3	3	0.183400005	-3.72259998	2.15350008
	4	4	0.798900008	-1.02330005	1.12730002
	5	5	-0.426200002	5.73999994E-02	0.125300005
	6	6	1.28320003	1.38290000	1.20599997
	7	7	0.442699999	-2.00550008	0.496300012
	8	8	-3.20140004	-2.35619998	-4.34000008E-02
	9	9	-0.762099981	3.08629990	-0.887099981
	10	10	-1.73969996	2.44840002	-1.32369995
11	11	1.8441	-1.9728	0.6675	Tot= 2.7817
12	12	-0.5171	2.8591	0.2999	Tot= 2.9209
13	13	0.2707	-0.9815	0.0516	Tot= 1.0194
14	14	-2.0504	2.3165	3.9850	Tot= 5.0448
15	15	2.3182	-0.4826	2.4949	Tot= 3.4397
16	16	-1.2268	1.7333	3.8022	Tot= 4.3550

Magnetic moments

1	-0.239999995	-2.84000002E-02	1.75999999E-02
2	8.35999995E-02	-0.442299992	-0.240899995
3	0.220500007	0.400200009	-6.43000007E-02
4	9.48999971E-02	-0.256099999	0.151600003
5	-0.192100003	9.60000008E-02	6.34000003E-02
6	0.409099996	0.490000010	0.131400004
7	0.159299999	-4.65000011E-02	-1.01300001
8	0.297600001	8.20999965E-02	-0.263999999
9	0.398799986	0.555499971	-0.109999999
10	0.232199997	6.76999986E-02	-0.136299998
11	-0.7003	-0.0343	0.4523
12	-0.3574	-0.0573	0.2048
13	-0.1022	-0.2423	0.4111
14	-0.2178	0.5478	-0.0389
15	0.0563	0.0856	0.0379
16	0.2458	-0.0046	0.3389

Ground energy

-686.908386

Excitation energy

6.45230007
6.57000017
6.89010000
7.00339985
7.27069998
7.29969978
7.40570021
7.43889999
7.60580015

7.63950014
7.8845
7.9111
8.0361
8.0898
8.1802
8.2244

Structure H-beta

Number of atoms: 24

1	-4.31513	-0.73695	0.16055
8	-3.3699	-0.9098	0.26262
6	-2.63702	0.19478	-0.24409
1	-3.03995	1.14968	0.10984
1	-2.64696	0.19081	-1.34322
6	-1.20644	0.07975	0.23284
1	-1.19991	0.05153	1.33476
6	-0.33368	1.23583	-0.27317
1	-0.36905	1.23369	-1.36993
8	-0.84465	2.49115	0.13576
1	-0.38361	2.79451	0.93117
6	1.11186	1.02884	0.18953
1	1.13539	1.12096	1.28554
8	1.96206	2.05764	-0.27128
1	2.28975	1.84631	-1.15753
6	1.62113	-0.36973	-0.15494
1	1.75608	-0.44732	-1.24415
8	2.84148	-0.58684	0.52483
1	3.46846	-1.03585	-0.05574
6	0.60328	-1.43833	0.23412
8	-0.67166	-1.13163	-0.2823
1	0.54444	-1.51355	1.3332
8	1.01945	-2.63918	-0.32939
1	0.31147	-3.29139	-0.21215

Electric dipoles

0	0	-0.935400009	-0.327199996	-0.812399983		
0	1	-3.37999985E-02	-3.31999995E-02	-0.116599999		
0	2	1.90999992E-02	7.85000026E-02	0.188500002		
0	3	0.157900006	-1.44999996E-02	-4.08000015E-02		
0	4	-4.19999985E-03	-0.116899997	0.267899990		
0	5	3.11999992E-02	-4.41000015E-02	-0.209299996		
0	6	-2.92000007E-02	0.123000003	-0.294900000		
0	7	-5.66999987E-02	8.81000012E-02	0.200700000		
0	8	-0.109700002	-0.127599999	0.210999995		
0	9	0.217899993	0.173600003	-5.05000018E-02		
0	10	5.57000004E-02	0.180800006	0.172399998		
0	11	0.0232	0.0453	-0.0514	0.0052	0.0010
0	12	-0.0729	0.1491	-0.3909	0.1804	0.0354
0	13	0.0509	-0.0685	0.0180	0.0076	0.0015
0	14	-0.1435	-0.0539	-0.0437	0.0254	0.0051
0	15	-0.1067	-0.0101	0.1717	0.0410	0.0083
0	16	0.1618	0.0770	-0.0721	0.0373	0.0075

1	1	5.90660000	-0.808399975	-0.250999987
2	2	-7.38019991	-0.498299986	3.73790002
3	3	-5.15990019	5.92000000E-02	3.53839993
4	4	-2.11330009	-4.89419985	-5.14540005
5	5	-0.175699994	5.86639977	-2.56940007
6	6	-0.763800025	-0.274500012	3.10260010
7	7	0.189500004	-4.32530022	-4.88880014
8	8	8.51109982	1.59619999	-1.29960001
9	9	-2.17960000	-1.76419997	-2.56340003
10	10	-0.853999972	-0.821799994	1.12170005
11 11	-1.4705	1.8414	-0.5525 Tot=	2.4204
12 12	-5.0484	-1.9405	-0.9566 Tot=	5.4925
13 13	-3.8534	0.4323	1.5641 Tot=	4.1811
14 14	-3.2916	-0.2605	0.0846 Tot=	3.3030
15 15	0.2330	-1.8398	0.8736 Tot=	2.0500
16 16	4.2883	-1.6473	-0.6043 Tot=	4.6334

Magnetic moments

1	-0.395399988	0.563199997	-0.358500004
2	0.333099991	-0.172900006	-0.289600015
3	5.68999983E-02	0.339199990	0.301099986
4	-0.301499993	0.202000007	-0.203999996
5	0.360100001	-0.345800012	-0.382699996
6	-0.567799985	-7.00000022E-03	-0.709500015
7	-0.263099998	-0.158099994	-0.109600000
8	0.165600002	0.207399994	-5.77999987E-02
9	0.269699991	0.290699989	0.120200001
10	-0.458299994	-0.268999994	-0.279300004
11	-0.3657	-0.1481	0.2937
12	-0.3195	0.4795	-0.0289
13	-0.2311	0.5159	0.1243
14	-0.0843	-0.1362	-0.1317
15	0.1462	0.1308	-0.3932
16	-0.0123	-0.4558	-0.0745

Ground energy

-686.909546

Excitation energies

6.65280008
6.72030020
6.95889997
7.01859999
7.07940006
7.39709997
7.59870005
7.63549995
7.81759977
7.89519978
7.9611
8.0167
8.0322
8.1402
8.2274
8.2504

Structure I-beta

Number of atoms: 24

1	2.01017	-1.15414	1.46561
8	2.85111	-0.87362	1.07386
6	2.63812	-0.61627	-0.30222
1	2.91896	-1.49924	-0.89125
1	3.27686	0.22157	-0.59155
6	1.19131	-0.27684	-0.62027
1	1.07729	-0.18984	-1.71134
6	0.70402	1.01351	0.03871
1	0.90799	0.95389	1.11883
8	1.42489	2.08475	-0.53285
1	1.08587	2.90733	-0.14598
6	-0.79604	1.21217	-0.1697
1	-0.98204	1.37893	-1.23722
8	-1.21301	2.41011	0.46846
1	-1.49419	2.222	1.37583
6	-1.553	-0.02584	0.27802
1	-1.43395	-0.16128	1.36423
8	-2.91999	0.10273	-0.06211
1	-3.455	-0.38224	0.58049
6	-0.9597	-1.26842	-0.39026
8	0.41532	-1.37134	-0.12793
1	-1.12991	-1.207	-1.47766
8	-1.55198	-2.41961	0.13606
1	-2.18105	-2.78393	-0.49965

Electric moments

	0	0	-3.5738	-0.6952	0.0590	
0	1	0.1226	0.0697	-0.0088		
0	2	-0.0485	-0.0082	-0.1031		
0	3	0.1724	-0.0524	0.2543		
0	4	-0.0507	0.2185	0.0486		
0	5	0.2003	-0.1275	0.1610		
0	6	0.0724	-0.0261	-0.1806		
0	7	0.0457	0.2589	0.2701		
0	8	0.0399	-0.0124	0.0242		
0	9	-0.2442	0.2243	0.3434		
0	10	0.2232	-0.0379	0.0837		
0	11	-0.0123	-0.1977	0.3588	0.1679	0.0325
0	12	0.0418	-0.0001	0.1759	0.0327	0.0064
0	13	0.0184	0.0172	0.0128	0.0008	0.0002
0	14	0.0905	0.1954	0.0007	0.0464	0.0092
0	15	0.0554	0.0621	-0.0589	0.0104	0.0021
0	16	0.1845	-0.0335	0.0781	0.0413	0.0083
1	1	2.7954	1.6324	-2.5168		
2	2	-0.8764	-2.6507	-5.0286		
3	3	-0.8448	1.6352	1.5639		
4	4	-0.9014	-0.7572	-4.2577		
5	5	-2.5055	-3.9624	-2.0718		
6	6	-1.1725	1.0540	3.0876		
7	7	-1.1252	-0.2122	-0.3808		

8 8	-2.4310	2.4185	0.3046		
9 8	-2.3898	-0.9685	1.0763		
10 10	3.6999	3.2659	-0.2157		
11 11	-2.7610	-4.8578	-1.0707	Tot=	5.6893
12 12	6.8788	1.7031	0.9743	Tot=	7.1532
13 13	3.4922	-0.4857	2.2734	Tot=	4.1951
14 14	5.6361	1.5318	-0.9529	Tot=	5.9178
15 15	-2.3813	3.3151	-0.1082	Tot=	4.0831
16 16	0.7503	1.3856	-1.4207	Tot=	2.1216

Magnetic moments

1	-0.3942	-0.1726	0.1635
2	0.0162	0.3829	-0.2490
3	-0.1224	-0.1334	-0.2130
4	0.6016	0.2109	-0.3561
5	-0.5917	0.2084	0.4015
6	-0.2116	0.4537	-0.7566
7	0.3853	-0.3446	0.4637
8	0.4190	0.1405	-0.2443
9	0.0229	0.2812	0.0274
10	-0.2001	-0.1638	0.5161
11	-0.2847	0.1846	-0.3264
12	-0.1210	-0.0116	-0.3761
13	0.2078	0.2902	0.0690
14	-0.0435	0.0106	0.3901
15	0.1255	-0.4070	0.2181
16	-0.3292	0.4224	-0.2089

Ground energy

-686.913747333

Excitation energies

6.6989
6.8369
6.9332
7.1430
7.3650
7.5693
7.5975
7.6623
7.7318
7.8570
7.8984
7.9707
8.0070
8.0765
8.1480
8.2153

Structure L-beta

Numer of atoms: 24

1	3.75242	-0.48807	1.21293
8	2.85902	-0.80313	1.02767
6	2.59645	-0.68849	-0.36284
1	2.82076	-1.63788	-0.86498

1	3.19017	0.10964	-0.82082
6	1.13459	-0.35854	-0.58574
1	0.97759	-0.28848	-1.67582
6	0.72578	0.97147	0.04475
1	0.95845	0.92086	1.11796
8	1.46925	2.00689	-0.57064
1	1.06342	2.85067	-0.31596
6	-0.7678	1.19607	-0.14679
1	-0.95714	1.36584	-1.21293
8	-1.17305	2.41358	0.48358
1	-1.35301	2.24696	1.42197
6	-1.58086	-0.00624	0.30035
1	-1.52378	-0.13649	1.39173
8	-2.93034	0.07399	-0.13032
1	-3.35972	0.84307	0.27078
6	-1.01829	-1.27957	-0.33757
8	0.34464	-1.40901	-0.05446
1	-1.17667	-1.22781	-1.43007
8	-1.62191	-2.41698	0.19543
1	-2.51261	-2.48922	-0.17792

Electric moments

0	0	-0.478700012	2.53850007	7.49999983E-03		
0	1	3.26999985E-02	-4.80999984E-02	7.24000037E-02		
0	2	0.108099997	-0.138200000	-1.33999996E-02		
0	3	-5.31999990E-02	0.101300001	0.241200000		
0	4	-0.121799998	8.91000032E-02	-0.130300000		
0	5	2.30999999E-02	-0.187500000	-2.89999996E-03		
0	6	0.327399999	7.63000026E-02	0.182300001		
0	7	-4.91999984E-02	0.127299994	-0.286799997		
0	8	0.132300004	6.62000030E-02	-0.146400005		
0	9	6.80000009E-03	5.40000014E-03	0.162200004		
0	10	0.142800003	-0.130500004	-0.143199995		
0	11	0.0374	-0.2320	-0.2075	0.0983	0.0191
0	12	0.0972	-0.0849	-0.2422	0.0753	0.0148
0	13	-0.1356	0.0292	0.2430	0.0783	0.0155
0	14	-0.1240	0.1062	-0.1098	0.0387	0.0077
0	15	0.0113	-0.2252	0.1234	0.0661	0.0132
0	16	0.0077	-0.0171	-0.1286	0.0169	0.0034
	1	1	3.36490011	-0.585399985	-4.55670023	
	2	2	-6.95060015	1.46190000	-1.39660001	
	3	3	4.50129986	-3.47079992	-4.55929995	
	4	4	4.45839977	6.25050020	3.69330001	
	5	5	1.43760002	-1.40030003	-2.52340007	
	6	6	1.80209994	-1.29260004	-2.85780001	
	7	7	-2.69429994	1.53970003	3.78049994	
	8	8	2.43470001	1.14269996	0.711000025	
	9	9	-3.90899992	0.370900005	-2.76220012	
	10	10	2.94589996	0.243599996	3.29999998E-02	
11	11	-0.5324	-1.0242	-0.4369	Tot=	1.2342
12	12	-0.5092	1.6315	-0.9209	Tot=	1.9414
13	13	-0.6990	2.5132	-0.4400	Tot=	2.6455
14	14	1.5993	0.0043	-1.9312	Tot=	2.5074

15	15	0.4621	0.5944	-0.1513	Tot=	0.7679
16	16	4.4124	2.9995	0.2734	Tot=	5.3423

Magnetic moments

1	9.22999978E-02	-0.478700012	0.129600003
2	-0.472999990	-0.170300007	0.398299992
3	0.259000003	-5.79000004E-02	-4.58000004E-02
4	0.410299987	-6.92000017E-02	0.151400000
5	-0.440800011	2.05000006E-02	-0.256999999
6	-0.238800004	0.195099995	0.754400015
7	0.191599995	0.300099999	-0.117399998
8	0.239999995	-0.472999990	-0.117899999
9	0.482699990	-0.535600007	0.151700005
10	-0.382699996	-0.316100001	0.490500003
11	0.0967	-0.1434	-0.0999
12	-0.1254	-0.5080	0.5180
13	0.1144	-0.3297	-0.5135
14	0.3617	-0.0333	-0.0326
15	-0.2656	-0.3287	-0.1876
16	-0.1890	-0.2585	-0.0726

Ground energy

-686.912781

Excitation energies

6.63110018
6.75180006
6.95539999
7.04920006
7.17439985
7.32740021
7.59420013
7.63180017
7.74940014
7.82490015
7.9265
8.0130
8.0812
8.0979
8.1479
8.2420

Structure M-beta

Number of atoms: 24

8	0.33161	-1.41254	-0.1097
6	1.12673	-0.34809	-0.60831
6	0.71218	0.96036	0.0621
6	-0.77921	1.21414	-0.14358
6	-1.59869	0.00664	0.27244
6	-1.04708	-1.27256	-0.36794
6	2.58325	-0.69356	-0.3825
8	2.82613	-0.77259	1.01393
8	1.47718	2.01288	-0.51457
8	-1.20874	2.33916	0.60584
8	-2.93222	0.21035	-0.14361

8	-1.68964	-2.4065	0.12426
1	3.75811	-0.97747	1.16494
1	2.78924	-1.65585	-0.8684
1	3.19466	0.08768	-0.84871
1	0.97762	-0.25288	-1.69705
1	0.92262	0.87978	1.13409
1	1.56082	2.72833	0.12987
1	-0.9566	1.39242	-1.21449
1	-0.97192	3.1433	0.12423
1	-1.53807	-0.09579	1.36712
1	-3.50194	-0.42739	0.30913
1	-1.24527	-1.2569	-1.44811
1	-1.40693	-2.53292	1.04493

Electric moments

0	0	2.75679994	0.881299973	0.435200006		
0	1	-6.36000037E-02	-0.163000003	-1.95000004E-02		
0	2	-2.45999992E-02	-0.114200003	-1.30000003E-02		
0	3	3.06000002E-02	9.83999968E-02	-0.170000002		
0	4	0.257200003	-4.06000018E-02	0.145999998		
0	5	1.16999997E-02	-3.70999984E-02	0.192399994		
0	6	-0.104000002	4.28000018E-02	0.228100002		
0	7	-0.224299997	0.202900007	0.105899997		
0	8	-2.39000004E-02	0.102899998	0.358000010		
0	9	3.70999984E-02	-6.41999990E-02	0.258300006		
0	10	-0.267100006	1.74000002E-02	-0.316199988		
0	11	0.1408	-0.3039	0.0930	0.1208	0.0236
0	12	-0.0290	0.1600	0.0182	0.0268	0.0053
0	13	0.1468	0.0508	-0.0638	0.0282	0.0056
0	14	-0.0356	-0.0242	0.0212	0.0023	0.0005
0	15	0.0133	0.1570	0.0250	0.0254	0.0051
	1	1	1.16069996	-5.94280005	-0.169799998	
	2	2	-3.85190010	2.17659998	-0.718299985	
	3	3	7.56829977	3.88409996	-4.50089979	
	4	4	1.59360003	-3.36279988	1.14069998	
	5	5	-1.62520003	2.63969994	5.25309992	
	6	6	3.56570005	-1.26839995	-1.51820004	
	7	7	-3.96160007	-5.57350016	-2.20009995	
	8	8	2.53660011	1.99140000	-2.69449997	
	9	9	0.668200016	2.91930008	1.12849998	
	10	10	4.77010012	-0.631900012	-1.34230006	
11	11	3.9230	-1.0552	1.7379	Tot=	4.4186
12	12	2.6306	-2.1540	1.8831	Tot=	3.8867
13	13	1.0141	-0.4850	0.7136	Tot=	1.3315
14	14	-3.2371	0.5905	-0.0715	Tot=	3.2912
15	15	3.4093	4.9077	-1.9359	Tot=	6.2815

Magnetic moments

1	0.126699999	0.330900013	1.60000008E-02
2	-0.535600007	0.127399996	0.423900008
3	-0.342299998	-0.153699994	0.127200007
4	-0.274399996	-0.225999996	0.702199996
5	-4.54999991E-02	-0.209000006	-0.485000014
6	0.380800009	-0.361900002	9.69000012E-02

7	0.334600002	-0.393999994	-0.132400006
8	0.157600001	-0.188999996	0.858600020
9	-0.429199994	-0.201499999	-1.20999999E-02
10	0.134900004	-0.220200002	0.246299997
11	-0.3924	-0.1690	0.5282
12	-0.1067	-0.0892	-0.3008
13	-0.0199	-0.0715	-0.3726
14	0.2486	0.0896	-0.2095
15	0.0059	0.0812	0.3421

Ground energies

-686.915222

Excitation energies

6.61899982

6.68550014

6.78919983

7.21280003

7.29180002

7.33750010

7.52720022

7.65910006

7.74329996

7.90719986

7.9729

8.0239

8.0831

8.1406

8.1532

D-galactose

Structure A-alpha

Number of atoms : 24

1	-4.25772	-0.13224	-0.35469
8	-3.33559	-0.16198	-0.64017
6	-2.57542	0.65188	0.23164
1	-2.64765	0.31059	1.27096
1	-2.8803	1.70658	0.18515
6	-1.12511	0.5377	-0.19862
1	-1.01515	0.97384	-1.19994
6	-0.65306	-0.91787	-0.27348
1	-1.16535	-1.40263	-1.10974
8	-0.98055	-1.62095	0.91041
1	-0.16008	-1.87924	1.35069
6	0.85509	-0.92533	-0.51906
1	1.03086	-0.55431	-1.54021
8	1.31869	-2.25478	-0.37578
1	2.26632	-2.23934	-0.57856
6	1.60975	-0.01706	0.45132
1	1.55148	-0.43296	1.46037
8	2.98505	0.0389	0.12673

1	3.0345	0.42651	-0.76203
6	0.99213	1.37663	0.47084
8	-0.37962	1.31599	0.73682
1	1.42107	1.97844	1.2788
8	1.28494	1.94791	-0.78574
1	1.05851	2.88837	-0.75466

Electric moments

0	0	0.274899989	3.36190009	-0.648899972
0	1	-0.107100002	2.38000005E-02	-2.48000007E-02
0	2	-7.02999979E-02	-4.50999998E-02	9.92999971E-02
0	3	-3.72000001E-02	1.72000006E-02	-0.123700000
0	4	5.90999983E-02	0.150700003	4.50999998E-02
0	5	7.94000030E-02	9.48000029E-02	0.149399996
0	6	-5.07999994E-02	-0.367000014	-0.284999996
0	7	0.158999994	-7.24000037E-02	-7.71000013E-02
0	8	0.121900000	6.52000010E-02	-3.75999995E-02
0	9	0.261799991	-7.69999996E-03	0.146500006
0	10	2.09999997E-02	2.59000007E-02	-0.226099998
0	11	-6.67999983E-02	-0.174099997	-6.31000027E-02
0	12	4.10000002E-03	6.44999966E-02	-0.138500005
0	13	1.73000004E-02	1.35000004E-02	1.53999999E-02
0	14	-6.09999988E-03	0.240700006	-0.234799996
0	15	1.62000004E-02	3.48999985E-02	0.127200007
0	16	0.136600003	0.255100012	-0.111100003
1	1	2.24659991	2.00920010	0.132799998
2	2	0.886600018	1.77610004	0.642899990
3	3	-2.68339992	-0.663900018	-4.17999998E-02
4	4	-1.41970003	4.45639992	-3.96359992
5	5	-0.969200015	2.46749997	0.359200001
6	6	-2.62639999	2.74099994	1.69620001
7	7	1.72230005	-2.94289994	0.225600004
8	8	5.90030003	1.40330005	-2.01889992
9	9	-2.46309996	-1.82729995	0.730700016
10	10	-1.28090000	0.166500002	-0.191499993
11	11	-5.09940004	-4.51580000	1.14779997
12	12	-1.78919995	0.227899998	-0.489100009
13	13	-1.53960001	5.99999987E-02	1.09440005
14	14	-1.62269998	1.21930003	-1.93840003
15	15	0.494300008	-1.80960000	-0.820900023
16	16	-4.29899979	3.69449997	2.30259991

Magnetic moments

1	-0.393999994	0.378800005	5.62000014E-02
2	0.103799999	-8.51999968E-02	-0.680400014
3	-0.326099992	-7.42999986E-02	0.172199994
4	0.238100007	-0.328000009	0.272799999
5	-0.268900007	-0.269100010	-0.176300004
6	-0.542400002	-0.466899991	0.491299987
7	-0.499199986	0.405800015	0.131200001
8	-0.493299991	7.00000022E-03	-0.137999997
9	0.539499998	8.20999965E-02	0.255400002
10	8.56999978E-02	-5.68999983E-02	-4.41999994E-02
11	-0.315299988	-0.143399999	-0.669900000

12	-0.241899997	-0.110600002	-0.174999997
13	-0.315200001	0.461400002	0.100199997
14	-8.88999999E-02	0.391900003	0.517400026
15	1.44999996E-02	-0.193000004	2.11999994E-02
16	-3.90000008E-02	0.163100004	0.235100001

Ground energy

-686.918701

Excitation energies

6.70289993

6.70919991

7.00150013

7.18069983

7.35290003

7.54949999

7.65329981

7.70310020

7.79820013

7.84240007

7.92749977

8.08520031

8.11789989

8.21560001

8.25189972

8.31130028

B.alpha

Number of atoms: 24

1	3.10312	0.94187	-0.72548
8	3.50647	0.09988	-0.47664
6	2.57731	-0.6352	0.29332
1	2.56787	-0.30091	1.33755
1	2.89671	-1.67912	0.26887
6	1.14668	-0.54956	-0.23074
1	1.09417	-0.97984	-1.2387
6	0.62091	0.89012	-0.31016
1	1.0846	1.37291	-1.18978
8	0.95184	1.61786	0.85319
1	0.16225	2.12054	1.10976
6	-0.89268	0.87636	-0.52097
1	-1.11387	0.49365	-1.52459
8	-1.45561	2.17543	-0.34507
1	-0.99042	2.79746	-0.92494
6	-1.57952	-0.02214	0.4882
1	-1.38785	0.36734	1.49768
8	-2.96888	-0.1106	0.25168
1	-3.24167	0.7162	-0.17327
6	-0.97696	-1.42076	0.40141
8	0.38823	-1.35099	0.66964
1	-1.40583	-2.06707	1.17492
8	-1.18085	-1.96622	-0.882
1	-2.07303	-2.33869	-0.90473

Electric moments

0	0	-2.98379993	2.15520000	-1.79310000
0	1	7.54999965E-02	0.141000003	6.57000020E-02
0	2	6.00000005E-03	5.79999993E-03	0.229599997
0	3	-0.100900002	0.177000001	-0.240300000
0	4	-1.99999995E-04	-3.17000002E-02	9.99999978E-03
0	5	-0.171299994	7.40000010E-02	0.255100012
0	6	0.170100003	0.247899994	-0.264899999
0	7	0.116999999	-5.31999990E-02	-0.144800007
0	8	4.03999984E-02	5.00000007E-02	2.12999992E-02
0	9	4.83000018E-02	-5.07999994E-02	0.125599995
0	10	7.64999986E-02	0.186600000	8.54000002E-02
0	11	6.70000017E-02	-2.67999992E-02	-1.32999998E-02
0	12	0.137500003	0.147599995	-0.148200005
0	13	-6.44000024E-02	-7.05000013E-02	-0.211099997
0	14	-2.25000009E-02	0.142299995	0.243799999
0	15	-0.126699999	-4.65999991E-02	0.197200000
0	16	-0.150000006	5.40000014E-02	-0.106700003
1	1	-2.06979990	-3.71620011	1.88479996
2	2	-1.96770000	-4.11040020	1.96389997
3	3	-1.81560004	-3.66849995	2.23320007
4	4	7.72999972E-02	2.31850004	-3.03000007E-02
5	5	0.123400003	1.70829999	0.182400003
6	6	-1.44480002	-1.27769995	-1.79310000
7	7	-2.20619988	-1.93219995	0.518899977
8	8	1.43519998	-3.08540010	1.93770003
9	9	0.749700010	0.377799988	-0.203400001
10	10	-1.12520003	-2.21679997	0.334800005
11	11	-0.226699993	1.11389995	-1.58260000
12	12	-2.16599989	-1.97479999	-1.12349999
13	13	-1.35730004	0.695699990	-2.92740011
14	14	-2.24040008	2.28360009	-0.388099998
15	15	-0.715799987	1.10270000	1.11510003
16	16	-1.23060000	1.07260001	1.57630002

Magnetic moments

1	-0.426699996	0.463400006	-0.171399996
2	0.218099996	0.407400012	-0.253600001
3	0.333400011	-7.97000006E-02	-0.405499995
4	0.559499979	-0.378399998	-0.150800005
5	-0.174199998	-0.256900012	0.239199996
6	0.177900001	-0.322800010	0.290199995
7	0.297300011	0.323700011	-0.304300010
8	-0.137600005	-0.143399999	-0.118500002
9	0.314500004	-0.584699988	-0.259499997
10	0.434700012	-0.513100028	-0.259600013
11	0.356599987	0.500500023	-0.221399993
12	-3.77000012E-02	-0.236200005	0.501399994
13	-0.488700002	-0.243200004	-0.219899997
14	-0.102799997	4.90000006E-03	0.288100004
15	-6.62000030E-02	0.151199996	-0.188199997
16	-0.222299993	-0.501100004	-0.168899998

Ground energy

-686.913208

Excitation energies

6.80079985
6.93510008
7.04160023
7.22940016
7.34159994
7.64709997
7.73699999
7.77750015
7.82180023
7.88539982
7.99529982
8.03499985
8.07310009
8.17980003
8.20139980
8.22140026

C-Alpha

Number of atoms: 24

1	3.48558	1.01057	-0.22845
8	3.40415	0.16606	-0.69267
6	2.60007	-0.68005	0.10423
1	2.72943	-0.48049	1.17394
1	2.91369	-1.71046	-0.08017
6	1.12725	-0.53299	-0.26094
1	0.94724	-0.94959	-1.25749
6	0.6483	0.91396	-0.21079
1	1.17004	1.52	-0.95404
8	0.93472	1.49353	1.0593
1	0.747	0.8047	1.7182
6	-0.84662	0.93816	-0.49412
1	-0.99164	0.57815	-1.5198
8	-1.40021	2.24002	-0.48614
1	-1.39955	2.54452	0.43547
6	-1.62315	0.01293	0.43857
1	-1.59856	0.42869	1.45801
8	-2.95737	-0.10995	-0.01221
1	-3.18199	0.74199	-0.42257
6	-0.9864	-1.38395	0.48229
8	0.39836	-1.27739	0.71907
1	-1.36218	-1.94979	1.34161
8	-1.25727	-2.08177	-0.69488
1	-1.95466	-1.59069	-1.15996

Electric moments

0	0	-0.982599974	1.56429994	1.48319995
0	1	0.152400002	-1.75999999E-02	4.12999988E-02
0	2	-0.192900002	1.68999992E-02	-4.67000008E-02
0	3	-0.165700004	-7.11999983E-02	-0.125200003
0	4	0.127000004	0.130199999	-1.15999999E-02
0	5	0.112099998	6.06999993E-02	-0.197200000
0	6	0.179600000	0.133900002	-0.126200005

0	7	-0.307700008	-2.62000002E-02	0.209199995
0	8	-7.85000026E-02	4.47999984E-02	5.27999997E-02
0	9	0.178900003	-7.33999982E-02	0.468600005
0	10	7.60000013E-03	-0.282200009	0.113899998
0	11	-3.20000015E-02	1.76999997E-02	0.137899995
0	12	0.202099994	-0.198300004	-0.193599999
0	13	5.02999984E-02	-0.112700000	8.79999995E-02
0	14	-0.172199994	0.245399997	0.119999997
0	15	9.20000002E-02	4.43000011E-02	9.30000022E-02
0	16	0.108700000	0.234300002	1.37000000E-02
1	1	0.269499987	-1.71010005	-2.22639990
2	2	-2.93219995	-2.17319989	-7.55999982E-02
3	3	1.31110001	0.214399993	-0.452699989
4	4	1.90149999	-0.328799993	1.67030001
5	5	4.30000015E-02	-3.83000001E-02	2.22889996
6	6	-7.90000036E-02	0.218099996	4.16069984
7	7	1.62769997	-0.370700002	-0.908800006
8	8	2.42379999	-1.12199998	0.640799999
9	9	2.56150007	7.18000010E-02	-2.69580007
10	10	-1.00230002	1.04380000	2.89310002
11	11	-2.56410003	0.605700016	2.35560012
12	12	-1.09000001E-02	1.14110005	-1.52590001
13	13	-3.55559993	3.37360001	0.305700004
14	14	-0.169200003	2.69000006	1.82040000
15	15	1.90100002	2.03609991	1.49790001
16	16	-0.499599993	-0.454200000	-1.13460004

Magnetic moments

1	-5.20999990E-02	-0.131600007	-7.46999979E-02
2	0.108700000	-0.359200001	-0.592199981
3	-0.243799999	0.607599974	-0.547399998
4	0.172700003	0.364600003	-0.356799990
5	-0.380199999	-0.424100012	0.126100004
6	-0.230700001	0.399699986	-2.83000004E-02
7	-6.53000027E-02	-0.289700001	-0.459899992
8	-0.502499998	0.206100002	-0.426699996
9	0.272199988	8.72000009E-02	0.249799997
10	-0.308800012	1.49999997E-02	7.90000036E-02
11	9.71999988E-02	6.03000000E-02	-9.04999971E-02
12	-1.75999999E-02	0.769400001	0.307000011
13	-0.140599996	0.100500003	9.32999998E-02
14	-6.44000024E-02	0.519800007	-0.181700006
15	-0.118199997	-0.120999999	-0.119300000
16	-0.261599988	-0.182999998	0.138999999

Ground energy

-686.919922

Excitation energy

6.91459990
7.11460018
7.26590014
7.51149988
7.63509989
7.66930008

7.83279991
7.97310019
8.06369972
8.13239956
8.16800022
8.24050045
8.38980007
8.42780018
8.47630024
8.49409962

D-Alpha

Number of atoms: 24

1	-3.19106	0.74285	1.12144
8	-3.52586	-0.07032	0.71872
6	-2.62636	-0.47724	-0.295
1	-2.73606	0.12784	-1.20233
1	-2.87691	-1.51242	-0.53499
6	-1.17718	-0.43658	0.16906
1	-1.10526	-0.90446	1.15688
6	-0.5657	0.96314	0.20106
1	-1.04387	1.56691	0.98045
8	-0.82129	1.66632	-1.00942
1	-0.22569	1.32943	-1.69387
6	0.92937	0.91315	0.52565
1	1.04376	0.50486	1.5335
8	1.48586	2.20355	0.58112
1	1.41502	2.59571	-0.30195
6	1.65534	-0.03331	-0.42919
1	1.68491	0.39027	-1.4459
8	2.97331	-0.22828	0.05646
1	3.34605	-1.01402	-0.37344
6	0.90904	-1.38132	-0.47031
8	-0.4391	-1.2189	-0.78131
1	1.30388	-2.01188	-1.28062
8	1.04834	-2.02802	0.76723
1	1.86807	-1.69694	1.1709

Electric moments

0	0	3.07380009	-0.365599990	-1.98080003
0	1	6.56000003E-02	5.95000014E-02	0.152300000
0	2	8.26999992E-02	-9.49999988E-02	0.103900000
0	3	-7.54000023E-02	7.09000006E-02	-0.138999999
0	4	-6.91000000E-02	-7.40000000E-03	-0.107900001
0	5	-0.183799997	3.90000008E-02	5.20000011E-02
0	6	0.213799998	-1.30000000E-03	-0.313499987
0	7	0.318100005	-7.20999986E-02	-0.295800000
0	8	-7.94999972E-02	0.402700007	-9.60000046E-03
0	9	1.60000008E-02	3.88999991E-02	-0.184900001
0	10	9.91000012E-02	-0.101400003	-1.46000003E-02
0	11	-9.13000032E-02	0.108400002	-1.43999998E-02
0	12	-4.01000008E-02	0.188899994	0.158800006
0	13	-1.55999996E-02	-0.178499997	9.25000012E-02

0	14	0.138099998	-0.176799998	0.194000006
0	15	3.70999984E-02	5.38000017E-02	0.111699998
0	16	-2.95000002E-02	-8.03000033E-02	5.31000011E-02
1	1	-0.839699984	-1.73329997	3.47390008
2	2	2.06080008	-2.94819999	-3.45070004
3	3	-1.25059998	1.20000001E-02	-0.376700014
4	4	0.994499981	-2.75950003	3.29380012
5	5	-1.85759997	3.20790005	-0.536599994
6	6	3.36260009	-1.13049996	-4.67549992
7	7	2.50020003	-1.21229994	-1.66779995
8	8	2.77080011	-0.255499989	-1.20630002
9	9	-3.10170007	-1.53830004	2.89750004
10	10	-5.64930010	3.62240005	0.856199980
11	11	1.93250000	-0.457800001	-1.54620004
12	12	8.69000033E-02	-2.28080010	1.67530000
13	13	2.61960006	-0.269600004	-1.80460000
14	14	-1.24030006	3.14280009	0.848399997
15	15	1.52470005	-0.583500028	-2.32850003
16	16	2.61649990	0.999800026	0.918399990

Magnetic moments

1	-0.144099995	9.52999964E-02	-0.171299994
2	-0.315600008	-0.273799986	-0.104000002
3	0.188199997	0.630599976	0.474299997
4	-0.324299991	-2.16000006E-02	-0.538500011
5	-6.23000003E-02	0.415399998	0.175699994
6	-8.39999989E-02	-0.127900004	-8.10000021E-03
7	-0.460200012	-0.107199997	0.550000012
8	-0.196700007	-8.89999978E-03	-5.10000018E-03
9	-1.62000004E-02	0.639599979	0.218400002
10	-1.32999998E-02	0.154300004	-0.199399993
11	-0.666999996	-0.354099989	-0.381599993
12	-9.62999985E-02	5.33000007E-02	7.16999993E-02
13	0.282700002	8.57999995E-02	-8.70999992E-02
14	0.153400004	1.39999995E-03	0.386500001
15	0.265899986	0.366400003	2.36000009E-02
16	3.35000008E-02	-0.371499985	0.160799995

Ground energy

-686.905090

Excitation energy

6.79430008
6.87050009
6.91039991
7.10680008
7.41249990
7.52199984
7.61590004
7.83500004
7.86089993
7.87069988
7.94339991
7.98769999
8.13319969

8.19349957
8.30249977
8.33290005

E-Alpha

Number of atoms: 24

1	3.29334	-0.30728	-1.45475
8	3.49309	0.08436	-0.59242
6	2.60553	-0.47467	0.35809
1	2.68158	0.13224	1.25996
1	2.87555	-1.51009	0.6072
6	1.16999	-0.47125	-0.14604
1	1.1353	-0.93223	-1.14378
6	0.57762	0.92999	-0.2505
1	1.10527	1.46024	-1.05294
8	0.76327	1.60734	0.98664
1	0.73423	2.5535	0.7908
6	-0.91896	0.88743	-0.5746
1	-1.07519	0.49156	-1.5813
8	-1.44868	2.20154	-0.56947
1	-1.72657	2.40182	0.33529
6	-1.61033	-0.02595	0.42378
1	-1.52245	0.4162	1.42657
8	-2.97058	-0.17514	0.04276
1	-3.42737	-0.65737	0.74778
6	-0.9218	-1.39673	0.43553
8	0.42425	-1.28259	0.76052
1	-1.36	-2.03855	1.21379
8	-1.03113	-1.99898	-0.83359
1	-1.96777	-2.19518	-0.98172

Electric moments

0	0	-2.61129999	-1.01030004	0.853799999
0	1	4.69999984E-02	0.109999999	-0.129700005
0	2	-9.73000005E-02	8.42000023E-02	5.68999983E-02
0	3	-8.70999992E-02	4.43000011E-02	-4.85999994E-02
0	4	0.116200000	-9.01999995E-02	-0.105200000
0	5	0.185399994	-0.100699998	0.140499994
0	6	-0.160300002	-6.23999983E-02	0.251100004
0	7	1.43999998E-02	-0.223299995	7.40000010E-02
0	8	0.386700004	0.150600001	-6.97000027E-02
0	9	-0.292499989	-0.273799986	0.245700002
0	10	0.123999998	-7.32000023E-02	-0.161899999
0	11	8.60000029E-02	9.60000008E-02	0.141000003
0	12	8.16000029E-02	-0.105099998	-9.67999995E-02
0	13	-5.55999987E-02	2.42999997E-02	0.184599996
0	14	0.139300004	-0.275799990	-7.47999996E-02
0	15	1.72000006E-02	-7.84000009E-02	0.124100000
0	16	-2.00999994E-02	0.209900007	4.19999985E-03
1	1	4.05700016	1.52980006	-2.90319991
2	2	-2.00990009	-5.27549982	-0.439399987
3	3	-2.96600008	-0.426200002	4.31689978

4	4	0.358200014	1.13220000	0.804400027
5	5	0.816999972	-1.84759998	-1.36039996
6	6	-1.46159995	1.17429996	1.01820004
7	7	-0.845399976	-3.11540008	-0.549600005
8	8	2.43400002	1.29709995	-2.47679996
9	9	-0.465700001	-2.70560002	-0.108900003
10	10	1.65090001	1.71120000	-1.71889997
11	11	0.883199990	2.98070002	0.459500015
12	12	-4.06739998	-1.79929996	2.95910001
13	13	1.18589997	-2.67750001	-2.50830007
14	14	-2.38470006	-0.635800004	2.41240001
15	15	-1.00549996	-0.523800015	1.53849995
16	16	2.75359988	0.766900003	-1.12189996

Magnetic moments

1	6.76999986E-02	-0.102600001	0.483900011
2	-0.329899997	4.98000011E-02	1.37000000E-02
3	-0.300300002	-0.455100000	-0.410299987
4	0.208000004	0.230299994	-0.331600010
5	0.375000000	-0.294400007	0.263399988
6	0.259200007	-0.294600010	0.564899981
7	-0.254500002	0.126499996	0.290199995
8	-8.57999995E-02	-0.173199996	0.597700000
9	-0.122800000	-0.222100005	-0.833100021
10	0.134499997	-0.136500001	2.81000007E-02
11	3.07999998E-02	-9.12000015E-02	0.112300001
12	0.335500002	-0.397899985	9.13000032E-02
13	-4.82000001E-02	0.150700003	6.71000034E-02
14	0.302500010	-0.286199987	0.314799994
15	-0.376100004	0.278400004	0.382299989
16	5.88999987E-02	9.31999981E-02	0.331600010

Ground energy

-686.910461

Excitation energy

6.46339989
6.76270008
6.82200003
7.19649982
7.31580019
7.46129990
7.56090021
7.58419991
7.63430023
7.82800007
7.86180019
7.94780016
8.00520039
8.16269970
8.20219994
8.25409985

F_alpha

Number of atoms: 24

1	2.73308	-0.99348	-0.69824
8	3.19801	-0.14313	-0.6429
6	2.64586	0.57901	0.42247
1	2.91955	1.62911	0.28591
1	3.06994	0.25313	1.38937
6	1.12555	0.51713	0.56284
1	0.85912	0.98403	1.52062
6	0.53436	-0.8928	0.5719
1	0.84983	-1.39506	1.49913
8	0.98915	-1.62918	-0.55235
1	0.48295	-2.45824	-0.55349
6	-0.9918	-0.85369	0.54563
1	-1.35465	-0.44413	1.49955
8	-1.39343	-2.20977	0.39258
1	-2.35734	-2.26249	0.44375
6	-1.49214	0.01864	-0.59469
1	-1.19953	-0.43447	-1.54421
8	-2.90074	0.16537	-0.59911
1	-3.23021	0.03077	0.30003
6	-0.82561	1.39227	-0.48699
8	0.57214	1.28937	-0.50403
1	-1.08149	2.00454	-1.35764
8	-1.30056	1.98073	0.70137
1	-0.98515	2.89587	0.72389

Electric moments

0	0	-2.99710011	-0.151899993	3.61299992
0	1	0.149700001	1.72000006E-02	0.100400001
0	2	-8.60999972E-02	9.14999992E-02	0.194199994
0	3	3.42999995E-02	0.132900000	9.49999969E-03
0	4	-7.97000006E-02	0.209199995	-4.10000011E-02
0	5	0.149599999	-8.63000005E-02	-0.158800006
0	6	-0.122000001	-4.96000014E-02	-2.67999992E-02
0	7	0.167999998	-0.223000005	0.363599986
0	8	-1.89999994E-02	-8.10000002E-02	4.30999994E-02
0	9	-1.37000000E-02	-0.101300001	0.268999994
0	10	8.03000033E-02	-6.15000017E-02	0.197799996
0	11	-0.186000004	5.27999997E-02	-0.222200006
0	12	3.40999998E-02	0.134399995	-9.22999978E-02
0	13	6.06999993E-02	0.102100000	0.205599993
0	14	-6.98999986E-02	-9.30000003E-03	3.81000005E-02
0	15	0.199300006	-7.93000013E-02	0.118400000
0	16	-1.57999992E-02	3.22999991E-02	0.103200004
1	1	2.83620000	3.49880004	-0.186800003
2	2	-1.33879995	1.03199995	-0.656199992
3	3	1.33539999	1.86409998	0.664200008
4	4	-2.27690005	-5.80249977	1.58800006
5	5	-0.432999998	3.73469996	1.51390004
6	6	-1.10450006	-1.14800000	1.39859998
7	7	0.227799997	-0.647499979	1.07889998
8	8	7.61759996	1.56750000	0.830699980
9	9	1.71039999	-1.92600000	1.01010001
10	10	0.319700003	-1.46089995	2.62680006

11	11	-0.707300007	-1.97700000	1.38600004
12	12	-0.907800019	-0.231900007	0.819899976
13	13	0.229599997	1.14489996	0.294200003
14	14	-0.287800014	1.06710005	1.28020000
15	15	0.169100001	-3.74489999	0.961600006
16	16	3.23920012	3.66969991	0.808300018

Magnetic moments

1	0.180099994	-9.60000046E-03	0.567799985
2	-0.223499998	-9.35999975E-02	-8.47999975E-02
3	-0.497200012	0.146699995	0.461199999
4	7.41999969E-02	-2.71000005E-02	-0.174400002
5	0.370999992	-5.35999984E-02	-0.132400006
6	0.149399996	-0.454499990	-0.320699990
7	-9.20000020E-03	0.363599986	-0.255400002
8	-4.80000023E-03	0.225299999	-5.90000004E-02
9	0.627300024	0.676599979	-0.195999995
10	-0.377700001	0.503799975	-0.231199995
11	6.93000033E-02	0.302399993	-7.51999989E-02
12	0.247999996	0.515600026	6.84999973E-02
13	0.515200019	-0.541400015	0.251100004
14	-0.281100005	-0.454600006	0.411300004
15	9.64000002E-02	-0.244599998	0.139100000
16	0.229599997	3.22000012E-02	-3.24000008E-02

Ground energy

-686.918457

Excitation energy

6.51959991
6.91169977
6.99760008
7.09110022
7.45270014
7.49139977
7.56790018
7.61129999
7.70340014
7.82730007
7.87190008
7.89639997
7.97279978
8.03190041
8.12500000
8.16079998

G-Alpha

Number of atoms: 24

1	3.11323	-1.33575	-0.36872
8	3.58096	-0.49696	-0.2636
6	2.62442	0.50219	0.03635
1	2.87388	1.39391	-0.54893
1	2.6697	0.77624	1.09648
6	1.20953	0.07238	-0.29615
1	1.2191	-0.42431	-1.27729

6	0.21834	1.22718	-0.36447
1	0.47765	1.87457	-1.20655
8	0.31812	2.06228	0.78315
1	-0.01892	1.5729	1.54791
6	-1.20824	0.70851	-0.57355
1	-1.2428	0.21016	-1.54851
8	-2.13382	1.76221	-0.6584
1	-2.18134	2.18668	0.21105
6	-1.5565	-0.33503	0.49362
1	-1.57854	0.13676	1.4843
8	-2.82613	-0.909	0.33012
1	-2.84041	-1.31665	-0.5496
6	-0.47207	-1.41954	0.51939
8	0.81426	-0.88138	0.70092
1	-0.62628	-2.08859	1.37207
8	-0.59651	-2.11611	-0.69653
1	-0.01333	-2.88841	-0.66868

Electric moments

0	0	-0.263000011	-2.50720000	0.198400006
0	1	-0.115300000	-7.15999976E-02	-0.204500005
0	2	-3.40000005E-03	-7.45000020E-02	-6.58999979E-02
0	3	8.32000002E-02	-4.03999984E-02	-3.88999991E-02
0	4	-6.03000000E-02	4.98999991E-02	-4.69999984E-02
0	5	0.177599996	-7.81999975E-02	-3.55000012E-02
0	6	0.178299993	0.258399993	-0.293399990
0	7	1.97000001E-02	0.186600000	-0.103699997
0	8	-0.163599998	-4.45999987E-02	0.132499993
0	9	-0.214100003	-5.73999994E-02	-3.90999988E-02
0	10	2.96999998E-02	0.224399999	-0.150900006
0	11	-7.45000020E-02	-0.175500005	0.158099994
0	12	3.80000006E-03	-3.33999991E-02	0.275099993
0	13	-4.74999994E-02	0.267100006	-9.70000029E-03
0	14	-2.63999999E-02	0.125400007	-0.112700000
0	15	5.95999993E-02	0.176200002	1.41000003E-02
0	16	-0.117600001	7.19999988E-03	-0.125200003
1	1	3.92000005E-02	3.43039989	0.790400028
2	2	0.738799989	-3.41370010	-4.29320002
3	3	-0.134800002	1.39279997	-0.983799994
4	4	-2.86999997E-02	-2.65580010	-1.99199998
5	5	0.650500000	0.297899991	2.71259999
6	6	-1.33130002	1.15709996	-0.206900001
7	7	0.677500010	-1.15579998	2.64770007
8	8	-0.705299973	0.806999981	0.753700018
9	9	-2.65660000	2.63190007	1.12860000
10	10	-0.330599993	-3.76270008	-0.754400015
11	11	-1.36469996	-0.123800002	-1.03670001
12	12	3.08890009	-1.12609994	-1.46519995
13	13	-9.79000032E-02	0.393599987	0.482400000
14	14	4.46560001	-0.947899997	-0.217700005
15	15	1.36210001	-1.15590000	1.75610006
16	16	-0.883700013	-3.29520011	-1.06340003

Magnetic moments

1	-0.374799997	-0.358399987	0.147400007
2	-0.201000005	-0.298799992	0.174400002
3	-0.137999997	-0.619199991	-0.233400002
4	-0.154899999	-0.279799998	-0.432099998
5	0.166299999	-2.98999995E-02	0.477899998
6	0.201900005	-8.34999979E-02	0.524100006
7	-0.130199999	0.320100009	0.649699986
8	0.254099995	6.44999966E-02	-0.142800003
9	0.555700004	-1.67999994E-02	0.342700005
10	-2.52999999E-02	0.319299996	-6.49000034E-02
11	-0.693400025	-0.322299987	0.378399998
12	0.314799994	0.208600000	-8.89999978E-03
13	-0.173199996	6.47000000E-02	-0.214000002
14	0.153500006	-0.626999974	3.35000008E-02
15	-0.143500000	0.259099990	-0.188899994
16	0.231800005	2.05000006E-02	0.156200007

Ground energy

-686.914124

Excitation energy

6.73050022

6.85540009

6.93400002

7.13159990

7.35790014

7.53109980

7.53520012

7.70030022

7.77610016

7.85370016

7.96210003

8.04539967

8.08139992

8.17899990

8.19610023

8.25689983

A-Beta

Number of atoms: 24

1	-4.25772	-0.13224	-0.35469
8	-3.33559	-0.16198	-0.64017
6	-2.57542	0.65188	0.23164
1	-2.64765	0.31059	1.27096
1	-2.8803	1.70658	0.18515
6	-1.12511	0.5377	-0.19862
1	-1.01515	0.97384	-1.19994
6	-0.65306	-0.91787	-0.27348
1	-1.16535	-1.40263	-1.10974
8	-0.98055	-1.62095	0.91041
1	-0.16008	-1.87924	1.35069
6	0.85509	-0.92533	-0.51906

1	1.03086	-0.55431	-1.54021
8	1.31869	-2.25478	-0.37578
1	2.26632	-2.23934	-0.57856
6	1.60975	-0.01706	0.45132
1	1.55148	-0.43296	1.46037
8	2.98505	0.0389	0.12673
1	3.0345	0.42651	-0.76203
6	0.99213	1.37663	0.47084
8	-0.37962	1.31599	0.73682
1	1.42107	1.97844	1.2788
8	1.28494	1.94791	-0.78574
1	1.05851	2.88837	-0.75466

Electric moments

0	0	0.274899989	3.36190009	-0.648899972
0	1	-0.107100002	2.38000005E-02	-2.48000007E-02
0	2	-7.02999979E-02	-4.50999998E-02	9.92999971E-02
0	3	-3.72000001E-02	1.72000006E-02	-0.123700000
0	4	5.90999983E-02	0.150700003	4.50999998E-02
0	5	7.94000030E-02	9.48000029E-02	0.149399996
0	6	-5.07999994E-02	-0.367000014	-0.284999996
0	7	0.158999994	-7.24000037E-02	-7.71000013E-02
0	8	0.121900000	6.52000010E-02	-3.75999995E-02
0	9	0.261799991	-7.69999996E-03	0.146500006
0	10	2.09999997E-02	2.59000007E-02	-0.226099998
0	11	-6.67999983E-02	-0.174099997	-6.31000027E-02
0	12	4.10000002E-03	6.44999966E-02	-0.138500005
0	13	1.73000004E-02	1.35000004E-02	1.53999999E-02
0	14	-6.09999988E-03	0.240700006	-0.234799996
0	15	1.62000004E-02	3.48999985E-02	0.127200007
0	16	0.136600003	0.255100012	-0.111100003
1	1	2.24659991	2.00920010	0.132799998
2	2	0.886600018	1.77610004	0.642899990
3	3	-2.68339992	-0.663900018	-4.17999998E-02
4	4	-1.41970003	4.45639992	-3.96359992
5	5	-0.969200015	2.46749997	0.359200001
6	6	-2.62639999	2.74099994	1.69620001
7	7	1.72230005	-2.94289994	0.225600004
8	8	5.90030003	1.40330005	-2.01889992
9	9	-2.46309996	-1.82729995	0.730700016
10	10	-1.28090000	0.166500002	-0.191499993
11	11	-5.09940004	-4.51580000	1.14779997
12	12	-1.78919995	0.227899998	-0.489100009
13	13	-1.53960001	5.99999987E-02	1.09440005
14	14	-1.62269998	1.21930003	-1.93840003
15	15	0.494300008	-1.80960000	-0.820900023
16	16	-4.29899979	3.69449997	2.30259991

Magnetic moments

1	-0.393999994	0.378800005	5.62000014E-02
2	0.103799999	-8.51999968E-02	-0.680400014
3	-0.326099992	-7.42999986E-02	0.172199994
4	0.238100007	-0.328000009	0.272799999
5	-0.268900007	-0.269100010	-0.176300004

6	-0.542400002	-0.466899991	0.491299987
7	-0.499199986	0.405800015	0.131200001
8	-0.493299991	7.00000022E-03	-0.137999997
9	0.539499998	8.20999965E-02	0.255400002
10	8.56999978E-02	-5.68999983E-02	-4.41999994E-02
11	-0.315299988	-0.143399999	-0.669900000
12	-0.241899997	-0.110600002	-0.174999997
13	-0.315200001	0.461400002	0.100199997
14	-8.88999999E-02	0.391900003	0.517400026
15	1.44999996E-02	-0.193000004	2.11999994E-02
16	-3.90000008E-02	0.163100004	0.235100001

Ground energy

-686.918701

Exccitation energy

6.70289993

6.70919991

7.00150013

7.18069983

7.35290003

7.54949999

7.65329981

7.70310020

7.79820013

7.84240007

7.92749977

8.08520031

8.11789989

8.21560001

8.25189972

8.31130028

B-Beta

Number of atoms: 24

1	3.10312	0.94187	-0.72548
8	3.50647	0.09988	-0.47664
6	2.57731	-0.6352	0.29332
1	2.56787	-0.30091	1.33755
1	2.89671	-1.67912	0.26887
6	1.14668	-0.54956	-0.23074
1	1.09417	-0.97984	-1.2387
6	0.62091	0.89012	-0.31016
1	1.0846	1.37291	-1.18978
8	0.95184	1.61786	0.85319
1	0.16225	2.12054	1.10976
6	-0.89268	0.87636	-0.52097
1	-1.11387	0.49365	-1.52459
8	-1.45561	2.17543	-0.34507
1	-0.99042	2.79746	-0.92494
6	-1.57952	-0.02214	0.4882
1	-1.38785	0.36734	1.49768
8	-2.96888	-0.1106	0.25168
1	-3.24167	0.7162	-0.17327

6	-0.97696	-1.42076	0.40141
8	0.38823	-1.35099	0.66964
1	-1.40583	-2.06707	1.17492
8	-1.18085	-1.96622	-0.882
1	-2.07303	-2.33869	-0.90473

Electric moments

0	0	-2.98379993	2.15520000	-1.79310000
0	1	7.54999965E-02	0.141000003	6.57000020E-02
0	2	6.00000005E-03	5.79999993E-03	0.229599997
0	3	-0.100900002	0.177000001	-0.240300000
0	4	-1.99999995E-04	-3.17000002E-02	9.99999978E-03
0	5	-0.171299994	7.40000010E-02	0.255100012
0	6	0.170100003	0.247899994	-0.264899999
0	7	0.116999999	-5.31999990E-02	-0.144800007
0	8	4.03999984E-02	5.00000007E-02	2.12999992E-02
0	9	4.83000018E-02	-5.07999994E-02	0.125599995
0	10	7.64999986E-02	0.186600000	8.54000002E-02
0	11	6.70000017E-02	-2.67999992E-02	-1.32999998E-02
0	12	0.137500003	0.147599995	-0.148200005
0	13	-6.44000024E-02	-7.05000013E-02	-0.211099997
0	14	-2.25000009E-02	0.142299995	0.243799999
0	15	-0.126699999	-4.65999991E-02	0.197200000
0	16	-0.150000006	5.40000014E-02	-0.106700003
1	1	-2.06979990	-3.71620011	1.88479996
2	2	-1.96770000	-4.11040020	1.96389997
3	3	-1.81560004	-3.66849995	2.23320007
4	4	7.72999972E-02	2.31850004	-3.03000007E-02
5	5	0.123400003	1.70829999	0.182400003
6	6	-1.44480002	-1.27769995	-1.79310000
7	7	-2.20619988	-1.93219995	0.518899977
8	8	1.43519998	-3.08540010	1.93770003
9	9	0.749700010	0.377799988	-0.203400001
10	10	-1.12520003	-2.21679997	0.334800005
11	11	-0.226699993	1.11389995	-1.58260000
12	12	-2.16599989	-1.97479999	-1.12349999
13	13	-1.35730004	0.695699990	-2.92740011
14	14	-2.24040008	2.28360009	-0.388099998
15	15	-0.715799987	1.10270000	1.11510003
16	16	-1.23060000	1.07260001	1.57630002

Magnetic moments

1	-0.426699996	0.463400006	-0.171399996
2	0.218099996	0.407400012	-0.253600001
3	0.333400011	-7.97000006E-02	-0.405499995
4	0.559499979	-0.378399998	-0.150800005
5	-0.174199998	-0.256900012	0.239199996
6	0.177900001	-0.322800010	0.290199995
7	0.297300011	0.323700011	-0.304300010
8	-0.137600005	-0.143399999	-0.118500002
9	0.314500004	-0.584699988	-0.259499997
10	0.434700012	-0.513100028	-0.259600013
11	0.356599987	0.500500023	-0.221399993
12	-3.77000012E-02	-0.236200005	0.501399994

13	-0.488700002	-0.243200004	-0.219899997
14	-0.102799997	4.900000006E-03	0.288100004
15	-6.62000030E-02	0.151199996	-0.188199997
16	-0.222299993	-0.501100004	-0.168899998

Ground energy

-686.913208

Excitation energy

6.80079985

6.93510008

7.04160023

7.22940016

7.34159994

7.64709997

7.73699999

7.77750015

7.82180023

7.88539982

7.99529982

8.03499985

8.07310009

8.17980003

8.20139980

8.22140026

C-Beta

Number of atoms: 24

1	3.48558	1.01057	-0.22845
8	3.40415	0.16606	-0.69267
6	2.60007	-0.68005	0.10423
1	2.72943	-0.48049	1.17394
1	2.91369	-1.71046	-0.08017
6	1.12725	-0.53299	-0.26094
1	0.94724	-0.94959	-1.25749
6	0.6483	0.91396	-0.21079
1	1.17004	1.52	-0.95404
8	0.93472	1.49353	1.0593
1	0.747	0.8047	1.7182
6	-0.84662	0.93816	-0.49412
1	-0.99164	0.57815	-1.5198
8	-1.40021	2.24002	-0.48614
1	-1.39955	2.54452	0.43547
6	-1.62315	0.01293	0.43857
1	-1.59856	0.42869	1.45801
8	-2.95737	-0.10995	-0.01221
1	-3.18199	0.74199	-0.42257
6	-0.9864	-1.38395	0.48229
8	0.39836	-1.27739	0.71907
1	-1.36218	-1.94979	1.34161
8	-1.25727	-2.08177	-0.69488
1	-1.95466	-1.59069	-1.15996

Electric moments

0	0	-0.982599974	1.56429994	1.48319995
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0	1	0.152400002	-1.75999999E-02	4.12999988E-02
0	2	-0.192900002	1.68999992E-02	-4.67000008E-02
0	3	-0.165700004	-7.11999983E-02	-0.125200003
0	4	0.127000004	0.130199999	-1.15999999E-02
0	5	0.112099998	6.06999993E-02	-0.197200000
0	6	0.179600000	0.133900002	-0.126200005
0	7	-0.307700008	-2.62000002E-02	0.209199995
0	8	-7.85000026E-02	4.47999984E-02	5.27999997E-02
0	9	0.178900003	-7.33999982E-02	0.468600005
0	10	7.60000013E-03	-0.282200009	0.113899998
0	11	-3.20000015E-02	1.76999997E-02	0.137899995
0	12	0.202099994	-0.198300004	-0.193599999
0	13	5.02999984E-02	-0.112700000	8.79999995E-02
0	14	-0.172199994	0.245399997	0.119999997
0	15	9.20000002E-02	4.43000011E-02	9.30000022E-02
0	16	0.108700000	0.234300002	1.37000000E-02
1	1	0.269499987	-1.71010005	-2.22639990
2	2	-2.93219995	-2.17319989	-7.55999982E-02
3	3	1.31110001	0.214399993	-0.452699989
4	4	1.90149999	-0.328799993	1.67030001
5	5	4.30000015E-02	-3.83000001E-02	2.22889996
6	6	-7.90000036E-02	0.218099996	4.16069984
7	7	1.62769997	-0.370700002	-0.908800006
8	8	2.42379999	-1.12199998	0.640799999
9	9	2.56150007	7.18000010E-02	-2.69580007
10	10	-1.00230002	1.04380000	2.89310002
11	11	-2.56410003	0.605700016	2.35560012
12	12	-1.09000001E-02	1.14110005	-1.52590001
13	13	-3.55559993	3.37360001	0.305700004
14	14	-0.169200003	2.69000006	1.82040000
15	15	1.90100002	2.03609991	1.49790001
16	16	-0.499599993	-0.454200000	-1.13460004

Magnetic moments

1	-5.20999990E-02	-0.131600007	-7.46999979E-02
2	0.108700000	-0.359200001	-0.592199981
3	-0.243799999	0.607599974	-0.547399998
4	0.172700003	0.364600003	-0.356799990
5	-0.380199999	-0.424100012	0.126100004
6	-0.230700001	0.399699986	-2.83000004E-02
7	-6.53000027E-02	-0.289700001	-0.459899992
8	-0.502499998	0.206100002	-0.426699996
9	0.272199988	8.72000009E-02	0.249799997
10	-0.308800012	1.49999997E-02	7.90000036E-02
11	9.71999988E-02	6.03000000E-02	-9.04999971E-02
12	-1.75999999E-02	0.769400001	0.307000011
13	-0.140599996	0.100500003	9.32999998E-02
14	-6.44000024E-02	0.519800007	-0.181700006
15	-0.118199997	-0.120999999	-0.119300000
16	-0.261599988	-0.182999998	0.138999999

Ground energy

-686.919922

Excitation energy

6.91459990
7.11460018
7.26590014
7.51149988
7.63509989
7.66930008
7.83279991
7.97310019
8.06369972
8.13239956
8.16800022
8.24050045
8.38980007
8.42780018
8.47630024
8.49409962

D-Beta

Number of atoms: 24

1	-3.19106	0.74285	1.12144
8	-3.52586	-0.07032	0.71872
6	-2.62636	-0.47724	-0.295
1	-2.73606	0.12784	-1.20233
1	-2.87691	-1.51242	-0.53499
6	-1.17718	-0.43658	0.16906
1	-1.10526	-0.90446	1.15688
6	-0.5657	0.96314	0.20106
1	-1.04387	1.56691	0.98045
8	-0.82129	1.66632	-1.00942
1	-0.22569	1.32943	-1.69387
6	0.92937	0.91315	0.52565
1	1.04376	0.50486	1.5335
8	1.48586	2.20355	0.58112
1	1.41502	2.59571	-0.30195
6	1.65534	-0.03331	-0.42919
1	1.68491	0.39027	-1.4459
8	2.97331	-0.22828	0.05646
1	3.34605	-1.01402	-0.37344
6	0.90904	-1.38132	-0.47031
8	-0.4391	-1.2189	-0.78131
1	1.30388	-2.01188	-1.28062
8	1.04834	-2.02802	0.76723
1	1.86807	-1.69694	1.1709

Electric moments

0	0	3.07380009	-0.365599990	-1.98080003
0	1	6.56000003E-02	5.95000014E-02	0.152300000
0	2	8.26999992E-02	-9.49999988E-02	0.103900000
0	3	-7.54000023E-02	7.09000006E-02	-0.138999999
0	4	-6.91000000E-02	-7.40000000E-03	-0.107900001
0	5	-0.183799997	3.90000008E-02	5.20000011E-02
0	6	0.213799998	-1.30000000E-03	-0.313499987
0	7	0.318100005	-7.20999986E-02	-0.295800000

0	8	-7.94999972E-02	0.402700007	-9.60000046E-03
0	9	1.60000008E-02	3.88999991E-02	-0.184900001
0	10	9.91000012E-02	-0.101400003	-1.46000003E-02
0	11	-9.13000032E-02	0.108400002	-1.43999998E-02
0	12	-4.01000008E-02	0.188899994	0.158800006
0	13	-1.55999996E-02	-0.178499997	9.25000012E-02
0	14	0.138099998	-0.176799998	0.194000006
0	15	3.70999984E-02	5.38000017E-02	0.111699998
0	16	-2.95000002E-02	-8.03000033E-02	5.31000011E-02
1	1	-0.839699984	-1.73329997	3.47390008
2	2	2.06080008	-2.94819999	-3.45070004
3	3	-1.25059998	1.20000001E-02	-0.376700014
4	4	0.994499981	-2.75950003	3.29380012
5	5	-1.85759997	3.20790005	-0.536599994
6	6	3.36260009	-1.13049996	-4.67549992
7	7	2.50020003	-1.21229994	-1.66779995
8	8	2.77080011	-0.255499989	-1.20630002
9	9	-3.10170007	-1.53830004	2.89750004
10	10	-5.64930010	3.62240005	0.856199980
11	11	1.93250000	-0.457800001	-1.54620004
12	12	8.69000033E-02	-2.28080010	1.67530000
13	13	2.61960006	-0.269600004	-1.80460000
14	14	-1.24030006	3.14280009	0.848399997
15	15	1.52470005	-0.583500028	-2.32850003
16	16	2.61649990	0.999800026	0.918399990

Magnetic moments

1	-0.144099995	9.52999964E-02	-0.171299994
2	-0.315600008	-0.273799986	-0.104000002
3	0.188199997	0.630599976	0.474299997
4	-0.324299991	-2.16000006E-02	-0.538500011
5	-6.23000003E-02	0.415399998	0.175699994
6	-8.39999989E-02	-0.127900004	-8.10000021E-03
7	-0.460200012	-0.107199997	0.550000012
8	-0.196700007	-8.89999978E-03	-5.10000018E-03
9	-1.62000004E-02	0.639599979	0.218400002
10	-1.32999998E-02	0.154300004	-0.199399993
11	-0.666999996	-0.354099989	-0.381599993
12	-9.62999985E-02	5.33000007E-02	7.16999993E-02
13	0.282700002	8.57999995E-02	-8.70999992E-02
14	0.153400004	1.39999995E-03	0.386500001
15	0.265899986	0.366400003	2.36000009E-02
16	3.35000008E-02	-0.371499985	0.160799995

Ground energy

-686.905090

Excitation energy

6.79430008
6.87050009
6.91039991
7.10680008
7.41249990
7.52199984
7.61590004

7.83500004
7.86089993
7.87069988
7.94339991
7.98769999
8.13319969
8.19349957
8.30249977
8.33290005

E-Beta

Number of atoms: 24

1	3.29334	-0.30728	-1.45475
8	3.49309	0.08436	-0.59242
6	2.60553	-0.47467	0.35809
1	2.68158	0.13224	1.25996
1	2.87555	-1.51009	0.6072
6	1.16999	-0.47125	-0.14604
1	1.1353	-0.93223	-1.14378
6	0.57762	0.92999	-0.2505
1	1.10527	1.46024	-1.05294
8	0.76327	1.60734	0.98664
1	0.73423	2.5535	0.7908
6	-0.91896	0.88743	-0.5746
1	-1.07519	0.49156	-1.5813
8	-1.44868	2.20154	-0.56947
1	-1.72657	2.40182	0.33529
6	-1.61033	-0.02595	0.42378
1	-1.52245	0.4162	1.42657
8	-2.97058	-0.17514	0.04276
1	-3.42737	-0.65737	0.74778
6	-0.9218	-1.39673	0.43553
8	0.42425	-1.28259	0.76052
1	-1.36	-2.03855	1.21379
8	-1.03113	-1.99898	-0.83359
1	-1.96777	-2.19518	-0.98172

Electric moments

0	0	-2.61129999	-1.01030004	0.853799999
0	1	4.69999984E-02	0.109999999	-0.129700005
0	2	-9.73000005E-02	8.42000023E-02	5.68999983E-02
0	3	-8.70999992E-02	4.43000011E-02	-4.85999994E-02
0	4	0.116200000	-9.01999995E-02	-0.105200000
0	5	0.185399994	-0.100699998	0.140499994
0	6	-0.160300002	-6.23999983E-02	0.251100004
0	7	1.43999998E-02	-0.223299995	7.40000010E-02
0	8	0.386700004	0.150600001	-6.97000027E-02
0	9	-0.292499989	-0.273799986	0.245700002
0	10	0.123999998	-7.32000023E-02	-0.161899999
0	11	8.60000029E-02	9.60000008E-02	0.141000003
0	12	8.16000029E-02	-0.105099998	-9.67999995E-02
0	13	-5.55999987E-02	2.42999997E-02	0.184599996
0	14	0.139300004	-0.275799990	-7.47999996E-02

0	15	1.72000006E-02	-7.84000009E-02	0.124100000
0	16	-2.00999994E-02	0.209900007	4.19999985E-03
1	1	4.05700016	1.52980006	-2.90319991
2	2	-2.00990009	-5.27549982	-0.439399987
3	3	-2.96600008	-0.426200002	4.31689978
4	4	0.358200014	1.13220000	0.804400027
5	5	0.816999972	-1.84759998	-1.36039996
6	6	-1.46159995	1.17429996	1.01820004
7	7	-0.845399976	-3.11540008	-0.549600005
8	8	2.43400002	1.29709995	-2.47679996
9	9	-0.465700001	-2.70560002	-0.108900003
10	10	1.65090001	1.71120000	-1.71889997
11	11	0.883199990	2.98070002	0.459500015
12	12	-4.06739998	-1.79929996	2.95910001
13	13	1.18589997	-2.67750001	-2.50830007
14	14	-2.38470006	-0.635800004	2.41240001
15	15	-1.00549996	-0.523800015	1.53849995
16	16	2.75359988	0.766900003	-1.12189996

Magnetic moments

1	6.76999986E-02	-0.102600001	0.483900011
2	-0.329899997	4.98000011E-02	1.37000000E-02
3	-0.300300002	-0.455100000	-0.410299987
4	0.208000004	0.230299994	-0.331600010
5	0.375000000	-0.294400007	0.263399988
6	0.259200007	-0.294600010	0.564899981
7	-0.254500002	0.126499996	0.290199995
8	-8.57999995E-02	-0.173199996	0.597700000
9	-0.122800000	-0.222100005	-0.833100021
10	0.134499997	-0.136500001	2.81000007E-02
11	3.07999998E-02	-9.12000015E-02	0.112300001
12	0.335500002	-0.397899985	9.13000032E-02
13	-4.82000001E-02	0.150700003	6.71000034E-02
14	0.302500010	-0.286199987	0.314799994
15	-0.376100004	0.278400004	0.382299989
16	5.88999987E-02	9.31999981E-02	0.331600010

Ground energy

-686.910461

Excitation energy

6.46339989
6.76270008
6.82200003
7.19649982
7.31580019
7.46129990
7.56090021
7.58419991
7.63430023
7.82800007
7.86180019
7.94780016
8.00520039
8.16269970

8.20219994

8.25409985

F-Beta

Number of atoms: 24

1	2.73308	-0.99348	-0.69824
8	3.19801	-0.14313	-0.6429
6	2.64586	0.57901	0.42247
1	2.91955	1.62911	0.28591
1	3.06994	0.25313	1.38937
6	1.12555	0.51713	0.56284
1	0.85912	0.98403	1.52062
6	0.53436	-0.8928	0.5719
1	0.84983	-1.39506	1.49913
8	0.98915	-1.62918	-0.55235
1	0.48295	-2.45824	-0.55349
6	-0.9918	-0.85369	0.54563
1	-1.35465	-0.44413	1.49955
8	-1.39343	-2.20977	0.39258
1	-2.35734	-2.26249	0.44375
6	-1.49214	0.01864	-0.59469
1	-1.19953	-0.43447	-1.54421
8	-2.90074	0.16537	-0.59911
1	-3.23021	0.03077	0.30003
6	-0.82561	1.39227	-0.48699
8	0.57214	1.28937	-0.50403
1	-1.08149	2.00454	-1.35764
8	-1.30056	1.98073	0.70137
1	-0.98515	2.89587	0.72389

Electric moments

0	0	-2.99710011	-0.151899993	3.61299992
0	1	0.149700001	1.72000006E-02	0.100400001
0	2	-8.60999972E-02	9.14999992E-02	0.194199994
0	3	3.42999995E-02	0.132900000	9.49999969E-03
0	4	-7.97000006E-02	0.209199995	-4.10000011E-02
0	5	0.149599999	-8.63000005E-02	-0.158800006
0	6	-0.122000001	-4.96000014E-02	-2.67999992E-02
0	7	0.167999998	-0.223000005	0.363599986
0	8	-1.89999994E-02	-8.10000002E-02	4.30999994E-02
0	9	-1.37000000E-02	-0.101300001	0.268999994
0	10	8.03000033E-02	-6.15000017E-02	0.197799996
0	11	-0.186000004	5.27999997E-02	-0.222200006
0	12	3.40999998E-02	0.134399995	-9.22999978E-02
0	13	6.06999993E-02	0.102100000	0.205599993
0	14	-6.98999986E-02	-9.30000003E-03	3.81000005E-02
0	15	0.199300006	-7.93000013E-02	0.118400000
0	16	-1.57999992E-02	3.22999991E-02	0.103200004
1	1	2.83620000	3.49880004	-0.186800003
2	2	-1.33879995	1.03199995	-0.656199992
3	3	1.33539999	1.86409998	0.664200008
4	4	-2.27690005	-5.80249977	1.58800006
5	5	-0.432999998	3.73469996	1.51390004

6	6	-1.10450006	-1.14800000	1.39859998
7	7	0.227799997	-0.647499979	1.07889998
8	8	7.61759996	1.56750000	0.830699980
9	9	1.71039999	-1.92600000	1.01010001
10	10	0.319700003	-1.46089995	2.62680006
11	11	-0.707300007	-1.97700000	1.38600004
12	12	-0.907800019	-0.231900007	0.819899976
13	13	0.229599997	1.14489996	0.294200003
14	14	-0.287800014	1.06710005	1.28020000
15	15	0.169100001	-3.74489999	0.961600006
16	16	3.23920012	3.66969991	0.808300018

Magnetic moments

1	0.180099994	-9.60000046E-03	0.567799985
2	-0.223499998	-9.35999975E-02	-8.47999975E-02
3	-0.497200012	0.146699995	0.461199999
4	7.41999969E-02	-2.71000005E-02	-0.174400002
5	0.370999992	-5.35999984E-02	-0.132400006
6	0.149399996	-0.454499990	-0.320699990
7	-9.20000020E-03	0.363599986	-0.255400002
8	-4.80000023E-03	0.225299999	-5.90000004E-02
9	0.627300024	0.676599979	-0.195999995
10	-0.377700001	0.503799975	-0.231199995
11	6.93000033E-02	0.302399993	-7.51999989E-02
12	0.247999996	0.515600026	6.84999973E-02
13	0.515200019	-0.541400015	0.251100004
14	-0.281100005	-0.454600006	0.411300004
15	9.64000002E-02	-0.244599998	0.139100000
16	0.229599997	3.22000012E-02	-3.24000008E-02

Ground energy

-686.918457

Excitation energy

6.51959991
6.91169977
6.99760008
7.09110022
7.45270014
7.49139977
7.56790018
7.61129999
7.70340014
7.82730007
7.87190008
7.89639997
7.97279978
8.03190041
8.12500000
8.16079998

G-Beta

Number of atoms: 24

1	3.11323	-1.33575	-0.36872
8	3.58096	-0.49696	-0.2636

6	2.62442	0.50219	0.03635
1	2.87388	1.39391	-0.54893
1	2.6697	0.77624	1.09648
6	1.20953	0.07238	-0.29615
1	1.2191	-0.42431	-1.27729
6	0.21834	1.22718	-0.36447
1	0.47765	1.87457	-1.20655
8	0.31812	2.06228	0.78315
1	-0.01892	1.5729	1.54791
6	-1.20824	0.70851	-0.57355
1	-1.2428	0.21016	-1.54851
8	-2.13382	1.76221	-0.6584
1	-2.18134	2.18668	0.21105
6	-1.5565	-0.33503	0.49362
1	-1.57854	0.13676	1.4843
8	-2.82613	-0.909	0.33012
1	-2.84041	-1.31665	-0.5496
6	-0.47207	-1.41954	0.51939
8	0.81426	-0.88138	0.70092
1	-0.62628	-2.08859	1.37207
8	-0.59651	-2.11611	-0.69653
1	-0.01333	-2.88841	-0.66868

Electric moments

0	0	-0.263000011	-2.50720000	0.198400006
0	1	-0.115300000	-7.15999976E-02	-0.204500005
0	2	-3.40000005E-03	-7.45000020E-02	-6.58999979E-02
0	3	8.32000002E-02	-4.03999984E-02	-3.88999991E-02
0	4	-6.03000000E-02	4.98999991E-02	-4.69999984E-02
0	5	0.177599996	-7.81999975E-02	-3.55000012E-02
0	6	0.178299993	0.258399993	-0.293399990
0	7	1.97000001E-02	0.186600000	-0.103699997
0	8	-0.163599998	-4.45999987E-02	0.132499993
0	9	-0.214100003	-5.73999994E-02	-3.90999988E-02
0	10	2.96999998E-02	0.224399999	-0.150900006
0	11	-7.45000020E-02	-0.175500005	0.158099994
0	12	3.80000006E-03	-3.33999991E-02	0.275099993
0	13	-4.74999994E-02	0.267100006	-9.70000029E-03
0	14	-2.63999999E-02	0.125400007	-0.112700000
0	15	5.95999993E-02	0.176200002	1.41000003E-02
0	16	-0.117600001	7.19999988E-03	-0.125200003
1	1	3.92000005E-02	3.43039989	0.790400028
2	2	0.738799989	-3.41370010	-4.29320002
3	3	-0.134800002	1.39279997	-0.983799994
4	4	-2.86999997E-02	-2.65580010	-1.99199998
5	5	0.650500000	0.297899991	2.71259999
6	6	-1.33130002	1.15709996	-0.206900001
7	7	0.677500010	-1.15579998	2.64770007
8	8	-0.705299973	0.806999981	0.753700018
9	9	-2.65660000	2.63190007	1.12860000
10	10	-0.330599993	-3.76270008	-0.754400015
11	11	-1.36469996	-0.123800002	-1.03670001
12	12	3.08890009	-1.12609994	-1.46519995

13	13	-9.79000032E-02	0.393599987	0.482400000
14	14	4.46560001	-0.947899997	-0.217700005
15	15	1.36210001	-1.15590000	1.75610006
16	16	-0.883700013	-3.29520011	-1.06340003

Magnetic moments

1	-0.374799997	-0.358399987	0.147400007
2	-0.201000005	-0.298799992	0.174400002
3	-0.137999997	-0.619199991	-0.233400002
4	-0.154899999	-0.279799998	-0.432099998
5	0.166299999	-2.98999995E-02	0.477899998
6	0.201900005	-8.34999979E-02	0.524100006
7	-0.130199999	0.320100009	0.649699986
8	0.254099995	6.44999966E-02	-0.142800003
9	0.555700004	-1.67999994E-02	0.342700005
10	-2.52999999E-02	0.319299996	-6.49000034E-02
11	-0.693400025	-0.322299987	0.378399998
12	0.314799994	0.208600000	-8.89999978E-03
13	-0.173199996	6.47000000E-02	-0.214000002
14	0.153500006	-0.626999974	3.35000008E-02
15	-0.143500000	0.259099990	-0.188899994
16	0.231800005	2.05000006E-02	0.156200007

Ground energy

-686.914124

Excitation energy

6.73050022
6.85540009
6.93400002
7.13159990
7.35790014
7.53109980
7.53520012
7.70030022
7.77610016
7.85370016
7.96210003
8.04539967
8.08139992
8.17899990
8.19610023
8.25689983

H-Beta

Number of atoms: 24

1	-2.80894	1.39213	-1.15073
8	-3.30209	0.96183	-0.43949
6	-2.65164	-0.24647	-0.1103
1	-3.0846	-1.09817	-0.65734
1	-2.81481	-0.41971	0.95514
6	-1.16024	-0.22197	-0.39663
1	-0.98465	-0.19508	-1.48292
6	-0.41017	-1.4196	0.19711
1	-0.746	-2.34392	-0.27995

8	-0.68673	-1.55943	1.57604
1	-0.44834	-0.72232	2.00363
6	1.09105	-1.26639	-0.07017
1	1.62162	-2.0621	0.46752
8	1.27374	-1.38675	-1.46986
1	2.20701	-1.58728	-1.62446
6	1.59637	0.08907	0.41337
1	1.50285	0.15796	1.50807
8	2.94304	0.214	0.01437
1	3.20489	1.13218	0.1823
6	0.72615	1.18709	-0.17509
8	-0.62403	0.97212	0.18769
1	0.8113	1.18517	-1.2731
8	1.14241	2.39773	0.37347
1	0.42	3.03465	0.2642

Electric moments

0	0	1.83130002	0.671100020	-1.37839997
0	1	-3.07000000E-02	5.48000000E-02	-7.22000003E-02
0	2	0.119400002	0.101099998	0.171000004
0	3	9.30999964E-02	2.79999990E-03	4.45999987E-02
0	4	-0.268700004	3.92999984E-02	7.22000003E-02
0	5	9.76999998E-02	-0.179199994	-0.170699999
0	6	-7.94000030E-02	0.221100003	-0.368099988
0	7	-4.28000018E-02	8.00000038E-03	-0.169300005
0	8	6.36000037E-02	-8.85000005E-02	-4.16000001E-02
0	9	-2.15000007E-02	-5.70000000E-02	-0.187800005
0	10	-2.97999997E-02	-0.105700001	-2.86999997E-02
0	11	5.70000010E-03	-0.265500009	-0.112899996
0	12	-1.98999997E-02	0.139200002	3.88000011E-02
0	13	7.66000003E-02	8.95999968E-02	0.117899999
0	14	-0.149200007	5.16000018E-02	0.190300003
0	15	-0.134800002	-0.259600013	0.404199988
0	16	-0.169200003	-0.199200004	4.60000001E-02
1	1	1.43859994	-3.52259994	2.68549991
2	2	2.35290003	-5.20069981	1.92429996
3	3	-1.92040002	1.63320005	0.140300006
4	4	0.456000000	1.22239995	-5.02899981
5	5	-1.56930006	0.766799986	-1.75469995
6	6	1.58270001	-0.557200015	1.98800004
7	7	1.96459997	1.59809995	-6.62470007
8	8	-1.84060001	2.39569998	0.754599988
9	9	2.27430010	-2.99460006	1.48300004
10	10	1.14590001	0.802800000	-0.139100000
11	11	2.06150007	3.20740008	-0.967800021
12	12	-1.56389999	0.604099989	-4.04239988
13	13	1.29380000	-1.54869998	-0.823300004
14	14	3.25959992	0.857800007	0.114500001
15	15	1.23080003	0.258599997	-4.86880016
16	16	1.91199994	2.10920000	1.12329996

Magnetic moments

1	0.646799982	0.284500003	-0.309899986
2	0.170200005	0.178700000	0.219699994

3	-0.497799993	0.128600001	-4.90000006E-03
4	3.55000012E-02	0.483599991	0.265899986
5	0.361999989	0.112000003	0.129500002
6	0.422300011	-0.367000014	-0.116200000
7	0.389400005	0.564599991	0.172399998
8	0.225400001	-0.667699993	0.252099991
9	0.297199994	-0.276199996	0.255100012
10	-0.263500005	-0.174199998	-0.486499995
11	-0.157600001	0.352499992	-7.09000006E-02
12	-9.39999968E-02	-7.86999986E-02	0.445100009
13	-0.326599985	0.246900007	0.197099999
14	-0.502799988	-0.163399994	-0.230100006
15	-5.04000001E-02	0.317000002	6.98999986E-02
16	-2.71000005E-02	0.109099999	-2.09999997E-02

Ground energy

-686.917236

Excitation energies

6.74109983

6.86040020

7.12519979

7.24580002

7.25589991

7.52199984

7.69939995

7.78859997

7.87410021

8.00479984

8.02280045

8.12860012

8.17889977

8.22910023

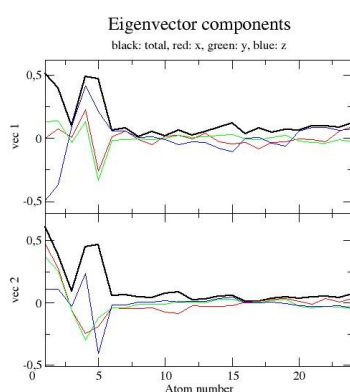
8.32590008

8.35179996

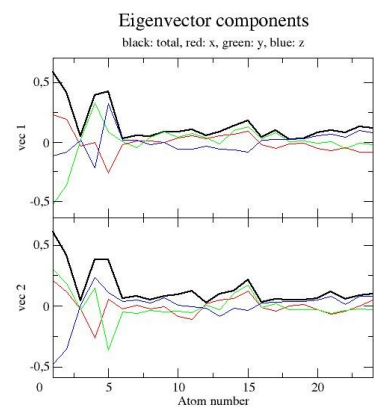
S2. Composition of the essential eigenvectors of the covariance matrix

Composition of the first two eigenvectors (number of atoms are reported at the end of this paragraph) of the covariance matrix for:

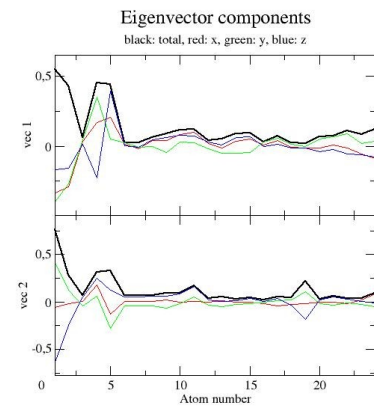
D-glucose-Alpha



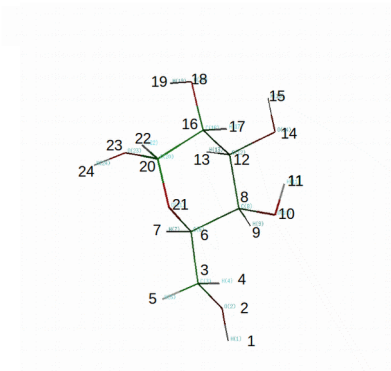
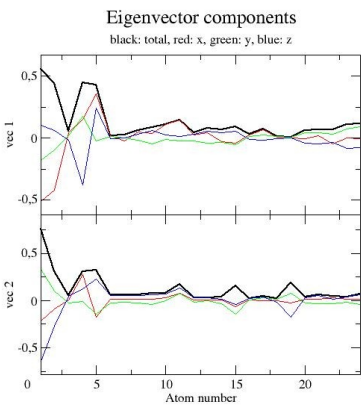
D-glucose-Beta



D-galactose-Alpha

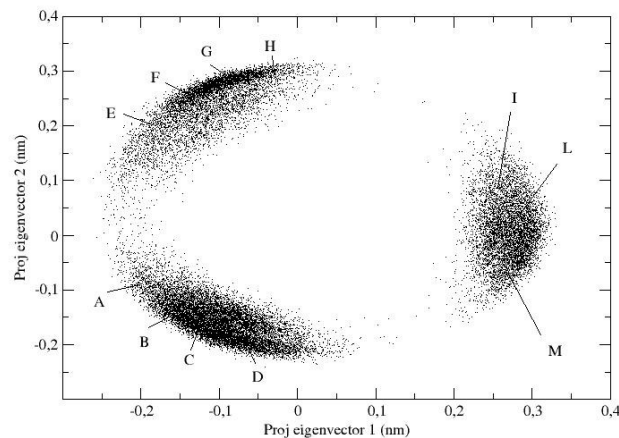


D-galactose-Beta

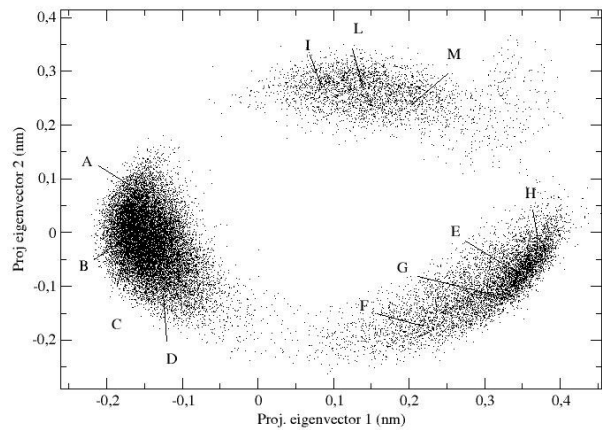


S3. Location of the Representative Conformations on the Essential plane

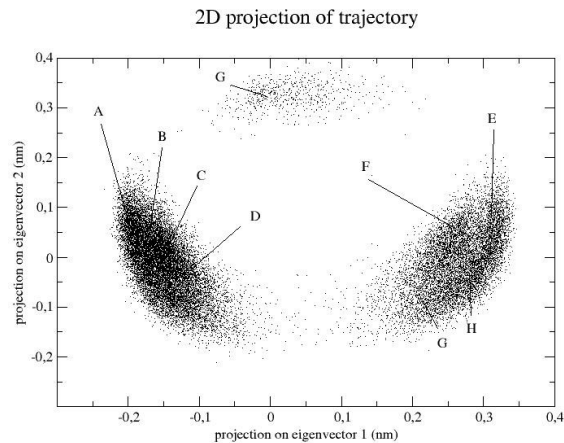
D-Glucose-Alpha



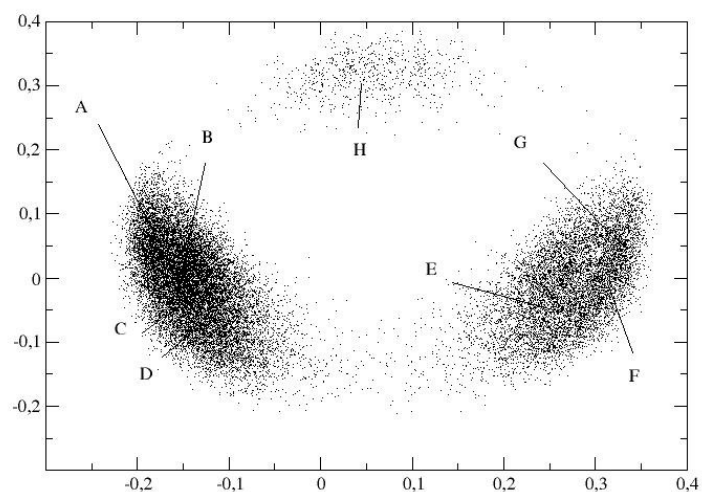
D-Glucose-Beta



D-Galactose-Alpha

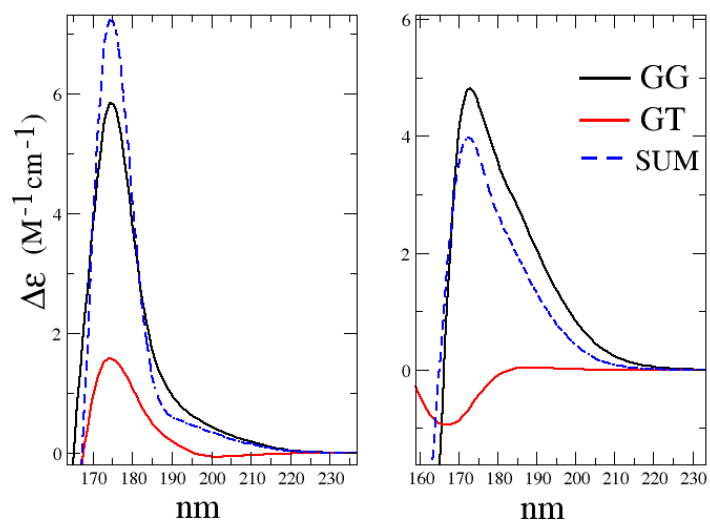


D-Galactose-Beta



S4. Spectra of the GG and GT rotamers for Alpha and Beta D-glucose

Spectra of the GG and GT rotamers for Alpha and Beta D-glucose



S5. Eigenvalues of the D-Galactose covariance matrix

Spectra of the eigenvalues from the diagonalization of the covariance matrix for Alpha (black) and Beta (red) D-galactose.

