Supplementary data for article:

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2-Alkylidene-4-oxothiazolidine-*S*-oxides: Synthesis and Stereochemistry

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[†]*1946-2012*

Supplementary Data

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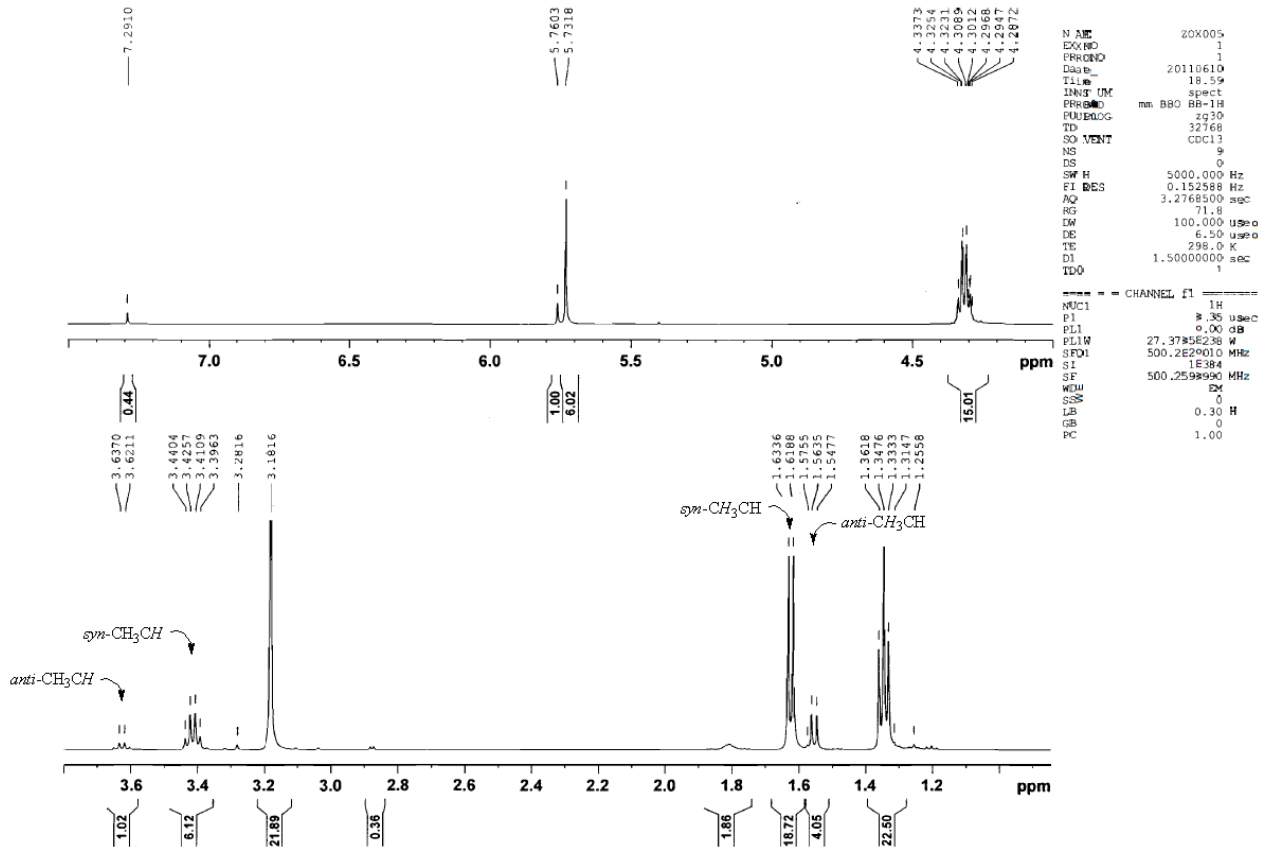
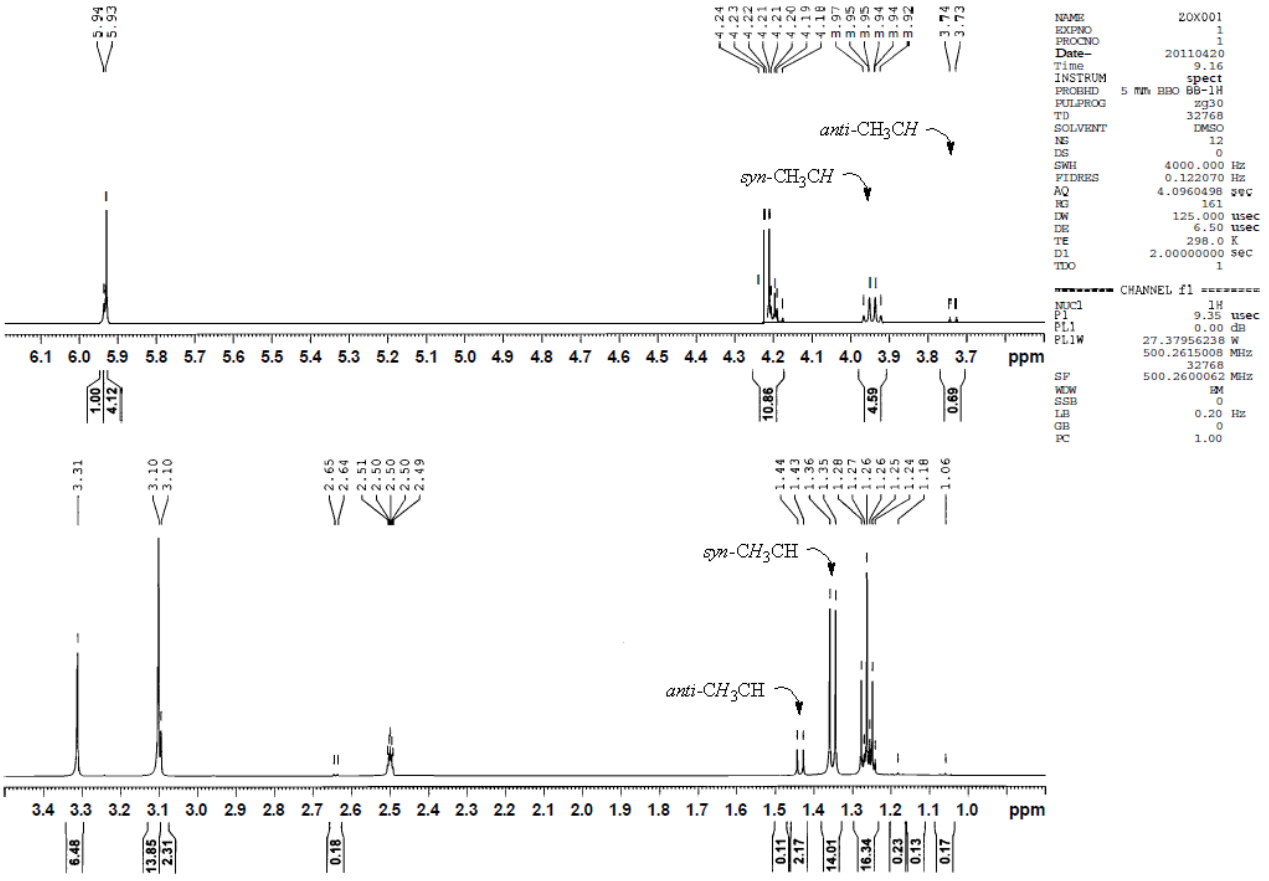


(a)



(b)

Figure S1. ^{1}H NMR spectra of **5l** in $CDCl_3$ (a) and DMSO-d_6 solutions (b).

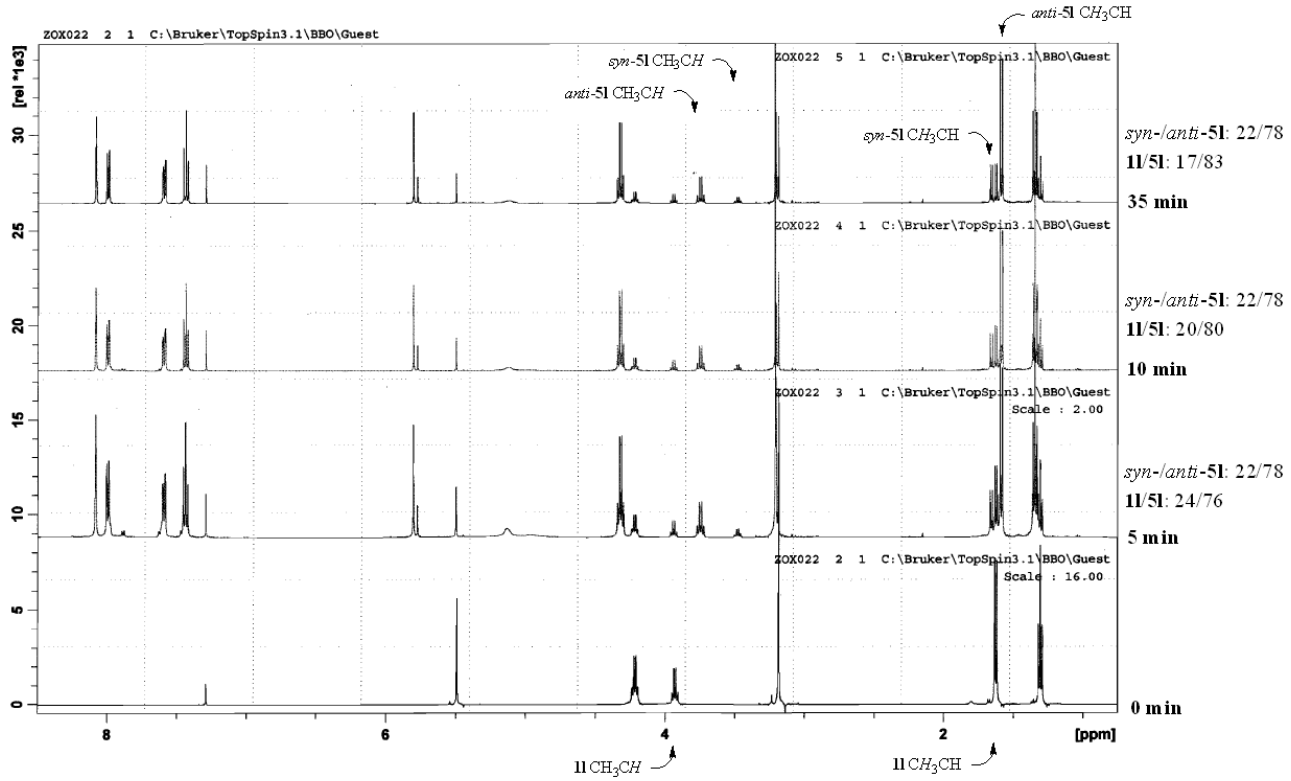


Figure S2. Monitoring of the oxidation course of **1l** by ^{1}H NMR spectroscopy: $CDCl_3$ solution, at 0 °C.

Absolute energies (atomic units) and x, y, z coordinates (Å) of the optimized structures

1c

E = -990.1131439 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.913833	-1.304458	0.000178
2	6	0	3.130746	0.199426	-0.000219
3	7	0	1.915410	0.874978	-0.000279
4	6	0	0.753607	0.113621	-0.000334
5	16	0	1.107740	-1.626272	-0.000263
6	6	0	-0.495471	0.646213	-0.000261
7	8	0	4.216495	0.745237	0.000650
8	6	0	-1.672494	-0.207691	0.000048
9	8	0	-2.817351	0.519504	-0.000274
10	8	0	-1.657766	-1.432044	0.000473
11	6	0	1.890526	2.331963	-0.000028
12	6	0	-4.043104	-0.242048	-0.000050
13	6	0	-5.193649	0.747312	0.000310
14	1	0	3.389557	-1.735631	-0.885185
15	1	0	3.389117	-1.735267	0.885952
16	1	0	-0.643741	1.718213	-0.000328
17	1	0	2.927311	2.668405	0.000104
18	1	0	1.377774	2.704106	0.892599
19	1	0	1.377916	2.704392	-0.892616
20	1	0	-4.059367	-0.890069	-0.882755
21	1	0	-4.058937	-0.890253	0.882517
22	1	0	-6.147743	0.208959	0.000433
23	1	0	-5.159116	1.387405	0.887905
24	1	0	-5.159479	1.387641	-0.887127

5c

E = -1065.2700862 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.827436	-0.965408	-0.611147
2	6	0	-3.031995	0.476998	-0.191832
3	7	0	-1.798845	1.091409	0.039429
4	6	0	-0.668911	0.305797	-0.066056
5	16	0	-1.110943	-1.505905	-0.166828
6	6	0	0.600907	0.755138	-0.001734
7	8	0	-4.099075	1.048053	-0.107465
8	6	0	1.767429	-0.136218	-0.095845
9	8	0	2.912248	0.579857	-0.023948
10	8	0	1.738070	-1.347762	-0.224818
11	6	0	-1.737337	2.510898	0.368530
12	8	0	-1.177645	-2.035861	1.240272
13	6	0	4.137643	-0.185294	-0.096323
14	6	0	5.291918	0.793518	0.007061
15	1	0	-3.532054	-1.629369	-0.106743
16	1	0	-2.959711	-1.054545	-1.695782
17	1	0	0.809067	1.812568	0.121839
18	1	0	-2.763595	2.868994	0.449994
19	1	0	-1.214152	3.064215	-0.418944
20	1	0	-1.213080	2.652131	1.318719
21	1	0	4.142511	-0.917652	0.717225
22	1	0	4.150696	-0.740262	-1.039962
23	1	0	6.242538	0.251788	-0.044478
24	1	0	5.264522	1.519684	-0.811749
25	1	0	5.258165	1.340194	0.954882

1j

E = -1161.9871828 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.770073	-1.073095	-0.299561
2	6	0	-3.996229	0.423727	-0.135430
3	7	0	-2.795601	1.117756	-0.050925
4	6	0	-1.620101	0.375199	-0.086568
5	16	0	-1.947457	-1.359720	-0.235803
6	6	0	-0.381285	0.926745	-0.009312
7	8	0	-5.091648	0.951423	-0.083534
8	6	0	0.818607	0.089655	-0.041120
9	7	0	2.006078	0.796681	0.030611
10	8	0	0.767102	-1.141247	-0.123757
11	6	0	-2.800352	2.566390	0.098752
12	6	0	3.330932	0.319849	0.031955
13	6	0	4.356740	1.277366	0.106151
14	6	0	5.691946	0.885513	0.114853
15	6	0	6.028500	-0.467886	0.049743
16	6	0	5.008647	-1.417487	-0.024244
17	6	0	3.665106	-1.042680	-0.034236
18	6	0	-4.552049	-1.878138	0.743147
19	1	0	-4.122778	-1.339578	-1.302674
20	1	0	-0.282685	2.003205	0.079355
21	1	0	1.919488	1.802182	0.088591
22	1	0	-3.843601	2.882185	0.110866
23	1	0	-2.314294	2.855683	1.036329
24	1	0	-2.279390	3.039592	-0.740086
25	1	0	4.102805	2.334976	0.157301
26	1	0	6.469468	1.642630	0.172723
27	1	0	7.069929	-0.776446	0.056458
28	1	0	5.255921	-2.474709	-0.075692
29	1	0	2.877155	-1.779867	-0.092123
30	1	0	-4.432877	-2.952192	0.572187
31	1	0	-5.614323	-1.624732	0.669619
32	1	0	-4.204819	-1.650822	1.755746

syn-**5j**

E = -1237.1463937 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.622916	-0.774942	-0.666922
2	6	0	-3.850159	0.661201	-0.221800
3	7	0	-2.634160	1.305265	0.015460
4	6	0	-1.488711	0.536605	-0.062050
5	16	0	-1.908633	-1.279289	-0.106349
6	6	0	-0.227685	1.011360	-0.002534
7	8	0	-4.930664	1.207600	-0.122283
8	6	0	0.963644	0.134022	-0.045242
9	7	0	2.152995	0.832797	-0.009113
10	8	0	0.895698	-1.091874	-0.109424
11	6	0	-2.607514	2.725020	0.343415
12	8	0	-2.049509	-1.738864	1.322499
13	6	0	3.475432	0.342324	-0.027764
14	6	0	4.508781	1.293467	-0.008144
15	6	0	5.840360	0.889836	-0.020646
16	6	0	6.162587	-0.468262	-0.053385
17	6	0	5.134158	-1.411106	-0.072878
18	6	0	3.793897	-1.024507	-0.060674
19	6	0	-4.686608	-1.740772	-0.163004
20	1	0	-3.572075	-0.770163	-1.764960
21	1	0	-0.074021	2.084498	0.083140
22	1	0	2.079076	1.840019	0.037211
23	1	0	-3.642324	3.056954	0.428660
24	1	0	-2.103061	3.294279	-0.445624
25	1	0	-2.084855	2.880389	1.292631
26	1	0	4.264830	2.354282	0.017491
27	1	0	6.625782	1.640578	-0.004601
28	1	0	7.201168	-0.786005	-0.063050
29	1	0	5.371488	-2.471374	-0.097228
30	1	0	2.999207	-1.756498	-0.074828
31	1	0	-4.603394	-2.711824	-0.660014
32	1	0	-5.676830	-1.321819	-0.362461
33	1	0	-4.574494	-1.891499	0.914223

anti-**5j**

=-1237.1437563

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.693404	-0.952368	0.174619
2	6	0	3.917009	0.537713	-0.015560
3	7	0	2.705559	1.225010	-0.107836
4	6	0	1.544802	0.476558	-0.069128
5	16	0	1.909620	-1.347171	-0.210265
6	6	0	0.295127	0.982912	-0.033284
7	8	0	5.002546	1.083937	-0.031715
8	6	0	-0.911485	0.126907	-0.001641
9	7	0	-2.088115	0.846562	0.038866
10	8	0	-0.864186	-1.101705	-0.003972
11	6	0	2.698221	2.678751	-0.214202
12	8	0	1.861063	-1.709205	-1.672116
13	6	0	-3.418090	0.377892	0.072192
14	6	0	-4.434443	1.345756	0.128396
15	6	0	-5.772162	0.964028	0.160814
16	6	0	-6.117556	-0.388560	0.138288
17	6	0	-5.105981	-1.348033	0.082437
18	6	0	-3.759916	-0.983512	0.049237
19	1	0	4.267719	-1.497485	-0.579911
20	6	0	4.079751	-1.394967	1.591285
21	1	0	0.162523	2.062083	-0.022562
22	1	0	-1.997175	1.853441	0.037205
23	1	0	3.737091	3.004081	-0.268218
24	1	0	2.217352	3.125734	0.663112
25	1	0	2.161388	2.986046	-1.117432
26	1	0	-4.172250	2.402402	0.146045
27	1	0	-6.544159	1.727549	0.203511
28	1	0	-7.160939	-0.689290	0.163322
29	1	0	-5.361440	-2.404191	0.062910
30	1	0	-2.978461	-1.728397	0.004496
31	1	0	3.986427	-2.479748	1.696889
32	1	0	3.441852	-0.921917	2.346609
33	1	0	5.116571	-1.109246	1.792760

1k

E = -1240.6120965 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.397341	1.379453	-0.182749
2	1	0	4.852202	1.677514	-1.134474
3	7	0	3.826336	-0.948300	0.068154
4	16	0	2.567454	1.305086	-0.417288
5	6	0	2.550412	-0.453182	-0.185846
6	6	0	1.439232	-1.229501	-0.241774
7	1	0	1.524919	-2.300923	-0.095797
8	6	0	4.873087	-0.037242	0.109374
9	8	0	6.027627	-0.337508	0.352815
10	6	0	0.123307	-0.641697	-0.503310
11	8	0	-0.042991	0.571029	-0.686920
12	6	0	4.834769	2.355005	0.914634
13	1	0	5.923462	2.312836	1.020459
14	1	0	4.544187	3.378879	0.660973
15	1	0	4.376986	2.096092	1.874396
16	7	0	-0.928117	-1.524846	-0.553921
17	1	0	-0.771448	-2.476375	-0.252826
18	6	0	-2.300173	-1.063011	-0.695546
19	1	0	-2.292842	-0.233634	-1.406883
20	1	0	-2.893738	-1.873873	-1.131762
21	6	0	-2.932681	-0.592177	0.633956
22	1	0	-2.928447	-1.425166	1.348813
23	1	0	-2.291364	0.194846	1.045255
24	6	0	-4.341839	-0.077625	0.441158
25	6	0	-5.451048	-0.908997	0.644728
26	6	0	-4.565258	1.238667	0.011886
27	6	0	-6.748445	-0.441126	0.429512
28	1	0	-5.296513	-1.931761	0.983291
29	6	0	-5.859972	1.710514	-0.205052
30	1	0	-3.714397	1.897593	-0.147747
31	6	0	-6.956758	0.871442	0.003258
32	1	0	-7.595855	-1.100613	0.599111
33	1	0	-6.012788	2.735624	-0.532761
34	1	0	-7.966020	1.239251	-0.161795
35	6	0	4.078618	-2.360585	0.316349
36	1	0	3.518625	-2.700722	1.193785
37	1	0	3.787186	-2.959780	-0.552569
38	1	0	5.148391	-2.466948	0.496875

syn-**5k**

E = -1315.7720967 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.336474	-1.089083	-0.493626
2	6	0	-4.760092	0.276047	0.025853
3	7	0	-3.667886	1.141520	0.094381
4	6	0	-2.421573	0.609275	-0.180441
5	16	0	-2.488653	-1.252043	-0.231111
6	6	0	-1.277830	1.314115	-0.284845
7	6	0	0.036425	0.678717	-0.537459
8	8	0	-5.896340	0.602827	0.307385
9	6	0	-3.860518	2.538172	0.461830
10	7	0	1.089442	1.552859	-0.605337
11	8	0	0.186338	-0.533965	-0.696340
12	6	0	2.459615	1.079298	-0.747505
13	6	0	3.096024	0.636066	0.588834
14	6	0	4.500050	0.106794	0.396271
15	6	0	5.615364	0.940822	0.549348
16	6	0	6.907342	0.457879	0.335235
17	6	0	7.103438	-0.872365	-0.038958
18	6	0	6.000269	-1.714078	-0.196240
19	6	0	4.710822	-1.227271	0.019278
20	8	0	-2.302663	-1.738456	1.184424
21	6	0	-5.099548	-2.242629	0.143080
22	1	0	-4.466977	-1.075565	-1.584951
23	1	0	-1.309515	2.396057	-0.179108
24	1	0	-4.915486	2.666118	0.704588
25	1	0	-3.243530	2.785533	1.331708
26	1	0	-3.591865	3.197095	-0.371603
27	1	0	0.940243	2.514844	-0.334901
28	1	0	3.052546	1.877640	-1.206397
29	1	0	2.441019	0.234346	-1.439850
30	1	0	2.452847	-0.135987	1.024602
31	1	0	3.103362	1.486199	1.283005
32	1	0	5.470474	1.977324	0.848143
33	1	0	7.760075	1.119342	0.465608
34	1	0	8.108563	-1.251874	-0.202544
35	1	0	6.143838	-2.752880	-0.482133
36	1	0	3.855071	-1.888496	-0.099173
37	1	0	-4.915591	-3.179009	-0.392007
38	1	0	-6.170468	-2.022562	0.118998
39	1	0	-4.785607	-2.369902	1.182820

anti-**5k**

E = -1315.7695549 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.156673	-1.259636	0.418774
2	6	0	-4.738877	0.133970	0.263081
3	7	0	-3.740499	1.084547	0.057697
4	6	0	-2.441739	0.630138	-0.096908
5	16	0	-2.370277	-1.228965	-0.136018
6	6	0	-1.351525	1.410090	-0.227593
7	6	0	-0.020658	0.846091	-0.552963
8	8	0	-5.923384	0.404073	0.318520
9	6	0	-4.086699	2.496403	-0.056598
10	7	0	1.028238	1.715446	-0.401866
11	8	0	0.134580	-0.301166	-0.973019
12	6	0	2.404399	1.271782	-0.583365
13	6	0	2.971828	0.514572	0.638002
14	6	0	4.386388	0.037113	0.394210
15	6	0	5.489082	0.793533	0.812389
16	6	0	6.792434	0.369306	0.548144
17	6	0	7.013173	-0.822606	-0.143526
18	6	0	5.922921	-1.586397	-0.565869
19	6	0	4.622115	-1.159167	-0.298576
20	8	0	-1.565591	-1.750222	1.023923
21	1	0	-4.073346	-1.473735	1.492068
22	6	0	-4.978652	-2.331559	-0.291606
23	1	0	-1.445216	2.489288	-0.133976
24	1	0	-5.173336	2.569117	-0.016355
25	1	0	-3.648116	3.066156	0.769863
26	1	0	-3.716557	2.896586	-1.006142
27	1	0	0.868821	2.568385	0.116792
28	1	0	3.019478	2.149457	-0.809344
29	1	0	2.421489	0.616595	-1.457467
30	1	0	2.310219	-0.334187	0.841761
31	1	0	2.939976	1.173167	1.515470
32	1	0	5.324918	1.720972	1.357869
33	1	0	7.634578	0.967713	0.886498
34	1	0	8.026976	-1.156693	-0.347797
35	1	0	6.085282	-2.519254	-1.099688
36	1	0	3.776024	-1.760607	-0.624052
37	1	0	-4.579242	-3.327830	-0.080060
38	1	0	-4.976770	-2.180487	-1.376309
39	1	0	-6.014867	-2.284445	0.055369

1l

E = -1029.4297355 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.741515	-0.928336	-0.314785
2	6	0	-2.819326	0.583962	-0.142977
3	7	0	-1.557354	1.155937	-0.047576
4	6	0	-0.461000	0.302674	-0.081761
5	16	0	-0.957036	-1.390756	-0.247189
6	6	0	0.825361	0.728520	0.008918
7	8	0	-3.858881	1.214472	-0.094630
8	6	0	1.932509	-0.214080	-0.024293
9	8	0	3.128762	0.419413	0.069636
10	8	0	1.826323	-1.429633	-0.123088
11	6	0	-1.416577	2.597681	0.110558
12	6	0	-3.602660	-1.657160	0.721407
13	6	0	4.292254	-0.433635	0.047260
14	6	0	5.514282	0.461119	0.142662
15	1	0	-3.114876	-1.153568	-1.320399
16	1	0	1.056969	1.780894	0.109214
17	1	0	-2.422285	3.018017	0.114614
18	1	0	-0.840408	3.017629	-0.720024
19	1	0	-0.912106	2.830874	1.053717
20	1	0	-3.593664	-2.736491	0.542816
21	1	0	-4.633220	-1.295751	0.648075
22	1	0	-3.235901	-1.473090	1.735877
23	1	0	4.233385	-1.137874	0.883923
24	1	0	4.285277	-1.021280	-0.876733
25	1	0	6.424397	-0.148534	0.129062
26	1	0	5.554309	1.159066	-0.699896
27	1	0	5.502572	1.042162	1.070544

syn-**5l**

E = -1104.5889584 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.624801	-0.622700	-0.656226
2	6	0	-2.700333	0.825927	-0.195416
3	7	0	-1.423326	1.341327	0.034601
4	6	0	-0.363374	0.463082	-0.065212
5	16	0	-0.962410	-1.299440	-0.127143
6	6	0	0.939980	0.806392	-0.015196
7	8	0	-3.719498	1.476589	-0.081058
8	6	0	2.031598	-0.177459	-0.087985
9	8	0	3.229576	0.449456	-0.041423
10	8	0	1.908686	-1.386290	-0.180187
11	6	0	-1.246217	2.748970	0.372035
12	8	0	-1.122140	-1.766235	1.297558
13	6	0	-3.771819	-1.482671	-0.143095
14	6	0	4.390941	-0.410616	-0.096574
15	6	0	5.618706	0.477795	-0.029135
16	1	0	-2.590816	-0.612034	-1.754761
17	1	0	1.234787	1.845822	0.083588
18	1	0	-2.240124	3.185994	0.467839
19	1	0	-0.689489	3.266214	-0.417047
20	1	0	-0.702181	2.840525	1.317187
21	1	0	-3.798100	-2.449401	-0.654507
22	1	0	-4.716947	-0.961023	-0.317306
23	1	0	-3.655819	-1.660257	0.929655
24	1	0	4.345232	-1.116437	0.738903
25	1	0	4.353874	-0.993227	-1.022782
26	1	0	6.523950	-0.137642	-0.069331
27	1	0	5.641465	1.179152	-0.869431
28	1	0	5.634945	1.053579	0.901781

anti-**5l**

E = -1104.5863464 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.714877	-0.802882	0.095915
2	6	0	2.786500	0.705049	-0.079078
3	7	0	1.513955	1.275243	-0.127726
4	6	0	0.430416	0.423542	-0.051864
5	16	0	0.953624	-1.361637	-0.163161
6	6	0	-0.859686	0.812388	0.008813
7	8	0	3.815259	1.350323	-0.121285
8	6	0	-1.975179	-0.142429	0.093369
9	8	0	-3.156210	0.516589	0.124579
10	8	0	-1.880916	-1.356534	0.138619
11	6	0	1.363320	2.723138	-0.220879
12	8	0	0.843100	-1.787315	-1.604363
13	1	0	3.273772	-1.280096	-0.714692
14	6	0	-4.337003	-0.314991	0.199175
15	6	0	-5.542990	0.605163	0.190071
16	6	0	3.255480	-1.230524	1.465509
17	1	0	-1.124235	1.864345	0.000140
18	1	0	2.364231	3.148915	-0.289355
19	1	0	0.854647	3.111228	0.668120
20	1	0	0.782395	2.983118	-1.111320
21	1	0	-4.335986	-1.003449	-0.651778
22	1	0	-4.285611	-0.918250	1.111498
23	1	0	-6.462038	0.011911	0.247133
24	1	0	-5.521035	1.289195	1.044598
25	1	0	-5.574047	1.200563	-0.728041
26	1	0	3.273014	-2.320856	1.551978
27	1	0	2.641019	-0.832073	2.280777
28	1	0	4.273913	-0.850278	1.589008

1m

E = -1106.6203188 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.473288	-0.800274	-0.330472
2	1	0	-3.865403	-0.957224	-1.342191
3	7	0	-2.111463	1.160185	-0.001887
4	16	0	-1.732926	-1.419618	-0.287001
5	6	0	-1.096691	0.215739	-0.080467
6	6	0	0.229373	0.523510	0.001429
7	1	0	0.519660	1.554327	0.151151
8	6	0	-3.421403	0.704002	-0.104858
9	8	0	-4.399288	1.423416	-0.024050
10	6	0	1.239328	-0.519079	-0.073440
11	8	0	0.912941	-1.710562	-0.176064
12	6	0	-4.391691	-1.491140	0.682535
13	1	0	-5.389113	-1.043866	0.626577
14	1	0	-4.471801	-2.560635	0.466268
15	1	0	-4.010218	-1.374244	1.701620
16	6	0	2.694451	-0.153165	-0.010101
17	6	0	3.617917	-1.194451	0.173453
18	6	0	3.172587	1.159605	-0.140140
19	6	0	4.982559	-0.929534	0.239766
20	1	0	3.235829	-2.206029	0.261041
21	6	0	4.540614	1.424692	-0.080933
22	1	0	2.486356	1.983246	-0.310555
23	6	0	5.448217	0.382214	0.113570
24	1	0	5.685615	-1.744821	0.388193
25	1	0	4.897471	2.445338	-0.189813
26	1	0	6.513769	0.590424	0.163025
27	6	0	-1.846792	2.578949	0.199961
28	1	0	-1.315785	2.738476	1.143871
29	1	0	-1.246327	2.976324	-0.624649
30	1	0	-2.813314	3.082050	0.229799

syn-**5m**

E = -1181.7774511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.284420	-0.440608	-0.737415
2	6	0	-3.242430	0.963355	-0.155011
3	7	0	-1.929536	1.335338	0.151216
4	6	0	-0.953153	0.372723	0.006203
5	16	0	-1.711164	-1.314421	-0.220046
6	6	0	0.377978	0.587519	0.108489
7	8	0	-4.198202	1.698375	-0.010232
8	6	0	1.373842	-0.495173	0.001148
9	6	0	2.828625	-0.133448	-0.037976
10	6	0	-1.638110	2.688372	0.610355
11	8	0	-1.978042	-1.877317	1.152693
12	6	0	-4.525209	-1.226972	-0.336838
13	6	0	3.300291	1.160843	-0.307340
14	6	0	4.670066	1.419856	-0.346853
15	6	0	5.583513	0.391412	-0.109826
16	8	0	1.033726	-1.678006	-0.040926
17	6	0	5.123582	-0.901913	0.155528
18	1	0	-3.208111	-0.339327	-1.829376
19	1	0	0.730066	1.595183	0.299085
20	1	0	-1.014154	3.216263	-0.119411
21	1	0	-2.591355	3.205503	0.719804
22	1	0	-1.117572	2.652042	1.572279
23	1	0	-4.618444	-2.141841	-0.929445
24	1	0	-5.411973	-0.607183	-0.496086
25	1	0	-4.467868	-1.502276	0.719834
26	6	0	3.757511	-1.163143	0.184402
27	1	0	2.606641	1.969745	-0.514493
28	1	0	5.023402	2.423907	-0.564974
29	1	0	6.650542	0.595957	-0.134677
30	1	0	5.832359	-1.704914	0.338245
31	1	0	3.379466	-2.161041	0.379967

anti-**5m**

E = -1181.7748429 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.395978	-0.634809	0.268768
2	6	0	3.331090	0.836989	-0.098978
3	7	0	2.011006	1.260028	-0.279092
4	6	0	1.016033	0.314969	-0.144330
5	16	0	1.724407	-1.406061	-0.041632
6	6	0	-0.311510	0.572970	-0.163823
7	8	0	4.289155	1.579993	-0.176414
8	6	0	-1.328888	-0.484821	-0.026988
9	6	0	-2.773780	-0.091927	0.058985
10	6	0	1.727724	2.662912	-0.560855
11	8	0	1.777857	-1.969650	-1.438046
12	1	0	4.068737	-1.145282	-0.426329
13	6	0	-3.211670	1.213851	0.329856
14	6	0	-4.574185	1.500453	0.409912
15	6	0	-5.514810	0.488249	0.212940
16	8	0	-1.014004	-1.675157	0.006185
17	6	0	-5.088760	-0.816387	-0.053370
18	6	0	3.852540	-0.824553	1.720577
19	1	0	-0.642572	1.596280	-0.298829
20	1	0	1.149785	3.108120	0.256415
21	1	0	2.685767	3.173974	-0.654287
22	1	0	1.162019	2.750326	-1.493584
23	6	0	-3.729682	-1.104780	-0.123351
24	1	0	-2.497288	2.011832	0.505954
25	1	0	-4.900469	2.513609	0.628081
26	1	0	-6.576288	0.714245	0.269396
27	1	0	-5.818393	-1.607040	-0.205259
28	1	0	-3.377808	-2.111618	-0.321668
29	1	0	3.967141	-1.887074	1.954118
30	1	0	3.132403	-0.395305	2.426557
31	1	0	4.814853	-0.325466	1.869342

1n

E = -1393.0367721 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.642776	-2.860676	0.018535
2	6	0	-3.195911	-1.560149	-0.545437
3	7	0	-2.192909	-0.631495	-0.788131
4	6	0	-0.891190	-0.990713	-0.441469
5	16	0	-0.822747	-2.634973	0.219559
6	6	0	0.185152	-0.177419	-0.588821
7	8	0	-4.377638	-1.352490	-0.758757
8	6	0	1.524013	-0.627166	-0.205868
9	7	0	2.515152	0.320581	-0.391089
10	8	0	1.742959	-1.756521	0.243115
11	6	0	-2.534272	0.650899	-1.417694
12	6	0	3.895291	0.232053	-0.127633
13	6	0	4.672804	1.373104	-0.389100
14	6	0	6.044828	1.363901	-0.156839
15	6	0	6.666973	0.217134	0.340238
16	6	0	5.893689	-0.915205	0.599210
17	6	0	4.517435	-0.923793	0.372218
18	6	0	-3.356725	-3.262807	1.313173
19	1	0	-2.811462	-3.631785	-0.742228
20	1	0	0.043481	0.831499	-0.957379
21	1	0	2.209250	1.215709	-0.747617
22	1	0	-3.535390	0.499206	-1.831037
23	1	0	-1.843162	0.816696	-2.250570
24	1	0	4.195585	2.271863	-0.776447
25	1	0	6.626876	2.257644	-0.365729
26	1	0	7.737721	0.207471	0.522570
27	1	0	6.364227	-1.815313	0.986472
28	1	0	3.921350	-1.802003	0.574722
29	1	0	-2.997099	-4.233079	1.668450
30	1	0	-4.432493	-3.333104	1.123484
31	1	0	-3.184385	-2.523809	2.101853
32	6	0	-2.530372	1.840076	-0.474907
33	6	0	-1.831394	3.005018	-0.807763
34	6	0	-3.266043	1.807368	0.717057
35	6	0	-1.856788	4.117834	0.035917
36	1	0	-1.268074	3.046774	-1.738307
37	6	0	-3.286954	2.914431	1.563697
38	1	0	-3.830861	0.915522	0.974572
39	6	0	-2.581354	4.072570	1.226598
40	1	0	-1.308394	5.015573	-0.236735
41	1	0	-3.859897	2.875822	2.486242
42	1	0	-2.600041	4.934602	1.887749

syn-**5n**

E = -1468.1973153 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.754889	-2.606197	-0.410654
2	6	0	-3.270082	-1.244961	-0.855090
3	7	0	-2.223528	-0.324449	-0.944884
4	6	0	-0.971779	-0.770351	-0.551016
5	16	0	-1.150169	-2.297573	0.493591
6	6	0	0.193026	-0.125651	-0.753044
7	8	0	-4.424337	-0.984118	-1.130680
8	6	0	1.492327	-0.627816	-0.249639
9	7	0	2.552842	0.182855	-0.596650
10	8	0	1.609823	-1.661590	0.405595
11	6	0	-2.488266	1.037491	-1.410472
12	8	0	-1.543905	-1.805285	1.867989
13	6	0	3.923889	0.031823	-0.302365
14	6	0	4.795661	1.011494	-0.805631
15	6	0	6.162833	0.934324	-0.558661
16	6	0	6.682695	-0.120797	0.193529
17	6	0	5.814595	-1.092592	0.692506
18	6	0	4.441362	-1.031036	0.454763
19	6	0	-3.748702	-3.376980	0.446674
20	1	0	-2.474093	-3.168816	-1.312385
21	1	0	0.180170	0.822538	-1.284499
22	1	0	2.325745	1.011999	-1.128847
23	1	0	-3.544886	1.032745	-1.695664
24	1	0	-1.904680	1.224392	-2.320900
25	1	0	4.397312	1.837150	-1.392948
26	1	0	6.820989	1.702153	-0.956221
27	1	0	7.749482	-0.183196	0.387848
28	1	0	6.206117	-1.918412	1.280589
29	1	0	3.771351	-1.784388	0.843458
30	1	0	-3.417259	-4.408043	0.602022
31	1	0	-4.723072	-3.385956	-0.049499
32	1	0	-3.854282	-2.892779	1.421533
33	6	0	-2.216165	2.118167	-0.376720
34	6	0	-1.923540	3.414272	-0.818742
35	6	0	-2.300159	1.868794	0.998003
36	6	0	-1.731235	4.450783	0.094990
37	1	0	-1.852604	3.616446	-1.886096
38	6	0	-2.098499	2.905100	1.911200
39	1	0	-2.495008	0.863727	1.362104
40	6	0	-1.818385	4.197619	1.464938
41	1	0	-1.507951	5.452206	-0.263466
42	1	0	-2.157549	2.696495	2.975812
43	1	0	-1.663061	5.001085	2.179788

anti-**5n**

E = -1468.1945148 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.767780	-2.663815	0.062650
2	6	0	-3.324276	-1.370309	-0.508581
3	7	0	-2.302935	-0.440300	-0.719858
4	6	0	-1.025954	-0.823051	-0.340924
5	16	0	-1.127357	-2.254811	0.841570
6	6	0	0.113550	-0.170881	-0.640447
7	8	0	-4.487388	-1.176232	-0.801368
8	6	0	1.442747	-0.608748	-0.155630
9	7	0	2.469303	0.204303	-0.588762
10	8	0	1.610286	-1.597295	0.556178
11	6	0	-2.614058	0.859524	-1.315927
12	8	0	-1.453338	-1.639643	2.183232
13	6	0	3.852241	0.106927	-0.329319
14	6	0	4.679656	1.085937	-0.903724
15	6	0	6.055164	1.059086	-0.695135
16	6	0	6.627902	0.055731	0.088865
17	6	0	5.803864	-0.915567	0.658361
18	6	0	4.423109	-0.904028	0.459990
19	1	0	-3.406687	-2.997170	0.884427
20	6	0	-2.634926	-3.745140	-1.017398
21	1	0	0.056988	0.734132	-1.239702
22	1	0	2.202314	0.996621	-1.157325
23	1	0	-3.679624	0.805596	-1.560123
24	1	0	-2.066621	0.958914	-2.261961
25	1	0	4.240126	1.871747	-1.515800
26	1	0	6.678357	1.825783	-1.147459
27	1	0	7.701264	0.032859	0.253369
28	1	0	6.236499	-1.701357	1.271957
29	1	0	3.787589	-1.656454	0.904352
30	1	0	-2.287017	-4.686489	-0.582155
31	1	0	-1.927356	-3.447345	-1.799493
32	1	0	-3.609083	-3.915300	-1.486196
33	6	0	-2.327552	2.047053	-0.411476
34	6	0	-2.077089	3.295121	-0.995075
35	6	0	-2.355640	1.940133	0.983847
36	6	0	-1.871616	4.423370	-0.200501
37	1	0	-2.049395	3.387260	-2.079451
38	6	0	-2.140953	3.068106	1.777547
39	1	0	-2.516825	0.975152	1.456504
40	6	0	-1.903093	4.311857	1.190580
41	1	0	-1.681592	5.385806	-0.668271
42	1	0	-2.156607	2.969447	2.859398
43	1	0	-1.737465	5.187259	1.812597

1o

E = -1260.4791728 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.092143	-0.729474	-0.817905
2	16	0	0.334507	-2.590586	0.366016
3	6	0	0.199671	-0.977427	-0.360044
4	6	0	1.225455	-0.094396	-0.458954
5	6	0	-2.037587	-1.725837	-0.625066
6	8	0	-3.210048	-1.620665	-0.941185
7	6	0	-1.439385	-2.962727	0.031369
8	6	0	2.553855	-0.429337	0.029416
9	8	0	2.871061	-1.487599	0.557020
10	1	0	-1.488475	-3.770272	-0.708152
11	1	0	1.074004	0.891244	-0.876168
12	6	0	-1.482901	0.514887	-1.500569
13	1	0	-2.397998	0.259985	-2.041491
14	8	0	3.428628	0.588688	-0.170130
15	6	0	4.776642	0.353394	0.286598
16	1	0	4.755661	0.130244	1.358503
17	1	0	5.176678	-0.529068	-0.223923
18	6	0	5.584701	1.601262	-0.018196
19	1	0	5.169054	2.472150	0.498993
20	1	0	6.619974	1.465016	0.313230
21	1	0	5.591615	1.810080	-1.092947
22	6	0	-2.225394	-3.370692	1.281600
23	1	0	-3.273696	-3.530033	1.009918
24	1	0	-1.825957	-4.296846	1.705411
25	1	0	-2.173274	-2.591386	2.048140
26	1	0	-0.707474	0.755988	-2.233441
27	6	0	-1.730532	1.688606	-0.571406
28	6	0	-1.004962	2.875668	-0.712747
29	6	0	-2.721763	1.611205	0.417033
30	6	0	-1.254413	3.966889	0.122581
31	1	0	-0.241450	2.952099	-1.484361
32	6	0	-2.967669	2.697341	1.255154
33	1	0	-3.307294	0.701336	0.517451
34	6	0	-2.233808	3.877953	1.111223
35	1	0	-0.680562	4.881664	0.001576
36	1	0	-3.738447	2.625375	2.017888
37	1	0	-2.428076	4.724001	1.764855

syn-**5o**

E = -1335.6392927 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.196326	-2.362426	-0.370432
2	6	0	-2.482247	-0.961073	-0.894007
3	7	0	-1.307031	-0.209728	-0.966329
4	6	0	-0.157048	-0.814856	-0.489665
5	16	0	-0.606918	-2.249443	0.601695
6	6	0	1.101035	-0.366186	-0.661911
7	8	0	-3.570976	-0.548469	-1.239984
8	6	0	2.278110	-1.030447	-0.077554
9	8	0	3.408584	-0.392564	-0.455632
10	8	0	2.269551	-2.012707	0.643761
11	6	0	-1.341072	1.154899	-1.496198
12	8	0	-0.981777	-1.649340	1.937745
13	6	0	-3.332114	-2.938641	0.463092
14	6	0	4.642512	-0.939481	0.063670
15	6	0	5.775740	-0.067981	-0.443592
16	1	0	-1.962178	-3.000633	-1.234317
17	1	0	1.290878	0.536484	-1.232455
18	1	0	-2.363893	1.285472	-1.862796
19	1	0	-0.670684	1.217380	-2.362161
20	1	0	-3.171561	-4.001641	0.666200
21	1	0	-4.273799	-2.816839	-0.079130
22	1	0	-3.403277	-2.406839	1.416022
23	1	0	4.588476	-0.952230	1.156831
24	1	0	4.737032	-1.976762	-0.274102
25	1	0	6.732254	-0.450715	-0.071451
26	1	0	5.808408	-0.064583	-1.537870
27	1	0	5.659820	0.964319	-0.098385
28	6	0	-0.994407	2.229709	-0.478435
29	6	0	-0.499798	3.456656	-0.937113
30	6	0	-1.203677	2.048540	0.893419
31	6	0	-0.231384	4.493525	-0.043526
32	1	0	-0.326607	3.604207	-2.001517
33	6	0	-0.925938	3.084009	1.787408
34	1	0	-1.557002	1.093886	1.273285
35	6	0	-0.444559	4.309064	1.323667
36	1	0	0.150873	5.440635	-0.414952
37	1	0	-1.084537	2.927240	2.850793
38	1	0	-0.230333	5.112578	2.023117

anti-**5o**

E = -1335.636451 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.944384	-2.619817	0.107802
2	6	0	-2.437344	-1.332035	-0.533500
3	7	0	-1.380869	-0.440283	-0.735921
4	6	0	-0.133633	-0.845910	-0.293006
5	16	0	-0.321993	-2.232902	0.930726
6	6	0	1.038126	-0.245183	-0.575569
7	8	0	-3.581133	-1.118157	-0.881710
8	6	0	2.326329	-0.705356	-0.031044
9	8	0	3.334749	0.055941	-0.512379
10	8	0	2.494041	-1.632971	0.741441
11	6	0	-1.625589	0.847438	-1.388150
12	8	0	-0.671383	-1.569664	2.242969
13	1	0	-2.622500	-2.898320	0.918574
14	6	0	4.658670	-0.282496	-0.039290
15	6	0	5.628065	0.711980	-0.649516
16	6	0	-1.811761	-3.747695	-0.923403
17	1	0	1.069067	0.633842	-1.210206
18	1	0	-2.673706	0.806919	-1.700555
19	1	0	-1.013855	0.907120	-2.296787
20	1	0	4.661249	-0.244518	1.054576
21	1	0	4.884830	-1.312583	-0.334034
22	1	0	6.647216	0.487920	-0.316321
23	1	0	5.604450	0.662506	-1.742919
24	1	0	5.382769	1.734338	-0.344777
25	1	0	-1.513363	-4.682258	-0.439546
26	1	0	-1.067568	-3.505698	-1.690598
27	1	0	-2.774585	-3.902420	-1.419995
28	6	0	-1.374921	2.054848	-0.499219
29	6	0	-1.085198	3.285350	-1.101284
30	6	0	-1.475809	1.984629	0.894800
31	6	0	-0.912946	4.432454	-0.326659
32	1	0	-0.997390	3.348104	-2.184373
33	6	0	-1.294424	3.131753	1.669308
34	1	0	-1.668201	1.033669	1.383821
35	6	0	-1.017824	4.358018	1.063378
36	1	0	-0.689883	5.380586	-0.808701
37	1	0	-1.366815	3.061558	2.751126
38	1	0	-0.878072	5.248596	1.670072

1p

E = -3679.1607033 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.197274	3.382022	-0.069827
2	6	0	-0.067456	2.780754	0.527937
3	7	0	0.053284	1.411085	0.728251
4	6	0	1.237018	0.804867	0.315512
5	16	0	2.364107	1.986949	-0.374968
6	6	0	1.494225	-0.523917	0.427480
7	8	0	-1.068493	3.416280	0.803035
8	6	0	2.761031	-1.085020	-0.017155
9	8	0	2.816573	-2.421711	0.204184
10	8	0	3.675608	-0.452575	-0.528742
11	6	0	-1.074989	0.674867	1.301871
12	6	0	0.891504	4.209568	-1.322257
13	6	0	4.037272	-3.074548	-0.204848
14	6	0	3.903418	-4.546383	0.139287
15	1	0	1.634161	4.032071	0.697115
16	1	0	0.764292	-1.203432	0.847407
17	1	0	-1.642276	1.405714	1.883044
18	1	0	-0.680149	-0.078419	1.990340
19	1	0	1.799488	4.687115	-1.702186
20	1	0	0.163708	4.986724	-1.068665
21	1	0	0.474918	3.581998	-2.116039
22	1	0	4.182463	-2.915667	-1.278594
23	1	0	4.881066	-2.606838	0.313158
24	1	0	4.812372	-5.081747	-0.156113
25	1	0	3.756507	-4.684638	1.215377
26	1	0	3.053464	-4.995250	-0.384814
27	6	0	-1.971688	0.042252	0.223058
28	1	0	-1.386954	-0.640714	-0.401689
29	1	0	-2.355380	0.834879	-0.427418
30	6	0	-3.133825	-0.708120	0.857410
31	1	0	-2.804244	-1.536247	1.486787
32	1	0	-3.789321	-0.052516	1.432242
33	35	0	-4.288430	-1.527881	-0.523624

syn-**5p**

E = -3754.3196333a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.500731	-3.144877	-0.302186
2	6	0	0.119072	-2.695016	-0.751133
3	7	0	0.058214	-1.304060	-0.867423
4	6	0	1.159581	-0.590797	-0.430867
5	16	0	2.316985	-1.687422	0.538273
6	6	0	1.352918	0.735631	-0.576901
7	8	0	-0.809964	-3.428783	-1.024200
8	6	0	2.541249	1.436423	-0.062959
9	8	0	2.480387	2.749549	-0.379642
10	8	0	3.461757	0.935680	0.558624
11	6	0	-1.162476	-0.679185	-1.385629
12	8	0	1.830868	-1.689972	1.965143
13	6	0	1.476254	-4.372916	0.597690
14	6	0	3.587513	3.558987	0.081297
15	6	0	3.321835	4.986443	-0.357384
16	1	0	2.096999	-3.321008	-1.208600
17	1	0	0.620328	1.352447	-1.086627
18	1	0	-1.687637	-1.462658	-1.936529
19	1	0	-0.876494	0.104688	-2.095441
20	1	0	2.482025	-4.781303	0.733238
21	1	0	0.838941	-5.137383	0.144765
22	1	0	1.072459	-4.109737	1.579233
23	1	0	3.659107	3.467428	1.169690
24	1	0	4.514398	3.161829	-0.345115
25	1	0	4.140864	5.633778	-0.025827
26	1	0	3.248889	5.054885	-1.447593
27	1	0	2.389347	5.362306	0.075657
28	6	0	-2.053724	-0.122301	-0.262032
29	1	0	-1.502685	0.616206	0.329288
30	1	0	-2.327755	-0.939290	0.412998
31	6	0	-3.310906	0.513453	-0.838966
32	1	0	-3.091069	1.358159	-1.493860
33	1	0	-3.934875	-0.206010	-1.370952
34	35	0	-4.457679	1.248171	0.594294

anti-**5p**

E = -3754.3170065a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.589072	-3.100253	0.209542
2	6	0	0.221901	-2.758168	-0.356284
3	7	0	0.094350	-1.389121	-0.600097
4	6	0	1.154764	-0.579017	-0.237857
5	16	0	2.422654	-1.524088	0.754419
6	6	0	1.254559	0.744665	-0.475062
7	8	0	-0.644543	-3.567357	-0.624086
8	6	0	2.422711	1.542838	-0.069774
9	8	0	2.255883	2.833738	-0.435707
10	8	0	3.412633	1.128505	0.507262
11	6	0	-1.137972	-0.884321	-1.213693
12	8	0	2.087201	-1.341439	2.211664
13	1	0	1.458883	-3.676165	1.130398
14	6	0	3.334270	3.731562	-0.083315
15	6	0	2.931742	5.123980	-0.530696
16	6	0	2.435973	-3.871827	-0.810287
17	1	0	0.462300	1.283388	-0.983535
18	1	0	-1.595948	-1.741081	-1.713127
19	1	0	-0.865438	-0.147035	-1.976422
20	1	0	3.498263	3.675479	0.997333
21	1	0	4.250921	3.389358	-0.574770
22	1	0	3.725706	5.836421	-0.282061
23	1	0	2.766469	5.156407	-1.612454
24	1	0	2.012345	5.444886	-0.030748
25	1	0	3.388852	-4.178103	-0.369047
26	1	0	2.648585	-3.263747	-1.696862
27	1	0	1.893098	-4.765694	-1.131803
28	6	0	-2.103334	-0.287815	-0.174367
29	1	0	-1.617292	0.527034	0.371969
30	1	0	-2.361014	-1.060668	0.556809
31	6	0	-3.367790	0.226476	-0.848304
32	1	0	-3.165437	1.024611	-1.564326
33	1	0	-3.930636	-0.568301	-1.339609
34	35	0	-4.608496	1.011890	0.474736

1q

E = -1660.2277378 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.561895	-0.129019	-1.201152
2	1	0	-2.964349	-0.475122	-2.158440
3	7	0	-0.802567	1.515153	-1.234036
4	16	0	-1.022273	-1.080102	-0.850114
5	6	0	-0.032675	0.390470	-0.933422
6	6	0	1.309731	0.426340	-0.737665
7	1	0	1.827937	1.377408	-0.767920
8	6	0	-2.170201	1.331581	-1.358692
9	8	0	-2.963058	2.235549	-1.563408
10	6	0	2.057324	-0.795591	-0.437906
11	8	0	1.518205	-1.904005	-0.367758
12	7	0	3.413055	-0.597433	-0.242616
13	1	0	3.734057	0.358762	-0.309995
14	6	0	4.418580	-1.536564	0.055404
15	6	0	5.724850	-1.046341	0.223283
16	6	0	4.179170	-2.914453	0.186203
17	6	0	6.774242	-1.912276	0.515509
18	1	0	5.915722	0.020992	0.123639
19	6	0	5.242908	-3.767819	0.479248
20	1	0	3.175150	-3.293085	0.058698
21	6	0	6.540599	-3.282556	0.645861
22	1	0	7.776746	-1.511747	0.641137
23	1	0	5.045968	-4.832267	0.577735
24	1	0	7.358110	-3.960510	0.873736
25	6	0	-3.644693	-0.288979	-0.130970
26	1	0	-3.258340	-0.052402	0.866489
27	1	0	-4.452244	0.425626	-0.336542
28	6	0	-4.225383	-1.691002	-0.119607
29	8	0	-5.068851	-1.853667	0.915025
30	8	0	-3.975477	-2.549805	-0.939445
31	6	0	-5.696931	-3.156134	1.023917
32	1	0	-6.268688	-3.345818	0.110005
33	1	0	-4.912856	-3.916635	1.089503
34	6	0	-6.579234	-3.133517	2.257164
35	1	0	-7.349140	-2.359750	2.174410
36	1	0	-7.075715	-4.102872	2.374254
37	1	0	-5.988306	-2.938243	3.157648
38	6	0	-0.230991	2.850120	-1.457924
39	1	0	0.620258	2.745405	-2.138084
40	1	0	-1.016248	3.405523	-1.978315
41	6	0	0.180283	3.584939	-0.195566
42	6	0	1.460204	4.137732	-0.083350
43	6	0	-0.731440	3.765850	0.852982
44	6	0	1.830838	4.852658	1.057834
45	1	0	2.171640	4.015701	-0.898215
46	6	0	-0.361133	4.473191	1.995534
47	1	0	-1.736145	3.361315	0.765387
48	6	0	0.921415	5.017823	2.102085
49	1	0	2.829030	5.276204	1.129949
50	1	0	-1.076945	4.605738	2.802331
51	1	0	1.207345	5.570081	2.993045

syn-**5q**

E = -1735.389511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.523612	0.066341	-0.902688
2	6	0	-2.069968	1.490160	-1.176826
3	7	0	-0.680721	1.590461	-1.120914
4	6	0	0.011910	0.445641	-0.757115
5	16	0	-1.141157	-0.779089	0.033979
6	6	0	1.346926	0.282749	-0.823918
7	8	0	-2.805449	2.422515	-1.439414
8	6	0	2.033561	-0.941825	-0.351469
9	7	0	3.399272	-0.900367	-0.538764
10	8	0	1.442726	-1.893856	0.154367
11	6	0	-0.031202	2.870964	-1.405322
12	8	0	-1.303674	-0.322482	1.467940
13	6	0	4.373290	-1.864701	-0.206013
14	6	0	5.709981	-1.549423	-0.500688
15	6	0	6.729570	-2.448136	-0.202339
16	6	0	6.432690	-3.675260	0.393816
17	6	0	5.103980	-3.986171	0.685018
18	6	0	4.069222	-3.097448	0.392812
19	6	0	-3.833654	0.008829	-0.133807
20	1	0	-2.607641	-0.476111	-1.852776
21	1	0	1.955370	1.097174	-1.208480
22	1	0	3.768176	-0.055346	-0.953581
23	1	0	-0.842613	3.529638	-1.729789
24	1	0	0.647802	2.744442	-2.257855
25	1	0	5.948729	-0.593988	-0.964921
26	1	0	7.757611	-2.185900	-0.437217
27	1	0	7.226829	-4.378316	0.627838
28	1	0	4.859328	-4.937701	1.149583
29	1	0	3.041339	-3.340280	0.620849
30	1	0	-4.499528	0.800263	-0.496860
31	1	0	-3.652939	0.210787	0.928782
32	6	0	0.709572	3.474893	-0.223119
33	6	0	1.748146	4.380896	-0.471410
34	6	0	0.352725	3.193015	1.100509
35	6	0	2.412400	5.007706	0.583099
36	1	0	2.035453	4.603448	-1.497598
37	6	0	1.024353	3.814170	2.154896
38	1	0	-0.429210	2.469869	1.315659
39	6	0	2.051226	4.724746	1.901504
40	1	0	3.214328	5.710857	0.374166
41	1	0	0.743448	3.579563	3.177860
42	1	0	2.570656	5.206260	2.725503
43	6	0	-4.522254	-1.334335	-0.276989
44	8	0	-4.122267	-2.249423	-0.968022
45	8	0	-5.642682	-1.379617	0.463137
46	6	0	-6.387408	-2.622373	0.417844
47	1	0	-5.723900	-3.437928	0.721433
48	1	0	-6.692978	-2.809503	-0.616583
49	6	0	-7.575720	-2.473241	1.348130
50	1	0	-8.220351	-1.647021	1.031655
51	1	0	-8.168065	-3.394688	1.342538
52	1	0	-7.246832	-2.281032	2.374260

anti-**5q**

E = -1735.3820964 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.386582	-0.717135	1.118659
2	6	0	-2.444318	0.565774	0.306319
3	7	0	-1.187767	0.887645	-0.210948
4	6	0	-0.142809	0.033653	0.105187
5	16	0	-0.604274	-1.019435	1.564998
6	6	0	1.087099	0.058797	-0.442530
7	8	0	-3.452888	1.204233	0.077782
8	6	0	2.170530	-0.859248	-0.022349
9	7	0	3.349521	-0.652040	-0.706239
10	8	0	2.026350	-1.719139	0.845000
11	6	0	-1.034207	2.069381	-1.060667
12	8	0	-0.336324	-0.157618	2.775840
13	6	0	4.584398	-1.321470	-0.576123
14	6	0	5.632530	-0.893425	-1.407429
15	6	0	6.881017	-1.504179	-1.340452
16	6	0	7.104051	-2.551241	-0.444204
17	6	0	6.061293	-2.974247	0.380783
18	6	0	4.803462	-2.373442	0.327215
19	1	0	1.307365	0.802252	-1.203995
20	1	0	3.347026	0.098560	-1.383717
21	1	0	-2.050834	2.453013	-1.191092
22	1	0	-0.674805	1.752894	-2.048114
23	1	0	5.465855	-0.076981	-2.108095
24	1	0	7.679669	-1.158624	-1.991213
25	1	0	8.077794	-3.029332	-0.389896
26	1	0	6.222223	-3.787147	1.083892
27	1	0	3.998560	-2.701351	0.969126
28	6	0	-0.123273	3.140907	-0.483397
29	6	0	0.491014	4.045776	-1.358163
30	6	0	0.080127	3.279147	0.894396
31	6	0	1.285174	5.081872	-0.866328
32	1	0	0.341735	3.943814	-2.431663
33	6	0	0.882188	4.311151	1.384539
34	1	0	-0.362877	2.569434	1.587530
35	6	0	1.482985	5.216823	0.508972
36	1	0	1.752656	5.778450	-1.557279
37	1	0	1.038563	4.402083	2.455794
38	1	0	2.105652	6.019298	0.894912
39	1	0	-2.912144	-0.579848	2.067328
40	6	0	-3.001167	-1.899442	0.348262
41	1	0	-2.768425	-2.829520	0.880402
42	1	0	-2.597068	-1.978693	-0.664668
43	6	0	-4.519238	-1.769136	0.307932
44	8	0	-5.208885	-1.640509	1.294884
45	8	0	-4.987028	-1.833118	-0.949975
46	6	0	-6.424210	-1.697182	-1.093413
47	1	0	-6.724075	-0.740169	-0.656409
48	1	0	-6.908908	-2.493632	-0.520163
49	6	0	-6.743382	-1.779267	-2.573569
50	1	0	-7.823670	-1.679132	-2.724516
51	1	0	-6.242948	-0.977871	-3.126291
52	1	0	-6.425127	-2.739761	-2.991619

1r

E = -1604.8609502 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.333801	0.119117	-1.218441
2	1	0	-2.814501	-0.166567	-2.159367
3	7	0	-0.167719	1.166561	-1.300213
4	16	0	-1.144262	-1.215106	-0.759701
5	6	0	0.227318	-0.104798	-0.889174
6	6	0	1.518850	-0.449608	-0.627404
7	1	0	2.293416	0.297263	-0.722644
8	6	0	-1.527323	1.383208	-1.466680
9	8	0	-2.013459	2.461101	-1.764909
10	6	0	1.861040	-1.804199	-0.225311
11	8	0	0.995722	-2.688635	-0.160911
12	6	0	-3.422510	0.366215	-0.170741
13	1	0	-2.990857	0.546284	0.819931
14	1	0	-3.977091	1.273095	-0.444855
15	6	0	-4.397582	-0.793595	-0.084659
16	8	0	-5.260044	-0.621498	0.932439
17	8	0	-4.409537	-1.744463	-0.838159
18	6	0	-6.250848	-1.665615	1.108968
19	1	0	-6.842013	-1.745425	0.191247
20	1	0	-5.731179	-2.617723	1.253677
21	6	0	-7.100817	-1.287813	2.306734
22	1	0	-7.604958	-0.329919	2.143544
23	1	0	-7.864374	-2.055014	2.474775
24	1	0	-6.489143	-1.206866	3.210889
25	6	0	0.777988	2.256820	-1.583759
26	1	0	1.580548	1.854609	-2.209416
27	1	0	0.206056	2.972644	-2.180387
28	6	0	1.347066	2.937246	-0.352655
29	6	0	2.730504	3.059451	-0.185228
30	6	0	0.494711	3.496175	0.608930
31	6	0	3.258447	3.718658	0.927371
32	1	0	3.402026	2.643776	-0.934155
33	6	0	1.020041	4.148982	1.722968
34	1	0	-0.581545	3.429158	0.474569
35	6	0	2.403312	4.260784	1.886478
36	1	0	4.335443	3.805628	1.043187
37	1	0	0.348650	4.577568	2.462199
38	1	0	2.810449	4.771107	2.755030
39	6	0	3.288960	-2.136924	0.096462
40	6	0	4.256226	-1.167434	0.402042
41	6	0	3.655812	-3.491519	0.112346
42	6	0	5.563534	-1.546009	0.707660
43	1	0	3.989748	-0.115242	0.434760
44	6	0	4.963235	-3.868032	0.405799
45	1	0	2.893807	-4.231342	-0.109765
46	6	0	5.921750	-2.895189	0.703433
47	1	0	6.301667	-0.787053	0.953135
48	1	0	5.236892	-4.919784	0.405668
49	1	0	6.942248	-3.187991	0.936165

syn-**5r**

E = -1680.0202246 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.225834	0.122690	-0.918040
2	6	0	-1.468890	1.382959	-1.300230
3	7	0	-0.094494	1.214283	-1.123349
4	6	0	0.319029	0.014769	-0.571490
5	16	0	-1.115521	-0.857257	0.226662
6	6	0	1.593443	-0.424591	-0.501892
7	8	0	-1.973108	2.400485	-1.734205
8	6	0	1.970721	-1.682940	0.172853
9	8	0	1.165639	-2.302418	0.868465
10	6	0	0.823583	2.297116	-1.482096
11	8	0	-1.295452	-0.213445	1.584443
12	6	0	-3.569075	0.421651	-0.272129
13	1	0	-2.355395	-0.504009	-1.809288
14	1	0	2.381208	0.192528	-0.918678
15	1	0	0.194431	3.046823	-1.971351
16	1	0	1.534513	1.926002	-2.230550
17	1	0	-4.033795	1.274507	-0.780140
18	1	0	-3.421895	0.717276	0.773587
19	6	0	1.563810	2.905894	-0.301747
20	6	0	2.773730	3.570362	-0.536961
21	6	0	1.048555	2.867224	0.998722
22	6	0	3.453640	4.198973	0.506135
23	1	0	3.185313	3.600761	-1.544209
24	6	0	1.734523	3.489407	2.043213
25	1	0	0.127503	2.330423	1.208372
26	6	0	2.934266	4.159838	1.801271
27	1	0	4.390941	4.711975	0.307749
28	1	0	1.328313	3.443651	3.049837
29	1	0	3.464848	4.642883	2.617249
30	6	0	-4.504990	-0.769838	-0.326556
31	8	0	-4.246972	-1.830765	-0.858511
32	8	0	-5.665778	-0.497162	0.292405
33	6	0	-6.641653	-1.568797	0.318105
34	1	0	-6.182617	-2.447399	0.781667
35	1	0	-6.898554	-1.832504	-0.712877
36	6	0	-7.842960	-1.070612	1.098066
37	1	0	-8.281032	-0.187312	0.622401
38	1	0	-8.607177	-1.854269	1.140328
39	1	0	-7.561820	-0.807454	2.122626
40	6	0	3.370934	-2.192701	0.013036
41	6	0	3.792284	-3.212925	0.881623
42	6	0	4.259781	-1.723751	-0.966824
43	6	0	5.075850	-3.739929	0.783501
44	1	0	3.091517	-3.573760	1.627057
45	6	0	5.543220	-2.259284	-1.070774
46	1	0	3.951994	-0.956790	-1.670530
47	6	0	5.955368	-3.263515	-0.193382
48	1	0	5.393171	-4.523196	1.466407
49	1	0	6.219939	-1.893595	-1.838118
50	1	0	6.957741	-3.675962	-0.271908

anti-**5r**

E = -1680.0186018 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.272772	0.520113	1.387909
2	6	0	-1.775440	1.533944	0.374343
3	7	0	-0.531151	1.184016	-0.139681
4	6	0	-0.004679	-0.036312	0.240345
5	16	0	-1.174190	-0.995108	1.326912
6	6	0	1.212209	-0.506384	-0.111344
7	8	0	-2.374730	2.547600	0.065834
8	6	0	1.652280	-1.877761	0.198123
9	8	0	0.871934	-2.712941	0.656626
10	6	0	0.087673	2.034119	-1.169420
11	8	0	-0.605219	-1.127600	2.714534
12	1	0	1.874661	0.135325	-0.678531
13	1	0	-0.713762	2.696080	-1.508350
14	1	0	0.376693	1.388165	-2.004727
15	6	0	1.275421	2.841819	-0.680494
16	6	0	2.488969	2.807962	-1.376251
17	6	0	1.162923	3.665158	0.447405
18	6	0	3.575534	3.576515	-0.951615
19	1	0	2.584362	2.181957	-2.261424
20	6	0	2.248027	4.427854	0.876205
21	1	0	0.219933	3.712431	0.985524
22	6	0	3.458123	4.384967	0.178761
23	1	0	4.511069	3.540105	-1.503347
24	1	0	2.148167	5.060046	1.754322
25	1	0	4.302555	4.980569	0.514507
26	1	0	-2.088859	0.914342	2.394077
27	6	0	-3.755560	0.207277	1.211974
28	1	0	-4.333313	1.134089	1.309040
29	1	0	-4.112173	-0.471872	1.994033
30	6	0	-4.047253	-0.391402	-0.152135
31	8	0	-3.215454	-0.533756	-1.027054
32	8	0	-5.337659	-0.732677	-0.271811
33	6	0	-5.733528	-1.304356	-1.546175
34	1	0	-5.126187	-2.195741	-1.730362
35	1	0	-5.511594	-0.579433	-2.335386
36	6	0	-7.213023	-1.624515	-1.459925
37	1	0	-7.551662	-2.060190	-2.406104
38	1	0	-7.412218	-2.343472	-0.658991
39	1	0	-7.799366	-0.720479	-1.267439
40	6	0	3.071904	-2.259093	-0.098446
41	6	0	3.388594	-3.626837	-0.114145
42	6	0	4.090328	-1.321407	-0.329451
43	6	0	4.688545	-4.049113	-0.373473
44	1	0	2.593928	-4.338882	0.082389
45	6	0	5.395589	-1.745644	-0.578689
46	1	0	3.881271	-0.256822	-0.288141
47	6	0	5.695983	-3.108393	-0.607714
48	1	0	4.920256	-5.110646	-0.390391
49	1	0	6.178671	-1.011105	-0.746077
50	1	0	6.712608	-3.436922	-0.807206