Electronic Supplementary Information

Halogen bond does not dictate the conformational preferences of *cis*-1,3-disubstituted cyclohexanes

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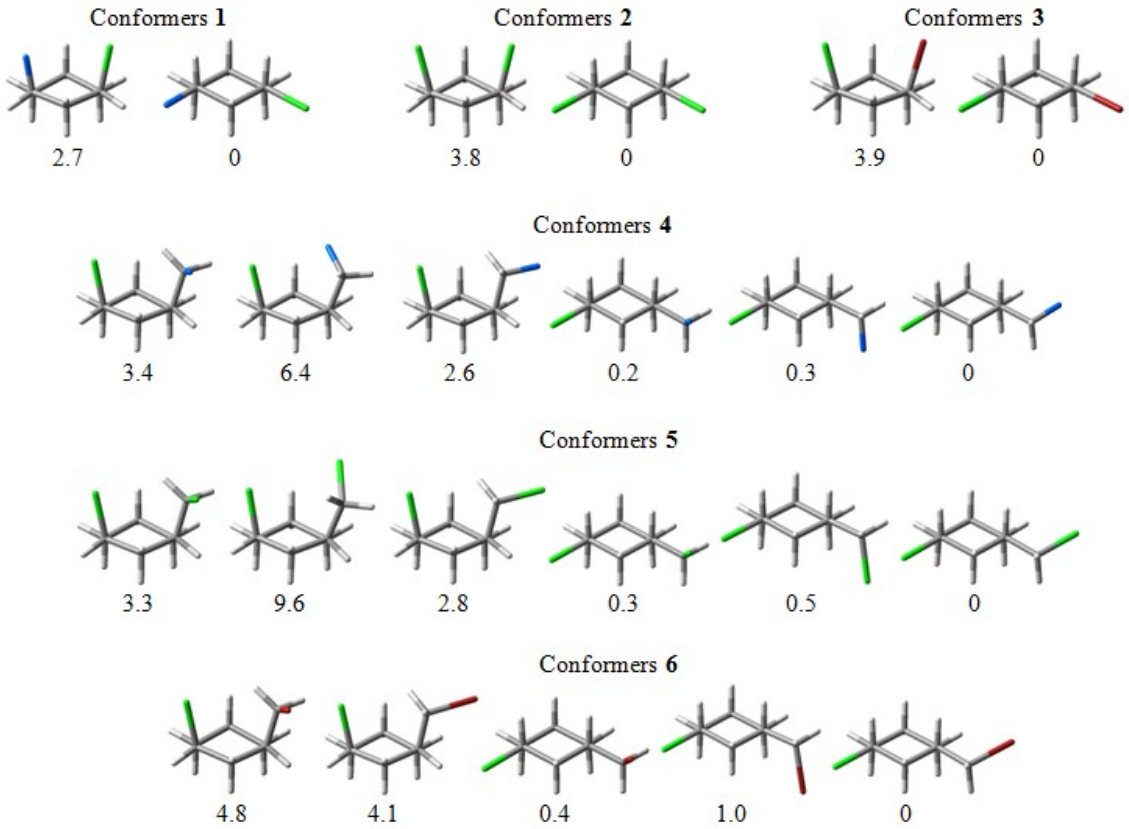

Figure S1. Diaxial and diequatorial structures for **1-6** (gas phase) and the corresponding relative Gibbs free energies.

Total electronic energies (hartrees) and standard coordinates for **1-6c** in gas phase and implicit DMSO, obtained at the ωB97X-D/6-311++G(2d,2p) level.

1(gas) E = -794.73876119
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004624	-0.000000698	0.000009434
2	6	-0.000000896	-0.000004890	0.000012448
3	6	-0.000000614	0.000001560	0.000005462
4	6	-0.000002451	-0.000005343	0.000002718
5	6	-0.000004035	0.000010157	-0.000019727
6	6	0.000003874	0.000001178	-0.000011005
7	1	0.000004641	-0.000001721	0.000008830
8	1	-0.000003020	0.000001484	0.000019279
9	1	0.000007408	-0.000011631	0.000015506
10	1	0.000006412	-0.000009959	-0.000005423
11	1	-0.000000371	-0.000005408	0.000009290
12	1	-0.000005865	0.000010436	0.000000151
13	1	-0.000001954	0.000007418	-0.000010881
14	1	-0.000009933	0.000008465	-0.000012146
15	1	-0.000008302	0.000009895	0.000004684
16	1	-0.000005532	0.000006294	-0.000011403
17	9	0.000002810	0.000002822	-0.000013116
18	17	0.000013204	-0.000020060	-0.000004101

2(gas) E = -1155.10371655
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000051104	-0.000027358	-0.000072667
2	6	0.000049847	-0.000139234	0.000019869
3	6	0.000100104	0.000095183	-0.000187459
4	6	0.000032337	0.000041055	0.000028085
5	6	-0.000128170	0.000184093	-0.000055965
6	6	-0.000076499	-0.000090696	0.000091851
7	1	-0.000062613	-0.000024786	0.000038289
8	1	0.000009533	0.000046937	-0.000066101
9	1	-0.000041294	0.000035486	0.000042338
10	1	0.000021502	0.000004598	0.000035687
11	1	0.000019951	0.000079378	-0.000019619
12	1	-0.000025141	0.000001557	-0.000046075
13	1	-0.000012446	-0.000073038	0.000028753
14	1	0.000038739	-0.000064558	-0.000018938
15	1	-0.000029264	0.000062238	-0.000044840
16	1	0.000065978	-0.000006235	-0.000018624
17	17	0.000018922	-0.000052873	0.000138148
18	17	0.000069618	-0.000071747	0.000107268

3(gas) E = -3269.06240547
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000023261	-0.000029379	0.000015147
2	6	-0.000027767	-0.000098700	0.000006556
3	6	0.000063263	0.000001170	0.000012386
4	6	0.000045277	0.000001444	-0.000013992
5	6	-0.000096114	0.000177911	-0.000070892
6	6	-0.000032660	-0.000082881	0.000040107
7	1	-0.000034357	-0.000025668	-0.000001067
8	1	-0.000000051	0.000023060	-0.000019298
9	1	-0.000052064	0.000008943	0.000038374
10	1	0.000007845	-0.000002939	0.000043455
11	1	-0.000021709	0.000029911	0.000006614
12	1	0.000017641	0.000020862	-0.000015377
13	1	-0.000002759	-0.000057181	-0.000028175
14	1	0.000054112	-0.000014513	-0.000008625
15	1	-0.000011611	0.000063410	-0.000006841
16	1	0.000045903	0.000026975	-0.000005726
17	17	0.000084493	-0.000043393	0.000039866
18	35	-0.000016182	0.000000968	-0.000032512

4a(gas) E = -834.04928579
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002816	0.000006586	0.000009436
2	6	0.000016743	-0.000022436	0.000003268
3	6	0.000027765	0.000024431	-0.000021757
4	6	-0.000013013	-0.000010208	0.000042586
5	6	-0.000063100	0.000045714	-0.000026538
6	6	0.000009055	-0.000002396	-0.000020290
7	1	0.000001268	0.000015832	0.000014081
8	1	-0.000010836	0.000009121	0.000006584
9	1	0.000018390	0.000005303	0.000008823
10	1	0.000013849	-0.000022246	-0.000007791
11	1	0.000007745	-0.000003369	-0.000007696
12	1	-0.000016673	0.000006536	-0.000003110
13	1	-0.000010514	0.000001383	-0.000004766
14	1	-0.000020607	-0.000008218	-0.000011354
15	1	-0.000014347	0.000001474	-0.000007497
16	1	-0.000006755	-0.000005377	-0.000019415
17	17	0.000002820	-0.000018982	0.000000083
18	6	0.000007926	-0.000016490	0.000032847
19	1	0.000022498	-0.000008738	0.000013579
20	1	0.000015205	-0.000009360	-0.000006648
21	9	0.000015396	0.000011441	0.000005574

4b(gas) E = -834.04395418
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001534	0.000011797	0.000003649
2	6	-0.000010274	-0.000014409	-0.000000775
3	6	0.000013710	0.000012660	-0.000005932
4	6	-0.000014691	-0.000012566	0.000011842
5	6	-0.000009187	0.000010149	-0.000011874
6	6	-0.000001850	-0.000009267	-0.000013638
7	1	-0.000002008	-0.000001719	0.000012547
8	1	-0.000005140	-0.000003144	0.000000267
9	1	0.000004753	0.000001387	-0.000007899
10	1	-0.000000083	-0.000002589	-0.000003458
11	1	-0.000000166	-0.000003977	-0.000011715
12	1	-0.000007238	-0.000008509	0.000006824
13	1	0.000001647	0.000003879	0.000010162
14	1	-0.000006590	-0.000002929	-0.000000119
15	1	-0.000006524	-0.000005648	-0.000007060
16	1	-0.000011221	-0.000002008	-0.000013116
17	17	0.000002868	0.000002699	0.000011985
18	6	0.000024922	0.000021805	0.000016432
19	1	-0.000000282	0.000005320	0.000009318
20	1	0.000011850	-0.000002882	0.000008339
21	9	0.000013971	-0.000000050	-0.000015779

4c(gas) E = -834.05080625
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000022643	-0.000093644	-0.000082855
2	6	0.000049644	0.000018533	-0.000006485
3	6	-0.000091520	0.000004086	0.000093385
4	6	0.000112146	-0.000000522	-0.000043435
5	6	-0.000104093	0.000159211	-0.000119404
6	6	-0.000070798	-0.000076968	0.000077758
7	1	-0.000003470	-0.000005303	0.000008729
8	1	-0.000004268	-0.000001148	-0.000033288
9	1	-0.000016788	0.000008263	0.000029932
10	1	0.000031903	0.000007369	0.000029094
11	1	0.000004578	0.000044832	-0.000014750
12	1	-0.000017181	0.000006070	-0.000004917
13	1	-0.000018983	-0.000043577	0.000012558
14	1	0.000019675	-0.000037786	-0.000005185
15	1	-0.000008548	0.000020801	-0.000035086
16	1	0.000038552	0.000009135	0.000002059
17	17	0.000058326	-0.000048114	0.000100012
18	6	0.000218834	-0.000083135	-0.000079676
19	1	-0.000001944	0.000058569	0.000020994
20	1	-0.000065353	-0.000006429	-0.000034045
21	9	-0.000108069	0.000059757	0.000084604

5a(gas) E = -1194.41892746
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001563	0.000022803	0.000026673
2	6	0.000025717	-0.000023757	0.000013989
3	6	0.000009510	0.000018869	-0.000032799
4	6	-0.000010756	0.000026509	0.000031652
5	6	-0.000071376	0.000016397	-0.000053882
6	6	0.000047162	-0.000011691	-0.000018842
7	1	0.000004085	0.000020231	0.000014056
8	1	0.000023822	0.000022019	0.000025053
9	1	0.000016972	0.000012609	0.000016236
10	1	0.000010792	-0.000035975	-0.000009004
11	1	0.000028975	-0.000019134	0.000014686
12	1	-0.000017795	0.000020553	-0.000002332
13	1	-0.000023090	0.000014001	-0.000028569
14	1	-0.000014688	-0.000001531	-0.000005764
15	1	-0.000002267	-0.000000178	0.000011969
16	1	-0.000002196	-0.000025947	-0.000009505
17	17	0.000012828	-0.000044282	0.000002191
18	6	-0.000038506	-0.000041884	0.000016962
19	1	0.000003546	-0.000003443	-0.000011106
20	1	0.000012001	0.000004631	0.000002657
21	17	-0.000013174	0.000029199	-0.000004319

5b(gas) E = -1194.40967649
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000090366	0.000362607	-0.000045970
2	6	0.000045890	-0.000165284	0.000088597
3	6	-0.000080349	0.000004042	0.000267062
4	6	-0.000186081	0.000102788	0.000233539
5	6	0.000085449	-0.000406062	-0.000055211
6	6	0.000050664	0.000246832	-0.000131852
7	1	0.000049112	0.000107864	-0.000160666
8	1	-0.000076084	-0.000016709	-0.000002192
9	1	0.000091424	0.000061319	-0.000097265
10	1	-0.000010581	-0.000067055	0.000061473
11	1	-0.000037296	-0.000132242	0.000121086
12	1	0.000112226	-0.000065134	0.000000374
13	1	0.000050631	-0.000052274	-0.000018007
14	1	-0.000074454	-0.000067365	0.000106329
15	1	0.000124386	-0.000106367	0.000044639
16	1	0.000015713	-0.000050434	0.000004085
17	17	-0.000127499	0.000122490	-0.000188772
18	6	0.000120170	0.000243588	-0.000064348
19	1	-0.000116932	-0.000045858	0.000043926
20	1	0.000042857	-0.000181173	-0.000053832
21	17	0.000011119	0.000104426	-0.000152994

5c(gas) E = -1194.41993852
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000007461	-0.000013217	0.000004283
2	6	-0.000006595	-0.000016886	0.000021170
3	6	0.000009426	0.000029967	-0.000005216
4	6	0.000026226	-0.000033087	-0.000011699
5	6	-0.000046763	0.000059647	-0.000024539
6	6	-0.000011609	-0.000025516	0.000005690
7	1	-0.000004225	0.000003009	0.000012244
8	1	-0.000003048	0.000001890	0.000003404
9	1	0.000004509	-0.000002471	0.000011852
10	1	0.000004844	-0.000001834	-0.000000988
11	1	0.000004574	0.000006625	0.000007517
12	1	-0.000010593	0.000020163	-0.000003340
13	1	-0.000008472	0.000011640	-0.000007155
14	1	-0.000009043	0.000001172	-0.000013351
15	1	-0.000004086	0.000023947	0.000000508
16	1	-0.000003420	0.000004480	-0.000010644
17	17	0.000013757	-0.000017333	0.000005189
18	6	0.000008859	-0.000047424	0.000015107
19	1	0.000007250	0.000005627	-0.000009605
20	1	0.000010710	-0.000003864	-0.000003151
21	17	0.000010237	-0.000006532	0.000002724

6a(gas) E = -3308.37874553
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000015141	0.000009077	0.000016251
2	6	-0.000011839	-0.000006937	-0.000002782
3	6	-0.000002697	-0.000006507	-0.000014498
4	6	0.000009924	0.000005263	-0.000000836
5	6	0.000007241	0.000018822	-0.000011446
6	6	0.000007654	0.000018186	0.000011383
7	1	0.000004219	-0.000019171	-0.000016940
8	1	-0.000012146	-0.000004216	0.000002299
9	1	-0.000024136	-0.000013307	0.000000539
10	1	-0.000015591	0.000006741	0.000011321
11	1	-0.000025124	0.000005908	0.000014579
12	1	0.000020123	-0.000004997	-0.000007187
13	1	0.000024075	-0.000004809	-0.000014851
14	1	0.000026455	0.000018094	0.000007869
15	1	-0.000000269	0.000013603	0.000010875
16	1	-0.000000936	0.000026062	0.000018521
17	17	0.000020000	0.000006225	0.000014393
18	6	-0.000017460	-0.000038408	0.000001534
19	1	0.000001578	-0.000000558	-0.000006935
20	1	-0.000011686	-0.000016373	-0.000012952
21	35	0.000015757	-0.000012699	-0.000021136

6c(gas) E = -3308.37963050
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000009129	-0.000017623	0.000010060
2	6	0.000005482	-0.000022993	0.000019916
3	6	0.000002175	0.000047788	-0.000001292
4	6	0.000031007	-0.000037437	-0.000023086
5	6	-0.000045423	0.000060750	-0.000019225
6	6	-0.000006319	-0.000031473	0.000022051
7	1	-0.000006779	0.000013044	-0.000007344
8	1	0.000011124	0.000009579	0.000000359
9	1	0.000005127	0.000002099	0.000008142
10	1	-0.000000093	-0.000013179	0.000008370
11	1	0.000016992	0.000005696	0.000022373
12	1	-0.000002733	0.000029606	-0.000014007
13	1	-0.000012056	0.000018215	-0.000015291
14	1	-0.000003414	-0.000005233	-0.000008256
15	1	0.000017744	0.000025374	0.000010583
16	1	0.000009535	-0.000006379	0.000007849
17	17	0.000000596	-0.000025962	0.000018269
18	6	-0.000024858	-0.000029554	0.000034735
19	1	-0.000011424	0.000001408	-0.000032467
20	1	0.000000109	-0.000010765	-0.000012122
21	35	0.000004076	-0.000012960	-0.000029617

1(dmso) E = -794.74634697
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004851	-0.000006796	0.000005798
2	6	0.000006460	-0.000006120	0.000016037
3	6	0.000000316	0.000002831	-0.000009552
4	6	-0.000005545	0.000003219	0.000002927
5	6	-0.000001066	0.000005824	-0.000018971
6	6	-0.000001540	0.000005557	-0.000007591
7	1	0.000003311	-0.000003718	0.000015344
8	1	-0.000001464	0.000005301	0.000023914
9	1	0.000011640	-0.000011676	0.000024577
10	1	0.000011514	-0.000016756	-0.000000987
11	1	0.000005021	-0.000006106	0.000014047
12	1	-0.000008547	0.000017175	0.000000547
13	1	-0.000008660	0.000003656	-0.000016086
14	1	-0.000013855	0.000010989	-0.000019577
15	1	-0.000010773	0.000015629	0.000001939
16	1	-0.000004730	0.000006167	-0.000012760
17	9	-0.000020903	0.000012701	-0.000005392
18	17	0.000033970	-0.000037878	-0.000014214

2(dmso) E = -1155.11111851
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000032706	-0.000023518	-0.000042378
2	6	0.000026267	-0.000128396	0.000010251
3	6	0.000081856	0.000078727	-0.000162684
4	6	0.000022415	0.000040918	0.000009493
5	6	-0.000112342	0.000154607	-0.000051463
6	6	-0.000069455	-0.000091846	0.000064712
7	1	-0.000050602	-0.000026427	0.000037763
8	1	0.000017404	0.000043098	-0.000052898
9	1	-0.000036460	0.000024438	0.000028126
10	1	0.000016021	0.000015172	0.000018380
11	1	0.000014932	0.000070026	-0.000021826
12	1	-0.000019290	0.000009847	-0.000041077
13	1	-0.000007210	-0.000049802	0.000021654
14	1	0.000033066	-0.000059350	-0.000009506
15	1	-0.000023902	0.000059626	-0.000030018
16	1	0.000047418	-0.000008411	-0.000019511
17	17	0.000039336	-0.000051923	0.000125184
18	17	0.000053252	-0.000056787	0.000115798

3(dmso) E = -3269.06977661
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000060649	0.000114789	-0.000029695
2	6	0.000031940	-0.000080675	0.000022988
3	6	-0.000104825	0.000118089	0.000008588
4	6	-0.000092658	-0.000004846	0.000239656
5	6	0.000156781	-0.000047249	-0.000055966
6	6	-0.000106976	-0.000013652	-0.000025696
7	1	-0.000033239	0.000028751	0.000012218
8	1	0.000019156	-0.000075318	-0.000032643
9	1	-0.000014399	0.000057144	-0.000034123
10	1	0.000004604	0.000003419	-0.000035238
11	1	0.000065754	-0.000003135	-0.000030472
12	1	-0.000024458	-0.000080333	-0.000111786
13	1	-0.000029334	-0.000025934	0.000003949
14	1	0.000015574	-0.000030154	-0.000015129
15	1	0.000033607	-0.000019354	0.000042597
16	1	0.000007069	-0.000028428	0.000021587
17	17	0.000012551	-0.000001621	0.000017643
18	35	-0.000001795	0.000088509	0.000001522

4a(dmso) E = -834.05558834
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004297	0.000025716	0.000036879
2	6	-0.000000841	-0.000054836	0.000009774
3	6	0.000026839	0.000055992	-0.000044310
4	6	-0.000032740	-0.000024204	0.000048364
5	6	-0.000071181	0.000044232	-0.000043909
6	6	0.000032386	0.000006586	-0.000045435
7	1	0.000013051	0.000028095	0.000020754
8	1	-0.000003811	0.000015843	0.000014376
9	1	0.000028517	-0.000000975	-0.000005965
10	1	0.000017813	-0.000017769	-0.000010915
11	1	0.000004037	-0.000023300	0.000006526
12	1	-0.000010640	0.000009479	0.000001511
13	1	-0.000008571	0.000027150	-0.000015025
14	1	-0.000029136	0.000001063	-0.000004353
15	1	-0.000001838	-0.000004408	0.000010582
16	1	-0.000020952	-0.000012635	-0.000022886
17	17	0.000015671	-0.000025090	-0.000020880
18	6	-0.000029961	-0.000034725	0.000029150
19	1	0.000021270	-0.000002421	0.000023831
20	1	0.000019787	-0.000024324	0.000002803
21	9	0.000026002	0.000010532	0.000009127

4b(dmso) E = -834.05087743
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002472	0.000038303	0.000003906
2	6	-0.000019954	-0.000009430	-0.000004053
3	6	0.000013879	0.000007919	0.000015529
4	6	-0.000058344	-0.000019777	0.000009643
5	6	0.000026493	-0.000014797	-0.000018683
6	6	0.000005683	0.000033404	-0.000021811
7	1	0.000003324	-0.000003005	0.000011438
8	1	-0.000012173	-0.000008522	0.000006527
9	1	0.000006056	-0.000004409	-0.000012337
10	1	-0.000000727	-0.000019365	-0.000008415
11	1	-0.000008074	-0.000014380	0.000000814
12	1	-0.000001902	-0.000011664	0.000014717
13	1	0.000018188	0.000009105	0.000006767
14	1	-0.000009802	0.000011850	0.000003207
15	1	-0.000012450	-0.000014953	0.000000196
16	1	-0.000021573	0.000002436	-0.000014803
17	17	-0.000008201	0.000020428	0.000002903
18	6	0.000096341	0.000021632	0.000007835
19	1	0.000004163	-0.000001603	0.000023929
20	1	-0.000000223	-0.000023211	0.000007205
21	9	-0.000018232	0.000000039	-0.000034513

4c(dmso) E = -834.05644686
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000026449	-0.000084711	-0.000072985
2	6	0.000052150	-0.000011093	-0.000005392
3	6	-0.000093258	0.000039418	0.000092693
4	6	0.000118247	-0.000013906	-0.000049522
5	6	-0.000098126	0.000142908	-0.000092597
6	6	-0.000073074	-0.000077802	0.000068424
7	1	-0.000008646	-0.000007712	0.000009525
8	1	-0.000006817	-0.000002835	-0.000031717
9	1	-0.000016099	0.000007701	0.000025959
10	1	0.000024905	0.000014207	0.000025297
11	1	0.000003298	0.000048782	-0.000014932
12	1	-0.000019109	0.000006662	-0.000009103
13	1	-0.000017019	-0.000033709	0.000014262
14	1	0.000019489	-0.000039941	-0.000008407
15	1	-0.000007133	0.000021862	-0.000031502
16	1	0.000033358	0.000009683	0.000000575
17	17	0.000062509	-0.000046990	0.000083861
18	6	0.000240243	-0.000096930	-0.000090993
19	1	-0.000003160	0.000058981	0.000018046
20	1	-0.000068415	0.000000940	-0.000031129
21	9	-0.000116894	0.000064484	0.000099638

5a(dmso) E = -1194.42508846
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000008513	-0.000009838	0.000011005
2	6	0.000009753	0.000006662	0.000008648
3	6	-0.000004735	0.000013377	0.000002460
4	6	-0.000005581	0.000013773	-0.000005366
5	6	-0.000025700	0.000016829	-0.000032403
6	6	0.000009858	-0.000002430	0.000003823
7	1	0.000001673	0.000015151	0.000001239
8	1	0.000011477	0.000013159	0.000020736
9	1	0.000016113	-0.000002416	0.000019420
10	1	0.000008591	-0.000018655	0.000005051
11	1	0.000017756	-0.000012569	0.000015172
12	1	-0.000006109	0.000018663	-0.000001888
13	1	-0.000016594	0.000012014	-0.000015648
14	1	-0.000010874	0.000005772	-0.000008735
15	1	0.000001562	0.000005741	0.000006239
16	1	0.000001232	-0.000009575	0.000000756
17	17	-0.000001742	-0.000030095	-0.000004233
18	6	-0.000018711	-0.000043929	-0.000004835
19	1	0.000001097	-0.000011279	-0.000006922
20	1	0.000006086	-0.000002979	0.000002864
21	17	-0.000003666	0.000022622	-0.000017384

5b(dmso) E = -1194.41672146
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000009722	0.000024772	0.000006355
2	6	0.000006324	0.000007485	0.000000863
3	6	-0.000042408	0.000025139	-0.000007677
4	6	-0.000022768	-0.000016157	-0.000015086
5	6	0.000035035	-0.000040708	0.000005777
6	6	0.000027774	0.000019556	-0.000016459
7	1	0.000022902	0.000002228	-0.000013006
8	1	0.000005117	-0.000013447	-0.000008224
9	1	-0.000008062	0.000004620	-0.000026298
10	1	-0.000012730	0.000009490	-0.000003407
11	1	-0.000006339	-0.000013369	0.000003507
12	1	0.000014670	-0.000012908	0.000012336
13	1	0.000017195	0.000003036	0.000002370
14	1	0.000004506	-0.000006453	0.000027198
15	1	0.000010256	-0.000019444	0.000011162
16	1	-0.000005550	-0.000008818	0.000002385
17	17	-0.000006124	0.000009539	0.000002796
18	6	-0.000000763	-0.000009088	0.000009337
19	1	-0.000010059	0.000011371	-0.000001955
20	1	-0.000009330	0.000003121	0.000007531
21	17	-0.000009923	0.000020035	0.000000496

5c(dmso) E = -1194.42538601
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000006133	-0.000010625	0.000001917
2	6	-0.000005088	-0.000016679	0.000020152
3	6	0.000008041	0.000028362	0.000000099
4	6	0.000019001	-0.000026329	-0.000010804
5	6	-0.000031449	0.000037242	-0.000010593
6	6	-0.000013978	-0.000015383	-0.000000819
7	1	-0.000005267	0.000000671	0.000015800
8	1	-0.000004608	0.000002622	0.000006383
9	1	0.000006315	-0.000002735	0.000011587
10	1	0.000005025	-0.000000894	-0.000001577
11	1	0.000004963	0.000005378	0.000005505
12	1	-0.000013581	0.000018926	-0.000002429
13	1	-0.000008178	0.000010706	-0.000004586
14	1	-0.000012630	0.000004883	-0.000017913
15	1	-0.000007456	0.000021536	-0.000000497
16	1	-0.000005125	0.000004011	-0.000013386
17	17	0.000006790	-0.000009213	-0.000008742
18	6	0.000020804	-0.000045060	0.000002005
19	1	0.000008599	0.000004177	-0.000005065
20	1	0.000014158	-0.000005200	-0.000002627
21	17	0.000007533	-0.000006396	0.000015589

6a(dmso) E = -3308.38486150
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000024850	0.000071015	0.000048472
2	6	-0.000022813	-0.000113492	0.000003693
3	6	0.000048204	0.000075056	-0.000114787
4	6	0.000041466	-0.000046755	0.000072520
5	6	-0.000128927	0.000177422	-0.000142995
6	6	0.000025199	-0.000021273	0.000013136
7	1	-0.000011524	-0.000026580	-0.000019238
8	1	-0.000028495	-0.000005032	-0.000022446
9	1	-0.000039012	-0.000018635	-0.000028982
10	1	-0.000018754	0.000007343	-0.000000420
11	1	-0.000035959	0.000021342	0.000027731
12	1	0.000012510	0.000000676	-0.000042969
13	1	0.000048979	0.000015849	-0.000025888
14	1	0.000050502	-0.000003930	0.000024753
15	1	0.000008374	0.000023770	0.000022773
16	1	-0.000013091	0.000021234	0.000022085
17	17	0.000117135	-0.000053282	0.000121705
18	6	-0.000046142	-0.000143102	0.000080307
19	1	-0.000003530	0.000024842	0.000003411
20	1	-0.000007930	-0.000003738	-0.000013784
21	35	0.000028658	-0.000002731	-0.000029077

6b(dmso) E = -3308.37566567
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001701	0.000004077	-0.000010519
2	6	0.000001593	0.000001816	-0.000008106
3	6	0.000002002	0.000000081	0.000011235
4	6	-0.000004080	-0.000010929	0.000003072
5	6	0.000001166	-0.000007347	0.000005256
6	6	-0.000004743	-0.000007976	-0.000009853
7	1	0.000001011	-0.000002279	0.000007775
8	1	-0.000003279	-0.000004202	-0.000008030
9	1	0.000002049	0.000006214	-0.000009885
10	1	0.000002026	0.000009110	-0.000012435
11	1	-0.000003158	0.000000977	-0.000020874
12	1	-0.000005289	-0.000013144	0.000011099
13	1	0.000001480	-0.000003370	0.000018417
14	1	-0.000006330	-0.000011633	0.000005192
15	1	-0.000008787	-0.000012974	-0.000009871
16	1	-0.000006919	-0.000005797	-0.000014046
17	17	0.000000154	0.000003932	0.000002863
18	6	0.000000535	0.000011838	0.000002398
19	1	0.000009431	0.000012285	0.000011701
20	1	0.000011073	0.000008570	0.000020082
21	35	0.000011766	0.000020747	0.000004528

6c(dmso) E = -3308.38504386
Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000009217	-0.000014356	0.000011856
2	6	0.000005784	-0.000034630	0.000022405
3	6	0.000003364	0.000065895	0.000001523
4	6	0.000032861	-0.000044276	-0.000028998
5	6	-0.000046645	0.000054642	-0.000010695
6	6	-0.000006239	-0.000028581	0.000018556
7	1	-0.000007474	0.000012739	-0.000005837
8	1	0.000011443	0.000011723	0.000001493
9	1	0.000005419	0.000005101	0.000008511
10	1	0.000001132	-0.000015238	0.000007336
11	1	0.000018767	0.000004298	0.000024745
12	1	-0.000003384	0.000032534	-0.000015116
13	1	-0.000014336	0.000018818	-0.000016317
14	1	-0.000007289	-0.000003897	-0.000011824
15	1	0.000018587	0.000027317	0.000012381
16	1	0.000010410	-0.000006845	0.000006487
17	17	-0.000001037	-0.000025348	0.000012595
18	6	-0.000029066	-0.000031632	0.000045856
19	1	-0.000011879	0.000001846	-0.000036743
20	1	0.000000628	-0.000012123	-0.000014696
21	35	0.000009737	-0.000017988	-0.000033516