Supplementary Material (ESI) for CrystEngComm

Chiral Selection in the Formation of Borates From Racemic Binaphthols and Related Diols.

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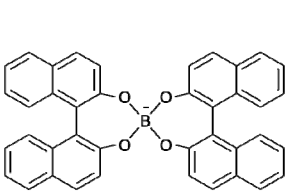
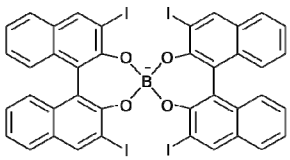
Supplementary Information

DFT-SI

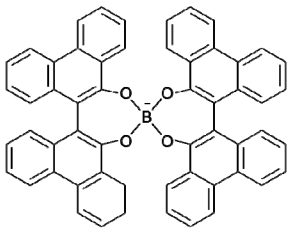
Computational work was carried out using Gaussian09, on both diastereomers of anions **2, 5 6** and **7** respectively. For the fast interconverting atropisomers of anion 7, the transition state was located. All the conclusions were unaltered by inclusion of diffusion functions in the B3LYP functional.



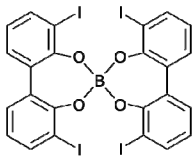
2



5



6



7

6-31G*

	HF	ZPE	SUM	kcal/mol	rel	IMAG
(R,*R*)ax-7	-1293.407	0.299631	-1293.107	-811437.7	**0.0**	
(R,*R*)ax-TS-(R,S)ax-7	-1293.395	0.299415	-1293.095	-811430.2	**7.5**	-70.1
(R,S)ax-7	-1293.401	0.299606	-1293.102	-811434.2	**3.5**	
(R,*R*)ax-2	-1864.751	0.529342	-1864.222	-1169818	**-0.1**	
(R,S)ax-2	-1864.751	0.529388	-1864.221	-1169818	**0.0**	
(R,*R*)ax-5	-1907.945	0.486345	-1907.459	-1196950	**4.3**	
(R,S)ax-5	-1907.952	0.486601	-1907.466	-1196954	**0.0**	
(R,*R*)ax-6	-2479.335	0.71747	-2478.618	-1555357	**3.1**	
(R,S)ax-6	-2479.34	0.717503	-2478.623	-1555360	**0.0**	

6-31+G*; ZPE from 6-31G*

(R,*R*)ax-7	-1293.458	0.299631	-1293.159	-811469.9	**0.0**	
(R,*R*)ax-TS-(R,S)ax-7	-1293.445	0.299415	-1293.146	-811462	**7.9**	
(R,S)ax-7	-1293.451	0.299606	-1293.152	-811465.7	**4.2**	
(R,*R*)ax-2	-1864.82	0.529342	-1864.291	-1169861	**0.4**	
(R,S)ax-2	-1864.821	0.529388	-1864.292	-1169862	**0.0**	
(R,*R*)ax-5	-1908.015	0.486345	-1907.528	-1196993	**4.9**	
(R,S)ax-5	-1908.023	0.486601	-1907.536	-1196998	**0.0**	
(R,*R*)ax-6	-2479.419	0.71747	-2478.701	-1555410	**3.2**	
(R,S)ax-6	-2479.424	0.717503	-2478.706	-1555413	**0.0**	

6-31+G*

						IMAG
(R,*R*)ax-7	-1293.458	0.299017	-1293.159	-811470.3	**0.0**	
(R,*R*)ax-TS-(R,S)ax-7	-1293.445	0.298966	-1293.146	-811462.3	**8.0**	-61.5
(R,S)ax-7	-1293.451	0.298904	-1293.152	-811466.1	**4.2**	

$(R,R)_{ax}$-**2**	
B3LYP/BS1	B3LYP/BS2

69
scf done: -1864.750857

B	0.000004	-0.000002	-0.000400
C	-6.202913	3.011937	-1.808598
C	-6.197032	1.600213	-1.897232
C	1.910018	1.445318	-0.433986
C	-5.161758	3.651881	-1.174727
C	3.021872	0.743551	0.043575
C	-5.178455	0.863721	-1.332460
C	4.097704	1.487096	0.642551
C	1.919959	2.867361	-0.482836
C	-1.910011	-1.445330	-0.433958
C	4.087911	2.923725	0.597875
C	3.021951	-0.743467	-0.043776
C	-3.021865	-0.743551	0.043586
C	5.178017	0.864061	1.332843
C	4.098025	-1.486900	-0.642454
C	-1.919955	-2.867374	-0.482781
C	-4.097705	-1.487081	0.642563
C	6.196355	1.600677	1.897884
C	5.161046	3.652219	1.175068
C	1.910039	-1.445351	0.433493
C	-4.087915	-2.923711	0.597916
C	-3.021942	0.743465	-0.043792
C	6.202100	3.012400	1.809230
C	2.984837	3.585249	-0.004001
C	4.088389	-2.923529	-0.597767
C	1.920149	-2.867398	0.482376
C	-2.984838	-3.585250	-0.003938
C	-5.178026	-0.864029	1.332826
C	-1.910029	1.445358	0.433463
C	-2.985225	3.585169	0.003764
C	5.178451	-0.863749	-1.332465
C	-6.196373	-1.600630	1.897871
C	-5.161059	-3.652190	1.175112
C	-1.920139	2.867405	0.482318
C	-4.098021	1.486886	-0.642475
C	2.985235	-3.585171	0.003833
C	6.202908	-3.011974	-1.808564
C	-4.088384	2.923516	-0.597817
C	-6.202119	-3.012355	1.809250
C	5.161759	-3.651905	-1.174670
C	6.197025	-1.600252	-1.897230
H	-2.984966	-4.672886	-0.049936
H	-1.048157	-3.352431	-0.911715
H	2.984962	4.672884	-0.050019
H	1.048161	3.352408	-0.911783
H	5.134733	4.739246	1.117098
H	-5.183901	0.215956	1.424189
H	6.999806	1.089860	2.424034
H	7.013714	3.584672	2.252650
H	5.183892	-0.215921	1.424231
H	-7.014713	3.584111	-2.251803
H	5.184228	0.216233	-1.423861
H	-6.999829	-1.089800	2.424000
H	-7.013739	-3.584616	2.252672
H	-5.134748	-4.739219	1.117166
H	-7.000569	1.089297	-2.423153
H	-5.135553	4.738913	-1.116775
H	7.000556	-1.089347	-2.423170
H	7.014705	-3.584157	-2.251765
H	5.135555	-4.738936	-1.116696
H	2.985473	-4.672805	0.049873
H	1.048295	-3.352538	0.911104
H	-1.048284	3.352554	0.911035
H	-2.985464	4.672805	0.049784
H	-5.184234	-0.216264	-1.423830
O	-0.822267	-0.818804	-0.910481
O	-0.822078	0.819000	0.909697
O	0.822276	0.818780	-0.910498
O	0.822087	-0.818985	0.909714

69
scf done: -1864.820165

B	0.000011	-0.000002	-0.000357
C	-6.207282	3.010054	-1.814276
C	-6.194892	1.597259	-1.910896
C	1.915376	1.446197	-0.440196
C	-5.171112	3.651672	-1.168835
C	3.025075	0.743496	0.040693
C	-5.175175	0.861438	-1.342281
C	4.100640	1.486715	0.643002
C	1.931498	2.868269	-0.502927
C	-1.915356	-1.446213	-0.440158
C	4.096974	2.923356	0.589399
C	3.025145	-0.743424	-0.040869
C	-3.025056	-0.743496	0.040706
C	5.174766	0.861752	1.342669
C	4.100927	-1.486544	-0.642913
C	-1.931483	-2.868286	-0.502852
C	-4.100639	-1.486695	0.643005
C	6.194258	1.597690	1.911536
C	5.170475	3.651983	1.169144
C	1.915390	-1.446229	0.439756
C	-4.096978	-2.923337	0.589439
C	-3.025124	0.743422	-0.040887
C	6.206537	3.010484	1.814875
C	2.999121	3.585764	-0.024740
C	4.097394	-2.923185	-0.589305
C	1.931654	-2.868304	0.502505
C	-2.999115	-3.585765	-0.024661
C	-5.174786	-0.861708	1.342615
C	-1.915367	1.446239	0.439715
C	-2.999445	3.585695	0.024496
C	5.175161	-0.861478	-1.342322
C	-6.194298	-1.597625	1.911475
C	-5.170497	-3.651944	1.169177
C	-1.931632	2.868315	0.502428
C	-4.100920	1.486525	-0.642924
C	2.999462	-3.585696	0.024581
C	6.207259	-3.010107	-1.814277
C	-4.097388	2.923167	-0.589353
C	-6.206575	-3.010422	1.814860
C	5.171105	-3.651707	-1.168791
C	6.194864	-1.597316	-1.910942
H	-3.003616	-4.673241	-0.080829
H	-1.065298	-3.356625	-0.940349
H	3.003618	4.673239	-0.080934
H	1.065316	3.356593	-0.940445
H	5.150024	4.739108	1.105491
H	-5.178446	0.218440	1.439135
H	6.992649	1.085753	2.444768
H	7.017879	3.582274	2.260051
H	5.178424	-0.218391	1.439226
H	-7.018799	3.581752	-2.259252
H	5.178737	0.218666	-1.438880
H	-6.992704	-1.085670	2.444666
H	-7.017932	-3.582197	2.260029
H	-5.150049	-4.739071	1.105554
H	-6.993377	1.085227	-2.443896
H	-5.150754	4.738801	-1.105214
H	6.993332	-1.085300	-2.443981
H	7.018765	-3.581819	-2.259257
H	5.150747	-4.738834	-1.105139
H	3.004053	-4.673170	0.080788
H	1.065418	-3.356711	0.939825
H	-1.065392	3.356734	0.939729
H	-3.004037	4.673171	0.080679
H	-5.178755	-0.218710	-1.438801
O	-0.824337	-0.817541	-0.912132
O	-0.824167	0.817715	0.911431
O	0.824360	0.817509	-0.912156
O	0.824190	-0.817694	0.911455

$(R,S)_{ax}$-**2**	
B3LYP/BS1	B3LYP/BS2

69
scf done: -1864.750803

B	0.000011	0.000699	-0.001540
C	-6.183134	-1.651136	3.121703
C	-6.190472	-0.401350	2.459212
C	1.905449	0.373556	1.456695
C	-5.135319	-2.519354	2.912359
C	3.020480	0.422019	0.613669
C	-5.177449	-0.060196	1.589493
C	4.091683	1.323489	0.942567
C	1.898537	1.080488	2.690570
C	-1.906635	1.457796	-0.374041
C	4.069102	2.035996	2.190684
C	3.020821	-0.421142	-0.614543
C	-3.021101	0.613963	-0.421891
C	5.178569	1.588704	0.059507
C	4.092058	-1.322845	-0.942692
C	-1.901122	2.691750	-1.080881
C	-4.093062	0.942127	-1.322722
C	6.192266	2.457652	0.400621
C	5.137675	2.911404	2.518772
C	1.906384	-0.372464	-1.458331
C	-4.071846	2.190288	-2.035188
C	-3.020162	-0.614255	0.421260
C	6.185552	3.120054	1.650458
C	2.957863	1.868213	3.059164
C	4.070164	-2.035398	-2.190794
C	1.900135	-1.079455	-2.692172
C	-2.961171	3.059601	-1.867973
C	-5.179459	0.058275	-1.587327
C	-1.905156	-1.457231	0.371978
C	-2.956209	-3.059602	1.867632
C	5.178306	-1.588243	-0.058900
C	-6.193910	0.398664	-2.455680
C	-5.141159	2.517610	-2.909973
C	-1.897515	-2.690997	1.079053
C	-4.090671	-0.943165	1.323551
C	2.959539	-1.867424	-3.060022
C	6.186033	-3.119867	-1.649119
C	-4.067418	-2.191226	2.036141
C	-6.188508	1.648522	-3.118056
C	5.138775	-2.911040	-2.518136
C	6.192052	-2.457413	-0.399306
H	2.946471	2.402973	4.007286
H	1.018579	0.972245	3.317113
H	5.102150	3.430433	3.475366
H	7.001618	2.640734	-0.302776
H	6.993415	3.799083	1.913488
H	5.194033	1.100892	-0.908235
H	5.193236	-1.100390	0.908829
H	7.000902	-2.640626	0.304635
H	6.993932	-3.799071	-1.911584
H	5.103779	-3.430101	-3.474732
H	2.948663	-2.402228	-4.008126
H	1.020618	-0.971055	-3.319307
H	-2.944314	-4.007651	2.402510
H	-5.099314	-3.475903	3.431440
H	-1.017568	-3.317451	0.970223
H	-6.990472	-1.914203	3.801343
H	-6.996958	1.910969	-3.796612
H	-5.106645	3.474252	-3.428983
H	-2.950803	4.007782	-2.402649
H	-1.021588	3.318968	-0.973080
H	-7.002845	-0.305329	-2.638314
H	-5.193941	-0.909492	-1.099534
H	-5.193366	0.907500	1.101607
H	-6.999768	0.301972	2.642828
O	0.827411	-0.373789	1.159776
O	-0.827785	-1.160148	-0.376351
O	0.828316	0.375154	-1.162153
O	-0.827899	1.161782	0.372592

69
scf done: -1864.820920

B	-0.000104	-0.000749	-0.000363
C	-6.182527	3.123529	1.659484
C	-6.186761	2.468933	0.403638
C	1.908760	1.461652	-0.361787
C	-5.137609	2.903567	2.532374
C	3.022535	0.617354	-0.416644
C	-5.173809	1.596282	0.061416
C	4.091828	0.948070	-1.320912
C	1.903250	2.703394	-1.056080
C	-1.909549	-0.362026	-1.462188
C	4.071408	2.201823	-2.024450
C	3.022692	-0.617783	0.416205
C	-3.023027	-0.416628	-0.617470
C	5.174537	0.061397	-1.595269
C	4.091982	-0.948140	1.320608
C	-1.904689	-1.056333	-2.703933
C	-4.092536	-1.320841	-0.947673
C	6.187988	0.403710	-2.467306
C	5.138958	2.532394	-2.902503
C	1.909206	-1.462448	0.361217
C	-4.072754	-2.024404	-2.201423
C	-3.022558	0.416329	0.617603
C	6.184051	1.659565	-3.121888
C	2.962981	3.074265	-1.845546
C	4.071882	-2.201889	2.024162
C	1.904005	-2.704176	1.055534
C	-2.964699	-1.845624	-3.074362
C	-5.174807	-1.595208	-0.060458
C	-1.908809	0.361026	1.461886
C	-2.962228	1.845462	3.074358
C	5.174374	-0.061116	1.595079
C	-6.188468	-2.467189	-0.402292
C	-5.140512	-2.902389	-2.531497
C	-1.902892	1.055438	2.703545
C	-4.091345	1.321259	0.948186
C	2.963757	-3.074690	1.845140
C	6.184221	-1.658937	3.121842
C	-4.070550	2.024880	2.201891
C	-6.185196	-3.121731	-1.658168
C	5.139434	-2.532105	2.902347
C	6.187832	-0.403090	2.467242
H	2.952152	4.027277	-2.372184
H	1.025930	3.333600	-0.943133
H	5.106322	3.492511	-3.415782
H	6.993934	-0.302141	-2.657339
H	6.990357	1.924090	-3.802605
H	5.190562	-0.909949	-1.113294
H	5.190148	0.910227	1.113090
H	6.993530	0.303022	2.657358
H	6.990533	-1.923194	3.802656
H	5.107047	-3.492225	3.415634
H	2.953169	-4.027696	2.371794
H	1.026901	-3.334665	0.942492
H	-2.951113	2.372211	4.027305
H	-5.104713	3.416881	3.492463
H	-1.025601	0.942144	3.333727
H	-6.988444	3.804733	1.923939
H	-6.991663	-3.802408	-1.922307
H	-5.108357	-3.415668	-3.491629
H	-2.954342	-2.372276	-4.027372
H	-1.027606	-0.943543	-3.334499
H	-6.994065	-2.657213	0.303961
H	-5.190332	-1.113289	0.910920
H	-5.190044	1.114321	-0.909929
H	-6.992540	2.659439	-0.302276
O	0.830511	1.156078	0.385749
O	-0.830914	-0.387035	1.156225
O	0.830958	-1.157225	-0.386477
O	-0.830976	0.385190	-1.157076

$(R,R)_{ax}$-**5**	
B3LYP/BS1	B3LYP/BS2

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   69                                                    69
scf done: -1907.945353                                scf done: -1908.014644
 C    -5.145837    -0.927710     1.298153              C    -5.144477    -0.929287     1.306391
 C    -4.124052    -1.502791     0.488226              C    -4.123155    -1.504995     0.495337
 C    -4.208737    -2.909256     0.223349              C    -4.202965    -2.913191     0.234708
 C    -5.305942    -3.659869     0.723548              C    -5.297409    -3.666349     0.741032
 C    -6.283197    -3.064855     1.488700              C    -6.275578    -3.071404     1.509373
 C    -6.188677    -1.684742     1.786429              C    -6.185099    -1.688300     1.801974
 C    -3.016964    -0.745304    -0.030771              C    -3.019501    -0.745386    -0.030064
 C    -1.931511    -1.423027    -0.602735              C    -1.935187    -1.424314    -0.600999
 C    -2.088862    -2.806985    -0.925006              C    -2.083143    -2.810191    -0.922800
 C    -3.187134    -3.528849    -0.542518              C    -3.180668    -3.532517    -0.533172
 C    -3.017021     0.744879     0.030655              C    -3.019541     0.745034     0.029969
 C    -1.931798     1.422631     0.602996              C    -1.935435     1.423970     0.601264
 C    -2.089237     2.806590     0.925167              C    -2.083447     2.809854     0.922961
 C    -3.187405     3.528427     0.542320              C    -3.180853     3.532174     0.532980
 C    -4.208760     2.908794    -0.223847              C    -4.202925     2.912826    -0.235182
 C    -4.123962     1.502330    -0.488702              C    -4.123036     1.504628    -0.495783
 C    -5.305837     3.659375    -0.724380              C    -5.297229     3.665973    -0.741831
 C    -6.282840     3.064333    -1.489830              C    -6.275166     3.071016    -1.510456
 C    -6.188189     1.684224    -1.787539              C    -6.184590     1.687913    -1.803032
 C    -5.145477     0.927221    -1.298947              C    -5.144109     0.928910    -1.307142
 O    -0.803017     0.806361     0.938688              O    -0.805569     0.804560     0.939259
 B     0.000000     0.000001     0.000344              B     0.000000     0.000002     0.000345
 O    -0.802585    -0.806828    -0.938008              O    -0.805167    -0.804995    -0.938580
 I    -0.578809     3.768347     2.117098              I    -0.583826     3.753867     2.127032
 I    -0.578097    -3.768708    -2.116544              I    -0.583218    -3.754188    -2.126511
 O     0.803025    -0.806360     0.938681              O     0.805577    -0.804557     0.939252
 C     1.931802    -1.422631     0.602978              C     1.935439    -1.423970     0.601246
 C     3.017020    -0.744881     0.030627              C     3.019540    -0.745035     0.029941
 C     4.123955    -1.502333    -0.488741              C     4.123028    -1.504632    -0.495823
 C     4.208754    -2.908797    -0.223886              C     4.202917    -2.912830    -0.235221
 C     3.187406    -3.528428     0.542291              C     3.180852    -3.532176     0.532951
 C     2.089242    -2.806590     0.925149              C     2.083451    -2.809853     0.922943
 C     5.145463    -0.927226    -1.298997              C     5.144093    -0.928916    -1.307192
 C     6.188169    -1.684230    -1.787599              C     6.184569    -1.687922    -1.803092
 C     6.282822    -3.064339    -1.489890              C     6.275145    -3.071025    -1.510516
 C     5.305825    -3.659379    -0.724430              C     5.297214    -3.665979    -0.741881
 C     3.016965     0.745302    -0.030799              C     3.019502     0.745384    -0.030092
 C     4.124059     1.502787     0.488188              C     4.123163     1.504991     0.495299
 C     4.208743     2.909253     0.223311              C     4.202973     2.913187     0.234671
 C     3.187133     3.528848    -0.542544              C     3.180670     3.532516    -0.533198
 C     2.088856     2.806986    -0.925023              C     2.083139     2.810193    -0.922816
 C     1.931507     1.423028    -0.602752              C     1.935184     1.424315    -0.601016
 C     5.305953     3.659864     0.723500              C     5.297424     3.666342     0.740985
 C     6.283216     3.064848     1.488642              C     6.275598     3.071395     1.509315
 C     6.188697     1.684735     1.786370              C     6.185120     1.688291     1.801917
 C     5.145852     0.927705     1.298104              C     5.144491     0.929280     1.306343
 I     0.578080     3.768712    -2.116543              I     0.583204     3.754193    -2.126511
 O     0.802577     0.806831    -0.938014              O     0.805159     0.804998    -0.938587
 I     0.578826    -3.768344     2.117096              I     0.583840    -3.753863     2.127030
 H    -3.280058     4.579633     0.796454              H    -3.271638     4.584556     0.785288
 H     3.280061    -4.579634     0.796426              H     3.271637    -4.584557     0.785259
 H     5.349289    -4.723259    -0.499551              H     5.339051    -4.731189    -0.521356
 H    -5.083485    -0.124972    -1.550452              H    -5.087724    -0.125539    -1.553354
 H     6.942351    -1.215562    -2.415335              H     6.938942    -1.218605    -2.430651
 H     7.113495    -3.650244    -1.875651              H     7.102769    -3.658874    -1.900753
 H     5.083469     0.124967    -1.550502              H     5.087708     0.125533    -1.553404
 H    -7.113974    -3.650783     1.874203              H    -7.103316    -3.659259     1.899359
 H     5.083972    -0.124491     1.549627              H     5.088192    -0.125168     1.552575
 H    -6.942377     1.215554    -2.415267              H    -6.938969     1.218595    -2.430582
 H    -7.113518     3.650237    -1.875583              H    -7.102795     3.658864    -1.900685
 H    -5.349300     4.723255    -0.499502              H    -5.339065     4.731183    -0.521306
 H    -6.943070    -1.216090     2.413923              H    -6.939666    -1.218987     2.429302
 H    -5.349303    -4.723750     0.498657              H    -5.339172    -4.731559     0.520490
 H     6.943096     1.216081     2.413856              H     6.939692     1.218976     2.429236
 H     7.113998     3.650774     1.874137              H     7.103341     3.659248     1.899294
 H     5.349314     4.723746     0.498611              H     5.339186     4.731552     0.520443
 H     3.279690     4.580048    -0.796743              H     3.271386     4.584886    -0.785577
 H    -3.279693    -4.580049    -0.796718              H    -3.271385    -4.584887    -0.785551
 H    -5.083957     0.124485     1.549677              H    -5.088177     0.125162     1.552623
```

$(R,S)_{ax}$-**5**	
B3LYP/BS1	B3LYP/BS2

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   69                                                    69
scf done: -1907.952500                                scf done: -1908.022744
 C     5.133755    -1.597200     0.046217               C     5.131641    -0.081551     1.603716
 C     4.079510    -1.288685     0.954293               C     4.076271     0.847508     1.367943
 C     4.102261    -1.933271     2.234814               C     4.090293     2.070053     2.118311
 C     5.178583    -2.797086     2.572564               C     5.162271     2.336568     3.014359
 C     6.191750    -3.052535     1.676886               C     6.178273     1.423430     3.199792
 C     6.155685    -2.452955     0.395274               C     6.149846     0.195821     2.492692
 C     2.998004    -0.403111     0.626959               C     2.999908     0.593828     0.451174
 C     1.896355    -0.305939     1.487624               C     1.898500     1.458424     0.422713
 C     1.968140    -0.934096     2.766973               C     1.956188     2.682809     1.154693
 C     3.035611    -1.706143     3.142624               C     3.021087     2.992073     1.962222
 C     2.997590     0.402727    -0.628024               C     2.999903    -0.593845    -0.451171
 C     1.895569     0.305186    -1.488152               C     1.898490    -1.458435    -0.422706
 C     1.966472     0.933375    -2.767519               C     1.956170    -2.682822    -1.154683
 C     3.033493     1.705802    -3.143681               C     3.021066    -2.992092    -1.962215
 C     4.100519     1.933278    -2.236399               C     4.090276    -2.070078    -2.118310
 C     4.078640     1.288667    -0.955875               C     4.076262    -0.847532    -1.367944
 C     5.176389     2.797453    -2.574678               C     5.162249    -2.336600    -3.014362
 C     6.189917     3.053228    -1.679503               C     6.178253    -1.423467    -3.199800
 C     6.154696     2.453628    -0.397876               C     6.149835    -0.195856    -2.492703
 C     5.133229     1.597527    -0.048318               C     5.131635     0.081522    -1.603723
 O     0.819221    -0.410548    -1.154461               O     0.822937    -1.179946     0.323892
 B     0.000028    -0.000359     0.000091               B     0.000000     0.000000     0.000001
 O     0.819579     0.409387     1.154582               O     0.822943     1.179944    -0.323884
 I     0.353892     0.640920    -4.160065               I     0.348525    -4.084250    -0.960696
 I     0.356088    -0.642273     4.160269               I     0.348548     4.084245     0.960713
 O    -0.819611    -1.154650     0.410135               O    -0.822944     0.323890     1.179942
 C    -1.896378    -1.487709    -0.305230               C    -1.898500    -0.422707     1.458425
 C    -2.998001    -0.627019    -0.402388               C    -2.999908    -0.451171     0.593827
 C    -4.079586    -0.954382    -1.287848               C    -4.076269    -1.367941     0.847508
 C    -4.102363    -2.234903    -1.932433               C    -4.090292    -2.118306     2.070056
 C    -3.035682    -3.142698    -1.705389               C    -3.021089    -1.962211     2.992077
 C    -1.968176    -2.767052    -0.933385               C    -1.956189    -1.154681     2.682812
 C    -5.133914    -0.046351    -1.596203               C    -5.131636    -1.603719    -0.081553
 C    -6.155925    -0.395434    -2.451850               C    -6.149840    -2.492698     0.195819
 C    -6.191993    -1.677032    -3.051462               C    -6.178268    -3.199793     1.423431
 C    -5.178765    -2.572677    -2.796140               C    -5.162269    -3.014355     2.336571
 C    -2.997519     0.627998     0.403392               C    -2.999904     0.451174    -0.593845
 C    -4.078638     0.955968     1.289197               C    -4.076264     1.367946    -0.847531
 C    -4.100504     2.236510     1.933768               C    -4.090276     2.118316    -2.070075
 C    -3.033402     3.143718     1.706357               C    -3.021064     1.962226    -2.992088
 C    -1.966351     2.767474     0.934013               C    -1.956168     1.154694    -2.682818
 C    -1.895447     1.488075     0.305870               C    -1.898490     0.422713    -1.458434
 C    -5.176444     2.574882     2.797819               C    -5.162250     3.014367    -2.336596
 C    -6.190076     1.679792     3.053484               C    -6.178257     3.199801    -1.423464
 C    -6.154900     0.398164     2.453882               C    -6.149840     2.492700    -0.195856
 C    -5.133357     0.048513     1.597909               C    -5.131639     1.603720     0.081521
 I    -0.353681     4.159934     0.641622               I    -0.348518     0.960718    -4.084243
 O    -0.819078     1.154388    -0.409801               O    -0.822936    -0.323886    -1.179948
 I    -0.356145    -4.160372    -0.641583               I    -0.348554    -0.960692     4.084252
 H    -3.067732    -4.121844    -2.172923               H    -3.047997    -2.510069     3.929430
 H    -5.176699    -3.554955    -3.264550               H    -5.155797    -3.565062     3.275574
 H    -6.939145     0.325444    -2.674131               H    -6.934558    -2.656408    -0.539410
 H    -7.006835    -1.943587    -3.720160               H    -6.988587    -3.893692     1.634963
 H    -5.115892     0.944514    -1.157751               H    -5.121557    -1.081168    -1.031569
 H    -5.116009    -0.942368     1.159466               H    -5.121569     1.081165     1.031535
 H    -6.938439    -0.322284     2.676429               H    -6.934564     2.656408     0.539367
 H    -7.004554     1.946801     3.722443               H    -6.988574     3.893702    -1.635001
 H    -5.173693     3.557166     3.266215               H    -5.155769     3.565078    -3.275597
 H    -3.064763     4.122892     2.173879               H    -3.047964     2.510091    -3.929437
 H     3.067635    -2.173680     4.121769               H     3.047994     3.929423     2.510084
 H     5.176498    -3.265486     3.554847               H     5.155798     3.275569     3.565069
 H     7.006526    -3.721321     1.943419               H     6.988593     1.634962     3.893690
 H     7.004337     3.722287    -1.946439               H     6.988570    -1.635004    -3.893702
 H     5.173659     3.265865    -3.556953               H     5.155769    -3.275603    -3.565069
 H     3.064870     2.173368    -4.122833               H     3.047967    -3.929444    -2.510074
 H     6.938139     2.676279     0.322645               H     6.934557     0.539368    -2.656415
 H     5.115839     1.159102     0.942569               H     5.121563     1.031538    -1.081170
 H     5.115732    -1.158794    -0.944667               H     5.121563    -1.031565     1.081161
 H     6.938841    -2.675349    -0.325639               H     6.934566    -0.539407     2.656399
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$(R,R)_{ax}$-**6**	
B3LYP/BS1	B3LYP/BS2

93
scf done: -2479.335195

B	0.000057	0.000489	-0.000357
C	-6.247813	-2.979458	1.703174
C	-6.155440	-1.591972	1.906386
C	1.935481	-1.430060	0.532832
C	-5.279635	-3.622217	0.953993
C	3.015343	-0.744405	0.011085
C	-5.113936	-0.878584	1.345173
C	4.117670	-1.505829	-0.553230
C	2.012981	-2.855245	0.790747
C	-1.935933	1.430658	0.532600
C	4.200281	-2.921020	-0.369185
C	3.015556	0.744671	-0.011034
C	-3.015556	0.744512	0.010969
C	5.114427	-0.878192	-1.344693
C	4.118029	1.505759	0.553453
C	-2.014114	2.855824	0.790508
C	-4.118297	1.505414	-0.553248
C	6.156141	-1.591459	-1.905656
C	5.280335	-3.621809	-0.953495
C	1.935984	1.430638	-0.532984
C	-4.201577	2.920563	-0.369190
C	-3.015174	-0.744567	-0.011117
C	6.248620	-2.978945	-1.702437
C	3.157359	-3.597132	0.387898
C	4.201101	2.920925	0.369412
C	2.013939	2.855802	-0.790844
C	-3.158902	3.597165	0.387783
C	-5.114852	0.877327	-1.344599
C	-1.935383	-1.430117	-0.533124
C	-3.156995	-3.597316	-0.387906
C	5.114481	0.877833	1.345075
C	-6.156981	1.590105	-1.905429
C	-5.282028	3.620851	-0.953335
C	-2.012793	-2.855296	-0.791028
C	-4.117294	-1.506104	0.553473
C	3.158485	3.597355	-0.387807
C	6.249292	2.978232	1.702913
C	-4.199801	-2.921308	0.369445
C	-6.250103	2.977538	-1.702171
C	5.281307	3.621386	0.953831
C	6.156344	1.590785	1.906167
C	0.970626	3.500205	-1.493697
C	-3.212180	-4.968292	-0.731651
C	-2.185066	-5.580381	-1.428377
C	1.053002	4.842565	-1.810341
C	-1.051178	-4.841635	-1.810692
C	-0.969284	-3.499254	-1.494011
C	2.185348	-5.580325	1.428076
C	1.051291	-4.841686	1.810128
C	0.969352	-3.499310	1.493446
C	3.212573	-4.968114	0.731628
C	-3.214767	4.968114	0.731530
C	-2.187782	5.580824	1.427874
C	-1.053308	4.842761	1.809810
C	-0.970757	3.500421	1.493110
C	2.187229	5.580843	-1.428100
C	3.214166	4.968328	-0.731509
H	-5.038527	0.187168	1.525834
H	2.261417	6.636427	-1.680105
H	5.345047	4.698335	0.834381
H	0.242701	5.325051	-2.350836
H	7.063859	3.546966	2.145152
H	-0.110687	2.907945	1.781168
H	6.896101	1.075865	2.514811
H	-0.242972	5.325399	2.350117
H	-5.342930	-4.699198	0.834582
H	-2.262140	6.636390	1.679906
H	-6.895348	-1.077339	2.515093
H	-4.084375	5.557543	0.458890
H	-5.345901	4.697794	-0.833876
H	4.081838	-5.558007	0.458901

93
scf done: -2479.418874

B	0.000050	0.000338	-0.000362
C	-6.246623	-2.982266	1.709380
C	-6.151121	-1.593886	1.917966
C	1.937973	-1.430234	0.538085
C	-5.282029	-3.624212	0.950844
C	3.016528	-0.744445	0.012763
C	-5.110109	-0.879722	1.352675
C	4.117594	-1.506706	-0.553920
C	2.018949	-2.853896	0.806160
C	-1.938287	1.430664	0.537901
C	4.202987	-2.921420	-0.364140
C	3.016656	0.744684	-0.012789
C	-3.016684	0.744514	0.012701
C	5.110638	-0.879300	-1.352171
C	4.117752	1.506736	0.554117
C	-2.019753	2.854344	0.805896
C	-4.118054	1.506383	-0.553926
C	6.151884	-1.593335	-1.917171
C	5.282773	-3.623773	-0.950297
C	1.938309	1.430660	-0.538298
C	-4.203931	2.921076	-0.364188
C	-3.016376	-0.744617	-0.012825
C	6.247493	-2.981715	-1.708563
C	3.163214	-3.596021	0.400857
C	4.203427	2.921440	0.364401
C	2.019556	2.854341	-0.806235
C	-3.164304	3.596054	0.400685
C	-5.110946	0.878622	-1.352075
C	-1.937887	-1.430287	-0.538407
C	-3.162838	-3.596216	-0.400874
C	5.110552	0.879134	1.352521
C	-6.152498	1.592282	-1.917005
C	-5.284003	3.623037	-0.950255
C	-2.018762	-2.853961	-0.806462
C	-4.117213	-1.507005	0.554161
C	3.163873	3.596254	-0.400711
C	6.247738	2.981332	1.709137
C	-4.202491	-2.921733	0.364404
C	-6.248578	2.980623	-1.708422
C	5.283252	3.623584	0.950735
C	6.151836	1.592968	1.917706
C	0.981220	3.497042	-1.520682
C	-3.223173	-4.966534	-0.752084
C	-2.201967	-5.577260	-1.462664
C	1.069362	4.838041	-1.848527
C	-1.068184	-4.837311	-1.849060
C	-0.980352	-3.496315	-1.521101
C	2.202278	-5.577189	1.462367
C	1.068319	-4.837363	1.848493
C	0.980428	-3.496375	1.520528
C	3.223599	-4.966341	0.752062
C	-3.225135	4.966372	0.751833
C	-2.203948	5.577608	1.461990
C	-1.069677	4.838198	1.848011
C	-0.981365	3.497223	1.520103
C	2.203397	5.577652	-1.462200
C	3.224525	4.966595	-0.751806
H	-5.035308	0.186407	1.535373
H	2.281688	6.631814	1.720013
H	5.352544	4.699627	0.825288
H	0.263614	5.318290	-2.398479
H	7.061052	3.551055	2.153100
H	-0.119402	2.906748	1.808972
H	6.888387	1.078727	2.531262
H	-0.263884	5.318581	2.397784
H	-5.351015	-4.700274	0.825387
H	-2.282379	6.631747	1.719852
H	-6.887751	-1.079866	2.531612
H	-4.091582	5.558230	0.473883
H	-5.353446	4.699070	-0.824803
H	4.089803	-5.558528	0.474050

H	-7.064878	3.546134	-2.144204	H	-7.062090	3.550225	-2.152178
H	0.109597	-2.906426	1.781588	H	0.118702	-2.905597	1.809484
H	-6.896806	1.075049	-2.513874	H	-6.889110	1.077901	-2.530370
H	0.240758	-5.323930	2.350500	H	0.262417	-5.317430	2.398380
H	5.038663	-0.187880	1.525788	H	5.035446	-0.186974	1.535206
H	2.259205	-6.635923	1.680094	H	2.280379	-6.631344	1.720264
H	-7.062086	-3.548530	2.145519	H	-7.059706	-3.552257	2.153422
H	-0.109658	-2.906273	-1.782350	H	-0.118760	-2.905438	-1.810259
H	5.038968	0.187554	-1.525371	H	5.035752	0.186820	-1.534884
H	-0.240742	-5.323780	-2.351298	H	-0.262372	-5.317284	-2.399161
H	6.896143	-1.076757	-2.514190	H	6.888630	-1.079241	-2.530616
H	-2.258892	-6.635988	-1.680383	H	-2.280021	-6.631419	-1.720557
H	-5.038925	-0.188377	-1.525330	H	-5.035720	-0.187475	-1.534787
H	-4.081333	-5.558254	-0.458726	H	-4.089248	-5.558813	-0.473865
H	5.343694	-4.698783	-0.834060	H	5.351843	-4.699826	-0.824816
H	0.110746	2.907560	-1.781977	H	0.119438	2.906409	-1.809771
H	7.063064	-3.547925	-2.144584	H	7.060771	-3.551598	-2.152386
H	4.083574	5.557941	-0.458647	H	4.090784	5.558621	-0.473628
O	0.813242	0.811880	-0.925256	O	0.814454	0.810398	-0.926813
O	-0.812957	0.812167	0.924527	O	-0.814202	0.810674	0.926080
O	0.812809	-0.810970	0.924815	O	0.814118	-0.809754	0.926318
O	-0.812889	-0.810877	-0.925399	O	-0.814206	-0.809664	-0.926920

$(R,S)_{ax}$-**6**	
B3LYP/BS1	B3LYP/BS2

93
scf done: -2479.340093

B	0.000071	0.000039	-0.000013
C	-6.195504	-1.350463	3.206449
C	-6.150291	-0.145218	2.484812
C	1.909452	0.443484	1.436167
C	-5.189190	-2.283137	3.036642
C	3.004231	0.449415	0.594340
C	-5.118467	0.089960	1.597030
C	4.086483	1.380394	0.859376
C	1.905296	1.196881	2.671803
C	-1.909343	1.436200	-0.443424
C	4.114973	2.142196	2.069549
C	3.004213	-0.449368	-0.594391
C	-3.004125	0.594376	-0.449326
C	5.118360	1.597411	-0.090337
C	4.086435	-1.380380	-0.859437
C	-1.905231	2.671864	-1.196779
C	-4.086502	0.859522	-1.380115
C	6.150088	2.485338	0.144709
C	5.189198	3.037013	2.282758
C	1.909427	-0.443405	-1.436208
C	-4.115035	2.069718	-2.141876
C	-3.004087	-0.594415	0.449371
C	6.195372	3.206959	1.349961
C	3.022202	2.004570	3.021660
C	4.114891	-2.142181	-2.069611
C	1.905238	-1.196797	-2.671847
C	-3.022201	3.021773	-2.004360
C	-5.118526	-0.090077	-1.596902
C	-1.909271	-1.436197	0.443429
C	-3.022010	-3.021813	2.004406
C	5.118313	-1.597428	0.090267
C	-6.150394	0.145063	-2.484642
C	-5.189396	2.283018	-3.036508
C	-1.905084	-2.671862	1.196782
C	-4.086416	-0.859601	1.380204
C	3.022117	-2.004520	-3.021713
C	6.195261	-3.207011	-1.350040
C	-4.114874	-2.069798	2.141965
C	-6.195682	1.350308	-3.206276
C	5.189085	-3.037034	-2.282828
C	6.150011	-2.485388	-0.144788
C	2.993669	-2.663044	-4.273805
C	2.993782	2.663099	4.273750
C	1.910526	2.546246	5.126587
C	1.910411	-2.546153	-5.126635
C	0.799061	1.765954	4.758398
C	0.799390	1.102007	3.547010
C	-0.799006	4.758461	-1.765869
C	-1.910533	5.126702	-2.546049
C	-2.993818	4.273893	-2.662836
C	-0.799303	3.547049	-1.101965
C	-0.798762	-4.758419	1.765826
C	-0.799128	-3.547006	1.101924
C	-1.910244	-5.126701	2.546050
C	-2.993556	-4.273931	2.662880
C	0.799329	-1.101886	-3.547046
C	0.798972	-1.765828	-4.758436
H	-6.920289	0.609046	2.629833
H	-0.041818	-0.494645	-3.234596
H	-5.080392	1.029611	1.058597
H	1.919812	-3.064366	-6.083035
H	-5.080395	-1.029728	-1.058473
H	-3.836969	-4.584330	3.271401
H	-6.920370	-0.609230	-2.629634
H	-1.919641	-6.083122	3.064223
H	-5.219455	3.193490	-3.626396
H	0.042052	-3.234494	0.494759
H	-7.004359	1.542685	-3.907427
H	0.056847	-5.424345	1.684998
H	-7.004146	-1.542870	3.907633

93
scf done: -2479.423979

B	0.000054	-0.000016	0.000069
C	6.189202	3.238169	-1.294195
C	6.140044	2.501753	-0.095910
C	-1.911933	1.435117	0.457866
C	5.188749	3.072461	-2.237162
C	-3.004407	0.589682	0.455539
C	5.110135	1.604547	0.121560
C	-4.084418	0.837811	1.394148
C	-1.915537	2.668869	1.215829
C	1.912059	-0.457804	1.435153
C	-4.117078	2.040138	2.168816
C	-3.004369	-0.589783	-0.455473
C	3.004507	-0.455493	0.589686
C	-5.110330	-0.121518	1.604089
C	-4.084324	-0.837942	-1.394139
C	1.915667	-1.215801	2.668882
C	4.084436	-1.394238	0.837700
C	-6.140398	0.095984	2.501106
C	-5.189133	2.237205	3.071994
C	-1.911872	-1.435186	-0.457744
C	4.117099	-2.168938	2.040009
C	3.004446	0.455584	-0.589733
C	-6.189642	1.294265	3.237525
C	-3.031141	3.002031	2.033945
C	-4.116906	-2.040269	-2.168812
C	-1.915397	-2.668936	-1.215707
C	3.031234	-2.033994	3.001972
C	5.110215	-1.604339	-0.121739
C	1.911945	0.457835	-1.435131
C	3.030930	2.034090	-3.002018
C	-5.110254	0.121357	-1.604131
C	6.140189	-2.501486	0.095666
C	5.189063	-3.072246	2.236979
C	1.915430	1.215832	-2.668859
C	4.084306	1.394390	-0.837815
C	-3.030946	-3.002128	-2.033886
C	-6.189436	-1.294456	-3.237627
C	4.116849	2.169094	-2.040124
C	6.189464	-3.237899	1.293949
C	-5.188907	-2.237367	-3.072046
C	-6.140268	-0.096176	-2.501203
C	-3.010603	-4.249655	-2.704083
C	-3.010872	4.249561	2.704138
C	-1.936578	5.116787	2.586205
C	-1.936291	-5.116850	-2.586093
C	-0.826811	4.766783	1.792348
C	-0.819299	3.558301	1.119388
C	0.826993	-1.792317	4.766824
C	1.936727	-2.586253	5.116757
C	3.010975	-2.704229	4.249480
C	0.819470	-1.119323	3.558362
C	0.826591	1.792292	-4.766731
C	0.819183	1.119292	-3.558270
C	1.936256	2.586294	-5.116730
C	3.010552	2.704329	-4.249521
C	-0.819139	-3.558338	-1.119206
C	-0.826579	-4.766818	-1.792171
H	6.904907	2.641085	0.665016
H	0.022660	-3.262916	-0.503621
H	5.072156	1.053372	1.054569
H	-1.951929	-6.068592	-3.113194
H	5.072146	-1.053167	-1.054746
H	3.850773	3.324397	-4.545756
H	6.905011	-2.640776	-0.665309
H	1.951866	3.113429	-6.068454
H	5.224898	-3.671298	3.141383
H	-0.022579	0.503645	-3.262873
H	6.995688	-3.945751	1.473304
H	-0.021396	1.708860	-5.442488
H	6.995375	3.946066	-1.473601

H	0.041912	3.234568	-0.494833	H	-0.022346	-0.503725	3.263015
H	-5.219192	-3.193609	3.626532	H	5.224495	3.671516	-3.141567
H	-3.837267	4.584261	-3.271323	H	3.851251	-3.324246	4.545664
H	5.219080	-3.626945	-3.193287	H	-5.224686	-3.141782	-3.671084
H	-1.919985	6.083122	-3.064222	H	1.952429	-3.113383	6.068482
H	7.003803	-3.908338	-1.542348	H	-6.995692	-1.473914	-3.945416
H	0.056582	5.424417	-1.685075	H	-0.020955	-1.708933	5.442635
H	6.919880	-2.630561	0.609579	H	-6.905204	0.664696	-2.640423
H	-0.041778	0.494791	3.234568	H	0.022542	3.262900	0.503850
H	5.080203	-1.059031	1.029934	H	-5.072270	1.054355	-1.052934
H	-0.056507	1.685112	5.424374	H	0.021171	5.442555	1.708994
H	7.003937	3.908260	1.542263	H	-6.995940	1.473698	3.945272
H	1.919949	3.064462	6.082985	H	-1.952274	6.068531	3.113301
H	6.919954	2.630488	-0.609665	H	-6.905318	-0.664911	2.640287
H	3.837176	3.271688	4.584070	H	-3.851179	4.545806	3.324083
H	5.219221	3.626923	3.193217	H	-5.224970	3.141621	3.671029
H	3.837041	-3.271658	-4.584133	H	-3.850867	-4.545922	-3.324077
H	5.080224	1.059015	-1.030004	H	-5.072288	-1.054516	1.052896
H	-0.056597	-1.684956	-5.424407	H	0.021418	-5.442566	-1.708772
O	0.827933	0.314513	-1.177676	O	-0.828412	-1.182253	0.300712
O	-0.827774	-1.177640	-0.314475	O	0.828499	-0.300635	-1.182191
O	-0.827810	1.177692	0.314447	O	0.828555	0.300605	1.182288
O	0.827937	-0.314409	1.177655	O	-0.828425	1.182227	-0.300528

$(R,R)_{ax}$-**7**	
B3LYP/BS1	B3LYP/BS2

45
scf done: -1293.401258

C	-1.947254	-1.417154	-0.672145
C	-3.065047	-0.734289	-0.117543
C	-4.239318	-1.458383	0.146656
C	-4.369642	-2.803982	-0.183742
C	-3.313095	-3.457274	-0.819457
C	-2.134028	-2.760960	-1.058590
C	-3.065083	0.734003	0.117318
C	-1.947519	1.416786	0.672448
C	-2.134316	2.760620	1.058738
C	-3.313220	3.457025	0.819046
C	-4.369533	2.803793	0.182879
C	-4.239176	1.458176	-0.147444
O	-0.795862	0.810170	0.935517
B	0.000002	-0.000027	0.000439
O	-0.795385	-0.810725	-0.934654
H	-5.065317	0.943015	-0.629055
H	-5.287253	3.340776	-0.042146
I	-0.555410	3.764103	2.128221
H	-5.065639	-0.943156	0.627886
H	-5.287509	-3.340893	0.040854
I	-0.554797	-3.764527	-2.127524
O	0.795873	-0.810219	0.935519
C	1.947534	-1.416829	0.672452
C	3.065091	-0.734040	0.117314
C	4.239192	-1.458203	-0.147438
C	4.369567	-2.803813	0.182911
C	3.313268	-3.457042	0.819104
C	2.134355	-2.760649	1.058784
C	3.065047	0.734253	-0.117540
C	4.239308	1.458354	0.146676
C	4.369614	2.803965	-0.183684
C	3.313053	3.457265	-0.819366
C	2.133996	2.760942	-1.058518
C	1.947246	1.417117	-0.672127
H	5.065635	0.943127	0.627896
H	5.287473	3.340883	0.040931
I	0.554718	3.764541	-2.127354
O	0.795382	0.810684	-0.934645
I	0.555495	-3.764108	2.128355
H	5.287296	-3.340786	-0.042101
H	5.065328	-0.943038	-0.629054
H	-3.401954	4.496943	1.115582
H	3.402023	-4.496948	1.115676
H	3.401718	4.497177	-1.115947
H	-3.401781	-4.497171	-1.116084

45
scf done: -1293.451389

C	-1.951723	-1.418048	-0.670720
C	-3.069396	-0.734547	-0.117859
C	-4.241509	-1.463346	0.151367
C	-4.365882	-2.811634	-0.177830
C	-3.306712	-3.462474	-0.816240
C	-2.127944	-2.763917	-1.058920
C	-3.069426	0.734211	0.117736
C	-1.951918	1.417656	0.670970
C	-2.128076	2.763613	1.058845
C	-3.306689	3.462262	0.815659
C	-4.365720	2.811428	0.177012
C	-4.241372	1.463088	-0.151995
O	-0.799142	0.807583	0.936082
B	0.000002	-0.000071	0.000384
O	-0.798753	-0.808144	-0.935333
H	-5.070225	0.952758	-0.635042
H	-5.280427	3.352709	-0.052111
I	-0.555134	3.746092	2.138588
H	-5.070496	-0.952973	0.634138
H	-5.280733	-3.352843	0.050886
I	-0.554922	-3.746309	-2.138634
O	0.799193	-0.807689	0.936086
C	1.951979	-1.417747	0.670972
C	3.069440	-0.734304	0.117638
C	4.241405	-1.463156	-0.152079
C	4.365829	-2.811454	0.177068
C	3.306883	-3.462249	0.815894
C	2.128248	-2.763630	1.059062
C	3.069389	0.734455	-0.117950
C	4.241483	1.463277	0.151297
C	4.365778	2.811610	-0.177747
C	3.306524	3.462495	-0.815972
C	2.127778	2.763910	-1.058677
C	1.951669	1.417963	-0.670705
H	5.070505	0.952894	0.633997
H	5.280607	3.352840	0.051010
I	0.554498	3.746472	-2.137861
O	0.798709	0.808047	-0.935322
I	0.555564	-3.745949	2.139326
H	5.280559	-3.352712	-0.052019
H	5.070222	-0.952832	-0.635193
H	-3.394030	4.502792	1.112217
H	3.394319	-4.502717	1.112641
H	3.393800	4.503017	-1.112579
H	-3.394083	-4.502931	-1.113046

$(R,S)_{ax}$-**7**	
B3LYP/BS1	B3LYP/BS2

45
scf done: -1293.406828

C	-2.378567	3.960895	-3.265420
C	-1.215054	4.771876	-3.370210
C	-1.345159	6.107023	-3.779546
C	-2.579546	6.651998	-4.122825
C	-3.722514	5.853475	-4.066435
C	-3.608150	4.533117	-3.643102
C	0.135871	4.211459	-3.113155
C	0.374309	3.346533	-2.009747
C	1.704221	2.956042	-1.763088
C	2.764046	3.348518	-2.574486
C	2.510645	4.161638	-3.679849
C	1.209037	4.584812	-3.935364
O	-0.606610	2.998178	-1.177093
B	-1.785161	2.235920	-1.614865
O	-2.299294	2.675819	-2.920187
H	1.007323	5.213039	-4.798655
H	3.325401	4.458192	-4.335293
I	2.133573	1.731636	-0.042282
H	-0.454076	6.727687	-3.816486
H	-2.656817	7.691597	-4.430468
I	-5.385755	3.315245	-3.603242
O	-2.848365	2.443230	-0.620706
C	-2.869072	1.810277	0.552249
C	-2.976793	0.394201	0.626940
C	-3.039047	-0.222722	1.884966
C	-3.035826	0.516002	3.065145
C	-2.975064	1.908737	3.003542
C	-2.893343	2.530535	1.761641
C	-3.085881	-0.432365	-0.601893
C	-3.967300	-1.523025	-0.627579
C	-4.037997	-2.383385	-1.719977
C	-3.208797	-2.165243	-2.820904
C	-2.344382	-1.075110	-2.814464
C	-2.267997	-0.173320	-1.736090
H	-4.615874	-1.686424	0.228739
H	-4.734116	-3.218130	-1.720109
I	-1.049949	-0.787371	-4.513388
O	-1.386348	0.826454	-1.741428
I	-2.839340	4.684089	1.698658
H	-3.077774	0.015365	4.028982
H	-3.080174	-1.307593	1.929496
H	-2.981510	2.502974	3.911261
H	-3.241596	-2.829814	-3.677866
H	-4.692234	6.256340	-4.339293
H	3.772680	3.016177	-2.352393

45
scf done: -1293.458131

C	-2.376462	3.964121	-3.267808
C	-1.213767	4.774841	-3.375916
C	-1.350043	6.110957	-3.785736
C	-2.590433	6.650548	-4.123360
C	-3.732789	5.847974	-4.058696
C	-3.615028	4.526911	-3.633423
C	0.138073	4.217440	-3.112208
C	0.372862	3.349950	-2.010782
C	1.697142	2.942136	-1.756979
C	2.761518	3.332943	-2.565866
C	2.516329	4.152966	-3.670728
C	1.217137	4.586337	-3.931517
O	-0.613484	3.006919	-1.176562
B	-1.787056	2.236348	-1.615738
O	-2.292660	2.674827	-2.925622
H	1.025053	5.216419	-4.796174
H	3.335732	4.445503	-4.322916
I	2.098835	1.713636	-0.044893
H	-0.462991	6.737835	-3.827085
H	-2.673272	7.690029	-4.431527
I	-5.374101	3.300479	-3.575952
O	-2.857148	2.437107	-0.626653
C	-2.871856	1.806816	0.551944
C	-2.981616	0.391625	0.629140
C	-3.041294	-0.219633	1.891884
C	-3.032112	0.528042	3.068582
C	-2.965556	1.922351	2.999742
C	-2.884537	2.540662	1.754316
C	-3.084303	-0.438504	-0.598888
C	-3.964086	-1.532464	-0.630216
C	-4.032000	-2.386458	-1.730121
C	-3.204741	-2.158048	-2.833193
C	-2.342540	-1.064238	-2.824202
C	-2.269570	-0.175402	-1.733713
H	-4.614181	-1.704663	0.223752
H	-4.725938	-3.223579	-1.735286
I	-1.054696	-0.751274	-4.511022
O	-1.384839	0.826361	-1.734325
I	-2.820576	4.683135	1.668009
H	-3.072134	0.032968	4.035873
H	-3.083647	-1.304458	1.945755
H	-2.967128	2.520438	3.905539
H	-3.237647	-2.818389	-3.694036
H	-4.705056	6.248975	-4.327163
H	3.768229	2.994090	-2.342495

$(R,R)_{ax}$-TS-$(R,S)_{ax}$-**7**	
B3LYP/BS1	B3LYP/BS2

45				45			
scf done: -1293.394735				scf done: -1293.445390			
C	4.048158	-0.196912	1.595255	C	4.055678	-0.202532	1.596998
C	2.981802	0.244309	0.796713	C	2.990405	0.239508	0.794673
C	2.144851	1.284074	1.278057	C	2.150769	1.274633	1.279901
C	2.482456	1.889291	2.501739	C	2.477852	1.883076	2.506231
C	3.557593	1.461057	3.273715	C	3.554432	1.454684	3.278850
C	4.336531	0.394257	2.822444	C	4.338041	0.388790	2.827342
C	2.797081	-0.323565	-0.564182	C	2.806140	-0.325817	-0.567997
C	1.510281	-0.627352	-1.096282	C	1.520373	-0.627974	-1.101978
C	1.468472	-1.283734	-2.344803	C	1.467840	-1.273159	-2.356943
C	2.609633	-1.584842	-3.080157	C	2.609948	-1.564767	-3.097722
C	3.859621	-1.231198	-2.572883	C	3.862952	-1.211901	-2.591403
C	3.937965	-0.613135	-1.328868	C	3.946503	-0.604210	-1.340539
C	-1.962142	1.354876	-1.238275	C	-1.965258	1.347251	-1.237556
C	-2.907357	0.388035	-0.754352	C	-2.907323	0.378911	-0.754041
C	-4.018796	0.146615	-1.594773	C	-4.009094	0.122913	-1.605537
C	-4.273327	0.825294	-2.777392	C	-4.259151	0.801361	-2.791113
C	-3.393624	1.818615	-3.202939	C	-3.386186	1.807639	-3.207202
C	-2.268697	2.052559	-2.434935	C	-2.265382	2.051518	-2.433235
C	-2.830282	-0.364122	0.556418	C	-2.837665	-0.362194	0.563059
C	-1.774799	-0.268397	1.524617	C	-1.780104	-0.275282	1.528783
C	-1.872026	-1.043629	2.706442	C	-1.874505	-1.045119	2.715738
C	-2.939674	-1.871982	3.004333	C	-2.953977	-1.858805	3.019509
C	-3.976203	-1.950633	2.078137	C	-4.000096	-1.924329	2.099875
C	-3.904853	-1.214694	0.903941	C	-3.925886	-1.193366	0.920588
H	-3.572144	2.379213	-4.113954	H	-3.565050	2.368831	-4.118371
O	0.382999	-0.406629	-0.424166	O	0.392415	-0.414880	-0.421902
B	-0.005818	0.874274	0.219138	B	-0.003205	0.865708	0.220063
O	1.122391	1.737119	0.548788	O	1.125882	1.728497	0.548848
O	-0.817018	1.692945	-0.668006	O	-0.816385	1.683727	-0.666561
O	-0.722122	0.535247	1.444372	O	-0.719171	0.522109	1.444581
I	-0.884524	3.555549	-3.132977	I	-0.892811	3.565702	-3.099392
I	-0.436517	-1.889260	-3.150256	I	-0.433435	-1.879019	-3.145742
H	4.908762	-0.331496	-0.931076	H	4.919703	-0.323653	-0.946736
H	4.759951	-1.435736	-3.146168	H	4.761511	-1.408101	-3.171173
H	4.654339	-1.026563	1.242539	H	4.665749	-1.031260	1.247493
H	5.164017	0.031798	3.426850	H	5.163022	0.025426	3.435395
H	-4.753694	-1.304383	0.242256	H	-4.781219	-1.269962	0.265228
H	-4.841269	-2.579560	2.271465	H	-4.874455	-2.538041	2.302409
H	-5.157602	0.585068	-3.361785	H	-5.132839	0.548802	-3.386884
H	-4.733979	-0.618106	-1.329640	H	-4.716381	-0.652248	-1.348302
H	2.521894	-2.079000	-4.042043	H	2.521116	-2.052780	-4.063165
H	3.776744	1.944328	4.220198	H	3.771298	1.937028	4.226872
I	1.308480	3.551999	3.200682	I	1.302262	3.540088	3.189794
H	-2.964207	-2.437039	3.929911	H	-2.981530	-2.421458	3.946974
I	-0.269350	-0.931559	4.146903	I	-0.268789	-0.942348	4.139292