Interrogating the Thionium Hydrogen Bond as a Noncovalent Stereocontrolling Interaction in Chiral Phosphate Catalysis

*Junshan Lai and Jolene P. Reid**

jreid@chem.ubc.ca

Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, British Columbia, V6T 1Z1, Canada

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Computational Details

For the study of the reaction catalyzed by buta-1,3-diene-1,4-diol-phosphoric acid, quantum mechanical calculations were performed using Gaussian 09 (revision D.01).[1] All geometries of the stationary points were obtained via unconstrained optimizations using the B3LYP density functional,[2,3] and split-valence polarized 6-31G(d,p) basis set.[4,5] Single point energies were taken using the M06-2X density functional,[6] and 6-31G(d,p) basis set. This energy was used to correct the gas phase energy obtained from the B3LYP calculations.

Calculations using the TRIP catalyst system was performed using B3LYP density functional, with the 6-31G(d,p) basis set implemented in Gaussian 09 (revision D.01). Single point energy calculations were performed on the resulting structures using M06-2X/6-31G(d,p). Free energies in solution were derived from structures optimized in the gas phase by means of a single point calculation using M06-2X/6-31G(d,p) with the polarizable continuum model (IEFPCM) using toluene.[7] These single point calculations were used to correct the gas phase energy.

For the QM/MM hybrid calculations on the full catalyst, transition states were located using the ONIOM method implemented in Gaussian 09 (revision D.01). The B3LYP density functional, and split-valence polarized 6-31G(d,p) basis set, were used for the high-layer, and the force field UFF,[8] was used for the low-layer. The reactants and the phosphoric acid moiety of the catalyst were included in the high-layer, and the remaining regions of the catalyst were treated as the low-layer. The combination of DFT and UFF has previously been shown to give excellent results when used to describe reactions catalyzed by chiral phosphoric acids.[9-15] Single point energy calculations were performed on the resulting structures using M06-2X density functional, and the 6- 31G(d,p) basis set. This energy was used to correct the gas-phase energy derived from the ONIOM calculations. Free energies in solution were derived from structures optimized in the gas phase at the ONIOM (B3LYP/6-31G(d,p):UFF), level of theory by means of a single point calculation using M06-2X/6-31G(d,p) with the polarizable continuum model (IEFPCM) using toluene. These values were used to correct the Gibbs free energy derived from the ONIOM calculations. All TS were verified by IRC.

Conformational searches were performed with Macromodel version 11.7[16] and the OPLS3 force field.[17] Structures were generated using the mixed torsional/Low-mode sampling method. For TS analysis, conformational searches were performed for each TS class i.e. guess structures generated separately for **TS-4Re**, **TS-4Si**, **TS-5Re**, and **TS-5Si,** etc. For each search, conformations generated within 21 kJ mol^{-1} were taken for optimization in Gaussian. For statistical modeling analysis, the energy window for conformer saving was reduced to 10 kJ mol^{-1}.

Cartesian coordinates and energies of the TS employing the model catalyst

TS-1
B3LYP/6-31G(d,p) Energy = -2993.101851
B3LYP/6-31G(d,p) Free Energy = -2992.759802
M06-2X/6-31G(d,p) Derived free energy = -2992.061936
Number of Imaginary Frequencies = 1 (-140.15)

B3LYP/6-31G(d,p) Geometry

C	-0.42812	5.15889	-1.48571
C	-0.68235	5.81232	-0.20746
C	-0.62942	3.87650	-1.82013
C	-1.00283	5.29345	0.99148
O	-1.15917	2.91005	-0.99121
O	-1.16732	3.98605	1.36094
P	-0.55113	2.69486	0.53636
O	-1.28920	1.49594	1.09503
O	0.94868	2.71922	0.52577
S	1.92959	-0.73583	3.18418
C	1.82211	-0.08176	1.57494
C	0.15606	-0.51147	3.56230
C	-0.61437	-1.29954	2.49017
N	-0.16986	-0.83306	1.17375
C	2.81454	-0.41078	0.57769
C	3.53321	-1.62549	0.57925
C	4.51168	-1.86065	-0.37341
C	4.76800	-0.88060	-1.33980
C	4.05752	0.32144	-1.37495
C	3.07353	0.55287	-0.42299
Cl	6.00401	-1.17877	-2.54106
S	-0.19422	-1.96972	-0.12628
O	0.22929	-1.20178	-1.29482
O	0.57858	-3.12252	0.34988
C	-1.90848	-2.49367	-0.30047
C	-2.16466	-3.80286	0.05825
C	-3.46865	-4.32877	-0.06034
C	-4.48626	-3.53179	-0.52913
C	-4.25623	-2.18216	-0.90498
C	-2.93321	-1.62475	-0.80340
C	-5.31805	-1.36915	-1.38224
C	-5.09755	-0.05918	-1.73799
C	-3.79950	0.48892	-1.63503
C	-2.74138	-0.27192	-1.18927
H	-0.03384	5.79187	-2.27579
H	-0.60670	6.89609	-0.21238
H	-0.41337	3.49640	-2.81345
H	-1.19214	5.94672	1.83724
H	1.36754	0.90476	1.47340
H	-0.10647	0.54816	3.52236
H	-0.03014	-0.90034	4.56539

H	-1.68756	-1.11372	2.60937
H	-0.41352	-2.36861	2.58863
H	-0.64018	0.11638	0.95137
H	3.29678	-2.39114	1.30973
H	5.06508	-2.79221	-0.38613
H	4.27284	1.05781	-2.14033
H	2.49989	1.47714	-0.42099
H	-1.35185	-4.42221	0.41856
H	-3.65614	-5.36045	0.21878
H	-5.49406	-3.92798	-0.62098
H	-6.31062	-1.80492	-1.45665
H	-5.91784	0.55610	-2.09492
H	-3.62053	1.52601	-1.89833
H	-1.76551	0.18573	-1.13028

Pre TS-1

B3LYP/6-31G(d,p) Energy = -2993.104178
B3LYP/6-31G(d,p) Free Energy = -2992.766144
M06-2X/6-31G(d,p) Derived free energy = -2992.062580
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	0.75004	4.84606	-1.49333
C	0.85880	5.59769	-0.24893
C	0.10930	3.68953	-1.71790
C	0.49865	5.26910	1.00504
O	-0.61126	2.97803	-0.78478
O	-0.06199	4.11423	1.47590
P	0.02881	2.65036	0.71155
O	-0.97300	1.76770	1.40748
O	1.46640	2.22204	0.57783
S	1.78718	-1.36809	2.94855
C	2.08306	-0.53278	1.51382
C	0.16006	-0.68795	3.44962
C	-0.96431	-1.29691	2.58600
N	-0.77719	-0.89491	1.20981
C	3.06546	-0.91077	0.55569
C	3.74451	-2.15611	0.56968
C	4.69397	-2.44357	-0.39029
C	4.97115	-1.48791	-1.38312
C	4.30697	-0.25962	-1.43166
C	3.35018	0.02896	-0.46947
Cl	6.16865	-1.85976	-2.59237
S	-0.97580	-1.94749	-0.06591
O	-0.33676	-1.30046	-1.21436
O	-0.51424	-3.25912	0.41278
C	-2.74645	-2.08591	-0.38506
C	-3.30414	-3.33176	-0.18942
C	-4.68443	-3.53660	-0.41084
C	-5.47649	-2.48796	-0.81275

C	-4.93349	-1.19171	-1.02059
C	-3.52829	-0.96509	-0.81742
C	-5.75949	-0.11035	-1.42721
C	-5.23378	1.14583	-1.62065
C	-3.85232	1.36892	-1.42331
C	-3.01808	0.34226	-1.04044
H	1.23884	5.28396	-2.35933
H	1.29321	6.58959	-0.33772
H	0.08125	3.22705	-2.69953
H	0.62261	5.98289	1.81349
H	1.57072	0.42147	1.33743
H	0.17321	0.39838	3.33285
H	0.04282	-0.94595	4.50525
H	-1.91394	-0.92396	2.99390
H	-0.95824	-2.38730	2.65230
H	-0.93896	0.12596	1.04354
H	3.49913	-2.90112	1.31974
H	5.21272	-3.39482	-0.39751
H	4.53655	0.45145	-2.21640
H	2.81072	0.97460	-0.46877
H	-2.66870	-4.14870	0.13176
H	-5.10920	-4.52372	-0.25827
H	-6.54048	-2.63538	-0.97855
H	-6.81926	-0.29708	-1.57920
H	-5.87635	1.96667	-1.92486
H	-3.43092	2.35845	-1.56665
H	-1.96499	0.55240	-0.92086

Post TS-1

B3LYP/6-31G(d,p) Energy = -2993.119624
B3LYP/6-31G(d,p) Free Energy = -2992.776912
M06-2X/6-31G(d,p) Derived free energy = -2992.093403
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-2.48491	4.83589	-1.22610
C	-3.11193	5.11386	0.06099
C	-2.02132	3.66153	-1.66850
C	-3.11487	4.40252	1.20034
O	-2.11671	2.47804	-0.94127
O	-2.49576	3.20795	1.49127
P	-1.42854	2.43540	0.53846
O	-1.68833	0.95689	1.01550
O	-0.04122	2.95190	0.57922
S	2.08489	-0.24369	3.13682
C	1.55275	0.14346	1.41382
C	0.37068	-0.72673	3.53316
C	-0.06009	-1.55470	2.32894
N	0.37027	-0.81426	1.09654
C	2.73178	0.22918	0.46838

C	3.75914	-0.72352	0.44404
C	4.85564	-0.56307	-0.39919
C	4.92548	0.56370	-1.21700
C	3.92193	1.52975	-1.20322
C	2.82883	1.35808	-0.35658
Cl	6.31262	0.77314	-2.27936
S	0.60159	-1.91022	-0.26688
O	0.74920	-1.05872	-1.44650
O	1.63112	-2.89712	0.08263
C	-0.97065	-2.80452	-0.33015
C	-0.91766	-4.09746	0.15462
C	-2.06731	-4.91460	0.14222
C	-3.24836	-4.42143	-0.35835
C	-3.33365	-3.10625	-0.88497
C	-2.17073	-2.25701	-0.89395
C	-4.55707	-2.61975	-1.41704
C	-4.64325	-1.35304	-1.94350
C	-3.49994	-0.52365	-1.96504
C	-2.29446	-0.96091	-1.46238
H	-2.39237	5.67330	-1.91138
H	-3.66308	6.04746	0.12592
H	-1.55812	3.52255	-2.63807
H	-3.65799	4.74663	2.07246
H	1.08464	1.12750	1.43549
H	-0.26145	0.15580	3.66617
H	0.35574	-1.32106	4.44881
H	-1.14442	-1.68928	2.29662
H	0.42678	-2.53373	2.37036
H	-0.91393	0.31762	0.89793
H	3.69906	-1.60043	1.07731
H	5.64830	-1.30210	-0.42090
H	3.99683	2.40363	-1.84026
H	2.04440	2.10872	-0.32949
H	0.02145	-4.48095	0.53502
H	-2.00747	-5.92703	0.52783
H	-4.14152	-5.04038	-0.36805
H	-5.42439	-3.27397	-1.40065
H	-5.58384	-0.98942	-2.34565
H	-3.56630	0.47758	-2.37677
H	-1.43110	-0.31392	-1.51524

TS-2

B3LYP/6-31G(d,p) Energy = -2993.098863
B3LYP/6-31G(d,p) Free Energy = -2992.757699
M06-2X/6-31G(d,p) Derived free energy = -2992.059798
Number of Imaginary Frequencies = 1 (-121.82)

B3LYP/6-31G(d,p) Geometry

C	3.68803	-4.84743	-0.28514

C	4.63126	-3.74137	-0.39258
C	2.34294	-4.84842	-0.25989
C	4.37629	-2.46011	-0.69163
O	1.46645	-3.79980	-0.30914
O	3.13190	-1.94601	-0.99064
P	1.85542	-2.22315	0.02286
O	0.69347	-1.43370	-0.56190
O	2.23179	-2.03770	1.45853
S	-1.82483	-0.98064	2.98620
C	-1.76847	-1.06522	1.26040
C	-0.02805	-0.69291	3.16898
C	0.32150	0.56857	2.35227
N	-0.24884	0.46313	1.00595
C	-2.93063	-0.88792	0.42365
C	-4.10855	-0.24840	0.86109
C	-5.20530	-0.14992	0.01935
C	-5.11901	-0.67603	-1.27519
C	-3.95261	-1.28632	-1.74398
C	-2.85896	-1.38452	-0.89598
Cl	-6.50218	-0.54934	-2.33579
S	-0.84542	1.90162	0.26490
O	-1.25732	1.48724	-1.07408
O	-1.80756	2.46627	1.21690
C	0.55766	3.02420	0.16896
C	0.43624	4.18944	0.89969
C	1.46324	5.15683	0.86625
C	2.59069	4.92983	0.11291
C	2.74805	3.73853	-0.64376
C	1.70752	2.74511	-0.64093
C	3.92445	3.51014	-1.40533
C	4.08340	2.34944	-2.12546
C	3.06275	1.37229	-2.12031
C	1.89855	1.56471	-1.40815
H	4.13123	-5.83698	-0.21613
H	5.67603	-3.98386	-0.21919
H	1.79961	-5.78691	-0.20998
H	5.16027	-1.71211	-0.75277
H	-0.97297	-1.66888	0.83157
H	0.54748	-1.54502	2.79435
H	0.17902	-0.54617	4.23106
H	1.41296	0.63223	2.29454
H	-0.08228	1.46071	2.83560
H	0.28102	-0.17286	0.32864
H	-4.15200	0.18408	1.85498
H	-6.11630	0.33748	0.34601
H	-3.90646	-1.66590	-2.75780
H	-1.92949	-1.82611	-1.24366
H	-0.45719	4.35277	1.49076
H	1.35417	6.07203	1.43883
H	3.38906	5.66669	0.08680

H	4.69974	4.27144	-1.40127
H	4.99051	2.18087	-2.69782
H	3.19145	0.44717	-2.67177
H	1.14004	0.79418	-1.44550

Pre TS-2

B3LYP/6-31G(d,p) Energy = -2993.101621
B3LYP/6-31G(d,p) Free Energy = -2992.764744
M06-2X/6-31G(d,p) Derived free energy = -2992.061110
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-0.60383	5.91623	-0.38561
C	-1.98056	5.50461	-0.13956
C	0.50776	5.18146	-0.56783
C	-2.50671	4.27213	-0.18542
O	0.66165	3.82151	-0.55915
O	-1.82700	3.11826	-0.50706
P	-0.37304	2.76940	0.19771
O	0.01905	1.40704	-0.34938
O	-0.39992	2.99983	1.67607
S	2.02156	-0.18964	2.95100
C	2.15306	0.09054	1.29995
C	0.30772	0.39353	3.25789
C	-0.74083	-0.58544	2.67933
N	-0.55854	-0.78069	1.25834
C	3.19474	-0.35997	0.44136
C	4.29763	-1.14605	0.85634
C	5.25842	-1.53422	-0.05654
C	5.11855	-1.14959	-1.40139
C	4.03348	-0.38778	-1.84253
C	3.07276	0.00648	-0.92313
Cl	6.33307	-1.64798	-2.54588
S	-0.56217	-2.27543	0.52765
O	0.20804	-2.11997	-0.70952
O	-0.15018	-3.24183	1.55544
C	-2.27427	-2.64386	0.09772
C	-2.81890	-3.76669	0.68358
C	-4.15437	-4.13672	0.40816
C	-4.91761	-3.36671	-0.43595
C	-4.38758	-2.20067	-1.05084
C	-3.02411	-1.81831	-0.80253
C	-5.18826	-1.40079	-1.90881
C	-4.67938	-0.26454	-2.49286
C	-3.33812	0.11012	-2.25183
C	-2.52502	-0.64881	-1.43883
H	-0.43788	6.98873	-0.43645
H	-2.67949	6.30011	0.10322
H	1.45589	5.66704	-0.77718
H	-3.55958	4.08866	0.00376

H	1.37963	0.70659	0.82855
H	0.19273	1.39618	2.82141
H	0.21450	0.45590	4.34532
H	-1.72041	-0.14293	2.90815
H	-0.67742	-1.55964	3.16909
H	-0.56618	0.03656	0.61890
H	4.38995	-1.45201	1.89383
H	6.10824	-2.13438	0.24630
H	3.94665	-0.11818	-2.88829
H	2.20656	0.58638	-1.23172
H	-2.20924	-4.35830	1.35635
H	-4.56864	-5.02629	0.87191
H	-5.94879	-3.63848	-0.64589
H	-6.21608	-1.70418	-2.08945
H	-5.30349	0.34477	-3.13972
H	-2.93638	1.01190	-2.70223
H	-1.49798	-0.33616	-1.30345

Post TS-2
B3LYP/6-31G(d,p) Energy = -2993.119138
B3LYP/6-31G(d,p) Free Energy = -2992.777272
M06-2X/6-31G(d,p) Derived free energy = -2992.094153
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	4.44858	-4.26324	-0.21282
C	5.22575	-3.03831	-0.36105
C	3.12580	-4.43920	-0.05954
C	4.77141	-1.82352	-0.68897
O	2.12119	-3.50382	0.03391
O	3.43860	-1.55770	-0.98614
P	2.31865	-1.88964	0.14574
O	0.98599	-1.40149	-0.54503
O	2.61014	-1.38180	1.50543
S	-1.93308	-0.96159	2.98488
C	-1.60455	-0.86007	1.17702
C	-0.17755	-0.54238	3.26428
C	0.11340	0.58342	2.27466
N	-0.56935	0.26205	0.96836
C	-2.86429	-0.86315	0.33980
C	-4.01332	-0.14828	0.70022
C	-5.16863	-0.22532	-0.07413
C	-5.17166	-1.02402	-1.21628
C	-4.04116	-1.74536	-1.59557
C	-2.89454	-1.66163	-0.81028
Cl	-6.62983	-1.12870	-2.19333
S	-1.17118	1.72598	0.18181
O	-1.52932	1.33959	-1.18263
O	-2.15582	2.37517	1.05680
C	0.29654	2.78112	0.15875

C	0.26863	3.83676	1.04874
C	1.34666	4.74459	1.11481
C	2.43250	4.57472	0.28981
C	2.48467	3.51288	-0.65094
C	1.38868	2.58508	-0.74955
C	3.60525	3.36127	-1.50990
C	3.65330	2.34569	-2.43526
C	2.57051	1.44460	-2.54457
C	1.46345	1.56144	-1.73267
H	5.01718	-5.18853	-0.22058
H	6.29695	-3.12009	-0.20185
H	2.69953	-5.43289	0.01221
H	5.40236	-0.94749	-0.78050
H	-1.04179	-1.75927	0.91817
H	0.46734	-1.40501	3.08162
H	-0.03910	-0.20370	4.29284
H	1.18675	0.67309	2.09826
H	-0.28342	1.52033	2.67275
H	0.51244	-0.67023	-0.03569
H	-4.00238	0.48216	1.58171
H	-6.05749	0.32867	0.20502
H	-4.06032	-2.36234	-2.48655
H	-2.00763	-2.21710	-1.10184
H	-0.59486	3.96306	1.69117
H	1.30923	5.56814	1.82021
H	3.27216	5.26279	0.33908
H	4.42399	4.07010	-1.42161
H	4.51448	2.23914	-3.08784
H	2.60588	0.64709	-3.27940
H	0.63672	0.87767	-1.86040

TS-3

B3LYP/6-31G(d,p) Energy = -2993.093931
B3LYP/6-31G(d,p) Free Energy = -2992.753121
M06-2X/6-31G(d,p) Derived free energy = -2992.057062
Number of Imaginary Frequencies = 1 (-121.59)

B3LYP/6-31G(d,p) Geometry

C	2.58438	3.13868	-0.02750
C	1.75845	4.13675	-0.37461
C	0.54917	4.59634	0.29615
C	-0.11522	4.07537	1.34403
O	0.15420	2.94801	2.06649
O	2.46891	2.32956	1.07840
P	1.02322	1.64895	1.51582
O	1.26670	0.74401	2.67533
O	0.35196	1.11607	0.25686
C	3.16329	-0.98731	0.55014
C	2.30823	-1.90110	-0.10647

C	2.52940	-2.20340	-1.46904
C	3.60782	-1.65609	-2.14513
C	4.46032	-0.78106	-1.46156
C	4.24091	-0.43348	-0.12535
H	2.93976	-0.66822	1.56431
C	1.20831	-2.53662	0.56998
H	1.84509	-2.86538	-1.98953
H	3.78951	-1.88856	-3.18771
Cl	5.81853	-0.08416	-2.31261
H	4.88885	0.28099	0.36785
S	1.23923	-2.77377	2.28173
N	-0.62557	-1.26491	0.57003
H	0.59953	-3.23096	0.00175
S	-1.56720	-1.89016	-0.72039
H	-0.22766	-0.25958	0.39063
O	-1.73020	-3.32362	-0.41786
O	-0.86924	-1.47735	-1.93821
C	-5.83541	-0.22295	-0.56353
C	-3.20268	-1.13876	-0.63383
C	-4.23485	-2.01182	-0.34854
C	-5.56717	-1.54807	-0.31467
H	-6.85858	0.14258	-0.53904
H	-4.01081	-3.05612	-0.16722
H	-6.36956	-2.24465	-0.09493
C	-4.79670	0.69998	-0.85497
C	-3.43006	0.25146	-0.90140
C	-2.41541	1.20327	-1.18353
C	-2.73740	2.52616	-1.39656
C	-4.07963	2.96582	-1.36126
C	-5.08750	2.06824	-1.09783
H	-1.37397	0.91643	-1.21126
H	-1.93761	3.23696	-1.57647
H	-4.31148	4.01189	-1.53732
H	-6.12435	2.39134	-1.06416
C	-1.10137	-1.47664	1.94020
H	-0.71120	-0.64594	2.53397
H	-2.19670	-1.47485	1.98870
C	-0.57239	-2.81241	2.50373
H	-0.76361	-2.89951	3.57558
H	-1.00302	-3.66599	1.97804
H	3.47085	2.90703	-0.60987
H	2.04185	4.68059	-1.27143
H	-0.98650	4.58308	1.74650
H	0.11717	5.51498	-0.09161

Pre TS-3
B3LYP/6-31G(d,p) Energy = -2993.096296
B3LYP/6-31G(d,p) Free Energy = -2992.758027
M06-2X/6-31G(d,p) Derived free energy = -2992.058225
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	2.24120	2.99158	-0.95210
C	1.64097	4.18883	-1.01837
C	1.01055	4.94456	0.05623
C	0.71136	4.58277	1.31750
O	0.89589	3.38738	1.95060
O	2.40304	2.23735	0.18731
P	1.11749	1.92928	1.19551
O	1.60519	0.97203	2.23770
O	-0.10541	1.62176	0.35716
C	3.49545	-0.91354	0.62576
C	2.61958	-1.93480	0.17597
C	2.85493	-2.55640	-1.07675
C	3.96811	-2.22332	-1.82651
C	4.83806	-1.23548	-1.34234
C	4.60056	-0.56819	-0.13532
H	3.23854	-0.33630	1.51142
C	1.47430	-2.33511	0.92134
H	2.15816	-3.30375	-1.44309
H	4.16485	-2.70060	-2.77909
Cl	6.23380	-0.80357	-2.29332
H	5.25777	0.23237	0.18210
S	1.28203	-2.04958	2.56344
N	-0.91811	-0.88181	0.68567
H	0.70337	-2.92190	0.42769
S	-1.65610	-1.75566	-0.51989
H	-0.59905	0.10360	0.44357
O	-1.57438	-3.17170	-0.09752
O	-1.02973	-1.33963	-1.77582
C	-6.15465	-0.84050	-0.58256
C	-3.40520	-1.31844	-0.53739
C	-4.29293	-2.34371	-0.28411
C	-5.68453	-2.10259	-0.30933
H	-7.22368	-0.64553	-0.60214
H	-3.90772	-3.33462	-0.07476
H	-6.37211	-2.91895	-0.11269
C	-5.26701	0.23754	-0.84339
C	-3.84656	0.01348	-0.83199
C	-2.98620	1.11489	-1.09089
C	-3.50677	2.36606	-1.33901
C	-4.90270	2.58550	-1.35576
C	-5.76302	1.54019	-1.11455
H	-1.91134	0.99774	-1.09007
H	-2.82561	3.19210	-1.51619
H	-5.29197	3.57916	-1.55636
H	-6.83879	1.69359	-1.12353
C	-1.26905	-1.08324	2.07886
H	-1.00501	-0.16007	2.59870
H	-2.34410	-1.26152	2.22005

C	-0.52443	-2.27760	2.72460
H	-0.72527	-2.32992	3.79757
H	-0.81227	-3.21594	2.24843
H	2.68890	2.52618	-1.82509
H	1.63770	4.65671	-1.99909
H	0.27216	5.30403	2.00015
H	0.74149	5.96929	-0.18522

Post TS-3
B3LYP/6-31G(d,p) Energy = -2993.127303
B3LYP/6-31G(d,p) Free Energy = -2992.786393
M06-2X/6-31G(d,p) Derived free energy = -2992.103943
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-3.17436	2.43364	-0.21093
C	-3.21892	3.72892	-0.54823
C	-2.69783	4.27809	-1.79288
C	-1.62152	3.81526	-2.44214
O	-0.78514	2.83541	-1.93558
O	-2.73964	1.44056	-1.07194
P	-1.23262	1.30232	-1.65441
O	-1.19179	0.35892	-2.79078
O	-0.27631	0.98904	-0.42491
C	-2.02887	-2.06014	-0.48671
C	-0.98186	-2.44525	0.36018
C	-1.21722	-2.50839	1.73995
C	-2.46358	-2.18330	2.27413
C	-3.48233	-1.78659	1.41067
C	-3.27716	-1.72157	0.03313
H	-1.87448	-2.01650	-1.55916
C	0.40563	-2.78508	-0.14837
H	-0.41588	-2.81441	2.40684
H	-2.64263	-2.23943	3.34196
Cl	-5.05736	-1.35989	2.07187
H	-4.07907	-1.40882	-0.62511
S	0.38070	-3.93650	-1.61727
N	1.20077	-1.56406	-0.54072
H	0.94122	-3.28068	0.65969
S	2.74009	-1.48511	0.33436
H	0.12103	0.08472	-0.41374
O	3.80159	-2.07755	-0.49049
O	2.47117	-2.02774	1.67135
C	3.74521	2.98714	0.43554
C	3.05289	0.28497	0.43340
C	4.02424	0.75630	-0.42811
C	4.37156	2.12363	-0.43062
H	4.00468	4.04230	0.44109
H	4.52779	0.06217	-1.09048
H	5.13413	2.47984	-1.11521

C	2.75670	2.53121	1.34653
C	2.38514	1.14233	1.36888
C	1.40179	0.72665	2.30716
C	0.82047	1.63306	3.16529
C	1.18342	2.99836	3.14025
C	2.13297	3.43428	2.24767
H	1.11656	-0.31473	2.35652
H	0.07176	1.29037	3.87299
H	0.71362	3.69667	3.82600
H	2.42555	4.48012	2.21667
C	1.39876	-1.52070	-2.02325
H	0.49671	-1.08815	-2.46272
H	2.23816	-0.86044	-2.25287
C	1.61747	-2.94238	-2.53411
H	1.40078	-3.01762	-3.60221
H	2.62873	-3.29657	-2.33119
H	-3.55890	2.03721	0.72213
H	-3.69520	4.40569	0.15570
H	-1.25796	4.23073	-3.37537
H	-3.20461	5.13342	-2.23126

Cartesian coordinates and energies of the TS employing TRIP

TS-4Re
B3LYP/6-31G(d,p) Energy = -4777.531976
B3LYP/6-31G(d,p) Free Energy = -4776.387011
M06-2X/6-31G(d,p) Derived free energy = -4774.910350
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.920965
Number of Imaginary Frequencies = 1 (-173.85)

B3LYP/6-31G(d,p) Geometry

C	2.96082	6.72310	-0.76986
C	4.21789	6.49581	-1.37668
C	4.67582	5.20847	-1.53026
C	3.90888	4.10046	-1.07922
C	2.65634	4.32740	-0.42288
C	2.20288	5.67118	-0.30515
C	4.35079	2.77100	-1.29245
C	3.58862	1.67743	-0.93896
C	2.34990	1.92101	-0.27407
C	1.90356	3.19509	0.05109
C	0.64408	3.37778	0.83083
C	-0.54124	2.80677	0.38434
C	-1.81736	3.13626	0.93203
C	-1.84209	3.97505	2.02681
C	-0.65619	4.45959	2.63478
C	0.61057	4.15715	2.03945
C	-0.70209	5.23844	3.82238
C	0.45285	5.68114	4.42410

C	1.70762	5.35502	3.85845
C	1.78467	4.61795	2.69738
O	-0.51673	1.96125	-0.70890
O	1.61249	0.82781	0.13892
C	-3.09684	2.65439	0.31135
C	4.07584	0.28969	-1.23903
C	4.09197	-0.18516	-2.57223
C	4.62880	-1.45513	-2.82671
C	5.14400	-2.27014	-1.81764
C	5.10357	-1.78393	-0.50702
C	4.58731	-0.52119	-0.19689
C	-3.93247	1.74494	1.00080
C	-5.16014	1.38623	0.42604
C	-5.59017	1.89066	-0.80185
C	-4.74215	2.77893	-1.46856
C	-3.50860	3.17257	-0.94251
C	4.65157	-0.04087	1.25284
C	3.58481	0.64399	-3.75443
C	5.78383	-3.61260	-2.15366
C	-3.56108	1.14400	2.35687
C	-6.95605	1.51700	-1.36516
C	-2.67747	4.18475	-1.73130
P	0.16703	0.46336	-0.58951
O	-0.55726	-0.40512	0.42318
O	0.33751	-0.05371	-1.98562
C	-3.40573	5.53834	-1.84944
C	-2.27549	3.64520	-3.11680
C	-3.60413	-0.39386	2.34564
C	-4.45195	1.70602	3.48266
C	-6.88056	0.97696	-2.80457
C	-7.93716	2.70250	-1.27678
C	6.11045	0.10463	1.72870
C	3.84370	-0.94542	2.19987
C	5.20551	-4.77994	-1.33423
C	7.31646	-3.54829	-2.00156
C	2.50515	-0.08389	-4.57620
C	4.75406	1.08767	-4.65646
H	2.58557	7.73781	-0.67396
H	4.80876	7.33488	-1.73179
H	5.62916	5.01473	-2.01505
H	1.23866	5.86600	0.14749
H	5.31104	2.61279	-1.77541
H	-2.79964	4.26609	2.44898
H	-1.67300	5.46785	4.25383
H	0.40543	6.27000	5.33535
H	2.61991	5.68617	4.34613
H	2.75351	4.37020	2.28029
H	4.65962	-1.81541	-3.85245
H	5.51223	-2.39130	0.29638
H	-5.80954	0.69963	0.96433

H	-5.05387	3.19305	-2.42338
H	4.20201	0.95386	1.29932
H	3.11720	1.54638	-3.35403
H	5.56845	-3.81522	-3.21139
H	-2.52953	1.43103	2.57649
H	-7.35709	0.71416	-0.73115
H	-1.75327	4.37238	-1.18029
H	-3.65346	5.94404	-0.86325
H	-2.77390	6.26809	-2.36785
H	-4.33910	5.44701	-2.41554
H	-1.71995	2.70878	-3.02487
H	-3.15268	3.46610	-3.74864
H	-1.63871	4.37043	-3.63555
H	-2.94991	-0.79867	1.57171
H	-3.26758	-0.78994	3.31001
H	-4.61679	-0.77618	2.17646
H	-4.39655	2.79789	3.53791
H	-5.50282	1.43697	3.32802
H	-4.14516	1.30197	4.45390
H	-6.20426	0.11960	-2.87742
H	-7.87051	0.65861	-3.14859
H	-6.52046	1.74158	-3.50097
H	-8.03237	3.06052	-0.24715
H	-7.59297	3.54210	-1.89060
H	-8.93227	2.41251	-1.63210
H	6.67350	0.78127	1.07817
H	6.14290	0.50718	2.74715
H	6.63043	-0.85952	1.73577
H	3.88978	-0.56586	3.22630
H	2.79188	-0.97513	1.90382
H	4.23299	-1.96989	2.21180
H	4.12239	-4.86977	-1.46988
H	5.66030	-5.72822	-1.64021
H	5.39679	-4.65437	-0.26315
H	7.73905	-2.74687	-2.61482
H	7.60002	-3.35574	-0.96101
H	7.77940	-4.49341	-2.30664
H	2.18527	0.54964	-5.41128
H	1.62918	-0.29207	-3.95827
H	2.87768	-1.02124	-5.00556
H	5.50839	1.64814	-4.09500
H	5.25476	0.22610	-5.11250
H	4.38999	1.72843	-5.46694
C	-3.20058	-4.40729	-1.94128
C	-2.65934	-3.12471	-1.72280
C	-3.51555	-2.06800	-1.35194
C	-4.88279	-2.27656	-1.23153
C	-5.39630	-3.55123	-1.48015
C	-4.56649	-4.62119	-1.83163
H	-2.54294	-5.23767	-2.17354

C	-1.24733	-2.83170	-1.86118
H	-3.10105	-1.08634	-1.14559
H	-5.53821	-1.46522	-0.93973
Cl	-7.11852	-3.82372	-1.33406
H	-4.99084	-5.60397	-1.99973
S	-0.18420	-3.80921	-2.82602
N	-0.17470	-3.00158	-0.05751
H	-0.95756	-1.78161	-1.82690
S	-0.94288	-4.09715	1.05493
H	-0.28444	-1.97900	0.24068
O	-2.15616	-3.40624	1.48233
O	-1.00531	-5.38122	0.35042
C	1.87233	-4.86745	4.59018
C	0.19195	-4.29406	2.44073
C	0.72423	-5.56026	2.58792
C	1.57501	-5.84990	3.67567
H	2.52484	-5.08254	5.43214
H	0.46947	-6.32909	1.86816
H	1.98359	-6.84932	3.78279
C	1.34205	-3.55621	4.46632
C	0.47136	-3.23542	3.36664
C	-0.03083	-1.91024	3.26758
C	0.30947	-0.96069	4.20673
C	1.15436	-1.27829	5.29392
C	1.65982	-2.55108	5.41775
H	-0.67613	-1.61921	2.45096
H	-0.07493	0.04835	4.09849
H	1.40543	-0.51560	6.02461
H	2.31443	-2.81007	6.24536
C	1.17380	-3.37525	-0.52007
H	1.92840	-2.78362	0.00772
H	1.33897	-4.43376	-0.31062
C	1.30822	-3.11355	-2.03529
H	1.35002	-2.04163	-2.24029
H	2.18870	-3.60781	-2.44691

Pre TS-4Re

B3LYP/6-31G(d,p) Energy = -4777.534806
B3LYP/6-31G(d,p) Free Energy = -4776.394197
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.925533
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	2.32016	6.93858	-0.72434
C	3.58226	6.83847	-1.35471
C	4.15259	5.60135	-1.54179
C	3.49684	4.41965	-1.10272
C	2.23934	4.51870	-0.42470
C	1.66847	5.81316	-0.27087
C	4.05447	3.13995	-1.34653

C	3.39894	1.97509	-1.00671
C	2.15053	2.09112	-0.32505
C	1.59909	3.31412	0.03481
C	0.34620	3.36724	0.84363
C	-0.79322	2.70301	0.40705
C	-2.07660	2.89059	1.00223
C	-2.14872	3.69488	2.12077
C	-0.99756	4.27665	2.70935
C	0.27468	4.10848	2.07416
C	-1.08309	5.01973	3.91756
C	0.04199	5.55335	4.50167
C	1.30573	5.35798	3.89691
C	1.41896	4.65909	2.71547
O	-0.71733	1.89938	-0.71481
O	1.51916	0.92834	0.06925
C	-3.32551	2.30174	0.41248
C	4.01174	0.64547	-1.33800
C	4.06596	0.20355	-2.68121
C	4.72847	-0.99859	-2.96819
C	5.33679	-1.77612	-1.98172
C	5.25527	-1.32600	-0.65969
C	4.61006	-0.13268	-0.31686
C	-4.03944	1.29376	1.10256
C	-5.25774	0.84595	0.57098
C	-5.79137	1.35218	-0.61550
C	-5.05718	2.33239	-1.28804
C	-3.84022	2.81955	-0.80246
C	4.62814	0.31513	1.14453
C	3.46351	0.99923	-3.84098
C	6.11251	-3.03517	-2.35201
C	-3.54968	0.68451	2.41690
C	-7.15240	0.88581	-1.11926
C	-3.13883	3.92537	-1.59135
P	0.08991	0.45687	-0.63626
O	-0.54203	-0.48890	0.36000
O	0.28255	-0.00696	-2.05127
C	-3.99714	5.20408	-1.65392
C	-2.73307	3.45449	-3.00061
C	-3.44991	-0.84991	2.35416
C	-4.43452	1.12383	3.60070
C	-7.13716	0.46989	-2.60083
C	-8.23199	1.95635	-0.86434
C	6.06395	0.61465	1.61862
C	3.93456	-0.69875	2.07159
C	5.63665	-4.28267	-1.58658
C	7.62852	-2.82806	-2.16572
C	2.43590	0.18540	-4.64943
C	4.56786	1.55948	-4.75954
H	1.85651	7.91300	-0.60095
H	4.08864	7.73461	-1.70084

H	5.11169	5.50465	-2.04404
H	0.69862	5.91025	0.20095
H	5.01915	3.07870	-1.84264
H	-3.11642	3.87942	2.57834
H	-2.05891	5.14703	4.37913
H	-0.03454	6.11328	5.42903
H	2.19664	5.75966	4.37090
H	2.39492	4.51151	2.26878
H	4.78779	-1.33009	-4.00241
H	5.73237	-1.90381	0.12765
H	-5.81914	0.08887	1.11436
H	-5.44922	2.74651	-2.21269
H	4.06812	1.25033	1.21798
H	2.92484	1.85069	-3.41910
H	5.93636	-3.21777	-3.42063
H	-2.53966	1.05952	2.60045
H	-7.42779	-0.00005	-0.53002
H	-2.21895	4.18979	-1.06521
H	-4.25354	5.55966	-0.65077
H	-3.45365	6.00371	-2.16923
H	-4.93349	5.03701	-2.19744
H	-2.08090	2.57954	-2.94481
H	-3.60909	3.19561	-3.60614
H	-2.19265	4.25002	-3.52562
H	-2.77800	-1.16847	1.55521
H	-3.04996	-1.24090	3.29570
H	-4.42791	-1.31978	2.20016
H	-4.47623	2.21362	3.69489
H	-5.46272	0.76375	3.48242
H	-4.04645	0.71724	4.54113
H	-6.37905	-0.29487	-2.79633
H	-8.11154	0.06647	-2.89650
H	-6.92327	1.32168	-3.25491
H	-8.28194	2.22186	0.19596
H	-8.01466	2.87100	-1.42678
H	-9.21960	1.59698	-1.17456
H	6.54168	1.36833	0.98460
H	6.05657	0.99142	2.64734
H	6.69102	-0.28352	1.59861
H	3.93096	-0.33433	3.10446
H	2.89517	-0.85310	1.77121
H	4.44646	-1.66789	2.06838
H	4.57083	-4.47321	-1.75109
H	6.18920	-5.17023	-1.91317
H	5.79257	-4.17670	-0.50781
H	7.98209	-1.96778	-2.74186
H	7.87424	-2.64759	-1.11355
H	8.18620	-3.71243	-2.49351
H	2.04459	0.79432	-5.47229
H	1.59510	-0.10338	-4.01492

H	2.88187	-0.71232	-5.09359
H	5.27938	2.17896	-4.20413
H	5.13582	0.75447	-5.23946
H	4.12983	2.17577	-5.55225
C	-3.02062	-4.38465	-2.56824
C	-2.48476	-3.17391	-2.06361
C	-3.34742	-2.24283	-1.43499
C	-4.70554	-2.50140	-1.32989
C	-5.20751	-3.69502	-1.85458
C	-4.37410	-4.64206	-2.47330
H	-2.36563	-5.12272	-3.02007
C	-1.10394	-2.83619	-2.11011
H	-2.93292	-1.33273	-1.01275
H	-5.36112	-1.79208	-0.84041
Cl	-6.91188	-4.03352	-1.72825
H	-4.79586	-5.56460	-2.85422
S	0.11960	-3.74189	-2.82847
N	0.49135	-3.06611	0.17735
H	-0.80233	-1.86552	-1.71923
S	-0.23204	-4.23333	1.12313
H	0.19269	-2.08597	0.36457
O	-1.57573	-3.73002	1.41727
O	-0.04318	-5.51062	0.41995
C	2.16071	-4.72121	5.01640
C	0.70346	-4.34082	2.66370
C	1.28931	-5.56062	2.93003
C	2.02407	-5.75430	4.12092
H	2.72693	-4.86004	5.93365
H	1.17383	-6.36702	2.21557
H	2.47606	-6.72113	4.31832
C	1.57215	-3.45177	4.77107
C	0.81124	-3.23608	3.57037
C	0.23811	-1.95237	3.35698
C	0.41735	-0.94181	4.27669
C	1.16325	-1.15512	5.45814
C	1.72550	-2.38684	5.69827
H	-0.34816	-1.74542	2.47211
H	-0.01879	0.03284	4.08182
H	1.29024	-0.34619	6.17126
H	2.30082	-2.56662	6.60254
C	1.70369	-3.32949	-0.57237
H	2.55414	-2.75877	-0.17843
H	1.93367	-4.39412	-0.49418
C	1.56666	-2.92102	-2.05944
H	1.41843	-1.84158	-2.16437
H	2.44481	-3.22712	-2.63079

Post TS-4Re

B3LYP/6-31G(d,p) Energy = -4777.547603

B3LYP/6-31G(d,p) Free Energy = -4776.401807

M06-2X/6-31G(d,p) Derived free energy in solution = -4774.947064
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	3.33448	6.54031	-0.85155
C	4.58437	6.24045	-1.44131
C	4.97957	4.93006	-1.57107
C	4.15342	3.86874	-1.11199
C	2.90757	4.16998	-0.47297
C	2.51991	5.53546	-0.37886
C	4.53189	2.51604	-1.30138
C	3.71418	1.46425	-0.94383
C	2.48700	1.78954	-0.29877
C	2.09403	3.08260	0.00709
C	0.83896	3.33712	0.77416
C	-0.37555	2.82875	0.33653
C	-1.63733	3.23504	0.86050
C	-1.61784	4.09640	1.93841
C	-0.41080	4.52186	2.54814
C	0.84118	4.13700	1.97052
C	-0.42143	5.32451	3.72084
C	0.75268	5.70906	4.32488
C	1.99104	5.29951	3.77763
C	2.03519	4.53883	2.63030
O	-0.39970	1.95374	-0.75104
O	1.66745	0.73525	0.11418
C	-2.93774	2.81927	0.23552
C	4.12657	0.04693	-1.21562
C	4.10070	-0.46103	-2.53621
C	4.54705	-1.77068	-2.75820
C	5.01745	-2.58945	-1.73075
C	5.03281	-2.06291	-0.43578
C	4.60159	-0.76242	-0.15593
C	-3.84178	1.98820	0.93889
C	-5.08026	1.69180	0.35291
C	-5.45604	2.18215	-0.89799
C	-4.54416	2.99708	-1.57368
C	-3.29716	3.32918	-1.03802
C	4.71768	-0.24433	1.27721
C	3.65422	0.37469	-3.73746
C	5.54466	-3.98746	-2.03097
C	-3.53638	1.41201	2.32229
C	-6.82775	1.86685	-1.48150
C	-2.39949	4.27505	-1.83683
P	0.26995	0.48118	-0.68329
O	-0.56182	-0.33405	0.38973
O	0.37839	-0.12222	-2.02975
C	-3.03826	5.67224	-1.96595
C	-2.03451	3.69993	-3.21816
C	-3.73730	-0.11269	2.38585

C	-4.37497	2.10590	3.41498
C	-6.74503	1.24668	-2.88804
C	-7.73320	3.11406	-1.48349
C	6.19245	-0.14790	1.71556
C	3.89654	-1.08469	2.27024
C	4.86690	-5.07726	-1.18171
C	7.07703	-4.04934	-1.87689
C	2.57513	-0.31797	-4.58960
C	4.86563	0.76607	-4.60851
H	3.01014	7.57386	-0.77519
H	5.21978	7.04335	-1.80261
H	5.92653	4.68186	-2.04279
H	1.56276	5.78586	0.06105
H	5.48815	2.30420	-1.77068
H	-2.55954	4.45291	2.34438
H	-1.38051	5.61798	4.13912
H	0.73261	6.31591	5.22508
H	2.91661	5.58450	4.26898
H	2.99151	4.22714	2.22777
H	4.53845	-2.16255	-3.77217
H	5.41084	-2.67296	0.38019
H	-5.78016	1.06206	0.89637
H	-4.81511	3.39956	-2.54562
H	4.31289	0.77079	1.30522
H	3.21056	1.29880	-3.35804
H	5.31225	-4.19855	-3.08315
H	-2.48240	1.60751	2.54026
H	-7.29541	1.12495	-0.82021
H	-1.46412	4.40867	-1.28837
H	-3.25749	6.10092	-0.98278
H	-2.36212	6.35528	-2.49194
H	-3.97683	5.63479	-2.52919
H	-1.54876	2.72571	-3.12190
H	-2.91985	3.57857	-3.85170
H	-1.34677	4.37442	-3.74007
H	-3.16391	-0.62776	1.61292
H	-3.41439	-0.49732	3.35927
H	-4.78806	-0.39457	2.26281
H	-4.21095	3.18784	3.43083
H	-5.44541	1.93784	3.25398
H	-4.12101	1.71029	4.40470
H	-6.12173	0.34752	-2.89433
H	-7.74299	0.96999	-3.24420
H	-6.32041	1.95051	-3.61187
H	-7.83155	3.53392	-0.47768
H	-7.32391	3.89595	-2.13269
H	-8.73526	2.86546	-1.84988
H	6.76794	0.48643	1.03400
H	6.26687	0.27911	2.72182
H	6.67056	-1.13325	1.73590

H	3.97357	-0.66807	3.28002
H	2.83889	-1.09563	1.99409
H	4.24942	-2.12085	2.31425
H	3.77977	-5.06620	-1.31000
H	5.22996	-6.07013	-1.46801
H	5.07719	-4.94481	-0.11500
H	7.56789	-3.30624	-2.51255
H	7.37651	-3.85192	-0.84170
H	7.45648	-5.03946	-2.15264
H	2.28709	0.33330	-5.42227
H	1.68198	-0.51906	-3.99517
H	2.93411	-1.25760	-5.02379
H	5.62390	1.30485	-4.03137
H	5.34642	-0.12004	-5.03776
H	4.55028	1.40937	-5.43719
C	-3.55660	-4.38004	-1.41953
C	-2.93688	-3.12792	-1.31920
C	-3.73463	-1.99005	-1.14624
C	-5.12058	-2.09289	-1.05507
C	-5.71231	-3.35019	-1.15557
C	-4.94255	-4.49675	-1.34052
H	-2.95288	-5.27156	-1.54312
C	-1.44216	-2.94485	-1.45283
H	-3.27398	-1.00943	-1.07305
H	-5.72861	-1.20837	-0.90845
Cl	-7.46329	-3.49143	-1.05205
H	-5.41968	-5.46692	-1.41857
S	-0.66436	-4.03571	-2.71386
N	-0.57151	-3.03493	-0.18271
H	-1.25221	-1.92606	-1.79690
S	-1.23661	-4.06724	1.09677
H	-0.55665	-1.33398	0.24739
O	-2.37911	-3.33706	1.64639
O	-1.40109	-5.43133	0.57939
C	2.06553	-4.56274	4.25909
C	0.08779	-4.13621	2.33176
C	0.74725	-5.34814	2.40200
C	1.75022	-5.56268	3.37068
H	2.83429	-4.71855	5.01121
H	0.47323	-6.13881	1.71348
H	2.25942	-6.52006	3.40900
C	1.39350	-3.31289	4.22976
C	0.36773	-3.07055	3.24924
C	-0.29267	-1.81258	3.26909
C	0.05209	-0.84987	4.19222
C	1.06139	-1.08735	5.15207
C	1.71470	-2.29673	5.16882
H	-1.08778	-1.61238	2.56733
H	-0.46473	0.10455	4.18051
H	1.31483	-0.31675	5.87356

H	2.48903	-2.49839	5.90384
C	0.82130	-3.46514	-0.57456
H	1.54764	-2.79650	-0.10482
H	1.00303	-4.48156	-0.22054
C	0.94868	-3.43977	-2.10073
H	1.13672	-2.42956	-2.46661
H	1.74467	-4.10617	-2.43685

TS-4Si

B3LYP/6-31G(d,p) Energy = -4777.530205
B3LYP/6-31G(d,p) Free Energy = -4776.384030
M06-2X/6-31G(d,p) Derived free energy = -4774.905504
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.916014
Number of Imaginary Frequencies = 1 (-185.26)

B3LYP/6-31G(d,p) Geometry

C	-3.47313	5.81989	2.50071
C	-4.80550	5.35407	2.59470
C	-5.17282	4.20513	1.93456
C	-4.23373	3.48008	1.15230
C	-2.89565	3.97017	1.01923
C	-2.54631	5.15069	1.73265
C	-4.58984	2.26804	0.51202
C	-3.66921	1.49413	-0.16418
C	-2.33403	1.98976	-0.27621
C	-1.96158	3.24090	0.20220
C	-0.62779	3.81730	-0.13187
C	0.53491	3.10756	0.13470
C	1.83782	3.67073	-0.01127
C	1.92369	4.96074	-0.49309
C	0.78406	5.69234	-0.90890
C	-0.51503	5.11249	-0.75099
C	0.91132	6.97974	-1.49706
C	-0.19277	7.66313	-1.94948
C	-1.47427	7.07558	-1.83577
C	-1.63194	5.83861	-1.25095
O	0.43289	1.82766	0.65513
O	-1.43189	1.23446	-0.99525
C	3.08652	2.92889	0.36293
C	-4.09915	0.19163	-0.77182
C	-4.20926	0.05980	-2.17653
C	-4.69559	-1.14148	-2.70843
C	-5.08491	-2.21525	-1.90503
C	-4.95972	-2.06534	-0.52098
C	-4.48124	-0.88680	0.06557
C	3.39228	2.69819	1.72416
C	4.60559	2.08327	2.05163
C	5.53298	1.69582	1.08439
C	5.20611	1.92453	-0.25484
C	4.00584	2.53335	-0.64099

C	-4.40194	-0.81881	1.59190
C	-3.88268	1.20329	-3.13749
C	-5.68989	-3.46968	-2.52543
C	2.47024	3.13897	2.86032
C	6.87140	1.09377	1.49445
C	3.75884	2.76957	-2.13299
P	-0.05101	0.59077	-0.32480
O	0.87629	0.34241	-1.47620
O	-0.38973	-0.55651	0.60769
C	3.73831	1.45803	-2.93901
C	4.78182	3.76292	-2.71864
C	3.14427	4.19456	3.75825
C	1.96761	1.94057	3.68662
C	8.03374	2.06225	1.20194
C	7.12784	-0.28035	0.85245
C	-3.37335	-1.81474	2.15464
C	-5.78354	-1.01319	2.24569
C	-7.20568	-3.54351	-2.25378
C	-4.99414	-4.76626	-2.07501
C	-5.14053	1.66444	-3.90052
C	-2.74293	0.84538	-4.10908
H	-3.17600	6.71241	3.04364
H	-5.52848	5.89620	3.19695
H	-6.18713	3.82227	2.01275
H	-1.52853	5.51737	1.67911
H	-5.61806	1.92380	0.58406
H	2.90194	5.42385	-0.58690
H	1.90575	7.40705	-1.59651
H	-0.08346	8.64272	-2.40530
H	-2.34349	7.60281	-2.21812
H	-2.62060	5.40196	-1.18113
H	-4.80085	-1.23349	-3.78716
H	-5.26363	-2.88113	0.12970
H	4.84628	1.91593	3.09886
H	5.91335	1.63738	-1.02896
H	-4.05249	0.17777	1.86720
H	-3.54233	2.05582	-2.54539
H	-5.55669	-3.38615	-3.61238
H	1.59097	3.61485	2.41987
H	6.83466	0.94385	2.58159
H	2.76925	3.21738	-2.24469
H	2.92306	0.81839	-2.59404
H	3.57539	1.67261	-4.00150
H	4.68599	0.91333	-2.85711
H	4.55285	3.97329	-3.76919
H	4.77867	4.71331	-2.17480
H	5.80104	3.36310	-2.67510
H	3.46765	5.06195	3.17400
H	2.44724	4.54454	4.52793
H	4.02515	3.78985	4.26819

H	1.43644	1.23296	3.04483
H	2.79603	1.41587	4.17622
H	1.27905	2.28011	4.46905
H	8.12438	2.25562	0.12738
H	8.98574	1.64494	1.54874
H	7.88000	3.02424	1.70029
H	6.31862	-0.98072	1.08105
H	7.21310	-0.19805	-0.23729
H	8.06476	-0.71227	1.22057
H	-2.37543	-1.58897	1.76956
H	-3.33267	-1.74464	3.24695
H	-3.63046	-2.85050	1.90194
H	-5.71070	-0.88858	3.33159
H	-6.51221	-0.28741	1.87002
H	-6.18639	-2.01407	2.05523
H	-7.71334	-2.64233	-2.61025
H	-7.65054	-4.40908	-2.75717
H	-7.40864	-3.63762	-1.18136
H	-3.92447	-4.75284	-2.30977
H	-5.09694	-4.92525	-0.99632
H	-5.43421	-5.63397	-2.57794
H	-4.90720	2.52855	-4.53202
H	-5.93922	1.95394	-3.21019
H	-5.53226	0.87487	-4.55115
H	-1.82234	0.61791	-3.56560
H	-3.00246	-0.01391	-4.73818
H	-2.53588	1.68903	-4.77658
S	0.85331	-4.21242	0.67478
N	0.11794	-2.99013	-0.33928
S	0.17401	-3.27443	-3.20526
C	-1.30628	-2.69924	-2.30913
H	-1.31984	-1.60877	-2.27325
H	-2.19787	-3.04506	-2.83260
C	-1.20897	-3.30946	-0.90210
H	-1.99112	-2.88566	-0.26681
H	-1.32171	-4.39349	-0.96035
H	0.07603	-2.02698	0.13145
O	2.09831	-3.60436	1.13514
O	0.84870	-5.42689	-0.14609
C	-1.91067	-5.23276	4.18228
C	-1.80061	-6.05340	3.08474
C	-0.95776	-5.68228	2.01697
C	-0.25406	-4.49346	2.06587
H	-2.55046	-5.51418	5.01440
H	-2.34530	-6.99044	3.03523
H	-0.83489	-6.33655	1.16237
C	-0.34138	-3.59845	3.18374
C	-1.19859	-4.00791	4.26524
C	-1.32361	-3.17554	5.40900
C	-0.64336	-1.98383	5.48994

C	0.18858	-1.57616	4.42327
C	0.34136	-2.35788	3.29941
H	-1.97119	-3.50161	6.21822
H	-0.74628	-1.35246	6.36707
H	0.71390	-0.62892	4.48246
H	0.98069	-2.01069	2.50052
C	1.27144	-2.61458	-2.01562
H	1.13141	-1.54880	-1.80921
C	5.30698	-3.88393	-1.89873
C	4.33565	-4.80102	-2.31119
C	3.00490	-4.40911	-2.32983
C	2.63925	-3.10309	-1.94885
C	3.63497	-2.20552	-1.51527
C	4.96949	-2.58974	-1.49759
Cl	6.98712	-4.37572	-1.87690
H	4.62425	-5.80482	-2.60015
H	2.23831	-5.12068	-2.61474
H	3.35348	-1.20366	-1.20714
H	5.73922	-1.90092	-1.17293

Pre TS-4Si
B3LYP/6-31G(d,p) Energy = -4777.534400
B3LYP/6-31G(d,p) Free Energy = -4776.391457
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.920017
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-3.81462	5.71119	2.44916
C	-5.12481	5.18317	2.52191
C	-5.42480	4.01424	1.86273
C	-4.43839	3.33033	1.10212
C	-3.12267	3.88286	0.99009
C	-2.84297	5.08240	1.70257
C	-4.72744	2.09995	0.46219
C	-3.76134	1.36848	-0.19707
C	-2.44906	1.92518	-0.28535
C	-2.14032	3.19147	0.19692
C	-0.81956	3.81498	-0.10389
C	0.36214	3.15024	0.19894
C	1.64378	3.77147	0.10402
C	1.69463	5.06491	-0.37325
C	0.54119	5.74859	-0.83056
C	-0.73723	5.11426	-0.71864
C	0.63449	7.04170	-1.41246
C	-0.48109	7.67980	-1.90158
C	-1.74018	7.03916	-1.83251
C	-1.86573	5.79500	-1.25514
O	0.30711	1.87475	0.72345
O	-1.49071	1.21063	-0.97373
C	2.90479	3.07941	0.52791

C	-4.11991	0.05204	-0.82121
C	-4.20495	-0.06719	-2.22862
C	-4.62400	-1.28379	-2.78279
C	-4.97712	-2.38301	-1.99738
C	-4.88128	-2.24353	-0.60959
C	-4.46101	-1.05350	-0.00148
C	3.15136	2.82786	1.89793
C	4.37584	2.26487	2.27310
C	5.36915	1.94561	1.34744
C	5.09831	2.18669	-0.00217
C	3.89064	2.74804	-0.43524
C	-4.40837	-1.00037	1.52679
C	-3.92167	1.10306	-3.17082
C	-5.50220	-3.66188	-2.63969
C	2.15512	3.19380	2.99762
C	6.71348	1.40293	1.81638
C	3.69615	2.98372	-1.93514
P	-0.16076	0.57911	-0.19160
O	0.80755	0.25630	-1.29737
O	-0.55792	-0.48685	0.79806
C	3.67189	1.66310	-2.72643
C	4.74925	3.95489	-2.50231
C	2.72752	4.27411	3.93644
C	1.69097	1.95598	3.78855
C	7.84037	2.43121	1.59908
C	7.07162	0.05426	1.16876
C	-3.43181	-2.03748	2.10908
C	-5.81284	-1.15186	2.14329
C	-6.99838	-3.86680	-2.33198
C	-4.68958	-4.90797	-2.24474
C	-5.19091	1.51665	-3.94198
C	-2.75622	0.81099	-4.13367
H	-3.57015	6.61975	2.99176
H	-5.88371	5.69354	3.10752
H	-6.42099	3.58386	1.92514
H	-1.84303	5.49690	1.66568
H	-5.73991	1.70965	0.51820
H	2.65522	5.56983	-0.42860
H	1.61286	7.51096	-1.47649
H	-0.39726	8.66458	-2.35164
H	-2.61718	7.53108	-2.24315
H	-2.83690	5.31688	-1.21881
H	-4.70853	-1.36736	-3.86414
H	-5.15719	-3.08038	0.02667
H	4.57058	2.08485	3.32763
H	5.85545	1.94911	-0.74542
H	-4.02927	-0.01833	1.81638
H	-3.62627	1.96207	-2.56434
H	-5.40584	-3.53771	-3.72670
H	1.26841	3.62328	2.52617

H	6.62871	1.23167	2.89748
H	2.71874	3.44804	-2.07963
H	2.84155	1.03760	-2.38822
H	3.53496	1.86505	-3.79524
H	4.61043	1.10702	-2.61504
H	4.54837	4.16123	-3.55941
H	4.74624	4.90891	-1.96489
H	5.76171	3.54187	-2.43346
H	3.02218	5.16859	3.37823
H	1.97952	4.56935	4.68066
H	3.60924	3.91388	4.47756
H	1.23002	1.22376	3.12086
H	2.52661	1.47594	4.31037
H	0.95123	2.24591	4.54353
H	7.97994	2.64337	0.53329
H	8.79179	2.05718	1.99370
H	7.61162	3.37746	2.09855
H	6.28586	-0.68770	1.34321
H	7.21295	0.16190	0.08682
H	8.00701	-0.33922	1.58121
H	-2.41798	-1.84580	1.75137
H	-3.41611	-1.97171	3.20234
H	-3.71838	-3.06268	1.84727
H	-5.76346	-1.04992	3.23284
H	-6.50489	-0.39296	1.76373
H	-6.24669	-2.13350	1.92209
H	-7.58782	-3.00112	-2.64853
H	-7.38478	-4.75188	-2.84949
H	-7.16406	-4.00764	-1.25837
H	-3.63304	-4.79868	-2.51140
H	-4.74325	-5.09770	-1.16749
H	-5.07314	-5.79767	-2.75578
H	-4.99142	2.39891	-4.56001
H	-6.00890	1.76029	-3.25668
H	-5.53954	0.71837	-4.60636
H	-1.83570	0.61259	-3.57892
H	-2.97110	-0.04770	-4.78047
H	-2.57600	1.67406	-4.78391
S	0.86775	-4.19233	0.56108
N	-0.03306	-2.98310	-0.15467
S	0.50983	-3.15287	-3.23908
C	-0.99578	-2.55450	-2.38753
H	-0.90180	-1.47471	-2.26066
H	-1.83898	-2.76718	-3.04762
C	-1.15714	-3.27096	-1.02575
H	-2.09215	-2.90291	-0.58909
H	-1.24036	-4.34899	-1.17794
H	-0.09486	-2.06527	0.34605
O	2.10174	-3.54899	1.02109
O	0.91503	-5.29282	-0.41406

C	-1.44445	-5.93052	4.13126
C	-1.22125	-6.66508	2.99174
C	-0.51059	-6.09228	1.91376
C	-0.03740	-4.79952	2.00001
H	-1.99139	-6.36241	4.96525
H	-1.58394	-7.68486	2.91079
H	-0.31996	-6.66368	1.01313
C	-0.23882	-3.99616	3.17004
C	-0.96983	-4.59720	4.25274
C	-1.20653	-3.84530	5.43401
C	-0.75084	-2.55310	5.55108
C	-0.03497	-1.96067	4.48631
C	0.22054	-2.66011	3.32757
H	-1.75792	-4.31424	6.24457
H	-0.93973	-1.98594	6.45758
H	0.31724	-0.93799	4.57549
H	0.77663	-2.17686	2.53640
C	1.68846	-2.38669	-2.31028
H	1.37393	-1.48628	-1.76395
C	5.77716	-3.34833	-2.15271
C	4.92306	-4.21281	-2.85577
C	3.57450	-3.91987	-2.91539
C	3.06358	-2.75574	-2.28964
C	3.94579	-1.91468	-1.56889
C	5.29986	-2.20588	-1.50474
Cl	7.47679	-3.72512	-2.07527
H	5.32348	-5.10282	-3.32649
H	2.90115	-4.60097	-3.42521
H	3.55012	-1.03682	-1.06885
H	5.97818	-1.56735	-0.95323

Post TS-4Si

B3LYP/6-31G(d,p) Energy = -4777.537241
B3LYP/6-31G(d,p) Free Energy = -4776.391941
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.934477
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-2.62196	6.13517	2.54240
C	-4.00848	5.86788	2.62804
C	-4.53766	4.79393	1.95183
C	-3.71143	3.94992	1.16145
C	-2.31615	4.24085	1.03698
C	-1.80019	5.34834	1.76631
C	-4.23764	2.81137	0.50451
C	-3.43813	1.91690	-0.17786
C	-2.04512	2.21641	-0.28263
C	-1.49676	3.39559	0.20856
C	-0.09919	3.78911	-0.12878
C	0.95990	2.92802	0.12029

C	2.32569	3.31140	-0.03184
C	2.57764	4.58501	-0.49941
C	1.54397	5.46803	-0.89639
C	0.18047	5.06587	-0.73371
C	1.83892	6.73431	-1.47015
C	0.83302	7.56485	-1.90464
C	-0.51481	7.15249	-1.78752
C	-0.83288	5.94045	-1.21600
O	0.68068	1.65830	0.61749
O	-1.26499	1.34603	-1.01717
C	3.47286	2.41252	0.32323
C	-4.05513	0.69471	-0.79048
C	-4.14595	0.56225	-2.19768
C	-4.80741	-0.55035	-2.73096
C	-5.39354	-1.53361	-1.93011
C	-5.28402	-1.38704	-0.54546
C	-4.63240	-0.29551	0.04366
C	3.76581	2.14793	1.68064
C	4.89308	1.38148	1.99444
C	5.75139	0.87864	1.01652
C	5.44211	1.15158	-0.31896
C	4.32451	1.90857	-0.69205
C	-4.57489	-0.23144	1.57143
C	-3.60971	1.61997	-3.16256
C	-6.18968	-2.66716	-2.56787
C	2.92950	2.71578	2.82647
C	7.00783	0.11380	1.41470
C	4.10356	2.19817	-2.17901
P	0.05886	0.54786	-0.42567
O	0.93860	0.24405	-1.59255
O	-0.39374	-0.61489	0.46574
C	3.96403	0.91914	-3.02351
C	5.22054	3.10368	-2.73643
C	3.75463	3.67085	3.71065
C	2.27900	1.60064	3.66458
C	8.27719	0.93988	1.12898
C	7.09906	-1.27449	0.75918
C	-3.71504	-1.36613	2.15384
C	-5.97992	-0.21611	2.20288
C	-7.69704	-2.33967	-2.56117
C	-5.93571	-4.04308	-1.93001
C	-4.75748	2.28468	-3.94892
C	-2.53782	1.05547	-4.11323
H	-2.19968	6.96763	3.09758
H	-4.64650	6.50223	3.23613
H	-5.59737	4.56274	2.02268
H	-0.73990	5.56434	1.71780
H	-5.30537	2.62048	0.56916
H	3.60808	4.91449	-0.59635
H	2.88084	7.02562	-1.57360

H	1.06923	8.52675	-2.34982
H	-1.30800	7.79580	-2.15710
H	-1.87048	5.63886	-1.14431
H	-4.89049	-0.64226	-3.81153
H	-5.73276	-2.13326	0.10415
H	5.12408	1.18660	3.03913
H	6.10114	0.78214	-1.10035
H	-4.08666	0.70275	1.85356
H	-3.13329	2.40697	-2.57409
H	-5.87379	-2.72806	-3.61811
H	2.11769	3.30696	2.39565
H	6.95479	-0.04067	2.50061
H	3.16073	2.73984	-2.28065
H	3.08829	0.34946	-2.70784
H	3.83229	1.18203	-4.07927
H	4.85244	0.28120	-2.95523
H	5.01919	3.35993	-3.78240
H	5.30716	4.03678	-2.17008
H	6.19550	2.60511	-2.69832
H	4.18666	4.48344	3.11809
H	3.12292	4.11577	4.48769
H	4.57800	3.14960	4.21057
H	1.64784	0.97368	3.02959
H	3.03252	0.96487	4.14274
H	1.65527	2.03292	4.45596
H	8.39119	1.12701	0.05553
H	9.17229	0.40964	1.47293
H	8.23956	1.91032	1.63343
H	6.20814	-1.87373	0.96893
H	7.20778	-1.19609	-0.32839
H	7.97149	-1.82147	1.13264
H	-2.68919	-1.29614	1.78145
H	-3.67659	-1.29645	3.24612
H	-4.11911	-2.35343	1.90018
H	-5.90740	-0.09729	3.28950
H	-6.58578	0.60796	1.81241
H	-6.52522	-1.14625	2.00901
H	-7.89555	-1.38650	-3.06003
H	-8.26938	-3.12061	-3.07417
H	-8.07313	-2.26320	-1.53496
H	-4.87187	-4.30268	-1.93250
H	-6.28482	-4.08008	-0.89262
H	-6.47147	-4.82324	-2.48065
H	-4.36831	3.08657	-4.58561
H	-5.50251	2.71829	-3.27411
H	-5.27225	1.56718	-4.59721
H	-1.68445	0.66306	-3.55448
H	-2.93924	0.25716	-4.74783
H	-2.16717	1.84504	-4.77586
S	0.46905	-4.21451	0.80696

N	-0.19377	-2.98832	-0.40492
S	-0.42152	-3.54199	-3.06981
C	-1.87064	-2.87082	-2.19094
H	-1.93726	-1.78737	-2.31035
H	-2.78355	-3.32349	-2.57901
C	-1.63897	-3.27204	-0.73804
H	-2.26445	-2.70670	-0.04637
H	-1.81787	-4.34202	-0.62225
H	-0.17967	-1.92851	0.04701
O	1.71209	-3.62598	1.28532
O	0.42394	-5.49119	0.09666
C	-2.53736	-4.79592	4.20381
C	-2.46418	-5.66508	3.14075
C	-1.55191	-5.41290	2.09776
C	-0.74987	-4.28486	2.12857
H	-3.22687	-4.98860	5.02124
H	-3.08729	-6.55219	3.10308
H	-1.45111	-6.11667	1.28064
C	-0.79354	-3.34224	3.21009
C	-1.72018	-3.63863	4.27269
C	-1.80749	-2.76356	5.38755
C	-1.02482	-1.63639	5.45919
C	-0.12692	-1.33829	4.41021
C	-0.00786	-2.16359	3.31330
H	-2.50793	-3.00595	6.18180
H	-1.09685	-0.97172	6.31439
H	0.47891	-0.44060	4.46186
H	0.68139	-1.89671	2.52547
C	0.64989	-2.87247	-1.74992
H	0.69998	-1.78600	-1.86768
C	4.70212	-4.26829	-1.92683
C	3.67632	-5.17009	-2.20616
C	2.35483	-4.73915	-2.12579
C	2.05545	-3.41731	-1.76957
C	3.10393	-2.52780	-1.49893
C	4.42926	-2.94848	-1.57285
Cl	6.37276	-4.80713	-2.03245
H	3.90887	-6.19203	-2.48267
H	1.55348	-5.43880	-2.33246
H	2.87962	-1.49831	-1.23862
H	5.23663	-2.25801	-1.36373

TS-5Re
B3LYP/6-31G(d,p) Energy = -4777.523919
B3LYP/6-31G(d,p) Free Energy = -4776.378766
M06-2X/6-31G(d,p) Derived free energy = -4774.902767
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.914582
Number of Imaginary Frequencies = 1 (-118.14)

B3LYP/6-31G(d,p) Geometry

C	0.93130	6.14454	2.38532
C	-0.35286	6.42957	2.90594
C	-1.43488	5.68619	2.49570
C	-1.28418	4.63589	1.55046
C	0.00746	4.36518	0.99638
C	1.10668	5.14399	1.45507
C	-2.38836	3.84839	1.14075
C	-2.25263	2.76709	0.29366
C	-0.94777	2.48082	-0.21103
C	0.14317	3.30706	0.03289
C	1.42270	3.09256	-0.70191
C	2.05745	1.85908	-0.64352
C	3.34942	1.63274	-1.20876
C	3.93880	2.67513	-1.89465
C	3.28980	3.91941	-2.09206
C	2.00555	4.13762	-1.49950
C	3.88596	4.94602	-2.87273
C	3.23385	6.13677	-3.09159
C	1.94815	6.34291	-2.53910
C	1.35152	5.37344	-1.76400
O	1.44279	0.83578	0.05579
O	-0.80367	1.40402	-1.06165
C	4.11090	0.34843	-1.03318
C	-3.47458	1.99342	-0.10839
C	-4.01031	2.15174	-1.41114
C	-5.23065	1.54224	-1.72199
C	-5.94447	0.78116	-0.79083
C	-5.38197	0.61616	0.47441
C	-4.16389	1.20370	0.84111
C	4.84370	0.13673	0.16097
C	5.65087	-1.00049	0.27305
C	5.75792	-1.93984	-0.75837
C	5.01679	-1.71468	-1.92035
C	4.19896	-0.58755	-2.08952
C	-3.64467	0.97253	2.26070
C	-3.33142	3.00698	-2.48152
C	-7.31135	0.19128	-1.11656
C	4.85170	1.17386	1.28606
C	6.71000	-3.12784	-0.66673
C	3.50400	-0.37215	-3.43525
P	0.11767	0.08723	-0.64487
O	0.48547	-0.62487	-1.90205
O	-0.52715	-0.66206	0.50899
C	2.75971	-1.61686	-3.94857
C	4.51664	0.11912	-4.49068
C	6.09175	2.08394	1.16856
C	4.76535	0.56558	2.69608
C	6.52722	-3.95960	0.61460
C	8.17471	-2.66890	-0.81223

C	-3.43980	-0.52265	2.56241
C	-4.56391	1.62648	3.31119
C	-7.29331	-0.71426	-2.36027
C	-8.37240	1.30007	-1.26068
C	-4.20390	4.21387	-2.87833
C	-2.93534	2.17432	-3.71491
H	1.78868	6.71849	2.72496
H	-0.47839	7.22604	3.63345
H	-2.42553	5.88338	2.89719
H	2.09792	4.93485	1.07077
H	-3.37540	4.09985	1.51847
H	4.93115	2.53562	-2.31413
H	4.86635	4.76460	-3.30567
H	3.69531	6.91228	-3.69570
H	1.42284	7.27367	-2.73257
H	0.36224	5.54580	-1.35804
H	-5.64563	1.68876	-2.71578
H	-5.91692	0.01751	1.20744
H	6.23175	-1.14299	1.17946
H	5.10395	-2.42610	-2.73772
H	-2.66435	1.44881	2.34065
H	-2.40782	3.41059	-2.06072
H	-7.60209	-0.43258	-0.26106
H	3.97076	1.80925	1.16085
H	6.48665	-3.78292	-1.51956
H	2.74885	0.40559	-3.30011
H	1.97350	-1.90559	-3.24995
H	2.27911	-1.38644	-4.90552
H	3.43282	-2.46466	-4.12172
H	5.29278	-0.63334	-4.67272
H	4.01129	0.31643	-5.44241
H	5.01568	1.04088	-4.17769
H	6.12339	2.58706	0.19793
H	6.08345	2.85277	1.94928
H	7.01449	1.50272	1.27631
H	3.88872	-0.07972	2.80262
H	5.65163	-0.02597	2.94914
H	4.68849	1.36375	3.44224
H	7.19484	-4.82797	0.60816
H	5.50059	-4.32663	0.71454
H	6.75869	-3.37545	1.51149
H	8.46333	-2.01303	0.01645
H	8.32265	-2.11330	-1.74306
H	8.85522	-3.52770	-0.81404
H	-2.70068	-0.95585	1.88662
H	-3.07613	-0.65439	3.58755
H	-4.37042	-1.09249	2.47125
H	-4.68379	2.69990	3.13167
H	-4.14913	1.49607	4.31695
H	-5.56330	1.17734	3.30347

H	-7.03055	-0.14961	-3.26192
H	-8.28121	-1.15749	-2.52767
H	-6.56938	-1.52667	-2.25007
H	-8.14096	1.95730	-2.10611
H	-8.42000	1.92083	-0.36071
H	-9.36530	0.86955	-1.43282
H	-3.67464	4.84717	-3.59888
H	-4.45306	4.82700	-2.00631
H	-5.14438	3.89842	-3.34313
H	-2.26495	1.35798	-3.43402
H	-3.81481	1.74813	-4.21161
H	-2.41597	2.80228	-4.44736
C	-0.11606	-2.66262	4.44616
C	0.62223	-2.12078	3.37054
C	0.78226	-0.71978	3.27660
C	0.26747	0.10819	4.26335
C	-0.42344	-0.45880	5.33908
C	-0.62913	-1.83958	5.43633
H	-0.27636	-3.73472	4.49960
C	1.19937	-3.02909	2.41374
H	1.26266	-0.28546	2.40755
H	0.37818	1.18387	4.19415
Cl	-1.06717	0.58396	6.58422
H	-1.18620	-2.24966	6.27031
S	2.62001	-2.62520	1.52575
N	-0.04046	-3.24967	0.58040
H	0.99757	-4.08692	2.55045
S	-1.20509	-4.45160	0.94424
H	-0.40323	-2.24196	0.53580
O	-2.20418	-3.77834	1.77390
O	-0.43155	-5.58159	1.48835
C	-2.94515	-6.03763	-2.98439
C	-1.90945	-4.99101	-0.61983
C	-1.75381	-6.33245	-0.91003
C	-2.28826	-6.86386	-2.10293
H	-3.34754	-6.43616	-3.91192
H	-1.21901	-6.96716	-0.21360
H	-2.16787	-7.92054	-2.31800
C	-3.11228	-4.65337	-2.71752
C	-2.60366	-4.09357	-1.49393
C	-2.79908	-2.70885	-1.25052
C	-3.43680	-1.91561	-2.17888
C	-3.92448	-2.46366	-3.38740
C	-3.77252	-3.80565	-3.64533
H	-2.44857	-2.25181	-0.33527
H	-3.56423	-0.85808	-1.97494
H	-4.42032	-1.82019	-4.10714
H	-4.14885	-4.24004	-4.56743
C	0.97713	-3.52998	-0.44114
H	0.67888	-4.37805	-1.06578

H	1.04938	-2.64226	-1.07571
C	2.34391	-3.85209	0.20753
H	2.35651	-4.85805	0.63408
H	3.15842	-3.74093	-0.51050

Pre TS-5Re

B3LYP/6-31G(d,p) Energy = -4777.524733
B3LYP/6-31G(d,p) Free Energy = -4776.383731
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.918390
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-2.19578	-6.00937	1.97136
C	-1.00174	-6.56105	2.49230
C	0.21079	-6.01437	2.14196
C	0.28480	-4.90356	1.25872
C	-0.91854	-4.36381	0.70177
C	-2.15597	-4.94404	1.09905
C	1.52752	-4.31282	0.92027
C	1.62048	-3.17947	0.13779
C	0.40715	-2.63356	-0.38114
C	-0.82682	-3.24824	-0.20021
C	-2.02486	-2.74519	-0.93225
C	-2.40613	-1.41562	-0.80392
C	-3.61860	-0.90726	-1.36256
C	-4.39057	-1.77122	-2.11182
C	-3.99435	-3.10544	-2.37989
C	-2.78790	-3.60615	-1.79489
C	-4.76662	-3.94778	-3.22412
C	-4.35677	-5.22880	-3.51069
C	-3.14612	-5.71571	-2.96467
C	-2.38441	-4.92911	-2.12940
O	-1.61908	-0.57395	-0.04138
O	0.48773	-1.51214	-1.17787
C	-4.10881	0.49156	-1.10960
C	2.97547	-2.61135	-0.17165
C	3.53372	-2.77523	-1.46326
C	4.85772	-2.38102	-1.68644
C	5.65386	-1.83110	-0.67680
C	5.06854	-1.64375	0.57532
C	3.74818	-2.01898	0.85466
C	-4.82247	0.76938	0.08251
C	-5.36861	2.04384	0.26915
C	-5.22933	3.05797	-0.68461
C	-4.51536	2.76192	-1.84765
C	-3.95607	1.49856	-2.09110
C	3.20976	-1.77816	2.26542
C	2.76074	-3.41137	-2.61843
C	7.12737	-1.50926	-0.89800
C	-5.08767	-0.31750	1.12613

C	-5.88975	4.42044	-0.50511
C	-3.28190	1.22830	-3.43725
P	-0.14711	-0.05977	-0.67769
O	-0.34447	0.78248	-1.89318
O	0.59820	0.46494	0.53063
C	-2.32060	2.34233	-3.88375
C	-4.34541	0.97603	-4.52688
C	-6.48634	-0.93420	0.91890
C	-4.92601	0.16235	2.57869
C	-5.50658	5.10748	0.81753
C	-7.42173	4.31561	-0.64001
C	3.27263	-0.29108	2.65729
C	3.93634	-2.65376	3.30537
C	7.37652	-0.58660	-2.10313
C	7.95796	-2.80254	-1.01867
C	3.42612	-4.71619	-3.09792
C	2.56191	-2.42325	-3.78297
H	-3.15422	-6.42844	2.26410
H	-1.04661	-7.40600	3.17307
H	1.13616	-6.41711	2.54570
H	-3.08010	-4.53049	0.71305
H	2.43844	-4.76178	1.30605
H	-5.32945	-1.41612	-2.52719
H	-5.68474	-3.55236	-3.65104
H	-4.95069	-5.86193	-4.16318
H	-2.81027	-6.71875	-3.21124
H	-1.45505	-5.31463	-1.72841
H	5.28582	-2.53692	-2.67315
H	5.66723	-1.20161	1.36788
H	-5.93682	2.24337	1.17301
H	-4.41705	3.53407	-2.60639
H	2.15483	-2.06347	2.27445
H	1.76620	-3.68043	-2.25557
H	7.47587	-0.97821	-0.00232
H	-4.35601	-1.11530	0.97065
H	-5.53267	5.05985	-1.32354
H	-2.67808	0.32422	-3.33057
H	-1.51959	2.47051	-3.15507
H	-1.85498	2.06229	-4.83457
H	-2.83240	3.29820	-4.04500
H	-4.97256	1.86273	-4.67639
H	-3.86435	0.74007	-5.48239
H	-5.00503	0.14288	-4.26824
H	-6.58830	-1.35471	-0.08545
H	-6.66812	-1.73683	1.64247
H	-7.26931	-0.17851	1.04823
H	-3.94296	0.61192	2.74825
H	-5.68495	0.90023	2.85954
H	-5.03119	-0.68389	3.26605
H	-5.96100	6.10205	0.88136

H	-4.42195	5.22770	0.90863
H	-5.85075	4.53282	1.68397
H	-7.84442	3.69204	0.15540
H	-7.70294	3.86833	-1.59805
H	-7.88780	5.30503	-0.57407
H	2.67655	0.31412	1.97259
H	2.87388	-0.15103	3.66878
H	4.29814	0.09270	2.65695
H	3.86257	-3.71842	3.06094
H	3.50411	-2.50534	4.30147
H	5.00102	-2.40220	3.36521
H	7.06051	-1.05639	-3.04124
H	8.44383	-0.35715	-2.19573
H	6.83512	0.35774	-1.99896
H	7.66124	-3.37825	-1.90237
H	7.81982	-3.44389	-0.14280
H	9.02566	-2.57329	-1.11034
H	2.82262	-5.18687	-3.88198
H	3.53357	-5.43200	-2.27654
H	4.42334	-4.53419	-3.51326
H	2.03318	-1.52821	-3.44592
H	3.52045	-2.11778	-4.21814
H	1.97060	-2.88773	-4.58005
C	0.26185	2.00901	4.66927
C	-0.48476	1.73410	3.49628
C	-0.91235	0.40588	3.24025
C	-0.65431	-0.59557	4.16104
C	0.04289	-0.28352	5.33522
C	0.51319	1.01122	5.59427
H	0.63166	3.01446	4.84366
C	-0.75279	2.81100	2.60492
H	-1.38272	0.15835	2.29481
H	-0.96140	-1.61635	3.96648
Cl	0.36274	-1.54453	6.49379
H	1.07271	1.21514	6.49935
S	-1.95701	2.78177	1.42670
N	0.92404	3.14392	0.50231
H	-0.22007	3.74797	2.74936
S	2.10997	4.09530	1.16555
H	1.04114	2.10187	0.50430
O	2.95077	3.20032	1.96488
O	1.42195	5.22947	1.81706
C	4.41657	6.00420	-2.31070
C	3.04410	4.77769	-0.21427
C	3.10306	6.15366	-0.29395
C	3.80722	6.77457	-1.34916
H	4.94728	6.47374	-3.13471
H	2.59809	6.74754	0.45877
H	3.85167	7.85781	-1.39755
C	4.36759	4.58546	-2.26067

C	3.68496	3.93223	-1.17728
C	3.67235	2.51153	-1.14580
C	4.26965	1.78021	-2.14870
C	4.92604	2.42438	-3.22293
C	4.98121	3.79740	-3.27010
H	3.19846	1.98510	-0.32852
H	4.23530	0.69637	-2.10758
H	5.38902	1.83056	-4.00492
H	5.49136	4.30421	-4.08476
C	-0.08536	3.67459	-0.39309
H	0.29452	4.53745	-0.95305
H	-0.32873	2.88059	-1.10499
C	-1.36231	4.13701	0.35629
H	-1.16188	5.01589	0.97244
H	-2.17650	4.34317	-0.34189

Post TS-5Re
B3LYP/6-31G(d,p) Energy = -4777.553232
B3LYP/6-31G(d,p) Free Energy = -4776.408665
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.954271
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	0.97958	5.71990	3.53770
C	-0.32098	5.95129	4.04354
C	-1.39935	5.32112	3.46831
C	-1.22694	4.44026	2.36674
C	0.08257	4.23080	1.83009
C	1.17672	4.88714	2.45867
C	-2.32848	3.76723	1.78300
C	-2.17915	2.83413	0.77722
C	-0.85650	2.60066	0.29887
C	0.24027	3.34561	0.70656
C	1.54333	3.24661	-0.01115
C	2.17463	2.02241	-0.15795
C	3.48699	1.87397	-0.69170
C	4.11153	3.01815	-1.14566
C	3.47620	4.28475	-1.14453
C	2.16645	4.41164	-0.58179
C	4.11293	5.42688	-1.70083
C	3.47587	6.64491	-1.73288
C	2.16646	6.76590	-1.21193
C	1.52996	5.68194	-0.64936
O	1.51474	0.88346	0.31707
O	-0.70099	1.65051	-0.71469
C	4.22350	0.56580	-0.72518
C	-3.39345	2.18738	0.17567
C	-3.85765	2.62409	-1.09063
C	-5.04971	2.09361	-1.59456
C	-5.80171	1.14785	-0.89077

C	-5.32186	0.73355	0.35122
C	-4.13600	1.23145	0.90710
C	4.81217	0.06913	0.46405
C	5.60039	-1.08411	0.39840
C	5.82979	-1.76227	-0.80325
C	5.23062	-1.25771	-1.95803
C	4.43005	-0.10722	-1.95189
C	-3.71852	0.74770	2.29625
C	-3.13638	3.69843	-1.90634
C	-7.11587	0.60416	-1.43688
C	4.68842	0.80765	1.79734
C	6.74291	-2.98055	-0.87262
C	3.85169	0.39408	-3.27643
P	0.24142	0.33837	-0.54640
O	0.56083	-0.28103	-1.84938
O	-0.49074	-0.58066	0.52109
C	3.06061	-0.68898	-4.03257
C	4.96021	0.98152	-4.17329
C	5.98567	1.58251	2.10643
C	4.30352	-0.11193	2.96877
C	6.36053	-4.07778	0.13621
C	8.22035	-2.57390	-0.70452
C	-3.70547	-0.78577	2.41592
C	-4.62093	1.35886	3.38814
C	-6.94732	-0.07218	-2.80923
C	-8.19912	1.69855	-1.49059
C	-3.99688	4.97040	-2.03907
C	-2.69085	3.18245	-3.28719
H	1.83252	6.19996	4.00813
H	-0.46219	6.61573	4.89061
H	-2.40254	5.47590	3.85624
H	2.18041	4.71443	2.08950
H	-3.32665	3.98933	2.14772
H	5.12220	2.94377	-1.53621
H	5.11177	5.31367	-2.11362
H	3.96827	7.50994	-2.16678
H	1.65518	7.72276	-1.26001
H	0.52441	5.79216	-0.26256
H	-5.40849	2.44331	-2.55904
H	-5.89549	-0.00026	0.91073
H	6.06502	-1.44990	1.30919
H	5.40332	-1.77187	-2.90033
H	-2.69701	1.09400	2.47865
H	-2.23046	3.98628	-1.36746
H	-7.45973	-0.16461	-0.73269
H	3.88939	1.54738	1.70178
H	6.63284	-3.40501	-1.87960
H	3.14602	1.19815	-3.05175
H	2.22006	-1.04164	-3.43225
H	2.65584	-0.27134	-4.96109

H	3.69104	-1.54200	-4.30742
H	5.69434	0.21564	-4.44749
H	4.53290	1.38169	-5.09926
H	5.50021	1.79152	-3.67310
H	6.22651	2.29043	1.30707
H	5.88587	2.14603	3.04080
H	6.83544	0.89949	2.21487
H	3.38720	-0.66681	2.75145
H	5.09040	-0.83873	3.19740
H	4.14035	0.48333	3.87376
H	6.99430	-4.96076	-0.00009
H	5.31722	-4.38740	0.02138
H	6.49012	-3.73791	1.16906
H	8.39776	-2.14248	0.28676
H	8.51275	-1.82767	-1.44963
H	8.87823	-3.44315	-0.81431
H	-3.06276	-1.24697	1.66477
H	-3.33166	-1.08079	3.40153
H	-4.70750	-1.21431	2.30897
H	-4.60701	2.45290	3.36664
H	-4.29245	1.03571	4.38195
H	-5.66115	1.03947	3.26026
H	-6.63915	0.64915	-3.57439
H	-7.89344	-0.51578	-3.13814
H	-6.19269	-0.86311	-2.77252
H	-7.91903	2.49818	-2.18528
H	-8.35351	2.15172	-0.50651
H	-9.15462	1.28260	-1.82879
H	-3.44617	5.75215	-2.57383
H	-4.27681	5.36339	-1.05655
H	-4.92052	4.77531	-2.59455
H	-2.03319	2.31453	-3.18803
H	-3.54849	2.89640	-3.90661
H	-2.14229	3.96242	-3.82659
C	-0.60902	-4.64316	3.46767
C	-0.03175	-3.60257	2.72978
C	-0.04482	-2.30660	3.26319
C	-0.62696	-2.05415	4.50265
C	-1.19442	-3.10894	5.21781
C	-1.19312	-4.40573	4.71110
H	-0.61690	-5.64864	3.05925
C	0.63274	-3.92884	1.40948
H	0.40553	-1.48823	2.71355
H	-0.63333	-1.05146	4.91466
Cl	-1.91922	-2.79474	6.78991
H	-1.63972	-5.21478	5.27758
S	2.34642	-3.23470	1.29952
N	-0.05533	-3.38963	0.17721
H	0.70069	-5.01501	1.31181
S	-1.58380	-4.30193	-0.06567

H	-0.37808	-1.56287	0.36822
O	-2.62705	-3.50901	0.58396
O	-1.33711	-5.68698	0.36618
C	-2.22754	-4.68123	-4.59239
C	-1.84446	-4.34531	-1.85118
C	-1.61360	-5.57352	-2.44008
C	-1.81074	-5.74406	-3.82640
H	-2.37463	-4.80112	-5.66240
H	-1.28904	-6.40397	-1.82485
H	-1.62918	-6.71466	-4.27607
C	-2.48177	-3.40958	-4.01573
C	-2.30334	-3.21410	-2.60086
C	-2.58738	-1.93373	-2.05732
C	-3.00618	-0.90214	-2.86833
C	-3.17030	-1.09203	-4.25920
C	-2.91684	-2.32195	-4.81798
H	-2.49075	-1.76534	-0.99411
H	-3.21712	0.06579	-2.42786
H	-3.49869	-0.26467	-4.88044
H	-3.04443	-2.48439	-5.88469
C	0.90042	-3.57858	-0.95796
H	1.02319	-4.64633	-1.18030
H	0.51746	-3.06182	-1.83836
C	2.23160	-2.97168	-0.51954
H	3.06552	-3.46093	-1.02431
H	2.27570	-1.90488	-0.73294

TS-5Si

B3LYP/6-31G(d,p) Energy = -4777.525584
B3LYP/6-31G(d,p) Free Energy = -4776.381920
M06-2X/6-31G(d,p) Derived free energy = -4774.906470
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.917257
Number of Imaginary Frequencies = 1 (-168.03)

B3LYP/6-31G(d,p) Geometry

C	0.15908	4.97988	3.72028
C	-1.06468	4.85744	4.41992
C	-2.08747	4.11122	3.88045
C	-1.93546	3.45864	2.62714
C	-0.70645	3.60044	1.90457
C	0.33187	4.37248	2.49572
C	-2.98104	2.67675	2.07035
C	-2.81974	1.95725	0.90422
C	-1.55516	2.04378	0.24724
C	-0.55958	2.92669	0.64286
C	0.61476	3.17178	-0.24545
C	1.41924	2.11661	-0.65702
C	2.63045	2.31354	-1.38660
C	2.94987	3.59934	-1.76928

C	2.10562	4.70317	-1.49015
C	0.91490	4.49582	-0.72249
C	2.42058	6.00689	-1.95861
C	1.58515	7.07003	-1.70769
C	0.39044	6.86441	-0.97931
C	0.06496	5.61533	-0.49895
O	1.09590	0.83364	-0.26774
O	-1.36585	1.28725	-0.89081
C	3.59914	1.19647	-1.65865
C	-3.97873	1.20836	0.30995
C	-4.44462	0.00740	0.89020
C	-5.59711	-0.59296	0.36645
C	-6.29891	-0.05494	-0.71187
C	-5.80619	1.12146	-1.28244
C	-4.66474	1.76577	-0.79761
C	3.62266	0.54560	-2.91427
C	4.62092	-0.40781	-3.15671
C	5.59225	-0.74051	-2.20770
C	5.53255	-0.09927	-0.96684
C	4.56111	0.86607	-0.67433
C	-4.21867	3.05904	-1.48051
C	-3.74163	-0.66089	2.07020
C	-7.57469	-0.71561	-1.21875
C	2.64050	0.90624	-4.02870
C	6.72017	-1.70247	-2.56913
C	4.59998	1.55530	0.69073
P	-0.25529	0.06008	-0.88480
O	-0.05881	-0.36694	-2.29967
O	-0.58815	-0.95300	0.19870
C	5.93656	2.28506	0.92468
C	4.29295	0.57674	1.83909
C	2.05427	-0.32091	-4.74618
C	3.29973	1.86456	-5.04201
C	7.03241	-2.73602	-1.47409
C	7.99396	-0.92212	-2.95316
C	-5.30400	4.15021	-1.40609
C	-3.77753	2.80578	-2.93485
C	-7.53036	-1.01270	-2.72797
C	-8.81707	0.12320	-0.86065
C	-3.40028	-2.13427	1.78522
C	-4.56462	-0.52929	3.36656
H	0.97099	5.55703	4.15337
H	-1.19193	5.34849	5.38024
H	-3.03006	4.00142	4.41049
H	1.27701	4.46878	1.97457
H	-3.93890	2.64571	2.58195
H	3.87921	3.77696	-2.30339
H	3.33380	6.14438	-2.53191
H	1.83215	8.06123	-2.07619
H	-0.28123	7.69925	-0.80157

H	-0.85927	5.47651	0.04829
H	-5.96031	-1.51288	0.81760
H	-6.33112	1.56076	-2.12631
H	4.65887	-0.89159	-4.12945
H	6.27759	-0.33190	-0.21096
H	-3.34813	3.44586	-0.94545
H	-2.79207	-0.14143	2.22430
H	-7.66578	-1.67793	-0.69784
H	1.79726	1.42824	-3.56914
H	6.39542	-2.25566	-3.46081
H	3.81636	2.31664	0.70457
H	6.13806	3.00747	0.12758
H	5.91391	2.82768	1.87616
H	6.78029	1.58742	0.96268
H	3.30090	0.13311	1.71821
H	5.03122	-0.23231	1.88905
H	4.30809	1.09780	2.80249
H	1.32015	0.00651	-5.49005
H	2.81968	-0.89639	-5.27951
H	1.53698	-0.96701	-4.03529
H	3.66006	2.77869	-4.56076
H	4.15473	1.38810	-5.53580
H	2.58199	2.15251	-5.81781
H	6.14766	-3.32016	-1.20101
H	7.80134	-3.43576	-1.81818
H	7.41104	-2.26031	-0.56331
H	7.79468	-0.21874	-3.76699
H	8.36929	-0.34686	-2.09963
H	8.78810	-1.60444	-3.27636
H	-5.59078	4.35490	-0.36954
H	-4.93814	5.08361	-1.84810
H	-6.20927	3.86032	-1.95032
H	-4.60839	2.43612	-3.54632
H	-3.41604	3.73375	-3.39212
H	-2.97078	2.06942	-2.97159
H	-6.66480	-1.63056	-2.98400
H	-8.43458	-1.54590	-3.04205
H	-7.47171	-0.09144	-3.31743
H	-8.87711	0.30054	0.21762
H	-8.78803	1.09940	-1.35724
H	-9.73532	-0.38546	-1.17542
H	-2.82355	-2.55955	2.61271
H	-2.79424	-2.21835	0.88115
H	-4.30198	-2.74502	1.66355
H	-4.76387	0.51819	3.61518
H	-5.53216	-1.03557	3.27418
H	-4.03045	-0.98238	4.20926
C	-1.55257	-3.24279	-2.07508
C	-0.95137	-4.21790	-1.24857
C	-1.75219	-5.21641	-0.65237

C	-3.11018	-5.28446	-0.92052
C	-3.67647	-4.33091	-1.77305
C	-2.91466	-3.30402	-2.33806
H	-0.96614	-2.41334	-2.46593
C	0.47198	-4.25712	-1.00810
H	-1.29814	-5.94181	0.01509
H	-3.72877	-6.05677	-0.47907
Cl	-5.38610	-4.42486	-2.12576
H	-3.38779	-2.55431	-2.96109
S	1.58893	-3.67559	-2.20191
N	1.10103	-2.91807	0.54625
H	0.83858	-5.05972	-0.37643
S	1.04226	-3.84396	2.00698
H	0.36041	-2.12898	0.48486
O	1.81550	-5.06060	1.70570
O	-0.37772	-3.93827	2.34096
C	3.42599	-1.80108	5.34447
C	1.94703	-2.93962	3.27518
C	3.06238	-3.58872	3.76993
C	3.80880	-3.01281	4.81928
H	3.99626	-1.35009	6.15218
H	3.34832	-4.54601	3.35127
H	4.67920	-3.53409	5.20380
C	2.28971	-1.10663	4.85303
C	1.50526	-1.67694	3.78968
C	0.38142	-0.95106	3.31461
C	0.05977	0.27363	3.85848
C	0.82638	0.83345	4.90516
C	1.91699	0.15294	5.39288
H	-0.22733	-1.33293	2.50675
H	-0.79193	0.82030	3.46889
H	0.55334	1.80280	5.30987
H	2.51811	0.56971	6.19642
C	2.42523	-2.48438	0.07131
H	2.32022	-1.47364	-0.32557
H	3.14410	-2.44583	0.89573
C	2.95643	-3.43217	-1.02216
H	3.78401	-2.97128	-1.56358
H	3.26694	-4.39122	-0.60193

Pre TS-5Si

B3LYP/6-31G(d,p) Energy = -4777.527850
B3LYP/6-31G(d,p) Free Energy = -4776.389251
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.921295
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	0.26144	4.90975	3.81742
C	-0.93479	4.75389	4.55645
C	-1.96849	4.01141	4.03319

C	-1.85535	3.39625	2.75714
C	-0.65521	3.57370	1.99483
C	0.39608	4.33959	2.57057
C	-2.91239	2.61829	2.21667
C	-2.78860	1.93829	1.02297
C	-1.55307	2.06405	0.31998
C	-0.54972	2.94002	0.70882
C	0.59547	3.20963	-0.20960
C	1.38869	2.16617	-0.67141
C	2.58090	2.38903	-1.42561
C	2.88859	3.68423	-1.78412
C	2.04800	4.77745	-1.45665
C	0.87900	4.54553	-0.66277
C	2.34438	6.09349	-1.90198
C	1.51120	7.14616	-1.60367
C	0.33777	6.91718	-0.84810
C	0.03113	5.65534	-0.38908
O	1.08862	0.87220	-0.30884
O	-1.39057	1.34353	-0.84640
C	3.53724	1.27708	-1.75187
C	-3.96007	1.19111	0.45125
C	-4.36888	-0.04797	0.99352
C	-5.53612	-0.64640	0.50093
C	-6.30481	-0.07142	-0.51104
C	-5.86618	1.14139	-1.04819
C	-4.71359	1.78632	-0.59045
C	3.53206	0.66929	-3.02887
C	4.50596	-0.29630	-3.31644
C	5.48524	-0.67670	-2.39323
C	5.45876	-0.07188	-1.13314
C	4.50902	0.90049	-0.79413
C	-4.32603	3.11997	-1.22979
C	-3.59065	-0.75398	2.10288
C	-7.59660	-0.73136	-0.97728
C	2.55042	1.09413	-4.12117
C	6.59080	-1.64322	-2.80827
C	4.59164	1.56027	0.58384
P	-0.29914	0.09576	-0.84664
O	-0.15717	-0.35666	-2.26525
O	-0.60499	-0.88310	0.26536
C	5.92448	2.31189	0.76727
C	4.35663	0.55959	1.73003
C	1.87858	-0.09136	-4.83392
C	3.24630	2.02178	-5.13833
C	6.95528	-2.68000	-1.73283
C	7.84639	-0.86471	-3.25240
C	-5.42982	4.18135	-1.05976
C	-3.94190	2.94386	-2.71142
C	-7.65441	-0.92083	-2.50319
C	-8.82966	0.04537	-0.47518

C	-3.27525	-2.21957	1.75445
C	-4.32785	-0.66053	3.45332
H	1.08293	5.48251	4.23811
H	-1.03186	5.21530	5.53483
H	-2.88984	3.87527	4.59364
H	1.32102	4.46092	2.01927
H	-3.84867	2.55916	2.76447
H	3.80292	3.87752	-2.33852
H	3.24153	6.24937	-2.49562
H	1.74381	8.14711	-1.95481
H	-0.33240	7.74413	-0.63191
H	-0.87710	5.49838	0.17975
H	-5.85918	-1.59394	0.92484
H	-6.44321	1.60983	-1.84086
H	4.52182	-0.74809	-4.30540
H	6.21370	-0.33841	-0.39870
H	-3.44166	3.50135	-0.71369
H	-2.62946	-0.24397	2.20661
H	-7.62882	-1.72971	-0.52089
H	1.74958	1.66398	-3.64275
H	6.22219	-2.19348	-3.68482
H	3.79562	2.30608	0.64578
H	6.07346	3.05226	-0.02495
H	5.93825	2.83641	1.72894
H	6.78105	1.62908	0.75029
H	3.36319	0.10877	1.65955
H	5.10303	-0.24321	1.72760
H	4.42151	1.06634	2.69891
H	1.17793	0.28271	-5.58843
H	2.60295	-0.72886	-5.35420
H	1.30866	-0.68698	-4.11886
H	3.67342	2.90473	-4.65320
H	4.05968	1.50009	-5.65590
H	2.53231	2.36480	-5.89507
H	6.08404	-3.26048	-1.41203
H	7.70047	-3.38309	-2.11937
H	7.38603	-2.20820	-0.84351
H	7.60963	-0.15967	-4.05469
H	8.26266	-0.29104	-2.41698
H	8.62300	-1.54782	-3.61431
H	-5.67820	4.32985	-0.00393
H	-5.10142	5.14274	-1.47016
H	-6.35034	3.89774	-1.58134
H	-4.78925	2.57966	-3.30341
H	-3.62339	3.90049	-3.14075
H	-3.11953	2.23142	-2.81569
H	-6.79369	-1.49091	-2.86528
H	-8.56458	-1.45922	-2.79010
H	-7.66395	0.04048	-3.02797
H	-8.81821	0.14231	0.61478

H	-8.85520	1.05560	-0.89847
H	-9.75658	-0.46314	-0.76396
H	-2.63964	-2.66634	2.52502
H	-2.73229	-2.27736	0.80930
H	-4.18470	-2.82733	1.68277
H	-4.50341	0.37900	3.74847
H	-5.30266	-1.15936	3.40639
H	-3.74336	-1.14327	4.24449
C	-1.69810	-3.14538	-2.41331
C	-1.06170	-4.16275	-1.65501
C	-1.83887	-5.20657	-1.09150
C	-3.19696	-5.28241	-1.33936
C	-3.79442	-4.29026	-2.12889
C	-3.06136	-3.21513	-2.64798
H	-1.13546	-2.26892	-2.73360
C	0.33859	-4.17165	-1.40905
H	-1.35917	-5.95298	-0.46642
H	-3.79825	-6.08286	-0.92528
Cl	-5.50415	-4.38752	-2.44592
H	-3.56513	-2.43365	-3.20430
S	1.46632	-3.30286	-2.31268
N	1.25819	-2.75273	0.70140
H	0.72978	-4.85640	-0.66168
S	1.18535	-3.86445	1.93541
H	0.48584	-2.03471	0.64079
O	1.95028	-5.03772	1.46551
O	-0.23277	-4.00947	2.27259
C	3.56530	-2.29297	5.53087
C	2.08391	-3.17592	3.33742
C	3.14365	-3.92462	3.80620
C	3.89022	-3.48039	4.91978
H	4.13844	-1.94056	6.38439
H	3.39178	-4.85566	3.31037
H	4.71841	-4.08098	5.28195
C	2.48419	-1.49585	5.06860
C	1.69905	-1.93700	3.94755
C	0.62353	-1.11535	3.51199
C	0.35379	0.07998	4.14231
C	1.12737	0.51453	5.24248
C	2.16727	-0.26195	5.69687
H	0.00260	-1.40885	2.67653
H	-0.46186	0.69839	3.78213
H	0.89769	1.46233	5.71931
H	2.76945	0.05748	6.54323
C	2.52079	-2.40570	0.07609
H	2.45822	-1.36451	-0.24539
H	3.35784	-2.48146	0.78027
C	2.86123	-3.31025	-1.13482
H	3.71816	-2.91067	-1.68057
H	3.05735	-4.33481	-0.81367

Post TS-5Si
B3LYP/6-31G(d,p) Energy = -4777.548594
B3LYP/6-31G(d,p) Free Energy = -4776.404006
M06-2X/6-31G(d,p) Derived free energy in solution = -4774.949230
Number of Imaginary Frequencies = 0

B3LYP/6-31G(d,p) Geometry

C	-0.47312	5.21594	3.79294
C	-1.71768	5.00124	4.42985
C	-2.63076	4.13609	3.87302
C	-2.34355	3.45131	2.66180
C	-1.09537	3.68692	2.00116
C	-0.17149	4.58071	2.60860
C	-3.28034	2.56138	2.07663
C	-2.98848	1.81925	0.95064
C	-1.69486	1.99360	0.37970
C	-0.81320	2.98748	0.77660
C	0.35719	3.34649	-0.07750
C	1.28812	2.38734	-0.43912
C	2.47446	2.67324	-1.17362
C	2.65416	3.97643	-1.58906
C	1.69300	4.99026	-1.34918
C	0.51650	4.68112	-0.59354
C	1.87402	6.30530	-1.85617
C	0.92195	7.27697	-1.65672
C	-0.25895	6.96550	-0.94368
C	-0.45643	5.70518	-0.42469
O	1.08343	1.07849	0.00937
O	-1.37394	1.18779	-0.71522
C	3.54239	1.64622	-1.42470
C	-4.05575	0.99330	0.28978
C	-4.49492	-0.22506	0.85307
C	-5.58060	-0.88789	0.26693
C	-6.24342	-0.39294	-0.85662
C	-5.77643	0.80232	-1.40807
C	-4.69986	1.50775	-0.86324
C	3.65063	1.00128	-2.67893
C	4.71388	0.11102	-2.88204
C	5.66683	-0.16119	-1.89760
C	5.53489	0.48918	-0.66790
C	4.49770	1.39230	-0.41247
C	-4.28979	2.82264	-1.52797
C	-3.83781	-0.84056	2.08731
C	-7.46330	-1.11284	-1.41769
C	2.69167	1.29648	-3.83296
C	6.83990	-1.08963	-2.18988
C	4.45453	2.09737	0.94291
P	-0.08999	0.20080	-0.70668
O	0.21762	-0.30036	-2.06200
O	-0.38754	-0.88712	0.41428

C	5.72284	2.93656	1.18980
C	4.20984	1.10533	2.09254
C	2.23632	0.03766	-4.59143
C	3.31953	2.31083	-4.81178
C	7.01270	-2.19387	-1.13228
C	8.14669	-0.29052	-2.36358
C	-5.42814	3.86061	-1.48673
C	-3.78981	2.59988	-2.96816
C	-7.41002	-1.29542	-2.94392
C	-8.76223	-0.39686	-0.99601
C	-3.40435	-2.29807	1.84592
C	-4.75858	-0.74257	3.31998
H	0.25317	5.88572	4.24379
H	-1.94568	5.51445	5.35923
H	-3.58713	3.95532	4.35646
H	0.78886	4.74863	2.13545
H	-4.26542	2.47054	2.52507
H	3.56187	4.23691	-2.12535
H	2.77806	6.52362	-2.41823
H	1.06692	8.27673	-2.05469
H	-1.02140	7.72672	-0.80781
H	-1.37108	5.48520	0.11142
H	-5.92422	-1.82293	0.70120
H	-6.27203	1.20934	-2.28463
H	4.81326	-0.37559	-3.84860
H	6.27008	0.30601	0.11103
H	-3.45721	3.24961	-0.96381
H	-2.93162	-0.26610	2.30306
H	-7.47655	-2.11399	-0.96834
H	1.79225	1.75208	-3.40929
H	6.62768	-1.58228	-3.14807
H	3.61199	2.79358	0.93525
H	5.87729	3.66699	0.38941
H	5.64193	3.48227	2.13638
H	6.61935	2.30977	1.24517
H	3.27616	0.55610	1.94381
H	5.02210	0.37558	2.17427
H	4.14209	1.63480	3.04953
H	1.49150	0.31399	-5.34527
H	3.06401	-0.44671	-5.12151
H	1.77273	-0.68269	-3.91568
H	3.58679	3.24732	-4.31348
H	4.23052	1.90358	-5.26490
H	2.61902	2.54706	-5.62022
H	6.10045	-2.78786	-1.01936
H	7.82415	-2.87273	-1.41528
H	7.26317	-1.77565	-0.15136
H	8.04560	0.46636	-3.14725
H	8.41736	0.22509	-1.43553
H	8.97591	-0.95377	-2.63346

H	-5.75715	4.04773	-0.45952
H	-5.09398	4.81179	-1.91569
H	-6.30005	3.52778	-2.05974
H	-4.58177	2.20000	-3.61072
H	-3.45332	3.54602	-3.40640
H	-2.95190	1.89783	-2.98715
H	-6.49857	-1.81641	-3.24956
H	-8.26833	-1.88315	-3.28699
H	-7.44395	-0.33434	-3.46846
H	-8.83045	-0.30727	0.09266
H	-8.80597	0.61406	-1.41662
H	-9.64199	-0.94618	-1.34948
H	-2.88930	-2.69602	2.72752
H	-2.72774	-2.36979	0.99147
H	-4.26063	-2.95190	1.65312
H	-5.02895	0.29500	3.54012
H	-5.68819	-1.30030	3.16312
H	-4.26839	-1.15988	4.20740
C	-1.37183	-3.27065	-1.90628
C	-0.76202	-4.25756	-1.11966
C	-1.55702	-5.25975	-0.54889
C	-2.93212	-5.29841	-0.76798
C	-3.51325	-4.31462	-1.56422
C	-2.74939	-3.29164	-2.12476
H	-0.77500	-2.48419	-2.35733
C	0.73366	-4.33112	-0.90968
H	-1.09676	-6.01698	0.07802
H	-3.54179	-6.08319	-0.33488
Cl	-5.24501	-4.37879	-1.87276
H	-3.22117	-2.52745	-2.73164
S	1.67203	-4.18374	-2.49940
N	1.31472	-3.29213	0.05889
H	0.96101	-5.31902	-0.50709
S	1.81691	-4.21199	1.48696
H	0.08770	-1.74873	0.29458
O	2.92821	-5.09409	1.09545
O	0.58318	-4.80403	2.01301
C	3.72811	-1.45550	4.61148
C	2.47895	-3.01708	2.66437
C	3.84848	-3.08225	2.83975
C	4.48052	-2.29139	3.82141
H	4.20443	-0.84566	5.37429
H	4.42743	-3.76633	2.23125
H	5.55583	-2.35776	3.94968
C	2.31918	-1.37070	4.46349
C	1.65018	-2.17233	3.47286
C	0.23577	-2.08285	3.38036
C	-0.46884	-1.23856	4.20971
C	0.18915	-0.44140	5.17294
C	1.55581	-0.51054	5.29638

H	-0.29535	-2.69745	2.66691
H	-1.54862	-1.18701	4.12118
H	-0.38697	0.22018	5.81217
H	2.07736	0.09075	6.03580
C	2.46042	-2.56382	-0.58315
H	2.04982	-1.67979	-1.07313
H	3.16064	-2.23192	0.18688
C	3.10890	-3.45409	-1.63782
H	3.68321	-2.85856	-2.35028
H	3.73702	-4.23117	-1.19855

Cartesian coordinates and energies of the TS employing AdDIP

TS-6Re

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.243931
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.716943
M06-2X/6-31G(d,p) Derived free energy = -5317.490003
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.500028
Number of Imaginary Frequencies = 1 (-163.18)

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.35299	5.29617	2.05566
C	-0.67042	4.46332	1.55513
C	0.13296	6.09134	3.18238
C	-1.91342	4.42589	2.23503
C	-0.48544	3.65768	0.40385
C	-2.12302	5.23931	3.35986
C	-2.93159	3.57857	1.78453
C	-1.10268	6.06784	3.82877
C	-1.46101	2.69745	0.06620
C	0.71147	3.79584	-0.47663
C	-2.70566	2.68958	0.72628
O	-1.24289	1.85016	-0.99015
C	-3.79839	1.77192	0.30124
C	1.55257	2.67780	-0.64892
C	1.02979	5.01485	-1.12872
C	2.26917	5.13649	-1.80734
C	0.14387	6.11379	-1.13249
C	3.15243	4.05221	-1.85097
C	2.61357	6.34719	-2.42914
C	2.79458	2.82017	-1.29281
C	3.76222	1.69519	-1.32646
O	1.23101	1.48389	-0.05733
C	0.49772	7.30889	-1.76253
C	1.73073	7.42751	-2.40326
P	-0.09007	0.71100	-0.70848
C	-4.23995	0.72724	1.16405
C	-4.45802	1.97660	-0.94259
C	4.47176	1.34196	-0.14717

C	4.02061	0.99919	-2.53998
C	-5.50507	1.11433	-1.31214
C	-4.11570	3.14172	-1.87569
C	-5.97270	0.09471	-0.46673
C	-5.33037	-0.07235	0.77322
C	-7.16289	-0.78248	-0.91768
C	-3.58919	0.45327	2.52295
C	4.95813	-0.05129	-2.53887
C	3.36689	1.40142	-3.86649
C	5.63584	-0.44756	-1.36911
C	5.37639	0.26835	-0.18920
C	6.67168	-1.59438	-1.34738
C	4.32902	2.12459	1.16095
C	-3.11507	-1.00072	2.64986
C	-4.54587	0.80459	3.66948
C	-5.30795	4.09591	-2.02596
C	-3.63901	2.64043	-3.24617
C	3.77828	1.23794	2.28299
C	5.66144	2.76520	1.57154
C	2.67927	0.22084	-4.56914
C	4.40047	2.04687	-4.79791
O	-0.53649	-0.18676	0.44263
O	0.23846	0.06489	-2.01950
C	7.43174	-4.48161	-1.59241
C	7.31276	-3.79320	-0.21806
C	7.86810	-3.44599	-2.64798
C	6.25647	-2.67023	-0.29502
C	8.67745	-3.19075	0.17949
C	6.81982	-2.31547	-2.72683
C	8.06977	-1.02448	-0.95998
C	9.23495	-2.84955	-2.25424
C	9.11633	-2.15808	-0.88083
C	-9.17642	-1.46177	-3.01113
C	-9.58857	-0.73340	-1.71348
C	-7.97475	-2.38851	-2.72615
C	-8.40512	0.11780	-1.20212
C	-9.97940	-1.77121	-0.64258
C	-6.78274	-1.54584	-2.22255
C	-7.59051	-1.84369	0.14989
C	-8.36509	-3.42383	-1.65217
C	-8.77555	-2.69140	-0.35843
C	-1.33326	-5.05328	-0.50730
C	-1.24338	-3.65939	-0.68505
C	-2.39723	-2.86422	-0.53391
C	-3.61953	-3.44780	-0.24024
C	-3.69068	-4.83381	-0.09479
C	-2.55625	-5.64383	-0.22187
C	-0.02280	-2.96557	-1.02817
S	1.33563	-3.70245	-1.80990
C	2.39932	-2.27151	-1.40753

C	2.40843	-2.12328	0.13051
N	1.03749	-2.23265	0.65608
S	0.84368	-3.15989	2.10178
C	1.84768	-2.33604	3.35644
Cl	-5.23483	-5.57234	0.26807
O	-0.57069	-3.05214	2.44453
O	1.45890	-4.46265	1.82562
C	1.52678	-1.04091	3.88540
C	2.37384	-0.54773	4.93903
C	3.46256	-1.33400	5.40005
C	3.73584	-2.56578	4.85556
C	2.91776	-3.07318	3.82338
C	0.47063	-0.20918	3.42639
C	0.27341	1.03910	3.97580
C	1.09271	1.51645	5.02217
C	2.11942	0.73378	5.49537
H	1.33052	5.32743	1.59286
H	0.92508	6.72668	3.55715
H	-3.07209	5.22597	3.88270
H	-3.89684	3.58633	2.27625
H	-1.26766	6.68750	4.70071
H	-0.82924	6.05518	-0.66344
H	4.11850	4.15892	-2.33049
H	3.56231	6.45526	-2.94150
H	-0.18877	8.14572	-1.75609
H	1.99977	8.35684	-2.88850
H	-5.98398	1.26535	-2.26802
H	-3.29417	3.76037	-1.46664
H	-5.66783	-0.83051	1.45941
H	-2.68203	1.07288	2.65695
H	5.15674	-0.54626	-3.47389
H	2.56912	2.15328	-3.70190
H	5.90573	0.00488	0.71423
H	3.61639	2.96593	1.05363
H	-2.47223	-1.26436	1.78938
H	-2.51961	-1.12472	3.57954
H	-3.96550	-1.71241	2.69035
H	-4.89450	1.85373	3.57510
H	-5.43279	0.13608	3.67034
H	-4.02419	0.70011	4.64484
H	-5.64335	4.44346	-1.02529
H	-5.00936	4.98633	-2.61969
H	-6.16061	3.60386	-2.53945
H	-2.80842	1.91413	-3.12378
H	-4.46125	2.14819	-3.80653
H	-3.26618	3.49352	-3.85237
H	4.48151	0.41839	2.54035
H	3.60236	1.84842	3.19366
H	2.81065	0.79395	1.97323
H	6.41852	1.99698	1.83467

H	6.05460	3.38817	0.73973
H	5.51044	3.42225	2.45469
H	1.95566	-0.26686	-3.89037
H	2.11769	0.58637	-5.45540
H	3.41120	-0.53656	-4.91791
H	4.88767	2.90767	-4.29379
H	5.18468	1.31670	-5.09087
H	3.90376	2.42141	-5.71839
H	6.45520	-4.93005	-1.87977
H	8.17418	-5.30816	-1.54081
H	7.00270	-4.54143	0.54365
H	7.95324	-3.94232	-3.63921
H	6.14405	-2.22815	0.71726
H	5.27483	-3.11203	-0.56570
H	9.43877	-3.99744	0.26130
H	8.60233	-2.70382	1.17669
H	7.14644	-1.59414	-3.50859
H	5.84454	-2.74908	-3.04243
H	8.03446	-0.50974	0.02399
H	8.39325	-0.26922	-1.71048
H	9.56654	-2.11637	-3.02214
H	10.00239	-3.65343	-2.21051
H	10.10280	-1.73178	-0.59589
H	-8.90722	-0.71978	-3.79478
H	-10.03134	-2.05790	-3.39947
H	-10.45797	-0.07211	-1.92068
H	-7.68555	-2.91725	-3.66042
H	-8.70415	0.65595	-0.27519
H	-8.17970	0.89093	-1.96651
H	-10.84465	-2.37468	-0.99512
H	-10.29346	-1.25507	0.29129
H	-5.91004	-2.20941	-2.03703
H	-6.48665	-0.84029	-3.02798
H	-7.89227	-1.34013	1.09536
H	-6.74869	-2.52927	0.38280
H	-7.50837	-4.10365	-1.45014
H	-9.20750	-4.05149	-2.01738
H	-9.05602	-3.43850	0.41577
H	-0.44030	-5.66619	-0.57592
H	-2.31161	-1.78611	-0.62142
H	-4.50184	-2.83712	-0.11332
H	-2.63831	-6.71563	-0.08517
H	-0.13575	-1.91132	-1.28038
H	1.95934	-1.38223	-1.86474
H	3.39524	-2.45449	-1.81006
H	2.82184	-1.14315	0.38466
H	3.02338	-2.90490	0.57973
H	0.44863	-1.31700	0.67327
H	4.08463	-0.93665	6.19764
H	4.57104	-3.15794	5.21502

H	3.11135	-4.05120	3.39886
H	-0.17384	-0.52248	2.61813
H	-0.52148	1.66767	3.58825
H	0.91457	2.50115	5.44376
H	2.76456	1.08839	6.29441

Pre TS-6Re

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.248027
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.722800
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.503935
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.44167	5.30880	1.48061
C	-0.60019	4.43891	1.09481
C	0.25973	6.21093	2.53090
C	-1.82346	4.47903	1.80947
C	-0.45031	3.51736	0.02894
C	-1.99518	5.39967	2.85518
C	-2.85650	3.59543	1.47709
C	-0.95627	6.26040	3.21217
C	-1.43719	2.53330	-0.18151
C	0.72013	3.55700	-0.89421
C	-2.66328	2.60241	0.50822
O	-1.25389	1.58529	-1.15600
C	-3.77784	1.66818	0.19238
C	1.55502	2.42374	-0.96862
C	1.01522	4.69565	-1.68717
C	2.22769	4.73494	-2.42147
C	0.13108	5.79227	-1.77922
C	3.10840	3.64898	-2.37590
C	2.54950	5.86732	-3.18643
C	2.77451	2.49071	-1.66637
C	3.75390	1.37894	-1.59498
O	1.24440	1.29935	-0.24746
C	0.46188	6.90825	-2.55103
C	1.66951	6.94848	-3.24740
P	-0.09170	0.47066	-0.79657
C	-4.21117	0.70714	1.15192
C	-4.47264	1.78590	-1.04340
C	4.54178	1.21135	-0.42544
C	3.95883	0.52342	-2.71204
C	-5.55868	0.93256	-1.30136
C	-4.13048	2.85610	-2.08468
C	-6.02829	0.00686	-0.35544
C	-5.33472	-0.09129	0.86477
C	-7.29221	-0.82481	-0.67141
C	-3.53314	0.54565	2.51592
C	4.93482	-0.48738	-2.62956
C	3.18751	0.69827	-4.02324

C	5.68642	-0.70526	-1.45867
C	5.47350	0.16140	-0.37389
C	6.73079	-1.83650	-1.33167
C	4.44036	2.15873	0.77255
C	-3.06140	-0.89350	2.76765
C	-4.46211	1.00840	3.64573
C	-5.29996	3.83009	-2.28061
C	-3.71318	2.22382	-3.41968
C	3.95048	1.42002	2.02157
C	5.77618	2.86516	1.03909
C	2.55236	-0.61435	-4.51104
C	4.10051	1.28195	-5.10817
O	-0.51438	-0.33905	0.42218
O	0.21528	-0.27510	-2.06135
C	7.49421	-4.73177	-1.24273
C	7.41294	-3.87900	0.03921
C	7.89428	-3.83386	-2.43078
C	6.35040	-2.77415	-0.14415
C	8.78671	-3.23201	0.31811
C	6.83877	-2.72231	-2.61559
C	8.13836	-1.22303	-1.06161
C	9.27009	-3.19366	-2.15529
C	9.19042	-2.33844	-0.87456
C	-9.47536	-1.50730	-2.58603
C	-9.75694	-0.66792	-1.32098
C	-8.31855	-2.49135	-2.30810
C	-8.49252	0.13439	-0.94457
C	-10.14069	-1.60191	-0.15600
C	-7.04497	-1.69959	-1.93792
C	-7.71321	-1.78096	0.49290
C	-8.70521	-3.42267	-1.14199
C	-8.98070	-2.57941	0.11943
C	-1.64459	-5.21284	-0.75396
C	-1.45820	-3.81211	-0.66441
C	-2.56192	-2.98012	-0.35462
C	-3.81352	-3.53037	-0.13069
C	-3.96940	-4.91513	-0.22373
C	-2.89375	-5.76274	-0.54032
C	-0.21206	-3.14510	-0.81967
S	1.26537	-3.83034	-1.21753
C	2.36295	-2.38834	-0.91214
C	2.64589	-2.18059	0.58950
N	1.42125	-2.03008	1.34893
S	1.29222	-2.60326	2.90499
C	2.12619	-1.41937	3.98964
Cl	-5.53284	-5.61993	0.07574
O	-0.13605	-2.59628	3.22387
O	2.07236	-3.84801	2.95547
C	1.65983	-0.07466	4.16508
C	2.41098	0.76343	5.06101

C	3.54940	0.24133	5.73114
C	3.95905	-1.05438	5.53224
C	3.24021	-1.89188	4.65038
C	0.54343	0.49273	3.49102
C	0.21034	1.81496	3.68506
C	0.94478	2.63772	4.56647
C	2.01959	2.11618	5.24623
H	1.40527	5.28606	0.98892
H	1.06649	6.87221	2.81963
H	-2.92788	5.44416	3.40495
H	-3.80740	3.65863	1.99250
H	-1.09130	6.96215	4.02502
H	-0.82337	5.79155	-1.26998
H	4.05812	3.69978	-2.89541
H	3.47830	5.91298	-3.74286
H	-0.22286	7.74434	-2.61154
H	1.92086	7.81677	-3.84271
H	-6.07265	1.02495	-2.24640
H	-3.27921	3.48316	-1.75832
H	-5.66637	-0.78246	1.62125
H	-2.62188	1.16766	2.57535
H	5.09394	-1.10257	-3.49862
H	2.34596	1.40862	-3.88990
H	6.05133	0.02873	0.52862
H	3.70820	2.96929	0.58693
H	-2.37981	-1.21977	1.96069
H	-2.49984	-0.94396	3.72505
H	-3.91163	-1.60365	2.82933
H	-4.81320	2.04428	3.45785
H	-5.34797	0.34431	3.73331
H	-3.91715	0.99888	4.61389
H	-5.59403	4.26991	-1.30351
H	-4.99522	4.65844	-2.95550
H	-6.18164	3.32358	-2.72638
H	-2.89386	1.49187	-3.25942
H	-4.56484	1.70339	-3.90573
H	-3.34390	3.01026	-4.11209
H	4.67514	0.64582	2.35034
H	3.80546	2.14179	2.85266
H	2.97626	0.93270	1.81163
H	6.55661	2.14906	1.37170
H	6.12548	3.37606	0.11632
H	5.64771	3.63264	1.83218
H	2.00314	-1.11385	-3.69053
H	1.83162	-0.40184	-5.32935
H	3.31529	-1.31847	-4.90375
H	4.53635	2.24434	-4.76839
H	4.92980	0.58302	-5.34897
H	3.51773	1.47428	-6.03425
H	6.51164	-5.21315	-1.44295

H	8.24154	-5.54507	-1.11182
H	7.12842	-4.52746	0.89636
H	7.95128	-4.44849	-3.35549
H	6.26494	-2.20911	0.80815
H	5.36154	-3.24430	-0.33289
H	9.55302	-4.02245	0.47637
H	8.73942	-2.62545	1.24925
H	7.13333	-2.10143	-3.49084
H	5.85701	-3.19534	-2.84215
H	8.13379	-0.59052	-0.14854
H	8.43573	-0.56701	-1.90981
H	9.57559	-2.56071	-3.01735
H	10.04145	-3.98610	-2.03614
H	10.18359	-1.88069	-0.67416
H	-9.21075	-0.83917	-3.43500
H	-10.38922	-2.06926	-2.87942
H	-10.59497	0.03449	-1.52206
H	-8.12419	-3.10036	-3.21771
H	-8.69697	0.75304	-0.04245
H	-8.26926	0.83745	-1.77463
H	-11.06344	-2.16830	-0.41058
H	-10.35970	-1.00357	0.75570
H	-6.20664	-2.40709	-1.75601
H	-6.75643	-1.07385	-2.80903
H	-7.92162	-1.19639	1.41666
H	-6.89969	-2.50230	0.72133
H	-7.88508	-4.14573	-0.94575
H	-9.60909	-4.01277	-1.40995
H	-9.25624	-3.25221	0.96060
H	-0.80319	-5.86241	-0.97450
H	-2.39863	-1.90969	-0.27148
H	-4.65346	-2.90141	0.12873
H	-3.05094	-6.83329	-0.59789
H	-0.22675	-2.06366	-0.68906
H	1.86265	-1.52456	-1.36562
H	3.28538	-2.60194	-1.45577
H	3.28728	-1.29205	0.65336
H	3.19543	-3.03132	0.99879
H	0.76076	-1.25900	1.10409
H	4.09851	0.89542	6.40332
H	4.83226	-1.44370	6.04612
H	3.55115	-2.91691	4.48693
H	-0.05145	-0.09652	2.80618
H	-0.63133	2.23288	3.14690
H	0.65883	3.67674	4.70183
H	2.59832	2.73386	5.92771

Post TS-6Re

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.264198

ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.737296

M06-2X/6-31G(d,p) Derived free energy in solution = -5317.526110
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.34006	5.25387	2.16346
C	-0.68673	4.41641	1.67701
C	0.15156	6.00679	3.32443
C	-1.89919	4.33003	2.40685
C	-0.53281	3.65105	0.49332
C	-2.07734	5.10138	3.56623
C	-2.92054	3.47996	1.96873
C	-1.05504	5.93569	4.02017
C	-1.50541	2.68184	0.16547
C	0.63251	3.83591	-0.42210
C	-2.72497	2.63832	0.86775
O	-1.31990	1.85610	-0.91572
C	-3.83213	1.74855	0.42414
C	1.48835	2.73980	-0.64487
C	0.91484	5.07725	-1.04728
C	2.13421	5.23752	-1.75504
C	0.01240	6.16096	-0.99552
C	3.03724	4.17144	-1.84521
C	2.44153	6.46998	-2.35292
C	2.71591	2.92143	-1.30522
C	3.71619	1.82601	-1.33969
O	1.18612	1.51967	-0.09883
C	0.32974	7.37821	-1.60222
C	1.54224	7.53419	-2.27367
P	-0.11363	0.77854	-0.77248
C	-4.23050	0.63606	1.21909
C	-4.54423	2.04552	-0.77096
C	4.43430	1.50026	-0.15872
C	3.97811	1.11513	-2.54273
C	-5.60138	1.20663	-1.16439
C	-4.24201	3.28112	-1.62401
C	-6.02104	0.11365	-0.38843
C	-5.32852	-0.14288	0.80858
C	-7.21739	-0.74246	-0.86207
C	-3.52961	0.27151	2.53026
C	4.90868	0.05711	-2.52191
C	3.34764	1.51960	-3.87935
C	5.58897	-0.31745	-1.34551
C	5.33699	0.42525	-0.18091
C	6.63128	-1.45825	-1.30317
C	4.29988	2.31489	1.13008
C	-3.06818	-1.19319	2.55049
C	-4.43907	0.55881	3.73136
C	-5.44385	4.23445	-1.66002
C	-3.81007	2.88839	-3.04343
C	3.75206	1.45543	2.27195

C	5.63558	2.96143	1.52058
C	2.64282	0.34978	-4.58067
C	4.40515	2.13820	-4.80176
O	-0.55923	-0.14575	0.43281
O	0.15525	0.11775	-2.06741
C	7.40411	-4.34695	-1.47586
C	7.29727	-3.62153	-0.11970
C	7.82387	-3.33895	-2.56446
C	6.23479	-2.50665	-0.21598
C	8.66268	-3.00123	0.24599
C	6.76938	-2.21573	-2.66391
C	8.03022	-0.87052	-0.94655
C	9.19177	-2.72521	-2.20205
C	9.08406	-1.99607	-0.84731
C	-9.32497	-1.26713	-2.90697
C	-9.68080	-0.67203	-1.52735
C	-8.09436	-2.18995	-2.77167
C	-8.48674	0.15357	-0.99811
C	-9.99750	-1.81422	-0.54126
C	-6.89282	-1.37167	-2.25134
C	-7.57015	-1.90842	0.11992
C	-8.40953	-3.32974	-1.78211
C	-8.76492	-2.73081	-0.40628
C	-1.24254	-5.05700	-0.16345
C	-1.16612	-3.70234	-0.51012
C	-2.35183	-2.97093	-0.65229
C	-3.59095	-3.56217	-0.42893
C	-3.64255	-4.90786	-0.07605
C	-2.47806	-5.66382	0.05446
C	0.12951	-2.99031	-0.80774
S	1.32675	-3.91179	-1.85809
C	2.43023	-2.47527	-1.62085
C	2.33365	-2.12516	-0.12770
N	0.93234	-2.40022	0.36021
S	0.91867	-3.34725	1.85562
C	2.08494	-2.46901	2.93124
Cl	-5.20755	-5.66186	0.20044
O	-0.43085	-3.21370	2.40113
O	1.49008	-4.67428	1.59656
C	1.75462	-1.25776	3.62464
C	2.72361	-0.76556	4.56779
C	3.94696	-1.46072	4.75498
C	4.22704	-2.61116	4.05769
C	3.27941	-3.12763	3.14863
C	0.55945	-0.51165	3.44480
C	0.33957	0.65131	4.14893
C	1.28550	1.12675	5.08414
C	2.45042	0.42663	5.29038
H	1.29715	5.32086	1.66336
H	0.94599	6.64598	3.68762

H	-3.00332	5.05106	4.12690
H	-3.86679	3.45599	2.49569
H	-1.19560	6.52272	4.91857
H	-0.94546	6.07322	-0.50013
H	3.99137	4.30770	-2.34144
H	3.37453	6.60815	-2.88651
H	-0.36908	8.20337	-1.55344
H	1.78295	8.48071	-2.74026
H	-6.12422	1.43155	-2.08203
H	-3.40940	3.87375	-1.19860
H	-5.63490	-0.95365	1.44692
H	-2.61181	0.87669	2.66505
H	5.10691	-0.45483	-3.44790
H	2.56501	2.29024	-3.73100
H	5.87233	0.18372	0.72508
H	3.58924	3.15590	1.00713
H	-2.44858	-1.40919	1.65939
H	-2.45676	-1.38338	3.45786
H	-3.92361	-1.89939	2.56839
H	-4.77569	1.61599	3.71774
H	-5.33482	-0.09791	3.72045
H	-3.88438	0.38502	4.67821
H	-5.74726	4.50052	-0.62474
H	-5.17014	5.17073	-2.19197
H	-6.31056	3.77725	-2.18200
H	-2.96337	2.17138	-3.00301
H	-4.64510	2.42189	-3.60693
H	-3.47394	3.78936	-3.59982
H	4.46717	0.65507	2.55518
H	3.56259	2.09043	3.16311
H	2.79255	0.98727	1.96919
H	6.39268	2.19788	1.79692
H	6.02596	3.56546	0.67366
H	5.48986	3.63771	2.39002
H	1.87422	-0.08767	-3.91793
H	2.12899	0.71393	-5.49599
H	3.35624	-0.44451	-4.88205
H	4.90131	2.99315	-4.29544
H	5.17853	1.39100	-5.08019
H	3.92775	2.51669	-5.73082
H	6.42645	-4.80731	-1.73976
H	8.15088	-5.16854	-1.40979
H	6.99925	-4.34974	0.66594
H	7.90113	-3.86239	-3.54231
H	6.13030	-2.03861	0.78541
H	5.25471	-2.96182	-0.46318
H	9.42923	-3.80140	0.34175
H	8.59557	-2.48726	1.23014
H	7.08603	-1.51471	-3.46785
H	5.79356	-2.66105	-2.95959

H	8.00208	-0.32890	0.02318
H	8.34168	-0.13460	-1.72096
H	9.51167	-2.01229	-2.99359
H	9.96364	-3.52394	-2.14398
H	10.07113	-1.55679	-0.58513
H	-9.10992	-0.44956	-3.62980
H	-10.18881	-1.84299	-3.30601
H	-10.57096	-0.01343	-1.62704
H	-7.84522	-2.62232	-3.76517
H	-8.74644	0.59651	-0.01089
H	-8.31181	0.99915	-1.69651
H	-10.86960	-2.40068	-0.90542
H	-10.27134	-1.39483	0.45186
H	-5.99988	-2.02924	-2.17469
H	-6.65271	-0.58813	-3.00120
H	-7.83429	-1.50294	1.12209
H	-6.70245	-2.59097	0.24538
H	-7.53123	-4.00594	-1.68786
H	-9.25862	-3.93935	-2.16215
H	-8.99191	-3.55298	0.30696
H	-0.33373	-5.63712	-0.04534
H	-2.30810	-1.92250	-0.92949
H	-4.50045	-2.98596	-0.53114
H	-2.53723	-6.71156	0.32604
H	-0.11298	-2.09728	-1.38788
H	2.07241	-1.64531	-2.22942
H	3.44765	-2.73129	-1.91516
H	2.56598	-1.07096	0.04746
H	3.03767	-2.73446	0.43867
H	0.01581	-0.97305	0.52289
H	4.66413	-1.06155	5.46708
H	5.16380	-3.13735	4.20871
H	3.47138	-4.05900	2.62857
H	-0.18841	-0.85918	2.75124
H	-0.57769	1.20776	3.98551
H	1.09078	2.04229	5.63425
H	3.19148	0.78149	6.00113

TS-7Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.242550
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.719334
M06-2X/6-31G(d,p) Derived free energy = -5317.488164
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.498770
Number of Imaginary Frequencies = 1 (-117.97)

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.31780	4.89331	1.68319
C	-0.72982	4.01680	1.33126
C	0.21935	5.69220	2.82438
C	-1.87494	3.94876	2.16475

C	-0.65885	3.18909	0.18418
C	-1.96397	4.76691	3.30167
C	-2.91978	3.07263	1.84605
C	-0.91909	5.63263	3.62845
C	-1.63193	2.19302	-0.01172
C	0.40919	3.34355	-0.84154
C	-2.80471	2.19502	0.76184
O	-1.49304	1.29605	-1.03832
C	-3.96169	1.34329	0.39140
C	1.30402	2.27623	-1.04083
C	0.56695	4.53685	-1.59004
C	1.71103	4.69316	-2.41396
C	-0.38891	5.57396	-1.54958
C	2.67654	3.68084	-2.46789
C	1.89096	5.87663	-3.14711
C	2.48633	2.48319	-1.77089
C	3.60425	1.51676	-1.67381
O	1.11212	1.08890	-0.38343
C	-0.19926	6.74203	-2.29138
C	0.93822	6.89466	-3.08435
P	-0.25334	0.22540	-0.83827
C	-4.30226	0.20870	1.17533
C	-4.78310	1.71167	-0.70777
C	3.86983	0.60335	-2.72585
C	4.43618	1.53081	-0.52375
C	-5.92375	0.94347	-0.99476
C	-4.49321	2.94030	-1.57500
C	-6.31772	-0.14147	-0.19354
C	-5.48763	-0.49333	0.88809
C	-7.62690	-0.89180	-0.52426
C	-3.42524	-0.26860	2.33257
C	5.48194	0.59932	-0.42524
C	4.23989	2.53633	0.61350
C	5.76133	-0.32271	-1.44717
C	4.95393	-0.28684	-2.60184
C	6.94048	-1.30637	-1.27675
C	3.02984	0.57591	-4.00292
C	-3.02737	-1.74307	2.17713
C	-4.11597	-0.03092	3.67967
C	-5.64166	3.95556	-1.50453
C	-4.20176	2.53658	-3.02581
C	2.49259	-0.83036	-4.30469
C	3.83546	1.11625	-5.18933
C	5.49515	3.39119	0.83300
C	3.82392	1.82412	1.90209
O	-0.49039	-0.60007	0.43055
O	-0.06492	-0.46249	-2.14866
C	9.23577	-2.27698	0.36413
C	9.46317	-1.46508	-0.92920
C	7.94005	-3.10624	0.23401

C	8.27219	-0.50642	-1.15254
C	9.58287	-2.42924	-2.12692
C	6.74211	-2.15765	0.01702
C	7.09258	-2.29690	-2.47681
C	8.05878	-4.06726	-0.96559
C	8.28459	-3.25217	-2.25476
C	-9.12737	-3.36126	-1.30518
C	-8.83782	-2.23782	-2.32105
C	-9.26601	-2.75423	0.10593
C	-7.52032	-1.52556	-1.94398
C	-9.99680	-1.21761	-2.30579
C	-7.95369	-2.03730	0.48853
C	-8.82773	0.10462	-0.50383
C	-10.42772	-1.74073	0.12187
C	-10.13853	-0.61509	-0.89102
C	-1.50917	-3.21092	-1.26349
C	-0.77759	-3.94588	-0.30062
C	-1.46117	-4.79167	0.60220
C	-2.82865	-4.97853	0.49062
C	-3.52181	-4.29145	-0.51276
C	-2.88126	-3.39152	-1.37002
C	0.65585	-3.90324	-0.23225
S	1.59502	-3.56951	-1.63619
C	3.07931	-3.00378	-0.74802
C	2.65367	-1.80564	0.13241
N	1.46534	-2.12882	0.92480
S	1.70386	-2.74232	2.48772
C	2.51484	-1.46863	3.47498
Cl	-5.23731	-4.56684	-0.68654
O	0.36496	-3.00877	3.01639
O	2.66678	-3.85005	2.33816
C	1.84559	-0.27265	3.89751
C	2.58557	0.60537	4.76505
C	3.91230	0.27315	5.14751
C	4.51852	-0.87578	4.70011
C	3.80933	-1.75903	3.85815
C	0.53565	0.11345	3.50356
C	-0.00436	1.29820	3.95476
C	0.71779	2.15709	4.81212
C	1.98805	1.81442	5.20873
H	1.22359	4.95287	1.09398
H	1.03087	6.35813	3.08792
H	-2.83668	4.72905	3.94280
H	-3.82388	3.06553	2.44408
H	-0.98944	6.25490	4.51116
H	-1.29191	5.48492	-0.95993
H	3.58961	3.82881	-3.03385
H	2.76695	6.01303	-3.77025
H	-0.93900	7.53126	-2.25293
H	1.08043	7.80338	-3.65487

H	-6.53113	1.22025	-1.84358
H	-3.59664	3.48489	-1.22095
H	-5.74709	-1.32080	1.52699
H	-2.47365	0.29508	2.35359
H	6.09737	0.60748	0.46180
H	3.42962	3.25636	0.38436
H	5.15033	-0.95454	-3.42360
H	2.13652	1.22574	-3.90080
H	-2.60474	-1.91689	1.16799
H	-2.25409	-2.00807	2.92871
H	-3.89429	-2.42093	2.32128
H	-4.38053	1.04170	3.78966
H	-5.04182	-0.63812	3.76711
H	-3.43152	-0.30504	4.51083
H	-5.84941	4.21940	-0.44538
H	-5.35970	4.88511	-2.04393
H	-6.56924	3.55449	-1.96407
H	-3.37447	1.79595	-3.05601
H	-5.09705	2.09343	-3.51031
H	-3.89001	3.42718	-3.61235
H	2.03078	-1.26420	-3.39654
H	1.71812	-0.77737	-5.09938
H	3.29728	-1.51132	-4.65244
H	4.18828	2.14671	-4.97105
H	4.71673	0.47369	-5.40009
H	3.19752	1.15328	-6.09813
H	5.79818	3.87152	-0.12195
H	5.28224	4.19333	1.57176
H	6.34171	2.78382	1.21584
H	2.90808	1.22427	1.71852
H	3.59774	2.57072	2.69284
H	4.62646	1.15034	2.26883
H	9.16217	-1.59057	1.23626
H	10.10114	-2.95164	0.54580
H	10.40071	-0.87495	-0.83537
H	7.78237	-3.69474	1.16407
H	8.44281	0.09277	-2.07457
H	8.23219	0.20882	-0.30320
H	10.45138	-3.10899	-1.98287
H	9.76353	-1.85434	-3.06179
H	5.81030	-2.75554	-0.05698
H	6.64134	-1.51530	0.91697
H	7.26733	-1.73667	-3.42221
H	6.16594	-2.90066	-2.59974
H	7.13321	-4.67734	-1.05784
H	8.90562	-4.77063	-0.80697
H	8.37016	-3.94543	-3.11975
H	-8.30475	-4.10930	-1.31970
H	-10.06346	-3.89347	-1.58369
H	-8.74363	-2.67566	-3.33864

H	-9.47281	-3.56491	0.83815
H	-7.30685	-0.75288	-2.71311
H	-6.67942	-2.25254	-1.97440
H	-10.94547	-1.71678	-2.60234
H	-9.80258	-0.41003	-3.04556
H	-8.05757	-1.62502	1.51705
H	-7.13628	-2.78850	0.50394
H	-8.67159	0.94356	-1.21425
H	-8.93205	0.55300	0.50924
H	-10.54718	-1.31376	1.14194
H	-11.38136	-2.25077	-0.13805
H	-10.97791	0.11392	-0.88192
H	-1.00820	-2.46528	-1.87976
H	-0.90546	-5.30522	1.37990
H	-3.35997	-5.64182	1.16262
H	-3.45626	-2.83207	-2.09854
H	1.14291	-4.48077	0.54571
H	3.80825	-2.71103	-1.50562
H	3.48409	-3.81215	-0.13675
H	2.40514	-0.94578	-0.49023
H	3.49733	-1.52399	0.77290
H	0.58930	-1.42775	0.78064
H	4.44742	0.95741	5.80045
H	5.53485	-1.11751	4.99355
H	4.26428	-2.68312	3.52214
H	-0.04321	-0.50385	2.83014
H	-1.00452	1.57936	3.64681
H	0.26841	3.08581	5.15046
H	2.56169	2.46661	5.86143

Pre TS-7Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.243570
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.720622
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.500858
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.34337	4.86044	1.63484
C	-0.70740	3.98786	1.28208
C	0.24676	5.66070	2.77530
C	-1.85233	3.92346	2.11570
C	-0.64011	3.16093	0.13379
C	-1.93953	4.74266	3.25208
C	-2.89764	3.04748	1.79974
C	-0.89254	5.60592	3.57839
C	-1.61831	2.17185	-0.06632
C	0.42953	3.31067	-0.89011
C	-2.78642	2.17039	0.71480
O	-1.48090	1.28085	-1.09821
C	-3.94422	1.31608	0.35636

C	1.32223	2.24058	-1.09013
C	0.59755	4.50883	-1.62865
C	1.75315	4.67105	-2.43452
C	-0.35856	5.54603	-1.59387
C	2.72070	3.66067	-2.47824
C	1.94275	5.85889	-3.15806
C	2.51875	2.45684	-1.79482
C	3.63418	1.48799	-1.69192
O	1.12557	1.04705	-0.44380
C	-0.15930	6.71864	-2.32585
C	0.98861	6.87609	-3.10271
P	-0.25749	0.19010	-0.87387
C	-4.26811	0.17725	1.14085
C	-4.79324	1.69680	-0.71679
C	3.93052	0.60593	-2.76260
C	4.43109	1.46573	-0.51654
C	-5.95056	0.94232	-0.97177
C	-4.51481	2.92492	-1.58809
C	-6.32758	-0.14651	-0.16761
C	-5.46500	-0.51617	0.88229
C	-7.65827	-0.87627	-0.45542
C	-3.36152	-0.31219	2.27021
C	5.47682	0.53404	-0.41778
C	4.19874	2.43261	0.64759
C	5.78461	-0.35877	-1.45752
C	5.00602	-0.29343	-2.63058
C	6.96580	-1.34014	-1.28713
C	3.13533	0.62382	-4.06881
C	-2.98358	-1.79034	2.09696
C	-4.01023	-0.07421	3.63799
C	-5.64699	3.95477	-1.47847
C	-4.27337	2.52211	-3.04816
C	2.56764	-0.76011	-4.41110
C	3.99644	1.15867	-5.21855
C	5.44291	3.28612	0.92695
C	3.75326	1.67899	1.90382
O	-0.50381	-0.61404	0.39475
O	-0.07946	-0.50751	-2.18721
C	9.22892	-2.34241	0.37909
C	9.48082	-1.49114	-0.88397
C	7.94338	-3.17685	0.19335
C	8.28814	-0.53497	-1.10735
C	9.63637	-2.41823	-2.10656
C	6.74299	-2.23140	-0.02470
C	7.15384	-2.29362	-2.51172
C	8.09868	-4.10103	-1.03080
C	8.34804	-3.24637	-2.28964
C	-9.22319	-3.31181	-1.21683
C	-8.96631	-2.17098	-2.22194
C	-9.28972	-2.73271	0.21102

C	-7.62452	-1.48135	-1.89143
C	-10.11071	-1.13812	-2.13311
C	-7.95270	-2.03898	0.54770
C	-8.84398	0.13333	-0.36070
C	-10.43670	-1.70617	0.30069
C	-10.18003	-0.56314	-0.70161
C	-1.61869	-3.19552	-1.45134
C	-0.88930	-3.95296	-0.49738
C	-1.57910	-4.80799	0.39790
C	-2.94481	-4.98773	0.28034
C	-3.63299	-4.28415	-0.71749
C	-2.98909	-3.36932	-1.55973
C	0.52726	-3.89219	-0.40222
S	1.51255	-3.32605	-1.64916
C	3.02176	-2.94395	-0.70191
C	2.75110	-1.74079	0.24036
N	1.60329	-1.96495	1.09657
S	1.78418	-2.68706	2.57714
C	2.53400	-1.47003	3.67523
Cl	-5.34453	-4.55316	-0.89798
O	0.43494	-3.00980	3.05043
O	2.77049	-3.76932	2.38876
C	1.85766	-0.26009	4.04163
C	2.55863	0.63038	4.92676
C	3.85475	0.28644	5.39609
C	4.46371	-0.88470	5.01548
C	3.79534	-1.77277	4.14377
C	0.57340	0.12818	3.57000
C	0.02315	1.32970	3.95863
C	0.71079	2.20509	4.82801
C	1.95311	1.85846	5.30316
H	1.25005	4.91642	1.04677
H	1.06043	6.32385	3.03912
H	-2.81212	4.70705	3.89345
H	-3.79949	3.03963	2.40116
H	-0.96139	6.22884	4.46078
H	-1.26932	5.45314	-1.01678
H	3.64294	3.81345	-3.02798
H	2.82736	5.99938	-3.76800
H	-0.89970	7.50751	-2.29244
H	1.13802	7.78810	-3.66612
H	-6.58492	1.23429	-1.79539
H	-3.59996	3.45588	-1.26119
H	-5.70968	-1.34823	1.52106
H	-2.40437	0.24408	2.26664
H	6.06800	0.51696	0.48550
H	3.39118	3.15581	0.41933
H	5.22274	-0.94038	-3.46379
H	2.25818	1.29791	-3.98923
H	-2.61239	-1.96953	1.06841

H	-2.17770	-2.06135	2.81108
H	-3.84846	-2.46063	2.28317
H	-4.25754	1.00095	3.76199
H	-4.94100	-0.67007	3.74843
H	-3.30567	-0.36220	4.44741
H	-5.81779	4.21761	-0.41247
H	-5.36978	4.88243	-2.02355
H	-6.59372	3.56752	-1.90987
H	-3.45506	1.77290	-3.10515
H	-5.18803	2.08954	-3.50530
H	-3.97061	3.41083	-3.64219
H	2.02757	-1.17375	-3.53778
H	1.85075	-0.67719	-5.25573
H	3.36751	-1.47123	-4.70510
H	4.37942	2.17069	-4.96716
H	4.85968	0.48878	-5.41803
H	3.38847	1.23832	-6.14498
H	5.76843	3.79772	-0.00403
H	5.20617	4.06357	1.68463
H	6.28233	2.67084	1.31290
H	2.84360	1.08292	1.68214
H	3.50549	2.40120	2.71043
H	4.54786	0.99602	2.27133
H	9.12891	-1.68260	1.26895
H	10.09506	-3.01580	0.56178
H	10.41118	-0.89734	-0.75029
H	7.76832	-3.79382	1.10159
H	8.47598	0.09269	-2.00682
H	8.22260	0.15435	-0.23838
H	10.50664	-3.09561	-1.96206
H	9.83445	-1.81437	-3.01939
H	5.81906	-2.83536	-0.14034
H	6.61426	-1.61699	0.89105
H	7.34621	-1.70451	-3.43592
H	6.23459	-2.89989	-2.67352
H	7.18085	-4.71536	-1.16314
H	8.94749	-4.80216	-0.87271
H	8.45955	-3.91294	-3.17245
H	-8.41174	-4.06895	-1.28416
H	-10.17762	-3.82723	-1.46275
H	-8.92396	-2.58874	-3.25138
H	-9.47309	-3.55595	0.93543
H	-7.43825	-0.69583	-2.65436
H	-6.79448	-2.21572	-1.97626
H	-11.07806	-1.62022	-2.39558
H	-9.94056	-0.31779	-2.86474
H	-8.00669	-1.64702	1.58793
H	-7.14327	-2.79862	0.51146
H	-8.70805	0.98450	-1.06093
H	-8.89665	0.56230	0.66472

H	-10.50405	-1.29902	1.33356
H	-11.40758	-2.19961	0.07474
H	-11.00894	0.17519	-0.63932
H	-1.11389	-2.42638	-2.03775
H	-1.02620	-5.32839	1.17323
H	-3.48277	-5.65341	0.94446
H	-3.56434	-2.79160	-2.27366
H	1.01536	-4.35267	0.44997
H	3.78286	-2.70666	-1.44858
H	3.32860	-3.81825	-0.12524
H	2.55040	-0.83994	-0.34066
H	3.66526	-1.57299	0.82235
H	0.72094	-1.36924	0.91044
H	4.36265	0.97801	6.06304
H	5.45524	-1.13646	5.37790
H	4.26026	-2.70310	3.83945
H	0.01666	-0.50485	2.89216
H	-0.95760	1.60727	3.59049
H	0.25681	3.14830	5.11643
H	2.49760	2.52185	5.96962

Post TS-7Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.271760
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.744998
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.528312
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.32983	4.88052	1.81438
C	-0.71663	3.99467	1.48212
C	0.28590	5.61488	3.00138
C	-1.80464	3.85275	2.38038
C	-0.69493	3.22350	0.29448
C	-1.83999	4.60716	3.56341
C	-2.85083	2.97306	2.07685
C	-0.79654	5.48152	3.87120
C	-1.65377	2.20740	0.11053
C	0.33198	3.42895	-0.76322
C	-2.78525	2.15681	0.94206
O	-1.54446	1.33244	-0.94264
C	-3.96152	1.33073	0.57487
C	1.23891	2.38540	-1.00616
C	0.43819	4.63366	-1.49988
C	1.53658	4.81322	-2.38085
C	-0.52473	5.65847	-1.39311
C	2.51438	3.81548	-2.49284
C	1.66318	6.00748	-3.10734
C	2.38023	2.61280	-1.79060
C	3.53751	1.69819	-1.68120
O	1.06715	1.18193	-0.37298

C	-0.38803	6.83762	-2.12912
C	0.70313	7.01292	-2.98079
P	-0.24879	0.34314	-0.90495
C	-4.25295	0.13267	1.27920
C	-4.85089	1.78811	-0.43418
C	3.79037	0.70746	-2.66440
C	4.40008	1.82203	-0.56200
C	-6.00759	1.04145	-0.71462
C	-4.61225	3.08597	-1.21158
C	-6.34213	-0.11972	0.00232
C	-5.44856	-0.55467	0.99970
C	-7.66063	-0.85722	-0.32011
C	-3.31141	-0.42984	2.34255
C	5.43236	0.88810	-0.39041
C	4.25289	2.95529	0.45844
C	5.69029	-0.12159	-1.33234
C	4.87953	-0.16817	-2.48497
C	6.84255	-1.11635	-1.07306
C	2.95600	0.61188	-3.94229
C	-2.93495	-1.89013	2.05598
C	-3.91833	-0.28928	3.74232
C	-5.75401	4.08709	-0.99081
C	-4.40513	2.80401	-2.70474
C	2.49193	-0.82342	-4.24033
C	3.74076	1.17991	-5.12935
C	5.53002	3.80159	0.54533
C	3.85961	2.40825	1.82973
O	-0.50611	-0.57776	0.35803
O	-0.05582	-0.30025	-2.22006
C	9.06442	-2.03549	0.69226
C	9.34994	-1.31867	-0.64545
C	7.74894	-2.83607	0.58091
C	8.19366	-0.34536	-0.96694
C	9.47394	-2.36386	-1.77229
C	6.58658	-1.87106	0.26794
C	6.99868	-2.18749	-2.20107
C	7.87128	-3.87790	-0.54896
C	8.15622	-3.15745	-1.88250
C	-9.17919	-3.25456	-1.27370
C	-8.98385	-2.01479	-2.16937
C	-9.22016	-2.81802	0.20475
C	-7.65261	-1.32019	-1.80889
C	-10.15287	-1.03004	-1.95023
C	-7.89352	-2.12027	0.57198
C	-8.86927	0.10287	-0.09720
C	-10.39145	-1.83940	0.42425
C	-10.19544	-0.59759	-0.46847
C	-1.32582	-3.20179	-1.43683
C	-0.72559	-3.93228	-0.40197
C	-1.52201	-4.76650	0.39283

C	-2.88929	-4.89259	0.15671
C	-3.46042	-4.16687	-0.88610
C	-2.69459	-3.31084	-1.67645
C	0.76558	-3.92112	-0.15122
S	1.72246	-4.18165	-1.71412
C	3.13700	-3.23047	-1.06593
C	2.47110	-2.10060	-0.28801
N	1.33092	-2.65346	0.51378
S	1.79601	-3.13261	2.16126
C	2.69982	-1.75165	2.90503
Cl	-5.17676	-4.35072	-1.21854
O	0.52757	-3.33721	2.86330
O	2.75309	-4.24499	2.04601
C	2.06475	-0.59655	3.47193
C	2.90913	0.29714	4.22123
C	4.29424	0.01984	4.36075
C	4.86359	-1.08456	3.77520
C	4.05511	-1.98434	3.05143
C	0.68699	-0.27123	3.35167
C	0.18672	0.88175	3.91747
C	1.01846	1.76502	4.64030
C	2.35119	1.47025	4.79553
H	1.19437	4.99665	1.17397
H	1.09647	6.28798	3.24914
H	-2.66966	4.51346	4.25405
H	-3.72014	2.91971	2.72240
H	-0.82508	6.05451	4.78896
H	-1.39138	5.55172	-0.75374
H	3.40118	3.98628	-3.09292
H	2.50363	6.16258	-3.77350
H	-1.13262	7.61813	-2.04001
H	0.80435	7.93029	-3.54621
H	-6.67188	1.39186	-1.49049
H	-3.69590	3.60339	-0.86715
H	-5.66620	-1.43651	1.57837
H	-2.35741	0.12977	2.34460
H	6.05384	0.96396	0.48939
H	3.45088	3.66302	0.17028
H	5.07757	-0.89085	-3.25818
H	2.03081	1.21744	-3.84796
H	-2.59197	-1.99150	1.00740
H	-2.11011	-2.21001	2.72664
H	-3.79212	-2.57620	2.21785
H	-4.16135	0.77435	3.94811
H	-4.84574	-0.89298	3.83799
H	-3.19002	-0.63204	4.50817
H	-5.90070	4.26028	0.09687
H	-5.50240	5.05974	-1.46533
H	-6.70661	3.72268	-1.42907
H	-3.57592	2.07756	-2.84232

H	-5.32487	2.39108	-3.16985
H	-4.13419	3.74227	-3.23450
H	2.05057	-1.28773	-3.33752
H	1.71636	-0.81013	-5.03560
H	3.32943	-1.46108	-4.59244
H	4.02994	2.23293	-4.92571
H	4.66124	0.58660	-5.31700
H	3.11286	1.16398	-6.04573
H	5.81097	4.16802	-0.46523
H	5.35614	4.68405	1.19771
H	6.37709	3.22049	0.96624
H	2.93747	1.79559	1.73902
H	3.65279	3.24458	2.53126
H	4.67341	1.78473	2.25235
H	8.98759	-1.29025	1.51444
H	9.90460	-2.71973	0.94306
H	10.30131	-0.74917	-0.56411
H	7.54872	-3.35590	1.54321
H	8.40487	0.18413	-1.92257
H	8.15642	0.42711	-0.16979
H	10.31800	-3.05586	-1.55827
H	9.69639	-1.85823	-2.73768
H	5.63623	-2.44158	0.20899
H	6.48465	-1.16338	1.11740
H	7.21002	-1.69467	-3.17613
H	6.06320	-2.77712	-2.31020
H	6.93049	-4.46640	-0.62725
H	8.69211	-4.59253	-0.31981
H	8.24472	-3.90918	-2.69686
H	-8.34864	-3.97616	-1.43547
H	-10.12554	-3.77298	-1.54333
H	-8.96016	-2.32976	-3.23534
H	-9.35980	-3.71240	0.85029
H	-7.51101	-0.46036	-2.49750
H	-6.80579	-2.01759	-1.98675
H	-11.11401	-1.51357	-2.23215
H	-10.02692	-0.13847	-2.60321
H	-7.93007	-1.83294	1.64654
H	-7.06347	-2.84738	0.44057
H	-8.77502	1.02076	-0.71545
H	-8.90372	0.42969	0.96594
H	-10.43962	-1.53611	1.49328
H	-11.35474	-2.33754	0.17719
H	-11.04201	0.10604	-0.31270
H	-0.73296	-2.53885	-2.05814
H	-1.07111	-5.32374	1.20841
H	-3.50114	-5.54624	0.76762
H	-3.15880	-2.74345	-2.47496
H	1.00332	-4.75904	0.50500
H	3.71196	-2.84770	-1.91018

H	3.76928	-3.85706	-0.43400
H	2.04691	-1.37583	-0.98375
H	3.15779	-1.56724	0.37337
H	0.10627	-1.36611	0.44062
H	4.90355	0.71309	4.93416
H	5.92489	-1.28502	3.87787
H	4.48515	-2.88610	2.63330
H	0.02354	-0.93112	2.81337
H	-0.86694	1.11722	3.81781
H	0.60071	2.66902	5.07286
H	3.00662	2.13615	5.34973

TS-6Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.238241
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.711941
M06-2X/6-31G(d,p) Derived free energy = -5317.486204
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.496343
Number of Imaginary Frequencies = 1 (-161.01)

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.28987	6.03261	1.76540
C	-1.16145	5.05195	1.24246
C	-0.76185	7.00440	2.65053
C	-2.51234	5.04741	1.67050
C	-0.72237	4.07166	0.31326
C	-2.97439	6.03634	2.55370
C	-3.38366	4.05146	1.22139
C	-2.10154	7.01151	3.03696
C	-1.57722	2.99386	-0.01288
C	0.61936	4.15301	-0.33745
C	-2.91755	3.00414	0.41844
O	-1.16223	2.01802	-0.88475
C	-3.85102	1.90639	0.05378
C	1.50978	3.07238	-0.17726
C	1.03117	5.29091	-1.07845
C	2.38612	5.40504	-1.47869
C	0.13023	6.31745	-1.43522
C	3.28964	4.37762	-1.18843
C	2.82066	6.54662	-2.17105
C	2.85358	3.19252	-0.58313
C	3.82532	2.08601	-0.36748
O	1.09915	1.95353	0.50018
C	0.57561	7.44291	-2.13193
C	1.91772	7.56097	-2.49193
P	0.04663	1.01871	-0.34618
C	-4.33729	1.78647	-1.27726
C	-4.31855	1.01074	1.05537
C	4.25143	1.75743	0.94945
C	4.38594	1.39206	-1.48039
C	-5.26457	0.03124	0.70976

C	-3.84745	1.08542	2.51023
C	-5.73515	-0.12687	-0.60359
C	-5.24775	0.75745	-1.58475
C	-6.78025	-1.22394	-0.90788
C	-3.96124	2.78185	-2.37884
C	5.36349	0.40450	-1.25073
C	4.01218	1.72269	-2.93103
C	5.78495	0.05735	0.04605
C	5.19315	0.73002	1.12735
C	6.87925	-1.00004	0.31802
C	3.77603	2.52422	2.18691
C	-5.19416	3.55523	-2.86471
C	-3.25393	2.08701	-3.55092
C	-3.23884	-0.24056	2.97805
C	-4.99398	1.50932	3.43698
C	3.05159	1.59811	3.17382
C	4.94418	3.24706	2.87057
C	3.50434	0.49464	-3.70060
C	5.20069	2.35773	-3.66550
O	-0.50940	0.04393	0.68278
O	0.66619	0.46447	-1.59817
C	9.70192	-1.99517	0.14069
C	8.56295	-2.66825	-0.65063
C	9.13596	-1.40011	1.44526
C	7.48147	-1.61950	-0.98637
C	7.93955	-3.79640	0.19642
C	8.05676	-0.34781	1.10823
C	6.28328	-2.16265	1.16824
C	8.50929	-2.52542	2.29686
C	7.37281	-3.20480	1.50262
C	-7.64541	-3.75915	-2.24851
C	-8.23256	-2.39428	-2.66077
C	-7.27014	-3.72486	-0.75341
C	-7.18487	-1.28686	-2.41689
C	-9.49396	-2.09937	-1.82376
C	-6.21521	-2.62381	-0.51300
C	-8.07492	-0.95164	-0.08317
C	-8.52857	-3.42616	0.08936
C	-9.11984	-2.06251	-0.32817
C	2.30603	-2.43841	-1.79057
C	1.11336	-3.09378	-2.15905
C	1.15970	-4.43976	-2.57111
C	2.37565	-5.10264	-2.65941
C	3.54853	-4.41939	-2.31956
C	3.52347	-3.09476	-1.88045
C	-0.09801	-2.30423	-2.10085
S	-1.50649	-2.68981	-3.04575
C	-2.59475	-1.66529	-1.99715
C	-2.47303	-2.23441	-0.57039
N	-1.05188	-2.31678	-0.20353

S	-0.56661	-3.70418	0.70920
C	-1.45622	-3.64677	2.27603
Cl	5.08495	-5.24949	-2.43940
O	-1.07287	-4.85881	-0.04184
O	0.86333	-3.52074	0.94493
C	-1.05446	-2.80707	3.36813
C	-1.80328	-2.94412	4.59009
C	-2.89159	-3.85270	4.65844
C	-3.25069	-4.62269	3.57812
C	-2.51751	-4.52584	2.37726
C	-0.00217	-1.85152	3.32748
C	0.29662	-1.09417	4.43846
C	-0.42231	-1.24655	5.64489
C	-1.45346	-2.15232	5.71560
H	0.76081	6.04833	1.50868
H	-0.08463	7.75311	3.04094
H	-4.00794	6.04781	2.87935
H	-4.42191	4.06121	1.53257
H	-2.46197	7.76762	3.72248
H	-0.92184	6.25336	-1.19142
H	4.33122	4.47975	-1.46890
H	3.85627	6.64932	-2.47325
H	-0.12389	8.22565	-2.39578
H	2.25725	8.43618	-3.03067
H	-5.63900	-0.62063	1.48464
H	-3.04136	1.83551	2.63280
H	-5.59194	0.68171	-2.60242
H	-3.25775	3.55061	-2.00400
H	5.80105	-0.07841	-2.10805
H	3.18131	2.45400	-2.97184
H	5.49652	0.47843	2.13255
H	3.05543	3.32003	1.91814
H	-5.69855	4.04392	-2.00364
H	-4.88804	4.34724	-3.58128
H	-5.91935	2.88575	-3.37330
H	-2.36255	1.53421	-3.18992
H	-3.92908	1.37564	-4.07063
H	-2.91114	2.84387	-4.28836
H	-2.44066	-0.55562	2.27892
H	-2.78692	-0.11093	3.98393
H	-3.99868	-1.04716	3.04074
H	-5.43192	2.46927	3.09207
H	-5.79575	0.74124	3.46156
H	-4.61355	1.65418	4.47070
H	3.75094	0.87120	3.63738
H	2.58464	2.19786	3.98402
H	2.24945	1.03445	2.65366
H	5.68077	2.52771	3.28618
H	5.45971	3.90770	2.14091
H	4.56528	3.87876	3.70237

H	2.61196	0.07439	-3.20231
H	3.20351	0.79031	-4.72844
H	4.27907	-0.29520	-3.78309
H	5.58060	3.23450	-3.10092
H	6.03031	1.62990	-3.78981
H	4.88445	2.70608	-4.67194
H	10.16986	-1.19346	-0.47207
H	10.49463	-2.73956	0.37432
H	8.97006	-3.09572	-1.59281
H	9.95797	-0.91736	2.01740
H	6.69189	-2.11595	-1.58807
H	7.93922	-0.82381	-1.61559
H	8.70793	-4.56602	0.42940
H	7.12972	-4.29937	-0.37528
H	7.70695	0.10405	2.06017
H	8.50877	0.47257	0.50743
H	5.45409	-2.65525	0.61517
H	5.85550	-1.78422	2.12110
H	8.11153	-2.10665	3.24742
H	9.28565	-3.27542	2.56486
H	6.92945	-4.01996	2.11501
H	-6.74610	-3.98784	-2.86192
H	-8.38853	-4.56522	-2.43580
H	-8.50205	-2.41860	-3.73915
H	-6.85066	-4.71052	-0.45559
H	-7.62085	-0.31601	-2.74206
H	-6.29154	-1.49302	-3.04793
H	-10.26228	-2.88303	-2.00454
H	-9.93555	-1.12546	-2.12982
H	-5.91373	-2.65525	0.55531
H	-5.30972	-2.85125	-1.11290
H	-8.50507	0.03485	-0.36621
H	-7.85673	-0.91011	1.00533
H	-8.26787	-3.41304	1.17058
H	-9.28400	-4.22878	-0.05955
H	-10.03023	-1.85386	0.27492
H	2.25234	-1.41046	-1.44546
H	0.24033	-4.96727	-2.80215
H	2.42431	-6.13752	-2.97720
H	4.44003	-2.58832	-1.61468
H	0.06060	-1.23373	-1.92148
H	-3.61350	-1.73686	-2.38078
H	-2.26842	-0.62391	-2.03591
H	-2.91820	-3.23019	-0.53401
H	-2.99192	-1.57431	0.12878
H	-0.71314	-1.35907	0.22262
H	-3.44166	-3.92853	5.59261
H	-4.08256	-5.31638	3.64278
H	-2.76201	-5.16016	1.53358
H	0.55811	-1.69474	2.41732

H	1.09560	-0.36327	4.38134
H	-0.16478	-0.64046	6.50808
H	-2.02598	-2.27248	6.63113

Pre TS-6Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.240690
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.716936
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.499257
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.30956	6.00751	1.76385
C	-1.17735	5.01563	1.25745
C	-0.78589	6.99237	2.63196
C	-2.52982	5.01480	1.68087
C	-0.73384	4.02261	0.34554
C	-2.99602	6.01640	2.54740
C	-3.40057	4.01588	1.23504
C	-2.12628	7.00149	3.01661
C	-1.58579	2.94270	0.02893
C	0.60199	4.09969	-0.31728
C	-2.93236	2.96250	0.44064
O	-1.14980	1.94934	-0.81091
C	-3.87679	1.88628	0.04003
C	1.50174	3.02570	-0.15240
C	0.99408	5.22500	-1.08834
C	2.34084	5.33870	-1.51503
C	0.08073	6.23849	-1.45197
C	3.25504	4.32247	-1.22124
C	2.75652	6.46808	-2.23822
C	2.83759	3.14882	-0.58200
C	3.82239	2.05548	-0.36222
O	1.12192	1.92421	0.57035
C	0.50723	7.35177	-2.17943
C	1.84229	7.47040	-2.56425
P	0.01916	0.95485	-0.17433
C	-4.32583	1.78998	-1.30655
C	-4.39797	0.99445	1.01890
C	4.29369	1.77114	0.94949
C	4.35631	1.33681	-1.47173
C	-5.36463	0.04871	0.63670
C	-3.95691	1.03260	2.48475
C	-5.79387	-0.08964	-0.69340
C	-5.25250	0.78814	-1.65085
C	-6.83770	-1.17291	-1.04619
C	-3.88638	2.77820	-2.39122
C	5.35647	0.37123	-1.24611
C	3.92714	1.61800	-2.91744
C	5.83576	0.07910	0.04452
C	5.26769	0.77353	1.12496

C	6.97217	-0.93550	0.30827
C	3.82972	2.55350	2.18142
C	-5.08082	3.58352	-2.91954
C	-3.15539	2.06638	-3.53844
C	-3.41993	-0.32568	2.95460
C	-5.10500	1.49711	3.38979
C	3.15563	1.63059	3.20692
C	4.99439	3.32310	2.81840
C	3.38907	0.36435	-3.62063
C	5.08491	2.22736	-3.71956
O	-0.56224	0.10960	0.93695
O	0.61183	0.27849	-1.38612
C	9.81188	-1.85702	0.03277
C	8.65668	-2.59654	-0.67119
C	9.29233	-1.22085	1.33737
C	7.52938	-1.59433	-0.99695
C	8.10924	-3.70327	0.25298
C	8.16556	-0.21568	1.01044
C	6.45541	-2.07540	1.23835
C	8.74388	-2.32538	2.26641
C	7.59093	-3.07095	1.56029
C	-7.67738	-3.67669	-2.46069
C	-8.25102	-2.30143	-2.85772
C	-7.33633	-3.67461	-0.95697
C	-7.20589	-1.20306	-2.56567
C	-9.53107	-2.02070	-2.04476
C	-6.28465	-2.58154	-0.66945
C	-8.15154	-0.91379	-0.24757
C	-8.61346	-3.39016	-0.13762
C	-9.19233	-2.01663	-0.54041
C	2.40464	-2.49670	-1.75562
C	1.28314	-3.08624	-2.38822
C	1.42917	-4.33278	-3.04291
C	2.66489	-4.94990	-3.09829
C	3.76483	-4.33105	-2.48116
C	3.64183	-3.11580	-1.80541
C	0.06763	-2.35562	-2.27886
S	-1.41567	-2.76460	-2.97059
C	-2.48520	-1.68044	-1.94834
C	-2.58132	-2.24876	-0.51233
N	-1.27546	-2.31327	0.11159
S	-0.76803	-3.70665	0.88252
C	-1.54161	-3.74639	2.51447
Cl	5.32359	-5.10847	-2.55502
O	-1.32785	-4.82799	0.11182
O	0.68112	-3.56758	1.04908
C	-1.15749	-2.85411	3.56952
C	-1.85059	-2.99497	4.82217
C	-2.86289	-3.98084	4.96427
C	-3.19902	-4.81225	3.92343

C	-2.52893	-4.69456	2.68594
C	-0.17040	-1.83707	3.45668
C	0.11167	-1.01227	4.52290
C	-0.55790	-1.16167	5.75790
C	-1.51922	-2.13411	5.90167
H	0.74089	6.02239	1.50552
H	-0.11174	7.75021	3.00988
H	-4.03079	6.03182	2.86899
H	-4.44290	4.03649	1.53101
H	-2.49011	7.76829	3.68829
H	-0.96707	6.17331	-1.19093
H	4.29048	4.42319	-1.52508
H	3.78615	6.57026	-2.56042
H	-0.20156	8.12442	-2.44813
H	2.16738	8.33620	-3.12658
H	-5.77688	-0.60257	1.39269
H	-3.12144	1.74621	2.63032
H	-5.56410	0.72732	-2.67995
H	-3.17849	3.52914	-1.99049
H	5.76837	-0.13458	-2.10309
H	3.09539	2.34858	-2.95276
H	5.61493	0.56351	2.12553
H	3.08060	3.32287	1.91381
H	-5.60458	4.08214	-2.07594
H	-4.72842	4.36961	-3.62123
H	-5.80309	2.93430	-3.45762
H	-2.30009	1.47949	-3.14511
H	-3.83284	1.38213	-4.09066
H	-2.75640	2.81529	-4.25544
H	-2.63616	-0.68503	2.26097
H	-2.96869	-0.22244	3.96400
H	-4.22146	-1.09121	3.01219
H	-5.49158	2.47983	3.04851
H	-5.94098	0.76593	3.38426
H	-4.74342	1.61136	4.43406
H	3.88581	0.93099	3.66498
H	2.69647	2.23567	4.01761
H	2.35328	1.03648	2.72155
H	5.75976	2.63383	3.23291
H	5.47428	3.97897	2.06067
H	4.61890	3.96479	3.64407
H	2.50942	-0.02589	-3.07647
H	3.05795	0.61962	-4.64997
H	4.15622	-0.43394	-3.69296
H	5.48401	3.12365	-3.20025
H	5.91034	1.49627	-3.85186
H	4.72879	2.54075	-4.72417
H	10.22494	-1.07036	-0.63633
H	10.63728	-2.56768	0.25815
H	9.03021	-3.05349	-1.61346

H	10.12606	-0.68983	1.84628
H	6.72693	-2.13688	-1.53885
H	7.93373	-0.81456	-1.68036
H	8.91056	-4.44071	0.47890
H	7.28692	-4.25257	-0.25556
H	7.84661	0.26724	1.95822
H	8.56238	0.59034	0.35381
H	5.61430	-2.61587	0.75409
H	6.06634	-1.66753	2.19546
H	8.38106	-1.87706	3.21748
H	9.55526	-3.04048	2.52594
H	7.20345	-3.87058	2.22853
H	-6.76495	-3.89579	-3.05798
H	-8.41831	-4.47626	-2.68160
H	-8.49491	-2.30213	-3.94244
H	-6.92599	-4.66737	-0.67025
H	-7.62780	-0.22286	-2.88135
H	-6.29883	-1.40253	-3.17915
H	-10.29671	-2.79820	-2.26015
H	-9.96288	-1.03927	-2.34049
H	-6.00648	-2.63492	0.40453
H	-5.36600	-2.79559	-1.25600
H	-8.57229	0.07946	-0.52083
H	-7.96149	-0.89554	0.84659
H	-8.37787	-3.40003	0.94939
H	-9.36681	-4.18769	-0.32052
H	-10.11632	-1.81856	0.04532
H	2.27212	-1.54949	-1.24069
H	0.56814	-4.81370	-3.49642
H	2.79283	-5.90263	-3.59835
H	4.49831	-2.66682	-1.32563
H	0.13406	-1.36739	-1.79112
H	-3.46389	-1.65614	-2.43337
H	-2.05665	-0.67605	-1.95071
H	-3.02262	-3.24703	-0.53899
H	-3.24812	-1.58592	0.04743
H	-0.91757	-1.39304	0.50935
H	-3.37205	-4.06426	5.92087
H	-3.97266	-5.56412	4.04299
H	-2.77245	-5.35565	1.86273
H	0.35321	-1.68368	2.52430
H	0.85470	-0.23077	4.40392
H	-0.31695	-0.50338	6.58727
H	-2.04856	-2.25646	6.84282

Post TS-6Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2839.258303
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2837.731566
M06-2X/6-31G(d,p) Derived free energy in solution = -5317.523036
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.27673	6.17001	1.62902
C	-1.14206	5.18161	1.10812
C	-0.76091	7.16190	2.48452
C	-2.49823	5.18711	1.51920
C	-0.69035	4.18198	0.20297
C	-2.97263	6.19594	2.37297
C	-3.36047	4.17465	1.09382
C	-2.10663	7.18103	2.84739
C	-1.54462	3.09398	-0.10917
C	0.67258	4.24699	-0.40753
C	-2.88299	3.10713	0.32694
O	-1.14277	2.09578	-0.96536
C	-3.79360	1.96918	0.03986
C	1.55031	3.16606	-0.19767
C	1.12576	5.37752	-1.13508
C	2.50070	5.48517	-1.46466
C	0.24762	6.40407	-1.54339
C	3.38533	4.45685	-1.12085
C	2.97377	6.62121	-2.14047
C	2.91277	3.27583	-0.53546
C	3.85664	2.15322	-0.28068
O	1.09056	2.03551	0.42524
C	0.73206	7.52395	-2.22294
C	2.09152	7.63594	-2.51378
P	0.11419	1.15466	-0.52282
C	-4.33116	1.78359	-1.26249
C	-4.18614	1.09903	1.09350
C	4.19227	1.79087	1.05365
C	4.45854	1.45600	-1.36945
C	-5.11722	0.08122	0.82948
C	-3.65344	1.24797	2.52103
C	-5.65076	-0.13310	-0.45149
C	-5.22824	0.72128	-1.48880
C	-6.69845	-1.25062	-0.65718
C	-4.02643	2.74551	-2.41416
C	5.38832	0.43400	-1.09914
C	4.16499	1.80234	-2.83415
C	5.70573	0.04075	0.21361
C	5.07689	0.72062	1.26958
C	6.70733	-1.09319	0.52916
C	3.67722	2.56170	2.27284
C	-5.29930	3.46342	-2.88173
C	-3.34083	2.02757	-3.58454
C	-2.99796	-0.04346	3.01796
C	-4.76739	1.69090	3.47796
C	2.86600	1.65559	3.21036
C	4.83329	3.23177	3.02694
C	3.68463	0.58426	-3.63726

C	5.39739	2.42762	-3.50092
O	-0.42566	0.12028	0.54967
O	0.72834	0.58667	-1.74335
C	9.46462	-2.27109	0.54249
C	8.35650	-2.83386	-0.36930
C	8.82865	-1.68912	1.82030
C	7.37752	-1.70207	-0.74676
C	7.59048	-3.94856	0.37232
C	7.85324	-0.55305	1.44132
C	5.96637	-2.24380	1.27400
C	8.05919	-2.80069	2.56667
C	6.95326	-3.37001	1.65179
C	-7.60978	-3.84236	-1.85115
C	-8.23315	-2.49893	-2.28095
C	-7.15227	-3.74802	-0.38168
C	-7.18545	-1.37355	-2.13770
C	-9.44931	-2.18391	-1.38633
C	-6.09776	-2.62964	-0.24336
C	-7.94859	-0.95882	0.22784
C	-8.36456	-3.42839	0.51869
C	-8.99321	-2.08714	0.08361
C	2.25707	-2.48248	-1.84512
C	1.05663	-3.16344	-2.08057
C	1.10072	-4.49293	-2.51473
C	2.32317	-5.13445	-2.70849
C	3.50414	-4.43554	-2.46536
C	3.48248	-3.11091	-2.03503
C	-0.22729	-2.39031	-1.90230
S	-1.52652	-2.75481	-3.15681
C	-2.63889	-1.72022	-2.14700
C	-2.38840	-2.17715	-0.70780
N	-0.91232	-2.41615	-0.52177
S	-0.63102	-3.89516	0.41034
C	-1.54707	-3.60600	1.94234
Cl	5.05290	-5.23372	-2.71443
O	-1.28133	-5.01872	-0.27670
O	0.79826	-3.93666	0.71335
C	-1.00037	-2.86774	3.04374
C	-1.77355	-2.85502	4.25793
C	-3.02392	-3.52514	4.31070
C	-3.51497	-4.20765	3.22371
C	-2.75810	-4.26405	2.03484
C	0.23096	-2.15594	3.02617
C	0.66884	-1.48221	4.14431
C	-0.08643	-1.47821	5.33842
C	-1.28267	-2.15258	5.39063
H	0.77910	6.17725	1.39554
H	-0.08794	7.91641	2.87114
H	-4.01038	6.21412	2.68474
H	-4.39862	4.18189	1.40612

H	-2.47650	7.95229	3.51063
H	-0.81558	6.34383	-1.35173
H	4.44003	4.55259	-1.34919
H	4.02400	6.71939	-2.38889
H	0.04982	8.30736	-2.52684
H	2.46125	8.50702	-3.03916
H	-5.43700	-0.54954	1.64526
H	-2.85839	2.01777	2.57537
H	-5.61644	0.59727	-2.48586
H	-3.33180	3.54719	-2.09434
H	5.86093	-0.04916	-1.93733
H	3.34489	2.54275	-2.91136
H	5.29979	0.43431	2.28640
H	3.00313	3.38727	1.97387
H	-5.78926	3.96599	-2.02030
H	-5.04343	4.23918	-3.63481
H	-6.01953	2.75463	-3.34175
H	-2.40298	1.54479	-3.24143
H	-4.00020	1.25478	-4.03177
H	-3.07577	2.76079	-4.37592
H	-2.24153	-0.39116	2.28789
H	-2.48573	0.14341	3.98551
H	-3.74544	-0.84923	3.17007
H	-5.23460	2.63000	3.11454
H	-5.55489	0.91262	3.56533
H	-4.34703	1.88211	4.48842
H	3.51258	0.90098	3.70511
H	2.37868	2.26657	3.99986
H	2.07194	1.12516	2.64501
H	5.52065	2.47952	3.46814
H	5.40981	3.88270	2.33518
H	4.43485	3.86562	3.84790
H	2.79981	0.13137	-3.15365
H	3.38628	0.90009	-4.65981
H	4.47571	-0.18777	-3.73405
H	5.75200	3.30161	-2.91610
H	6.22707	1.69323	-3.57751
H	5.14068	2.77738	-4.52367
H	10.03442	-1.48043	0.00644
H	10.18432	-3.07640	0.80825
H	8.81423	-3.25150	-1.29249
H	9.62824	-1.28622	2.47944
H	6.61217	-2.12356	-1.43056
H	7.93479	-0.91517	-1.30249
H	8.28431	-4.77744	0.63416
H	6.80147	-4.37238	-0.28660
H	7.45561	-0.11517	2.38057
H	8.40707	0.25649	0.91582
H	5.15822	-2.65610	0.62995
H	5.48265	-1.87223	2.20285

H	7.60932	-2.39232	3.49833
H	8.75928	-3.61179	2.86510
H	6.40695	-4.17573	2.18881
H	-6.74366	-4.08678	-2.50492
H	-8.35362	-4.66122	-1.96606
H	-8.56181	-2.56661	-3.34090
H	-6.70573	-4.71774	-0.07092
H	-7.64859	-0.41913	-2.47374
H	-6.32666	-1.59560	-2.80977
H	-10.21773	-2.98074	-1.49446
H	-9.91791	-1.22630	-1.70335
H	-5.73195	-2.61923	0.80520
H	-5.23039	-2.87161	-0.88987
H	-8.40456	0.01240	-0.06736
H	-7.67141	-0.87416	1.30027
H	-8.04360	-3.37133	1.58218
H	-9.11819	-4.24285	0.44323
H	-9.87089	-1.86369	0.72843
H	2.22634	-1.44886	-1.51750
H	0.17834	-5.03705	-2.68754
H	2.35927	-6.16470	-3.04369
H	4.40521	-2.57424	-1.86312
H	0.01494	-1.33555	-2.03405
H	-3.67619	-1.88116	-2.44397
H	-2.39323	-0.66415	-2.28214
H	-2.92762	-3.10941	-0.53688
H	-2.72139	-1.43045	0.01663
H	-0.46111	-0.82636	0.22179
H	-3.59023	-3.48836	5.23738
H	-4.46974	-4.72064	3.27467
H	-3.10794	-4.85057	1.19335
H	0.83865	-2.15894	2.13271
H	1.61446	-0.95180	4.10742
H	0.27954	-0.94199	6.20852
H	-1.87949	-2.15410	6.29847

TS-8Re

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.952293
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.378285
M06-2X/6-31G(d,p) Derived free energy = -4822.176033
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.186656
Number of Imaginary Frequencies = 1 (-90.78)

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.15828	5.59838	2.42865
C	-1.03487	4.65887	1.84421
C	-0.60937	6.46403	3.42756
C	-2.36917	4.58912	2.31215
C	-0.61832	3.78805	0.80567

C	-2.81123	5.47198	3.31037
C	-3.24917	3.64898	1.76897
C	-1.93309	6.40527	3.86295
C	-1.46401	2.73421	0.39647
C	0.67234	3.98154	0.08856
C	-2.80333	2.70583	0.83374
O	-1.03407	1.83596	-0.55151
C	-3.77941	1.71992	0.30048
C	1.59970	2.92156	0.08124
C	0.98167	5.19029	-0.58959
C	2.28429	5.37663	-1.11577
C	0.02692	6.21534	-0.76926
C	3.22947	4.35186	-1.01780
C	2.62166	6.58316	-1.74963
C	2.88175	3.11170	-0.46975
C	3.88448	2.02009	-0.46261
O	1.29552	1.75098	0.73197
C	0.37481	7.40671	-1.40958
C	1.67019	7.59381	-1.89036
P	0.15681	0.80862	-0.03753
C	-4.26217	1.84263	-1.03154
C	-4.34032	0.73556	1.16284
C	4.22954	1.35295	-1.67269
C	4.55808	1.68861	0.74261
C	-5.41955	-0.04410	0.70418
C	-3.83315	0.52016	2.59294
C	-5.93367	0.08913	-0.60002
C	-5.29659	0.99543	-1.46324
C	-7.16729	-0.69544	-1.10278
C	-3.75014	2.91083	-2.00209
C	5.50453	0.65056	0.73205
C	4.36525	2.49080	2.03321
C	5.82716	-0.05915	-0.43693
C	5.17474	0.31060	-1.62957
C	6.93393	-1.13763	-0.38926
C	3.71759	1.82348	-3.04231
C	-4.87133	3.87735	-2.40734
C	-3.10085	2.27219	-3.23722
C	-3.35200	-0.91911	2.81577
C	-4.90769	0.89284	3.62329
C	3.04728	0.70820	-3.85529
C	4.86133	2.45558	-3.84698
C	5.66426	3.19922	2.43971
C	3.84341	1.60866	3.17252
O	-0.38350	-0.08181	1.07673
O	0.75839	0.14642	-1.23721
C	9.03913	-2.56915	1.16894
C	9.40929	-1.53579	0.08329
C	7.71376	-3.26452	0.79053
C	8.29276	-0.47169	-0.01911

C	9.56841	-2.25247	-1.27338
C	6.59247	-2.20935	0.69088
C	7.12501	-1.88218	-1.75119
C	7.87201	-3.97760	-0.56654
C	8.24076	-2.94335	-1.64803
C	-9.02743	-1.36342	-3.33836
C	-9.47876	-0.46341	-2.16765
C	-7.97974	-2.38022	-2.83621
C	-8.25965	0.30108	-1.60584
C	-10.09808	-1.33460	-1.05729
C	-6.75212	-1.62393	-2.28313
C	-7.82804	-1.58209	0.00280
C	-8.59717	-3.24875	-1.72107
C	-9.04774	-2.34456	-0.55519
C	2.67834	-2.39169	-1.93420
C	2.90252	-2.89489	-0.63432
C	3.57101	-4.12621	-0.45973
C	4.06982	-4.79825	-1.56505
C	3.89139	-4.26433	-2.84821
C	3.18971	-3.07055	-3.03316
C	2.42178	-2.08613	0.45497
S	3.13611	-2.16154	2.03245
C	1.65997	-1.57137	2.93610
C	0.52822	-2.55816	2.60889
N	0.37345	-2.58793	1.15392
S	-0.19319	-4.04296	0.42379
C	-1.92591	-4.21042	0.90583
O	-0.11293	-3.81237	-1.01510
O	0.60972	-5.10219	1.04258
C	-2.31343	-5.17298	1.87072
C	-3.67848	-5.27425	2.16836
C	-4.64616	-4.48569	1.55107
C	-4.21941	-3.55737	0.60119
C	-2.87881	-3.37863	0.25914
H	0.87957	5.66187	2.12899
H	0.07107	7.18205	3.86692
H	-3.83345	5.43499	3.66819
H	-4.28468	3.63406	2.08795
H	-2.27780	7.07998	4.63591
H	-0.99430	6.10150	-0.43179
H	4.22963	4.49876	-1.40947
H	3.61769	6.73962	-2.14685
H	-0.36475	8.18684	-1.53635
H	1.93420	8.51963	-2.38502
H	-5.85671	-0.74958	1.39123
H	-2.95221	1.16010	2.80180
H	-5.64483	1.08551	-2.48121
H	-2.97315	3.54482	-1.53590
H	6.02812	0.42308	1.64826
H	3.61522	3.29561	1.89984

H	5.42859	-0.17204	-2.55724
H	2.94016	2.60402	-2.93298
H	-5.33934	4.31611	-1.50010
H	-4.45474	4.70706	-3.01772
H	-5.65511	3.36586	-3.00448
H	-2.62708	3.05687	-3.86500
H	-2.31242	1.55386	-2.92757
H	-3.84947	1.73429	-3.85590
H	-2.59406	-1.18833	2.05474
H	-2.87775	-1.01060	3.81618
H	-4.19227	-1.64177	2.76468
H	-5.26702	1.92829	3.45028
H	-5.77565	0.20242	3.56774
H	-4.48394	0.84127	4.64895
H	3.72699	-0.14994	-4.02949
H	2.13408	0.36089	-3.34034
H	2.73070	1.09974	-4.84573
H	5.34797	3.26003	-3.25596
H	5.62743	1.69738	-4.11543
H	4.46760	2.90634	-4.78301
H	6.03622	3.82131	1.59749
H	5.47729	3.86789	3.30710
H	6.45237	2.47080	2.72437
H	2.88102	1.14952	2.87607
H	4.56368	0.80480	3.43155
H	3.66273	2.22443	4.07932
H	8.93632	-2.06476	2.15494
H	9.84961	-3.32458	1.26635
H	10.36757	-1.04166	0.35444
H	7.45098	-4.01142	1.57108
H	8.56711	0.28457	-0.78792
H	8.22286	0.06307	0.95268
H	10.38487	-3.00532	-1.21252
H	9.85220	-1.51915	-2.06003
H	5.63913	-2.70831	0.43433
H	6.45897	-1.75361	1.69389
H	7.41181	-1.16379	-2.55075
H	6.17657	-2.37811	-2.05546
H	6.92554	-4.49280	-0.83904
H	8.66442	-4.75493	-0.49757
H	8.35466	-3.45770	-2.62711
H	-8.59395	-0.74082	-4.15177
H	-9.90357	-1.90048	-3.76382
H	-10.23676	0.26406	-2.53143
H	-7.66337	-3.03223	-3.67934
H	-8.58422	0.96188	-0.77141
H	-7.87090	0.96222	-2.40835
H	-10.98841	-1.87427	-1.44867
H	-10.44196	-0.69261	-0.21663
H	-5.98723	-2.35600	-1.94628

H	-6.29570	-1.03836	-3.10977
H	-8.15527	-0.95156	0.85949
H	-7.10832	-2.32853	0.38892
H	-7.85182	-3.99187	-1.36100
H	-9.46640	-3.81699	-2.11919
H	-9.49211	-2.97170	0.24823
H	2.09292	-1.48315	-2.03241
H	3.67774	-4.54375	0.53557
H	4.58850	-5.74290	-1.43761
H	3.03089	-2.68023	-4.03300
H	1.93902	-1.15648	0.16462
H	1.90423	-1.55886	4.00025
H	1.37352	-0.57584	2.59325
H	-0.39294	-2.19934	3.08123
H	0.76742	-3.55954	2.97126
H	-0.07792	-1.67118	0.84879
C	-6.10562	-4.61522	1.90838
H	-4.94539	-2.92769	0.10438
C	-2.56370	-2.28862	-0.74384
C	-1.39291	-6.12598	2.60618
H	-3.98790	-6.00771	2.90789
H	-1.98147	-6.72265	3.30720
H	-0.87503	-6.80021	1.92200
H	-0.61459	-5.60791	3.17048
H	-3.49402	-1.81954	-1.07101
H	-1.94396	-1.49835	-0.30806
H	-2.03488	-2.67132	-1.61640
H	-6.72370	-4.74964	1.01452
H	-6.28160	-5.46507	2.57253
H	-6.46506	-3.71320	2.41738
H	4.28660	-4.79650	-3.70881

Pre TS-8Re

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.956390
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.385038
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.185952
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.03897	5.57721	2.51505
C	-0.87066	4.66155	1.94581
C	-0.37582	6.45810	3.51648
C	-2.20498	4.63643	2.42250
C	-0.48840	3.77288	0.91028
C	-2.60918	5.53370	3.42362
C	-3.12488	3.73688	1.87218
C	-1.69622	6.43930	3.96657
C	-1.37194	2.75308	0.50999
C	0.77845	3.94173	0.14560
C	-2.71615	2.79177	0.92301

O	-0.95392	1.79765	-0.38316
C	-3.72820	1.89362	0.31465
C	1.69617	2.86999	0.09568
C	1.06414	5.14213	-0.56054
C	2.33997	5.31299	-1.15380
C	0.10833	6.17226	-0.70895
C	3.28118	4.28290	-1.09227
C	2.65377	6.50879	-1.81934
C	2.95311	3.05435	-0.50960
C	3.94590	1.95635	-0.53813
O	1.44604	1.70664	0.78252
C	0.43230	7.35268	-1.38116
C	1.70367	7.52449	-1.92651
P	0.17372	0.76432	0.24820
C	-4.15830	2.11255	-1.02261
C	-4.32429	0.85917	1.08435
C	4.18980	1.24597	-1.74548
C	4.68529	1.63927	0.63108
C	-5.34706	0.08039	0.51317
C	-3.88284	0.55128	2.51615
C	-5.76940	0.26428	-0.81697
C	-5.14608	1.27484	-1.56769
C	-6.87277	-0.59637	-1.47043
C	-3.61738	3.25738	-1.88429
C	5.60175	0.57513	0.58980
C	4.58296	2.47333	1.91156
C	5.82852	-0.17429	-0.57774
C	5.10773	0.17956	-1.73527
C	6.89519	-1.29246	-0.56754
C	3.56422	1.66613	-3.08205
C	-4.73556	4.23184	-2.27768
C	-2.89099	2.72338	-3.12588
C	-3.45450	-0.91345	2.66213
C	-4.98958	0.89579	3.51995
C	2.76130	0.53753	-3.73553
C	4.64167	2.19056	-4.03996
C	5.92258	3.14677	2.23800
C	4.08995	1.63245	3.09465
O	-0.32643	0.12661	1.52766
O	0.62162	-0.12581	-0.88028
C	9.01874	-2.78039	0.90907
C	9.37389	-1.78054	-0.21247
C	7.64988	-3.42863	0.60989
C	8.29602	-0.67473	-0.27845
C	9.43633	-2.52470	-1.56220
C	6.56630	-2.33179	0.54678
C	6.98827	-2.06517	-1.92406
C	7.71190	-4.16930	-0.74031
C	8.06566	-3.16806	-1.85767
C	-8.49740	-1.26258	-3.88036

C	-9.12159	-0.52664	-2.67477
C	-7.37258	-2.20005	-3.39009
C	-8.03662	0.31551	-1.96700
C	-9.70196	-1.55824	-1.68646
C	-6.27826	-1.36738	-2.68744
C	-7.48765	-1.64929	-0.49367
C	-7.95369	-3.22878	-2.39935
C	-8.57434	-2.48883	-1.19694
C	2.11076	-2.57885	-2.20714
C	2.69501	-3.05499	-1.01025
C	3.59437	-4.14715	-1.05213
C	3.93684	-4.70941	-2.26894
C	3.38222	-4.20355	-3.45547
C	2.46617	-3.15090	-3.42355
C	2.30270	-2.37210	0.18204
S	3.00332	-2.62191	1.68616
C	2.04203	-1.54696	2.82945
C	0.81047	-2.22860	3.45356
N	-0.31220	-2.38512	2.53910
S	-0.50084	-3.80826	1.68881
C	-2.29558	-3.98929	1.57891
O	0.02614	-3.68481	0.31349
O	0.07199	-4.87863	2.52189
C	-2.98800	-4.41396	2.74008
C	-4.35708	-4.66184	2.63169
C	-5.05426	-4.49723	1.43326
C	-4.34806	-4.02848	0.32794
C	-2.97470	-3.74752	0.36161
H	1.07409	5.60901	2.20037
H	0.32997	7.15722	3.94619
H	-3.62962	5.53206	3.78829
H	-4.16200	3.76331	2.18588
H	-2.01230	7.12609	4.74113
H	-0.89754	6.07088	-0.32526
H	4.26024	4.41453	-1.54006
H	3.62988	6.65266	-2.26754
H	-0.30790	8.13585	-1.48324
H	1.94917	8.44174	-2.44602
H	-5.79878	-0.67942	1.12881
H	-2.99454	1.15319	2.79582
H	-5.44906	1.43310	-2.59203
H	-2.87809	3.86753	-1.33047
H	6.17202	0.35228	1.47909
H	3.85310	3.29963	1.79616
H	5.27613	-0.34295	-2.66145
H	2.84027	2.49260	-2.94729
H	-5.25861	4.59557	-1.36734
H	-4.30524	5.11065	-2.80404
H	-5.47668	3.75144	-2.95038
H	-2.40725	3.56141	-3.67181

H	-2.09996	2.00367	-2.82699
H	-3.59367	2.21397	-3.81820
H	-2.79213	-1.19162	1.81874
H	-2.89937	-1.05832	3.61351
H	-4.32937	-1.59668	2.66308
H	-5.28264	1.96144	3.41661
H	-5.88825	0.26303	3.36001
H	-4.62479	0.73541	4.55698
H	3.39050	-0.35113	-3.94567
H	1.92204	0.25278	-3.07496
H	2.32458	0.88718	-4.69542
H	5.21591	3.00894	-3.55554
H	5.34570	1.38344	-4.33368
H	4.16980	2.59792	-4.95963
H	6.27382	3.73583	1.36376
H	5.79958	3.84178	3.09607
H	6.69907	2.39900	2.50366
H	3.08895	1.21639	2.86711
H	4.78638	0.79858	3.32226
H	3.99496	2.26823	4.00069
H	8.98541	-2.25616	1.88949
H	9.80308	-3.56577	0.97998
H	10.36317	-1.32064	0.00161
H	7.39810	-4.15176	1.41601
H	8.55995	0.05720	-1.07399
H	8.29760	-0.12179	0.68548
H	10.22486	-3.30840	-1.52847
H	9.70828	-1.81602	-2.37518
H	5.58209	-2.79615	0.34448
H	6.49934	-1.85378	1.54636
H	7.25892	-1.36979	-2.74938
H	6.00815	-2.52946	-2.17202
H	6.73349	-4.65116	-0.95546
H	8.47607	-4.97619	-0.69668
H	8.10968	-3.70225	-2.83175
H	-8.08886	-0.52537	-4.60613
H	-9.27771	-1.85160	-4.41067
H	-9.93562	0.14185	-3.03050
H	-6.93043	-2.73388	-4.25932
H	-8.48663	0.85925	-1.10675
H	-7.67292	1.08379	-2.68147
H	-10.49881	-2.15462	-2.18291
H	-10.16807	-1.03669	-0.82166
H	-5.45858	-2.03826	-2.34854
H	-5.83840	-0.66768	-3.42983
H	-7.94129	-1.14308	0.38752
H	-6.69712	-2.33418	-0.12597
H	-7.15197	-3.91681	-2.05226
H	-8.72665	-3.84881	-2.90435
H	-8.99080	-3.23071	-0.48112

H	1.39433	-1.76586	-2.13364
H	4.00038	-4.55667	-0.13243
H	4.62699	-5.54579	-2.30682
H	2.02839	-2.77926	-4.34410
H	1.56077	-1.56876	0.05577
H	2.76578	-1.27753	3.60444
H	1.72756	-0.64979	2.29128
H	0.48550	-1.56518	4.26452
H	1.05724	-3.19862	3.89037
H	-0.48977	-1.51161	1.98862
C	-6.53381	-4.78616	1.35962
H	-4.87399	-3.87118	-0.60936
C	-2.36451	-3.18483	-0.90588
C	-2.34704	-4.58322	4.09860
H	-4.89267	-4.99377	3.51759
H	-3.11886	-4.77245	4.84847
H	-1.63008	-5.40607	4.11005
H	-1.80302	-3.67931	4.38776
H	-3.16549	-2.93961	-1.60761
H	-1.77875	-2.28085	-0.72555
H	-1.68977	-3.89969	-1.38185
H	-6.86702	-4.91439	0.32655
H	-6.78881	-5.69437	1.91437
H	-7.11780	-3.96684	1.79663
H	3.66019	-4.64881	-4.40640

Post TS-8Re

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.979644
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.406659
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.220772
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.22110	5.66631	2.14809
C	-1.13496	4.69414	1.68600
C	-0.58421	6.55879	3.15905
C	-2.41372	4.62058	2.29181
C	-0.80595	3.78796	0.64442
C	-2.76740	5.53012	3.30113
C	-3.32871	3.65072	1.87260
C	-1.85506	6.49500	3.72968
C	-1.67470	2.71014	0.36059
C	0.42602	3.95662	-0.17593
C	-2.96554	2.69387	0.91855
O	-1.34897	1.77032	-0.58861
C	-3.97946	1.70812	0.47008
C	1.37275	2.91758	-0.16947
C	0.68399	5.13385	-0.92336
C	1.96073	5.31482	-1.51266
C	-0.29701	6.13142	-1.10819

C	2.94188	4.32724	-1.37084
C	2.24360	6.48897	-2.22835
C	2.65170	3.12411	-0.71728
C	3.72316	2.11136	-0.55916
O	1.07590	1.74106	0.46911
C	-0.00299	7.29035	-1.83005
C	1.26462	7.47146	-2.38313
P	-0.03553	0.84077	-0.31677
C	-4.59834	1.85675	-0.80045
C	-4.40157	0.66898	1.34274
C	4.14653	1.33271	-1.67084
C	4.38688	1.97677	0.68961
C	-5.47361	-0.15752	0.95588
C	-3.74004	0.43355	2.70348
C	-6.10942	-0.01665	-0.29369
C	-5.62473	0.97110	-1.16654
C	-7.30740	-0.88872	-0.73143
C	-4.22469	2.97905	-1.77306
C	5.43966	1.05306	0.80684
C	4.02743	2.83535	1.90597
C	5.87627	0.27176	-0.27678
C	5.21629	0.43315	-1.50958
C	7.06595	-0.69512	-0.08613
C	3.50967	1.47579	-3.05583
C	-5.41806	3.90772	-2.03403
C	-3.66992	2.41270	-3.08688
C	-3.19387	-0.99474	2.83090
C	-4.71197	0.74621	3.84783
C	3.04842	0.12550	-3.62270
C	4.47832	2.16071	-4.02747
C	5.21871	3.69369	2.35188
C	3.50693	1.97196	3.06215
O	-0.45486	-0.16109	0.85357
O	0.39366	0.20832	-1.57926
C	9.16760	-1.82641	1.70223
C	9.52647	-0.83433	0.57447
C	7.93913	-2.66315	1.28443
C	8.33356	0.11407	0.32416
C	9.84488	-1.61432	-0.71720
C	6.73782	-1.72447	1.03764
C	7.41609	-1.50435	-1.37785
C	8.26291	-3.44099	-0.00668
C	8.61384	-2.44639	-1.13036
C	-9.29645	-1.62334	-2.82924
C	-9.71801	-0.83103	-1.57257
C	-8.11715	-2.55763	-2.48193
C	-8.52820	0.02048	-1.07695
C	-10.14674	-1.81300	-0.46437
C	-6.91851	-1.71430	-1.99492
C	-7.77329	-1.89151	0.37193

C	-8.54537	-3.53700	-1.37009
C	-8.96501	-2.74012	-0.11793
C	3.16983	-3.40093	-2.06210
C	3.06249	-3.32121	-0.66845
C	3.87387	-4.15267	0.11582
C	4.75809	-5.04745	-0.47875
C	4.86986	-5.10640	-1.86971
C	4.07385	-4.27943	-2.65974
C	2.09854	-2.30324	-0.08039
S	2.91150	-1.27943	1.24755
C	1.75644	-1.81374	2.57386
C	1.08899	-3.07391	2.03415
N	0.83374	-2.79432	0.59993
S	0.07185	-4.13551	-0.24913
C	-1.57236	-4.21532	0.50689
O	-0.03546	-3.69944	-1.64047
O	0.79045	-5.37212	0.07134
C	-1.83167	-5.17490	1.51983
C	-3.13572	-5.24322	2.02393
C	-4.17091	-4.43640	1.55912
C	-3.87609	-3.51545	0.55335
C	-2.59748	-3.37171	0.00679
H	0.78094	5.73458	1.74579
H	0.12437	7.30107	3.50334
H	-3.74681	5.49006	3.76317
H	-4.32674	3.62918	2.29538
H	-2.13137	7.19040	4.51170
H	-1.29707	6.01824	-0.71094
H	3.93338	4.48620	-1.77878
H	3.21932	6.64341	-2.67378
H	-0.76246	8.04998	-1.96332
H	1.48689	8.37252	-2.94010
H	-5.80089	-0.91211	1.65193
H	-2.86322	1.09892	2.83821
H	-6.07737	1.08193	-2.14053
H	-3.43122	3.62908	-1.35719
H	5.93731	0.95692	1.76024
H	3.21775	3.55330	1.66979
H	5.53283	-0.12764	-2.37240
H	2.59938	2.10756	-3.00719
H	-5.81323	4.29615	-1.07093
H	-5.09690	4.77404	-2.65115
H	-6.23448	3.38104	-2.57129
H	-3.29324	3.23905	-3.72684
H	-2.82455	1.72288	-2.87960
H	-4.45028	1.86087	-3.65174
H	-2.55889	-1.24095	1.95636
H	-2.56967	-1.08255	3.74565
H	-4.01481	-1.73748	2.90143
H	-5.09465	1.78400	3.75269

H	-5.57453	0.04670	3.84517
H	-4.18991	0.65814	4.82452
H	3.90672	-0.51036	-3.92468
H	2.45383	-0.42068	-2.86765
H	2.40985	0.28864	-4.51701
H	4.79376	3.14595	-3.62529
H	5.38378	1.53892	-4.19335
H	3.98034	2.32977	-5.00608
H	5.59642	4.29209	1.49522
H	4.90152	4.39673	3.15163
H	6.04636	3.06826	2.74712
H	2.62183	1.38867	2.73245
H	4.28531	1.26900	3.42615
H	3.19403	2.61916	3.90913
H	8.94883	-1.27212	2.64140
H	10.03133	-2.49659	1.90690
H	10.41602	-0.23891	0.87482
H	7.68688	-3.38176	2.09441
H	8.59553	0.84108	-0.47652
H	8.15326	0.70165	1.24960
H	10.71814	-2.28309	-0.55210
H	10.11798	-0.90750	-1.53143
H	5.84952	-2.32435	0.75045
H	6.48987	-1.21713	1.99369
H	7.68221	-0.81296	-2.20811
H	6.54167	-2.11330	-1.70093
H	7.39281	-4.06093	-0.30783
H	9.11572	-4.13284	0.16951
H	8.84256	-3.00783	-2.06235
H	-8.99990	-0.92160	-3.63965
H	-10.15520	-2.22093	-3.20672
H	-10.57114	-0.16416	-1.82470
H	-7.82174	-3.13254	-3.38649
H	-8.83330	0.60380	-0.17977
H	-8.27688	0.75547	-1.87017
H	-11.01647	-2.41638	-0.80587
H	-10.46758	-1.25039	0.43988
H	-6.06099	-2.38407	-1.76578
H	-6.59598	-1.04909	-2.82422
H	-8.07387	-1.34380	1.29290
H	-6.94732	-2.57919	0.63606
H	-7.70474	-4.22198	-1.12153
H	-9.39259	-4.16554	-1.72241
H	-9.27152	-3.44654	0.68411
H	2.52662	-2.78643	-2.68209
H	3.83963	-4.07716	1.19715
H	5.37660	-5.68605	0.14519
H	4.15057	-4.31687	-3.74228
H	1.76432	-1.62954	-0.86930
H	2.32261	-2.01974	3.48468

H	1.02712	-1.02480	2.76760
H	0.13398	-3.26182	2.53230
H	1.73515	-3.94984	2.16037
H	-0.12831	-1.08018	0.67690
C	-5.56064	-4.55963	2.13241
H	-4.65939	-2.86997	0.17272
C	-2.44286	-2.34413	-1.09531
C	-0.84385	-6.16668	2.10249
H	-3.34477	-5.96915	2.80469
H	-1.31220	-6.68367	2.94356
H	-0.54199	-6.90813	1.36030
H	0.07718	-5.70241	2.45704
H	-3.27604	-1.63807	-1.04983
H	-1.51298	-1.78121	-1.05585
H	-2.45568	-2.82961	-2.07551
H	-6.28822	-4.82106	1.35620
H	-5.60450	-5.33204	2.90414
H	-5.88911	-3.61699	2.58397
H	5.57612	-5.79043	-2.33122

TS-8Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.942076
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.370579
M06-2X/6-31G(d,p) Derived free energy = -4822.174566
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.185377
Number of Imaginary Frequencies = 1 (-126.96)

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.96683	6.13887	1.80379
C	-1.76484	5.04769	1.39653
C	-1.46636	7.09075	2.69537
C	-3.06587	4.91487	1.94423
C	-1.29965	4.08065	0.46755
C	-3.55704	5.88472	2.83270
C	-3.85897	3.81439	1.60366
C	-2.75975	6.96855	3.20215
C	-2.05909	2.91213	0.24584
C	-0.02643	4.25888	-0.29135
C	-3.35255	2.79634	0.78769
O	-1.60546	1.95458	-0.62566
C	-4.19865	1.61163	0.49127
C	0.97428	3.27440	-0.16190
C	0.20813	5.38394	-1.12352
C	1.50295	5.58907	-1.66434
C	-0.81284	6.30563	-1.44069
C	2.52224	4.66510	-1.40916
C	1.76235	6.71865	-2.45671
C	2.25932	3.49589	-0.68667
C	3.35043	2.51153	-0.46900

O	0.73753	2.15676	0.59481
C	-0.54104	7.42009	-2.23725
C	0.74370	7.63008	-2.73748
P	-0.29847	1.07987	-0.10000
C	-4.75605	1.44032	-0.80608
C	-4.49399	0.66729	1.51453
C	3.84544	1.73982	-1.55706
C	3.94396	2.37629	0.81664
C	-5.32503	-0.42619	1.21361
C	-3.97621	0.81833	2.94914
C	-5.85516	-0.63559	-0.07076
C	-5.55579	0.31283	-1.06570
C	-6.74674	-1.86954	-0.33506
C	-4.56976	2.47311	-1.92202
C	5.01022	1.47523	0.98828
C	3.49766	3.21197	2.02008
C	5.53941	0.73274	-0.08294
C	4.93930	0.88403	-1.34428
C	6.75231	-0.21030	0.07416
C	3.25164	1.82970	-2.96594
C	-5.91140	3.10447	-2.31628
C	-3.87166	1.86178	-3.14527
C	-3.20637	-0.42177	3.42565
C	-5.13074	1.13286	3.90891
C	2.85716	0.45016	-3.51664
C	4.22865	2.52470	-3.92253
C	4.63214	4.11774	2.51695
C	2.96964	2.32029	3.15297
O	-0.69775	0.15878	1.03560
O	0.26209	0.45795	-1.34998
C	9.63874	-0.72246	0.68959
C	9.11517	-0.69479	-0.76015
C	8.51975	-1.21535	1.62882
C	7.91049	0.26693	-0.85508
C	8.67517	-2.11506	-1.17782
C	7.30919	-0.26233	1.53445
C	6.34591	-1.65911	-0.32871
C	8.08529	-2.63485	1.21589
C	7.55867	-2.61039	-0.23338
C	-8.04110	-4.34494	0.70815
C	-6.82777	-4.41848	-0.24363
C	-8.87102	-3.08155	0.39330
C	-5.93962	-3.17109	-0.04561
C	-7.31998	-4.47208	-1.70393
C	-7.99489	-1.82647	0.59874
C	-7.26245	-1.95472	-1.80917
C	-9.36024	-3.13636	-1.06798
C	-8.14397	-3.20581	-2.01339
C	2.48713	-3.01850	-1.69791
C	1.15736	-3.44503	-1.89516

C	0.91329	-4.77842	-2.28694
C	1.97150	-5.64956	-2.50943
C	3.28654	-5.20846	-2.33187
C	3.54145	-3.89744	-1.92328
C	0.08667	-2.47413	-1.74973
S	-1.38273	-2.70137	-2.63314
C	-2.37043	-1.60114	-1.56674
C	-2.27969	-2.19421	-0.15272
N	-0.85942	-2.34095	0.23996
S	-0.68079	-3.59066	1.46508
C	1.08257	-4.00486	1.52857
O	-1.06687	-3.01471	2.75635
O	-1.44231	-4.72450	0.92891
C	1.46886	-5.36243	1.39000
C	2.82095	-5.66547	1.59128
C	3.77436	-4.70777	1.92912
C	3.34959	-3.38746	2.07423
C	2.01756	-3.00276	1.89185
H	0.04846	6.25796	1.44995
H	-0.84630	7.92518	2.99680
H	-4.55369	5.79873	3.24943
H	-4.86398	3.72805	2.00011
H	-3.14176	7.71008	3.89189
H	-1.82640	6.16702	-1.08886
H	3.52045	4.84100	-1.79214
H	2.75055	6.89145	-2.86652
H	-1.33116	8.12242	-2.46973
H	0.94842	8.49645	-3.35309
H	-5.56106	-1.12754	1.99946
H	-3.25657	1.65707	3.02677
H	-5.95749	0.20323	-2.05884
H	-3.93264	3.31581	-1.59020
H	5.43682	1.38753	1.97329
H	2.66995	3.89660	1.75258
H	5.33311	0.33179	-2.18410
H	2.31822	2.42835	-2.96230
H	-6.40501	3.53619	-1.41927
H	-5.74535	3.92393	-3.04799
H	-6.59229	2.35801	-2.77663
H	-3.64302	2.65679	-3.88678
H	-2.91510	1.38627	-2.84601
H	-4.50897	1.09877	-3.63892
H	-2.37999	-0.64994	2.72766
H	-2.76133	-0.22944	4.42528
H	-3.86399	-1.31164	3.50779
H	-5.68314	2.03205	3.56427
H	-5.84169	0.28179	3.97212
H	-4.73536	1.33910	4.92645
H	3.74786	-0.16590	-3.76004
H	2.24162	-0.09860	-2.77963

H	2.25871	0.57081	-4.44483
H	4.50503	3.52601	-3.53251
H	5.15606	1.92678	-4.05026
H	3.75490	2.66027	-4.91822
H	5.00908	4.74555	1.68128
H	4.25648	4.79309	3.31525
H	5.47528	3.52539	2.93017
H	2.17246	1.64725	2.77332
H	3.77858	1.69975	3.59218
H	2.53566	2.94937	3.95924
H	9.97146	0.29428	0.99402
H	10.52088	-1.39595	0.76267
H	9.92361	-0.34367	-1.43779
H	8.89650	-1.23382	2.67470
H	7.58474	0.31265	-1.91589
H	8.22829	1.29418	-0.56863
H	9.54331	-2.80902	-1.13549
H	8.30909	-2.10662	-2.22810
H	6.52158	-0.61868	2.23574
H	7.63173	0.75109	1.86222
H	5.96299	-1.68718	-1.37000
H	5.52858	-2.02501	0.33107
H	7.29372	-2.99752	1.90442
H	8.94440	-3.33639	1.29759
H	7.24905	-3.63538	-0.53247
H	-7.69447	-4.31913	1.76471
H	-8.67233	-5.25286	0.58869
H	-6.23641	-5.33297	-0.01974
H	-9.74844	-3.03611	1.07458
H	-5.06699	-3.23129	-0.73077
H	-5.54383	-3.18021	0.99230
H	-7.94293	-5.37976	-1.86244
H	-6.45205	-4.54051	-2.39624
H	-8.59472	-0.91306	0.38863
H	-7.69857	-1.78072	1.66801
H	-6.40464	-2.00563	-2.51663
H	-7.86511	-1.05370	-2.06111
H	-9.97162	-2.23635	-1.29893
H	-10.01028	-4.02627	-1.21837
H	-8.49664	-3.24294	-3.06713
H	2.67794	-1.99787	-1.38256
H	-0.10977	-5.12059	-2.40356
H	1.77603	-6.67275	-2.81432
H	4.56429	-3.56806	-1.78441
H	0.33568	-1.42642	-1.53638
H	-1.95869	-0.59295	-1.62463
H	-3.39893	-1.60842	-1.93311
H	-2.76083	-3.17127	-0.12016
H	-2.76931	-1.51158	0.54375
H	-0.58521	-1.36990	0.62239

C	5.21782	-5.09402	2.13033
H	4.06791	-2.62262	2.35863
C	1.68881	-1.54029	2.07493
C	0.56154	-6.53476	1.07794
H	3.12939	-6.70302	1.49642
H	1.15824	-7.44992	1.05439
H	-0.22657	-6.65569	1.82363
H	0.05816	-6.42038	0.11707
H	1.61728	-1.02001	1.11528
H	0.74727	-1.36859	2.59547
H	2.48503	-1.05186	2.64142
H	5.67574	-4.51640	2.93819
H	5.31679	-6.15548	2.37285
H	5.80301	-4.91106	1.22116
H	4.11371	-5.89024	-2.50626

Pre TS-8Si
ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.947663
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.377358
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.188328
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.61688	6.08923	-1.59027
C	1.46958	5.03080	-1.20708
C	1.08160	7.11103	-2.42112
C	2.79072	5.00433	-1.71761
C	1.04017	3.99535	-0.33604
C	3.24669	6.04329	-2.54465
C	3.64005	3.94124	-1.39931
C	2.39449	7.09252	-2.89053
C	1.85783	2.86073	-0.14959
C	-0.24775	4.08170	0.41087
C	3.17432	2.85372	-0.65080
O	1.42889	1.83160	0.65138
C	4.09344	1.71517	-0.39533
C	-1.21159	3.07132	0.21508
C	-0.54466	5.17288	1.26806
C	-1.86738	5.33739	1.74865
C	0.44010	6.10546	1.65981
C	-2.85294	4.40492	1.41154
C	-2.18889	6.43692	2.56031
C	-2.52748	3.25541	0.68073
C	-3.58888	2.25595	0.39238
O	-0.92388	1.99497	-0.58514
C	0.10721	7.18938	2.47518
C	-1.20427	7.35863	2.91833
P	0.17660	0.93192	0.02641
C	4.64368	1.51619	0.90104
C	4.50382	0.87691	-1.46984

C	-4.15671	1.48995	1.44994
C	-4.08852	2.10521	-0.93163
C	5.46122	-0.12312	-1.22804
C	3.96291	1.04001	-2.89430
C	5.99253	-0.35985	0.05060
C	5.56365	0.47077	1.10237
C	7.01903	-1.49740	0.24881
C	4.31829	2.43641	2.08139
C	-5.12552	1.18675	-1.17298
C	-3.58749	2.95523	-2.10373
C	-5.71905	0.44041	-0.13908
C	-5.20826	0.60164	1.16043
C	-6.92530	-0.49668	-0.37616
C	-3.70649	1.63739	2.90842
C	5.57284	3.17270	2.56962
C	3.65431	1.66294	3.22928
C	3.32729	-0.25455	-3.42064
C	5.06703	1.51994	-3.84528
C	-3.20629	0.31245	3.49539
C	-4.83400	2.22001	3.77104
C	-4.70583	3.84951	-2.65518
C	-2.98687	2.08013	-3.21393
O	0.65596	0.14489	-1.17056
O	-0.37085	0.19065	1.22401
C	-9.76271	-0.98704	-1.20329
C	-9.34974	-0.94908	0.28167
C	-8.58154	-1.50174	-2.05059
C	-8.14459	0.00101	0.45888
C	-8.95904	-2.36952	0.74430
C	-7.37234	-0.55928	-1.87382
C	-6.56730	-1.94514	0.07052
C	-8.19477	-2.92139	-1.59270
C	-7.77964	-2.88573	-0.10818
C	8.62458	-3.71350	-0.93629
C	7.40940	-4.00419	-0.02942
C	9.28861	-2.38826	-0.50411
C	6.38131	-2.85989	-0.16170
C	7.87367	-4.11121	1.43702
C	8.27148	-1.23428	-0.64185
C	7.51033	-1.63440	1.72711
C	9.75043	-2.49719	0.96305
C	8.53210	-2.78375	1.86402
C	-2.20682	-2.68996	1.96465
C	-0.96145	-3.20129	2.40051
C	-0.92639	-4.37028	3.19959
C	-2.10736	-4.98781	3.57301
C	-3.33708	-4.45956	3.14955
C	-3.38519	-3.31953	2.34553
C	0.19486	-2.46822	1.99383
S	1.77112	-2.82058	2.45827

C	2.69981	-1.76294	1.28265
C	2.68287	-2.38334	-0.12509
N	1.32814	-2.42424	-0.65982
S	1.04200	-3.56836	-1.88626
C	-0.68983	-4.02595	-1.58828
O	1.13215	-2.94938	-3.21139
O	1.92471	-4.70552	-1.58625
C	-0.99132	-5.22984	-0.90536
C	-2.33963	-5.57449	-0.76234
C	-3.37686	-4.77929	-1.24731
C	-3.04142	-3.58785	-1.88828
C	-1.71433	-3.18024	-2.08311
H	-0.41430	6.12845	-1.26573
H	0.41946	7.91901	-2.70454
H	4.25881	6.03835	-2.93187
H	4.66112	3.93890	-1.76248
H	2.74955	7.88783	-3.53313
H	1.47185	5.99743	1.35232
H	-3.87247	4.54925	1.75050
H	-3.19953	6.57828	2.92496
H	0.87024	7.89973	2.76634
H	-1.45671	8.20150	3.54868
H	5.78753	-0.73613	-2.05464
H	3.15584	1.79878	-2.92913
H	5.95529	0.33397	2.09620
H	3.60480	3.23097	1.78985
H	-5.48260	1.09302	-2.18452
H	-2.78648	3.64999	-1.78702
H	-5.65333	0.04604	1.97231
H	-2.84928	2.33251	2.99700
H	6.04600	3.71660	1.72409
H	5.29806	3.91579	3.34861
H	6.31396	2.46973	3.00457
H	3.33262	2.36838	4.02491
H	2.75491	1.12655	2.86231
H	4.35060	0.92462	3.67893
H	2.54590	-0.60645	-2.72161
H	2.84536	-0.06764	-4.40404
H	4.07919	-1.06009	-3.55195
H	5.52798	2.45360	-3.46110
H	5.86162	0.75210	-3.95729
H	4.63928	1.73318	-4.84818
H	-3.99513	-0.46775	3.48901
H	-2.33288	-0.04341	2.91726
H	-2.87406	0.46197	4.54495
H	-5.20248	3.17019	3.33012
H	-5.68494	1.51128	3.85342
H	-4.45782	2.43709	4.79362
H	-5.13326	4.46879	-1.83761
H	-4.29786	4.53311	-3.43027

H	-5.51930	3.24882	-3.11348
H	-2.21557	1.39993	-2.79588
H	-3.76538	1.46688	-3.71406
H	-2.50307	2.72156	-3.98118
H	-10.06028	0.02976	-1.54197
H	-10.64434	-1.65202	-1.33612
H	-10.20312	-0.58260	0.89280
H	-8.87855	-1.52709	-3.12171
H	-7.89699	0.05342	1.54055
H	-8.42875	1.02873	0.14056
H	-9.82927	-3.05464	0.64245
H	-8.67380	-2.35457	1.81929
H	-6.53735	-0.92820	-2.51080
H	-7.66197	0.45298	-2.23433
H	-6.27130	-1.96724	1.13886
H	-5.70421	-2.32306	-0.52007
H	-7.35809	-3.30348	-2.21608
H	-9.05416	-3.61371	-1.73097
H	-7.50682	-3.91074	0.22365
H	8.29963	-3.64786	-1.99802
H	9.35847	-4.54622	-0.86544
H	6.93799	-4.96262	-0.33811
H	10.16798	-2.18612	-1.15368
H	5.50530	-3.07756	0.48647
H	6.01435	-2.83642	-1.20977
H	8.59823	-4.94794	1.54658
H	7.00598	-4.33541	2.09589
H	8.75214	-0.27493	-0.34709
H	7.99275	-1.14155	-1.71294
H	6.65015	-1.84100	2.40264
H	7.99471	-0.69051	2.06315
H	10.24355	-1.55134	1.27825
H	10.50010	-3.31232	1.06632
H	8.86482	-2.86001	2.92213
H	-2.21377	-1.79948	1.34379
H	0.02690	-4.78130	3.51784
H	-2.08413	-5.88004	4.19010
H	-4.33864	-2.92165	2.02252
H	0.03445	-1.52011	1.44623
H	2.26194	-0.76310	1.30319
H	3.71832	-1.71712	1.67451
H	3.08692	-3.39753	-0.10345
H	3.34913	-1.77192	-0.74297
H	0.99664	-1.46017	-0.93681
C	-4.81489	-5.19389	-1.05709
H	-3.83307	-2.94854	-2.27084
C	-1.49410	-1.87290	-2.81486
C	0.01816	-6.19297	-0.31390
H	-2.58025	-6.50535	-0.25487
H	-0.51087	-6.96758	0.24776

H	0.62444	-6.67107	-1.08533
H	0.72208	-5.69664	0.35725
H	-0.85177	-1.17224	-2.27267
H	-1.02270	-2.04151	-3.78535
H	-2.45844	-1.38312	-2.97382
H	-5.46403	-4.74028	-1.80930
H	-4.92839	-6.28014	-1.12130
H	-5.18558	-4.88863	-0.07068
H	-4.26026	-4.94730	3.44865

Post TS-8Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.967988
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.393171
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.216194
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-1.38800	6.10034	1.96952
C	-2.11684	4.99397	1.48085
C	-1.96260	6.98034	2.88923
C	-3.42446	4.76782	1.98162
C	-1.57593	4.10149	0.51762
C	-3.99136	5.66648	2.89944
C	-4.14388	3.63881	1.57714
C	-3.26302	6.76946	3.34585
C	-2.27235	2.90813	0.21474
C	-0.27987	4.37557	-0.17680
C	-3.55899	2.68472	0.73758
O	-1.77075	2.02575	-0.70945
C	-4.29388	1.42732	0.43348
C	0.74767	3.41444	-0.07762
C	-0.05581	5.55378	-0.93566
C	1.24509	5.82139	-1.43476
C	-1.09325	6.46606	-1.22571
C	2.27944	4.90204	-1.22527
C	1.49295	7.00270	-2.15181
C	2.02968	3.68250	-0.58800
C	3.12261	2.68285	-0.46580
O	0.50869	2.23177	0.57173
C	-0.83226	7.63249	-1.94803
C	0.45788	7.90425	-2.40224
P	-0.42015	1.21676	-0.29785
C	-4.81444	1.19571	-0.87013
C	-4.50244	0.45750	1.45518
C	3.57063	1.97038	-1.61302
C	3.75959	2.46876	0.78730
C	-5.22246	-0.71064	1.15114
C	-4.00745	0.65335	2.89236
C	-5.71734	-0.97452	-0.13639
C	-5.49554	-0.00727	-1.13396

C	-6.50304	-2.27985	-0.39600
C	-4.71766	2.23763	-1.98820
C	4.81107	1.53548	0.87216
C	3.37877	3.26066	2.04164
C	5.29183	0.85026	-0.25970
C	4.66345	1.09808	-1.49055
C	6.48485	-0.12884	-0.20579
C	2.92133	2.13427	-2.98970
C	-6.10983	2.74404	-2.38691
C	-3.96514	1.68841	-3.20936
C	-3.13714	-0.51671	3.37082
C	-5.18877	0.86715	3.84713
C	2.59277	0.77858	-3.64251
C	3.82211	2.95993	-3.91678
C	4.56161	4.09725	2.54737
C	2.84501	2.34015	3.14691
O	-0.83359	0.18709	0.82880
O	0.18979	0.64126	-1.51395
C	9.37096	-0.75106	0.29851
C	8.81809	-0.59036	-1.13211
C	8.26049	-1.29786	1.21814
C	7.63307	0.39944	-1.11974
C	8.33746	-1.96013	-1.65808
C	7.07231	-0.31145	1.23121
C	6.03674	-1.53327	-0.71427
C	7.78809	-2.66908	0.69485
C	7.23196	-2.51135	-0.73238
C	-7.63463	-4.82648	0.66776
C	-6.39560	-4.82631	-0.25316
C	-8.54790	-3.63488	0.30762
C	-5.60881	-3.51228	-0.05912
C	-6.84464	-4.94381	-1.72347
C	-7.77304	-2.31379	0.50775
C	-6.97410	-2.43147	-1.87946
C	-8.99472	-3.75416	-1.16348
C	-7.75320	-3.74955	-2.07841
C	2.67522	-3.17840	-1.78615
C	1.34897	-3.58733	-1.59199
C	1.03451	-4.94968	-1.71033
C	2.03281	-5.88043	-1.99165
C	3.35335	-5.46422	-2.17538
C	3.67146	-4.11038	-2.07675
C	0.28971	-2.52302	-1.39881
S	-0.97723	-2.66439	-2.74551
C	-2.22662	-1.86616	-1.68389
C	-1.97474	-2.47953	-0.31547
N	-0.48228	-2.42294	-0.07998
S	-0.17126	-3.50464	1.29573
C	1.60908	-3.67105	1.63445
O	-0.75072	-2.75962	2.41992

O	-0.73597	-4.81754	0.95713
C	2.10651	-4.96470	1.94609
C	3.38297	-5.03864	2.51706
C	4.16004	-3.91752	2.80134
C	3.65165	-2.67138	2.44216
C	2.38524	-2.51247	1.87269
H	-0.36943	6.28733	1.65742
H	-1.39525	7.82783	3.25183
H	-4.99313	5.50845	3.28141
H	-5.14632	3.47197	1.95378
H	-3.70322	7.45533	4.05813
H	-2.11115	6.28143	-0.90988
H	3.27817	5.12003	-1.58378
H	2.48462	7.22247	-2.52947
H	-1.63513	8.32705	-2.15929
H	0.65386	8.81019	-2.96115
H	-5.40474	-1.42497	1.93959
H	-3.36089	1.54905	2.97325
H	-5.87299	-0.15988	-2.13096
H	-4.15922	3.13422	-1.65540
H	5.26664	1.37802	1.83570
H	2.57055	3.98777	1.82866
H	5.02670	0.60085	-2.37716
H	1.95547	2.67328	-2.90082
H	-6.64017	3.13715	-1.49313
H	-6.01721	3.56902	-3.12535
H	-6.72129	1.93571	-2.84037
H	-3.79146	2.50343	-3.94402
H	-2.97807	1.28247	-2.90631
H	-4.53958	0.88362	-3.71374
H	-2.31259	-0.69100	2.65616
H	-2.68872	-0.27612	4.35843
H	-3.72334	-1.45280	3.47788
H	-5.81429	1.71645	3.50128
H	-5.82526	-0.04124	3.90584
H	-4.81660	1.10438	4.86666
H	3.49833	0.30466	-4.07692
H	2.16289	0.07540	-2.90260
H	1.85614	0.92215	-4.46161
H	4.03586	3.95188	-3.47016
H	4.78754	2.44090	-4.09835
H	3.31663	3.12258	-4.89262
H	4.94678	4.74281	1.72913
H	4.23319	4.75441	3.38087
H	5.38713	3.45319	2.91654
H	1.96742	1.77005	2.77778
H	3.62095	1.62436	3.49033
H	2.51645	2.94496	4.01891
H	9.73319	0.22919	0.67932
H	10.23889	-1.44662	0.29490

H	9.61992	-0.19987	-1.79593
H	8.65776	-1.41341	2.25010
H	7.28540	0.53921	-2.16530
H	7.97978	1.39295	-0.75775
H	9.19075	-2.67254	-1.69578
H	7.94787	-1.85492	-2.69458
H	6.29330	-0.70117	1.92181
H	7.42854	0.66417	1.63068
H	5.62092	-1.47564	-1.74193
H	5.23152	-1.93625	-0.06035
H	7.00003	-3.07902	1.35786
H	8.63400	-3.39116	0.69775
H	6.89664	-3.50260	-1.10681
H	-7.31775	-4.75526	1.73156
H	-8.19326	-5.78122	0.55176
H	-5.74345	-5.68944	0.00351
H	-9.44306	-3.64249	0.96693
H	-4.71581	-3.52160	-0.71833
H	-5.24144	-3.47430	0.98822
H	-7.39339	-5.89876	-1.87848
H	-5.95652	-4.95908	-2.39303
H	-8.43438	-1.45223	0.26564
H	-7.50539	-2.22522	1.58214
H	-6.09750	-2.42714	-2.56537
H	-7.63907	-1.58549	-2.16322
H	-9.66594	-2.90743	-1.42737
H	-9.57226	-4.69326	-1.31064
H	-8.07560	-3.83320	-3.13916
H	2.92429	-2.12260	-1.72320
H	0.00747	-5.27284	-1.58712
H	1.77610	-6.93192	-2.08197
H	4.69126	-3.77948	-2.24167
H	0.74679	-1.53968	-1.51079
H	-2.10035	-0.78273	-1.69387
H	-3.22384	-2.11640	-2.05134
H	-2.31396	-3.51845	-0.30212
H	-2.47242	-1.92846	0.48451
H	-0.59220	-0.75160	0.56810
C	5.48076	-4.05715	3.51639
H	4.23817	-1.77877	2.63775
C	1.94526	-1.10292	1.56823
C	1.38781	-6.28424	1.75698
H	3.76624	-6.02282	2.77285
H	2.06109	-7.09789	2.03747
H	0.48666	-6.35410	2.36951
H	1.07369	-6.43094	0.72373
H	1.76759	-0.94739	0.50082
H	1.03428	-0.83568	2.10639
H	2.72981	-0.40549	1.86513
H	5.99897	-3.09814	3.59638

H	5.32969	-4.43760	4.53308
H	6.14230	-4.76506	3.00571
H	4.12711	-6.19058	-2.40633

TS-9Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.952901
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.380970
M06-2X/6-31G(d,p) Derived free energy = -4822.176132
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.185792
Number of Imaginary Frequencies = 1 (-61.70)

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.68620	5.08345	2.45692
C	-1.53076	4.08104	1.93157
C	-1.04108	5.77571	3.61665
C	-2.72534	3.76627	2.62609
C	-1.20826	3.37084	0.74638
C	-3.07252	4.47670	3.78624
C	-3.56320	2.75293	2.15139
C	-2.23323	5.47801	4.27573
C	-1.99113	2.25462	0.36902
C	-0.03859	3.74832	-0.09964
C	-3.20433	1.99348	1.03284
O	-1.64448	1.50431	-0.72692
C	-4.16327	0.97276	0.53843
C	0.98978	2.80420	-0.25665
C	0.08416	5.02023	-0.71186
C	1.30521	5.37071	-1.34422
C	-0.97654	5.95013	-0.71718
C	2.36589	4.45594	-1.37676
C	1.45292	6.63879	-1.92800
C	2.20935	3.16762	-0.85292
C	3.35161	2.21779	-0.86945
O	0.83506	1.55350	0.27566
C	-0.81591	7.20485	-1.30915
C	0.39591	7.55011	-1.90776
P	-0.24888	0.62306	-0.56910
C	-4.32864	-0.24609	1.24650
C	-5.05218	1.29345	-0.52236
C	3.76990	1.60636	-2.08415
C	4.04884	1.93450	0.33590
C	-6.11659	0.41818	-0.81428
C	-4.93268	2.59576	-1.31874
C	-6.36777	-0.73293	-0.04191
C	-5.44215	-1.05666	0.96403
C	-7.64146	-1.59440	-0.21075
C	-3.35485	-0.68758	2.33745
C	5.10508	1.00849	0.31393
C	3.72561	2.64136	1.65509

C	5.53146	0.38567	-0.87072
C	4.86011	0.71597	-2.06309
C	6.72218	-0.59777	-0.82483
C	3.10112	1.91521	-3.42636
C	-2.80961	-2.09717	2.06406
C	-4.01302	-0.62117	3.72054
C	-6.18598	3.46628	-1.15691
C	-4.63972	2.31604	-2.79707
C	2.69494	0.64080	-4.18330
C	4.01983	2.78049	-4.29739
C	4.91470	3.48399	2.13432
C	3.29456	1.63974	2.73234
O	-0.47863	-0.54943	0.37630
O	0.24644	0.36936	-1.95926
C	7.90839	-3.33089	-1.13295
C	7.59769	-2.73805	0.25550
C	8.25972	-2.19025	-2.10939
C	6.39724	-1.77438	0.14490
C	8.82923	-1.96934	0.77939
C	7.06534	-1.21780	-2.21858
C	7.99376	0.14434	-0.31206
C	9.49569	-1.42739	-1.59037
C	9.18544	-0.83200	-0.20196
C	-9.41436	-3.45244	-1.75415
C	-9.82481	-1.99029	-1.48760
C	-8.53292	-3.95657	-0.59377
C	-8.56064	-1.11021	-1.37921
C	-10.62049	-1.90897	-0.16891
C	-7.26432	-3.08187	-0.49377
C	-8.47723	-1.52975	1.10410
C	-9.32317	-3.87436	0.72957
C	-9.73994	-2.41173	0.99294
C	-2.21516	-3.77115	-1.39448
C	-1.21981	-2.99722	-2.04012
C	-1.59101	-1.82973	-2.75049
C	-2.93045	-1.48506	-2.85133
C	-3.90423	-2.27057	-2.23391
C	-3.54902	-3.40861	-1.49653
C	0.15044	-3.39894	-1.93436
S	1.31541	-2.83428	-3.07696
C	2.77649	-2.79054	-1.97920
C	2.39233	-1.90057	-0.77898
N	1.21172	-2.41833	-0.09506
S	1.41694	-3.67497	1.03716
C	2.68026	-3.10744	2.20752
O	0.12419	-3.83268	1.70330
O	1.95274	-4.81344	0.26746
C	3.97809	-3.68121	2.20912
C	4.91727	-3.14480	3.09821
C	4.62637	-2.08967	3.96091

C	3.32447	-1.59132	3.96580
C	2.32873	-2.06895	3.10863
H	0.25721	5.32988	1.98864
H	-0.38657	6.54397	4.00777
H	-3.98905	4.25182	4.31890
H	-4.50163	2.54749	2.65467
H	-2.50349	6.01866	5.17356
H	-1.93575	5.71177	-0.27661
H	3.31413	4.74047	-1.81684
H	2.38341	6.92246	-2.40547
H	-1.63561	7.91170	-1.30540
H	0.51435	8.52470	-2.36344
H	-6.77678	0.68459	-1.62269
H	-4.09026	3.21591	-0.95580
H	-5.60407	-1.93929	1.56420
H	-2.47033	-0.01734	2.36661
H	5.61931	0.79116	1.23835
H	2.88508	3.35312	1.53883
H	5.17587	0.28791	-2.99916
H	2.16302	2.48667	-3.27446
H	-2.39149	-2.15580	1.03859
H	-2.00303	-2.33528	2.78623
H	-3.59836	-2.87069	2.16928
H	-3.26985	-0.87262	4.50714
H	-4.38954	0.40441	3.91688
H	-4.86192	-1.33338	3.79553
H	-6.39433	3.63358	-0.07836
H	-6.02476	4.45595	-1.63546
H	-7.07392	2.99382	-1.62665
H	-3.69793	1.73581	-2.88928
H	-5.46446	1.74690	-3.27486
H	-4.50758	3.27245	-3.34672
H	3.57517	0.11989	-4.61468
H	2.17160	-0.05995	-3.50716
H	2.00750	0.89925	-5.01686
H	4.29451	3.71239	-3.76110
H	4.95182	2.23467	-4.55761
H	3.49920	3.06254	-5.23743
H	5.21539	4.20045	1.34005
H	4.62852	4.06641	3.03617
H	5.78678	2.84682	2.39203
H	4.14279	0.99408	3.04023
H	2.92460	2.18060	3.62928
H	2.47303	0.99818	2.35096
H	7.02886	-3.89837	-1.50973
H	8.75794	-4.04502	-1.06015
H	7.35080	-3.56092	0.95969
H	8.48284	-2.61735	-3.11132
H	6.15146	-1.40289	1.16149
H	5.51265	-2.33461	-0.22447

H	9.69216	-2.66289	0.88581
H	8.61466	-1.55007	1.78721
H	7.33107	-0.41700	-2.94409
H	6.18833	-1.77188	-2.62156
H	7.82019	0.59771	0.68707
H	8.25385	0.97514	-1.00514
H	9.76855	-0.61576	-2.30026
H	10.36689	-2.11557	-1.52303
H	10.07809	-0.28571	0.17325
H	-8.85738	-3.52270	-2.71437
H	-10.32029	-4.09076	-1.84883
H	-10.45923	-1.62624	-2.32491
H	-8.24051	-5.01216	-0.78464
H	-8.88155	-0.05817	-1.20989
H	-8.00978	-1.15202	-2.34539
H	-11.54260	-2.52659	-0.24220
H	-10.93832	-0.86005	0.02057
H	-6.61585	-3.49663	0.30611
H	-6.70073	-3.15909	-1.44617
H	-8.77437	-0.47805	1.31412
H	-7.88094	-1.87830	1.97464
H	-8.69817	-4.24935	1.56977
H	-10.22576	-4.52186	0.67339
H	-10.31507	-2.35630	1.94279
H	-1.92128	-4.63731	-0.80967
H	-0.82575	-1.16243	-3.12940
H	-3.21444	-0.58594	-3.38536
H	-4.31047	-3.99795	-0.99718
H	0.40080	-4.29298	-1.37583
H	3.05075	-3.79773	-1.66529
H	3.58575	-2.34675	-2.56481
H	2.13169	-0.89981	-1.13255
H	3.24572	-1.81763	-0.09696
H	0.46195	-1.65346	0.17171
C	5.69259	-1.49052	4.84276
H	3.06396	-0.79488	4.65760
C	0.94989	-1.46285	3.23909
C	4.44885	-4.84480	1.35936
H	5.91622	-3.57213	3.10724
H	5.46642	-5.11247	1.65326
H	3.80903	-5.72019	1.47427
H	4.45498	-4.61047	0.29226
H	0.55283	-1.05279	2.30591
H	0.23733	-2.21318	3.58766
H	0.98177	-0.64984	3.96815
H	6.17720	-0.64461	4.33923
H	5.27363	-1.11335	5.78000
H	6.47277	-2.21856	5.08197
H	-4.94359	-1.97369	-2.31746

Pre TS-9Si
ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.952948
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.383094
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.188011
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	0.44167	5.30880	1.48061
C	-0.60019	4.43891	1.09481
C	0.25973	6.21093	2.53090
C	-1.82346	4.47903	1.80947
C	-0.45031	3.51736	0.02894
C	-1.99518	5.39967	2.85518
C	-2.85650	3.59543	1.47709
C	-0.95627	6.26040	3.21217
C	-1.43719	2.53330	-0.18151
C	0.72013	3.55700	-0.89421
C	-2.66328	2.60241	0.50822
O	-1.25389	1.58529	-1.15600
C	-3.77784	1.66818	0.19238
C	1.55502	2.42374	-0.96862
C	1.01522	4.69565	-1.68717
C	2.22769	4.73494	-2.42147
C	0.13108	5.79227	-1.77922
C	3.10840	3.64898	-2.37590
C	2.54950	5.86732	-3.18643
C	2.77451	2.49071	-1.66637
C	3.75390	1.37894	-1.59498
O	1.24440	1.29935	-0.24746
C	0.46188	6.90825	-2.55103
C	1.66951	6.94848	-3.24740
P	-0.09170	0.47066	-0.79657
C	-4.21117	0.70714	1.15192
C	-4.47264	1.78590	-1.04340
C	4.54178	1.21135	-0.42544
C	3.95883	0.52342	-2.71204
C	-5.55868	0.93256	-1.30136
C	-4.13048	2.85610	-2.08468
C	-6.02829	0.00686	-0.35544
C	-5.33472	-0.09129	0.86477
C	-7.29221	-0.82481	-0.67141
C	-3.53314	0.54565	2.51592
C	4.93482	-0.48738	-2.62956
C	3.18751	0.69827	-4.02324
C	5.68642	-0.70526	-1.45867
C	5.47350	0.16140	-0.37389
C	6.73079	-1.83650	-1.33167
C	4.44036	2.15873	0.77255
C	-3.06140	-0.89350	2.76765
C	-4.46211	1.00840	3.64573

C	-5.29996	3.83009	-2.28061
C	-3.71318	2.22382	-3.41968
C	3.95048	1.42002	2.02157
C	5.77618	2.86516	1.03909
C	2.55236	-0.61435	-4.51104
C	4.10051	1.28195	-5.10817
O	-0.51438	-0.33905	0.42218
O	0.21528	-0.27510	-2.06135
C	7.49421	-4.73177	-1.24273
C	7.41294	-3.87900	0.03921
C	7.89428	-3.83386	-2.43078
C	6.35040	-2.77415	-0.14415
C	8.78671	-3.23201	0.31811
C	6.83877	-2.72231	-2.61559
C	8.13836	-1.22303	-1.06161
C	9.27009	-3.19366	-2.15529
C	9.19042	-2.33844	-0.87456
C	-9.47536	-1.50730	-2.58603
C	-9.75694	-0.66792	-1.32098
C	-8.31855	-2.49135	-2.30810
C	-8.49252	0.13439	-0.94457
C	-10.14069	-1.60191	-0.15600
C	-7.04497	-1.69959	-1.93792
C	-7.71321	-1.78096	0.49290
C	-8.70521	-3.42267	-1.14199
C	-8.98070	-2.57941	0.11943
C	-1.64459	-5.21284	-0.75396
C	-1.45820	-3.81211	-0.66441
C	-2.56192	-2.98012	-0.35462
C	-3.81352	-3.53037	-0.13069
C	-3.96940	-4.91513	-0.22373
C	-2.89375	-5.76274	-0.54032
C	-0.21206	-3.14510	-0.81967
S	1.26537	-3.83034	-1.21753
C	2.36295	-2.38834	-0.91214
C	2.64589	-2.18059	0.58950
N	1.42125	-2.03008	1.34893
S	1.29222	-2.60326	2.90499
C	2.12619	-1.41937	3.98964
Cl	-5.53284	-5.61993	0.07574
O	-0.13605	-2.59628	3.22387
O	2.07236	-3.84801	2.95547
C	1.65983	-0.07466	4.16508
C	2.41098	0.76343	5.06101
C	3.54940	0.24133	5.73114
C	3.95905	-1.05438	5.53224
C	3.24021	-1.89188	4.65038
C	0.54343	0.49273	3.49102
C	0.21034	1.81496	3.68506
C	0.94478	2.63772	4.56647

C	2.01959	2.11618	5.24623
H	1.40527	5.28606	0.98892
H	1.06649	6.87221	2.81963
H	-2.92788	5.44416	3.40495
H	-3.80740	3.65863	1.99250
H	-1.09130	6.96215	4.02502
H	-0.82337	5.79155	-1.26998
H	4.05812	3.69978	-2.89541
H	3.47830	5.91298	-3.74286
H	-0.22286	7.74434	-2.61154
H	1.92086	7.81677	-3.84271
H	-6.07265	1.02495	-2.24640
H	-3.27921	3.48316	-1.75832
H	-5.66637	-0.78246	1.62125
H	-2.62188	1.16766	2.57535
H	5.09394	-1.10257	-3.49862
H	2.34596	1.40862	-3.88990
H	6.05133	0.02873	0.52862
H	3.70820	2.96929	0.58693
H	-2.37981	-1.21977	1.96069
H	-2.49984	-0.94396	3.72505
H	-3.91163	-1.60365	2.82933
H	-4.81320	2.04428	3.45785
H	-5.34797	0.34431	3.73331
H	-3.91715	0.99888	4.61389
H	-5.59403	4.26991	-1.30351
H	-4.99522	4.65844	-2.95550
H	-6.18164	3.32358	-2.72638
H	-2.89386	1.49187	-3.25942
H	-4.56484	1.70339	-3.90573
H	-3.34390	3.01026	-4.11209
H	4.67514	0.64582	2.35034
H	3.80546	2.14179	2.85266
H	2.97626	0.93270	1.81163
H	6.55661	2.14906	1.37170
H	6.12548	3.37606	0.11632
H	5.64771	3.63264	1.83218
H	2.00314	-1.11385	-3.69053
H	1.83162	-0.40184	-5.32935
H	3.31529	-1.31847	-4.90375
H	4.53635	2.24434	-4.76839
H	4.92980	0.58302	-5.34897
H	3.51773	1.47428	-6.03425
H	6.51164	-5.21315	-1.44295
H	8.24154	-5.54507	-1.11182
H	7.12842	-4.52746	0.89636
H	7.95128	-4.44849	-3.35549
H	6.26494	-2.20911	0.80815
H	5.36154	-3.24430	-0.33289
H	9.55302	-4.02245	0.47637

H	8.73942	-2.62545	1.24925
H	7.13333	-2.10143	-3.49084
H	5.85701	-3.19534	-2.84215
H	8.13379	-0.59052	-0.14854
H	8.43573	-0.56701	-1.90981
H	9.57559	-2.56071	-3.01735
H	10.04145	-3.98610	-2.03614
H	10.18359	-1.88069	-0.67416
H	-9.21075	-0.83917	-3.43500
H	-10.38922	-2.06926	-2.87942
H	-10.59497	0.03449	-1.52206
H	-8.12419	-3.10036	-3.21771
H	-8.69697	0.75304	-0.04245
H	-8.26926	0.83745	-1.77463
H	-11.06344	-2.16830	-0.41058
H	-10.35970	-1.00357	0.75570
H	-6.20664	-2.40709	-1.75601
H	-6.75643	-1.07385	-2.80903
H	-7.92162	-1.19639	1.41666
H	-6.89969	-2.50230	0.72133
H	-7.88508	-4.14573	-0.94575
H	-9.60909	-4.01277	-1.40995
H	-9.25624	-3.25221	0.96060
H	-0.80319	-5.86241	-0.97450
H	-2.39863	-1.90969	-0.27148
H	-4.65346	-2.90141	0.12873
H	-3.05094	-6.83329	-0.59789
H	-0.22675	-2.06366	-0.68906
H	1.86265	-1.52456	-1.36562
H	3.28538	-2.60194	-1.45577
H	3.28728	-1.29205	0.65336
H	3.19543	-3.03132	0.99879
H	0.76076	-1.25900	1.10409
H	4.09851	0.89542	6.40332
H	4.83226	-1.44370	6.04612
H	3.55115	-2.91691	4.48693
H	-0.05145	-0.09652	2.80618
H	-0.63133	2.23288	3.14690
H	0.65883	3.67674	4.70183
H	2.59832	2.73386	5.92771

Post TS-9Si

ONIOM(B3LYP/6-31G(d,p):UFF) Energy = -2343.984411
ONIOM(B3LYP/6-31G(d,p):UFF) Free Energy = -2342.410350
M06-2X/6-31G(d,p) Derived free energy in solution = -4822.222249
Number of Imaginary Frequencies = 0

ONIOM(B3LYP/6-31G(d,p):UFF) Geometry

C	-0.27673	6.17001	1.62902
C	-1.14206	5.18161	1.10812

C	-0.76091	7.16190	2.48452
C	-2.49823	5.18711	1.51920
C	-0.69035	4.18198	0.20297
C	-2.97263	6.19594	2.37297
C	-3.36047	4.17465	1.09382
C	-2.10663	7.18103	2.84739
C	-1.54462	3.09398	-0.10917
C	0.67258	4.24699	-0.40753
C	-2.88299	3.10713	0.32694
O	-1.14277	2.09578	-0.96536
C	-3.79360	1.96918	0.03986
C	1.55031	3.16606	-0.19767
C	1.12576	5.37752	-1.13508
C	2.50070	5.48517	-1.46466
C	0.24762	6.40407	-1.54339
C	3.38533	4.45685	-1.12085
C	2.97377	6.62121	-2.14047
C	2.91277	3.27583	-0.53546
C	3.85664	2.15322	-0.28068
O	1.09056	2.03551	0.42524
C	0.73206	7.52395	-2.22294
C	2.09152	7.63594	-2.51378
P	0.11419	1.15466	-0.52282
C	-4.33116	1.78359	-1.26249
C	-4.18614	1.09903	1.09350
C	4.19227	1.79087	1.05365
C	4.45854	1.45600	-1.36945
C	-5.11722	0.08122	0.82948
C	-3.65344	1.24797	2.52103
C	-5.65076	-0.13310	-0.45149
C	-5.22824	0.72128	-1.48880
C	-6.69845	-1.25062	-0.65718
C	-4.02643	2.74551	-2.41416
C	5.38832	0.43400	-1.09914
C	4.16499	1.80234	-2.83415
C	5.70573	0.04075	0.21361
C	5.07689	0.72062	1.26958
C	6.70733	-1.09319	0.52916
C	3.67722	2.56170	2.27284
C	-5.29930	3.46342	-2.88173
C	-3.34083	2.02757	-3.58454
C	-2.99796	-0.04346	3.01796
C	-4.76739	1.69090	3.47796
C	2.86600	1.65559	3.21036
C	4.83329	3.23177	3.02694
C	3.68463	0.58426	-3.63726
C	5.39739	2.42762	-3.50092
O	-0.42566	0.12028	0.54967
O	0.72834	0.58667	-1.74335
C	9.46462	-2.27109	0.54249

C	8.35650	-2.83386	-0.36930
C	8.82865	-1.68912	1.82030
C	7.37752	-1.70207	-0.74676
C	7.59048	-3.94856	0.37232
C	7.85324	-0.55305	1.44132
C	5.96637	-2.24380	1.27400
C	8.05919	-2.80069	2.56667
C	6.95326	-3.37001	1.65179
C	-7.60978	-3.84236	-1.85115
C	-8.23315	-2.49893	-2.28095
C	-7.15227	-3.74802	-0.38168
C	-7.18545	-1.37355	-2.13770
C	-9.44931	-2.18391	-1.38633
C	-6.09776	-2.62964	-0.24336
C	-7.94859	-0.95882	0.22784
C	-8.36456	-3.42839	0.51869
C	-8.99321	-2.08714	0.08361
C	2.25707	-2.48248	-1.84512
C	1.05663	-3.16344	-2.08057
C	1.10072	-4.49293	-2.51473
C	2.32317	-5.13445	-2.70849
C	3.50414	-4.43554	-2.46536
C	3.48248	-3.11091	-2.03503
C	-0.22729	-2.39031	-1.90230
S	-1.52652	-2.75481	-3.15681
C	-2.63889	-1.72022	-2.14700
C	-2.38840	-2.17715	-0.70780
N	-0.91232	-2.41615	-0.52177
S	-0.63102	-3.89516	0.41034
C	-1.54707	-3.60600	1.94234
Cl	5.05290	-5.23372	-2.71443
O	-1.28133	-5.01872	-0.27670
O	0.79826	-3.93666	0.71335
C	-1.00037	-2.86774	3.04374
C	-1.77355	-2.85502	4.25793
C	-3.02392	-3.52514	4.31070
C	-3.51497	-4.20765	3.22371
C	-2.75810	-4.26405	2.03484
C	0.23096	-2.15594	3.02617
C	0.66884	-1.48221	4.14431
C	-0.08643	-1.47821	5.33842
C	-1.28267	-2.15258	5.39063
H	0.77910	6.17725	1.39554
H	-0.08794	7.91641	2.87114
H	-4.01038	6.21412	2.68474
H	-4.39862	4.18189	1.40612
H	-2.47650	7.95229	3.51063
H	-0.81558	6.34383	-1.35173
H	4.44003	4.55259	-1.34919
H	4.02400	6.71939	-2.38889

H	0.04982	8.30736	-2.52684
H	2.46125	8.50702	-3.03916
H	-5.43700	-0.54954	1.64526
H	-2.85839	2.01777	2.57537
H	-5.61644	0.59727	-2.48586
H	-3.33180	3.54719	-2.09434
H	5.86093	-0.04916	-1.93733
H	3.34489	2.54275	-2.91136
H	5.29979	0.43431	2.28640
H	3.00313	3.38727	1.97387
H	-5.78926	3.96599	-2.02030
H	-5.04343	4.23918	-3.63481
H	-6.01953	2.75463	-3.34175
H	-2.40298	1.54479	-3.24143
H	-4.00020	1.25478	-4.03177
H	-3.07577	2.76079	-4.37592
H	-2.24153	-0.39116	2.28789
H	-2.48573	0.14341	3.98551
H	-3.74544	-0.84923	3.17007
H	-5.23460	2.63000	3.11454
H	-5.55489	0.91262	3.56533
H	-4.34703	1.88211	4.48842
H	3.51258	0.90098	3.70511
H	2.37868	2.26657	3.99986
H	2.07194	1.12516	2.64501
H	5.52065	2.47952	3.46814
H	5.40981	3.88270	2.33518
H	4.43485	3.86562	3.84790
H	2.79981	0.13137	-3.15365
H	3.38628	0.90009	-4.65981
H	4.47571	-0.18777	-3.73405
H	5.75200	3.30161	-2.91610
H	6.22707	1.69323	-3.57751
H	5.14068	2.77738	-4.52367
H	10.03442	-1.48043	0.00644
H	10.18432	-3.07640	0.80825
H	8.81423	-3.25150	-1.29249
H	9.62824	-1.28622	2.47944
H	6.61217	-2.12356	-1.43056
H	7.93479	-0.91517	-1.30249
H	8.28431	-4.77744	0.63416
H	6.80147	-4.37238	-0.28660
H	7.45561	-0.11517	2.38057
H	8.40707	0.25649	0.91582
H	5.15822	-2.65610	0.62995
H	5.48265	-1.87223	2.20285
H	7.60932	-2.39232	3.49833
H	8.75928	-3.61179	2.86510
H	6.40695	-4.17573	2.18881
H	-6.74366	-4.08678	-2.50492

H	-8.35362	-4.66122	-1.96606
H	-8.56181	-2.56661	-3.34090
H	-6.70573	-4.71774	-0.07092
H	-7.64859	-0.41913	-2.47374
H	-6.32666	-1.59560	-2.80977
H	-10.21773	-2.98074	-1.49446
H	-9.91791	-1.22630	-1.70335
H	-5.73195	-2.61923	0.80520
H	-5.23039	-2.87161	-0.88987
H	-8.40456	0.01240	-0.06736
H	-7.67141	-0.87416	1.30027
H	-8.04360	-3.37133	1.58218
H	-9.11819	-4.24285	0.44323
H	-9.87089	-1.86369	0.72843
H	2.22634	-1.44886	-1.51750
H	0.17834	-5.03705	-2.68754
H	2.35927	-6.16470	-3.04369
H	4.40521	-2.57424	-1.86312
H	0.01494	-1.33555	-2.03405
H	-3.67619	-1.88116	-2.44397
H	-2.39323	-0.66415	-2.28214
H	-2.92762	-3.10941	-0.53688
H	-2.72139	-1.43045	0.01663
H	-0.46111	-0.82636	0.22179
H	-3.59023	-3.48836	5.23738
H	-4.46974	-4.72064	3.27467
H	-3.10794	-4.85057	1.19335
H	0.83865	-2.15894	2.13271
H	1.61446	-0.95180	4.10742
H	0.27954	-0.94199	6.20852
H	-1.87949	-2.15410	6.29847

Cartesian coordinates and energies for the truncated TS

4-ClC_6H_4 replaced for H

TS-4Re
M06-2X/6-31G(d,p) Energy = -4085.498203

C	-2.29697	6.45651	0.66559
C	-1.18172	7.23347	0.27486
C	0.01213	6.61384	-0.01028
C	0.14655	5.20282	0.09093
C	-0.96649	4.41592	0.53034
C	-2.19293	5.08891	0.79139
C	1.35766	4.55725	-0.26216
C	1.48903	3.18452	-0.25190
C	0.37527	2.41638	0.20123
C	-0.80613	2.99013	0.65218
C	-1.89898	2.13509	1.20196

C	-2.40625	1.08290	0.44968
C	-3.60116	0.38406	0.79731
C	-4.20140	0.70815	1.99623
C	-3.64169	1.65628	2.88985
C	-2.47020	2.38117	2.49907
C	-4.22131	1.89949	4.16421
C	-3.65737	2.79897	5.03876
C	-2.48027	3.49141	4.67034
C	-1.90530	3.29178	3.43468
O	-1.80181	0.75334	-0.74895
O	0.52336	1.04444	0.27374
C	-4.23285	-0.61774	-0.12565
C	2.77506	2.54658	-0.69056
C	3.13717	2.54498	-2.05878
C	4.38211	2.01329	-2.42372
C	5.27585	1.48272	-1.49225
C	4.88861	1.48310	-0.14845
C	3.66232	2.00833	0.27290
C	-4.28735	-1.98632	0.22755
C	-4.96202	-2.87661	-0.62004
C	-5.58155	-2.46545	-1.80081
C	-5.50448	-1.11041	-2.13335
C	-4.84686	-0.17841	-1.32574
C	3.35390	2.03501	1.76981
C	2.24525	3.13481	-3.15371
C	6.64841	0.98313	-1.92927
C	-3.65252	-2.53774	1.50462
C	-6.35105	-3.45655	-2.66578
C	-4.86022	1.28800	-1.75809
P	-0.30744	0.05185	-0.76422
O	-0.31415	-1.29838	-0.07053
O	0.20065	0.13221	-2.17167
C	-6.29362	1.85509	-1.77488
C	-4.16299	1.49472	-3.11583
C	-2.67666	-3.69260	1.22008
C	-4.72589	-2.96965	2.52358
C	-5.89832	-3.44185	-4.13686
C	-7.87108	-3.22430	-2.55922
C	4.34568	2.93897	2.52822
C	3.30966	0.62231	2.37814
C	6.95336	-0.44613	-1.44677
C	7.75845	1.95571	-1.48417
C	1.93144	2.12869	-4.27623
C	2.86299	4.42454	-3.73048
H	-3.24806	6.94228	0.86334
H	-1.27551	8.31178	0.18700
H	0.87264	7.19359	-0.33408
H	-3.06142	4.51126	1.08224
H	2.20004	5.16700	-0.57676
H	-5.12703	0.21313	2.27549

H	-5.11691	1.34842	4.43929
H	-4.10558	2.97149	6.01279
H	-2.02302	4.18515	5.36991
H	-0.99966	3.82443	3.16993
H	4.67129	2.02736	-3.47208
H	5.57181	1.09024	0.60005
H	-5.01766	-3.92598	-0.33967
H	-5.98346	-0.76035	-3.04351
H	2.36126	2.47187	1.90241
H	1.28926	3.40286	-2.69820
H	6.64938	0.96639	-3.02744
H	-3.06858	-1.73361	1.95968
H	-6.14586	-4.45943	-2.26643
H	-4.30174	1.86768	-1.01983
H	-6.77512	1.74801	-0.79751
H	-6.28010	2.92011	-2.03186
H	-6.92170	1.34425	-2.51282
H	-3.13261	1.13234	-3.08467
H	-4.68924	0.97131	-3.92198
H	-4.14276	2.55961	-3.37300
H	-1.89515	-3.38296	0.52423
H	-2.19104	-4.01621	2.14723
H	-3.18536	-4.56768	0.80087
H	-5.40138	-2.14605	2.77596
H	-5.33810	-3.78916	2.13083
H	-4.25770	-3.31956	3.45042
H	-4.82386	-3.62846	-4.22878
H	-6.42675	-4.21138	-4.70984
H	-6.10756	-2.47704	-4.61081
H	-8.20749	-3.28152	-1.51955
H	-8.14386	-2.23525	-2.94335
H	-8.42165	-3.97336	-3.13921
H	4.34593	3.95513	2.12143
H	4.07675	2.99761	3.58869
H	5.36985	2.55533	2.46587
H	3.06586	0.67060	3.44489
H	2.54397	0.01396	1.88980
H	4.27462	0.11091	2.28559
H	6.19879	-1.15896	-1.79622
H	7.92703	-0.77988	-1.82130
H	6.98432	-0.50457	-0.35352
H	7.56985	2.96585	-1.85966
H	7.81603	2.01228	-0.39160
H	8.73617	1.62918	-1.85577
H	1.29901	2.60462	-5.03422
H	1.38891	1.26841	-3.87861
H	2.83944	1.78246	-4.78358
H	3.04858	5.16887	-2.94951
H	3.81883	4.22139	-4.22654
H	2.19176	4.87178	-4.47170

C	0.82194	-2.93827	-2.82785
S	2.29298	-2.74424	-3.73067
N	1.69043	-2.84508	-0.91221
H	0.35131	-1.99271	-2.55907
S	1.79655	-4.41512	-0.16949
H	0.92868	-2.23775	-0.46777
O	0.41566	-4.77829	0.13601
O	2.61157	-5.22014	-1.08424
C	4.32340	-4.10572	3.64313
C	2.74182	-4.19694	1.34903
C	3.96920	-4.83037	1.37232
C	4.76954	-4.78356	2.53343
H	4.93237	-4.06659	4.54232
H	4.30177	-5.37368	0.49581
H	5.72986	-5.28851	2.54089
C	3.06732	-3.44382	3.65056
C	2.23189	-3.47722	2.47957
C	0.98716	-2.79369	2.51864
C	0.59431	-2.11925	3.65453
C	1.40854	-2.09656	4.80917
C	2.62068	-2.74579	4.80371
H	0.33311	-2.77887	1.65842
H	-0.35405	-1.59173	3.65218
H	1.07689	-1.56285	5.69449
H	3.26043	-2.73398	5.68183
C	2.96643	-2.15475	-1.17160
H	3.13279	-1.37882	-0.41777
H	3.77883	-2.88210	-1.12097
C	2.94030	-1.49439	-2.56648
H	2.27518	-0.62815	-2.57175
H	3.94069	-1.19992	-2.88506
H	0.17381	-3.77906	-2.96163

TS-4Si

M06-2X/6-31G(d,p) Energy = -4085.497369

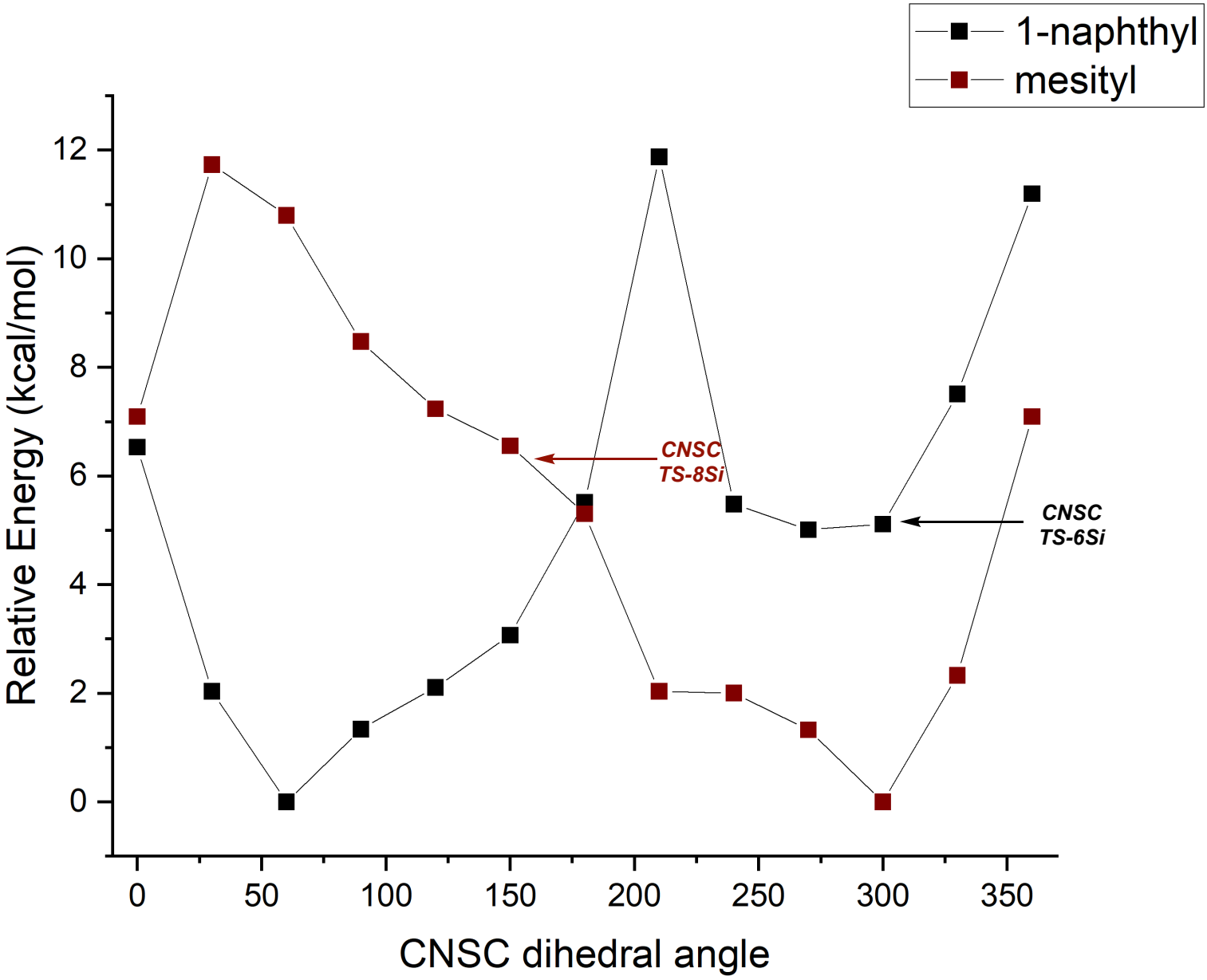
C	1.88075	5.11883	3.73609
C	0.62194	5.70393	4.00823
C	-0.46894	5.35622	3.24675
C	-0.34959	4.42046	2.18391
C	0.93012	3.85787	1.87705
C	2.03199	4.22549	2.69888
C	-1.47784	4.01738	1.42867
C	-1.40501	3.03404	0.46353
C	-0.12303	2.47173	0.17850
C	1.04249	2.93176	0.78089
C	2.37860	2.48233	0.29547
C	2.67851	1.13014	0.20436
C	3.98624	0.64444	-0.09561

C	4.96770	1.57803	-0.35784
C	4.69752	2.96764	-0.41163
C	3.38060	3.43637	-0.10373
C	5.70439	3.89837	-0.78510
C	5.42367	5.24040	-0.88943
C	4.11282	5.70323	-0.62896
C	3.12108	4.82836	-0.24417
O	1.69362	0.20453	0.50875
O	-0.05024	1.52482	-0.82121
C	4.32420	-0.81683	-0.10509
C	-2.64916	2.61274	-0.26116
C	-2.83964	2.96438	-1.61866
C	-4.04905	2.63065	-2.24192
C	-5.08115	1.96945	-1.57289
C	-4.86747	1.62489	-0.23521
C	-3.67913	1.93458	0.43848
C	4.38896	-1.53671	1.11033
C	4.79307	-2.87593	1.08429
C	5.14475	-3.52842	-0.09736
C	5.06420	-2.80095	-1.28774
C	4.66396	-1.45967	-1.32196
C	-3.55433	1.52982	1.90857
C	-1.80307	3.75681	-2.41569
C	-6.41237	1.70507	-2.26745
C	4.08168	-0.89581	2.46315
C	5.64609	-4.96705	-0.06593
C	4.64216	-0.74288	-2.67422
P	0.45416	-0.03873	-0.55372
O	0.90338	-0.54982	-1.88950
O	-0.59395	-0.81792	0.21754
C	3.67299	-1.40244	-3.67216
C	6.05919	-0.63119	-3.27069
C	5.32151	-0.88503	3.37833
C	2.88155	-1.56834	3.15523
C	7.14595	-5.04461	-0.41082
C	4.82636	-5.90310	-0.97035
C	-3.54946	0.00115	2.08095
C	-4.64433	2.18661	2.77723
C	-7.51397	2.63500	-1.72102
C	-6.85646	0.23374	-2.18965
C	-2.35470	5.13628	-2.82777
C	-1.28278	2.97822	-3.63806
H	2.73677	5.37296	4.35440
H	0.51848	6.41352	4.82375
H	-1.44750	5.78093	3.45552
H	3.00164	3.78110	2.51048
H	-2.43833	4.47930	1.64080
H	5.97877	1.23637	-0.56095
H	6.70084	3.52287	-1.00293
H	6.19836	5.94210	-1.18405

H	3.88370	6.75929	-0.73821
H	2.12152	5.20126	-0.05768
H	-4.20305	2.92123	-3.27876
H	-5.65669	1.11773	0.31359
H	4.85399	-3.42671	2.02000
H	5.33790	-3.28350	-2.22269
H	-2.59075	1.88711	2.27592
H	-0.94517	3.94135	-1.76517
H	-6.27463	1.95073	-3.32898
H	3.80783	0.14772	2.29100
H	5.52752	-5.32427	0.96559
H	4.27603	0.27297	-2.51207
H	2.65144	-1.35760	-3.28849
H	3.69984	-0.86978	-4.62978
H	3.93989	-2.44675	-3.87140
H	6.03733	-0.05871	-4.20457
H	6.74843	-0.13033	-2.58287
H	6.47950	-1.61760	-3.49627
H	6.16229	-0.37384	2.89866
H	5.10007	-0.36612	4.31771
H	5.64865	-1.89978	3.62940
H	1.99481	-1.51028	2.51878
H	3.08563	-2.62223	3.37648
H	2.65864	-1.06563	4.10349
H	7.33338	-4.69875	-1.43334
H	7.51115	-6.07483	-0.33337
H	7.73839	-4.41984	0.26452
H	3.76370	-5.87315	-0.71059
H	4.92991	-5.62434	-2.02541
H	5.17088	-6.93823	-0.87184
H	-2.69952	-0.43838	1.55224
H	-3.45587	-0.26296	3.13982
H	-4.47682	-0.45233	1.71068
H	-4.48927	1.93857	3.83291
H	-4.63289	3.27721	2.68077
H	-5.64691	1.84143	2.50154
H	-7.22263	3.68557	-1.81230
H	-8.45260	2.49109	-2.26764
H	-7.70796	2.43430	-0.66167
H	-6.10750	-0.43736	-2.62343
H	-7.02753	-0.08163	-1.15490
H	-7.79328	0.08496	-2.73712
H	-1.57944	5.71988	-3.33601
H	-2.69133	5.70547	-1.95544
H	-3.20376	5.04487	-3.51403
H	-0.80006	2.04654	-3.33216
H	-2.08995	2.74273	-4.34129
H	-0.54097	3.57558	-4.17941
S	-2.36141	-4.15689	-0.58415
N	-2.00598	-2.56204	-1.21117

S	-2.21078	-2.04940	-4.03838
C	-2.81210	-0.86910	-2.78519
H	-2.03620	-0.13511	-2.56201
H	-3.68702	-0.34856	-3.17517
C	-3.16455	-1.71189	-1.54944
H	-3.39379	-1.04950	-0.71060
H	-4.02379	-2.34827	-1.76842
H	-1.33547	-2.00678	-0.58420
O	-1.05329	-4.72942	-0.27958
O	-3.24988	-4.75831	-1.58300
C	-4.96649	-3.83802	3.17020
C	-5.49569	-4.18209	1.94884
C	-4.65811	-4.23944	0.81597
C	-3.31336	-3.93948	0.92810
H	-5.60179	-3.79989	4.05104
H	-6.54886	-4.42259	1.84791
H	-5.05536	-4.54339	-0.14492
C	-2.71457	-3.56637	2.17732
C	-3.58954	-3.52844	3.31974
C	-3.06165	-3.17808	4.59065
C	-1.73066	-2.86824	4.73881
C	-0.87433	-2.89371	3.61537
C	-1.34623	-3.23438	2.36687
H	-3.73479	-3.15868	5.44330
H	-1.33574	-2.59935	5.71366
H	0.17286	-2.63544	3.73118
H	-0.66346	-3.23653	1.52940
C	-0.95788	-2.67386	-2.99182
H	-0.28521	-1.91306	-2.58340
H	-0.51723	-3.62585	-3.20266

Relaxed scans for 1-naphthyl and mesityl substituted sulfonamides



Examination of other computational methods

Although ONIOM calculations have shown to give excellent results with similar reactions and catalysts we tested some additional methods routinely employed in studies of this type (using Gaussian 16 rev C.01). Each test confirmed TS-6Re to be the lowest transition state structure, thus, validating the ONIOM calculations used for our analysis.

As a first step we re-evaluated the geometry of the transition state structures by performing a re-optimization at the B3LYP/6-31G(d) level of theory. Single point energy calculations with the IEFPCM(toluene) model and two different functionals/basis sets were performed on these structures.

Table S1. Comparison of DFT functionals with the 6-31G(d,p) and 6-311G(d,p) basis sets.

	Solvent Derived Relative Free Energies			
Transition State	M06-2X/6-31G(d,p)	ωB97XD/6-31G(d,p)	M06-2X/6-311G(d,p)	ωB97XD/6-311G(d,p)
TS-6Re	0	0	0	0
TS-6Si	2.2	2	1.7	1.6
TS-7Si	3.3	1.5	2.1	0.6

We also re-evaluated the geometry of the transition state structures by performing a re-optimization at the ωB97XD/6-31G(d) level of theory. Single point energies were then performed on these structures to confirm TS-6Re to be lowest in energy. However, the computed ee is much lower when moving from a B3LYP to a ωB97XD optimization as the monocoordination TS is more stabilized (compare TS-6Re to TS-7Si), in line with previous studies on similar systems.[18]

Table S2. Comparison of DFT functionals with the 6-31G(d,p) basis set with a ωB97XD/6-31G(d) optimized TS.

	Solvent Derived Free Energies	
Transition State	M06-2X/6-31G(d,p)	ωB97XD/6-31G(d,p)
TS-6Re	0	0
TS-6Si	3.1	3.4
TS-7Si	0.4	0.3

As a final validation we re-evaluated the geometry of the transition state structures (TS-8Re, TS-8Si and TS-9Si) by performing a re-optimization at the B3LYP/6-31G(d) level of theory. These trends mirror those observed from the ONIOM calculations and a decrease in enantioselectivity is expected.

Table S3. Comparison of DFT functionals with the 6-31G(d,p) basis set with a B3LYP/6-31G(d) optimized TS.

	Solvent Derived Free Energies	
Transition State	M06-2X/6-31G(d,p)	ωB97XD/6-31G(d,p)
TS-8Re	0	0
TS-8Si	2.3	1.1
TS-9Si	0.6	0.3

As part of our investigation we also tested larger basis sets in the single point energy evaluation with the smaller TRIP system. Our analysis with 6-311+G(d,p) and def2-TZVP showed that the TS energy ordering remained unaltered.

Table S4. Comparing larger basis sets with the TRIP TS in the gas phase.

	Gas Derived Free Energies		
Transition State	M06-2X/6-311+G(d,p)	M06-2X/def2-TZVP	M06-2X/6-31G(d,p)
TS-4Re	0	0	0
TS-4Si	2.6	3.1	3.0
TS-5Re	4.1	4.0	4.8
TS-5Si	1.0	2.1	2.4

Table S5. Comparing larger basis sets with the TRIP TS in the solution phase.

	Solvent Derived Free Energies		
Transition State	M06-2X/6-311+G(d,p)	M06-2X/def2-TZVP	M06-2X/6-31G(d,p)
TS-4Re	0	0	0
TS-4Si	2.9	3.4	3.1
TS-5Re	3.3	3.2	4.0
TS-5Si	0.9	2.0	2.3

Cartesian coordinates and energies of the re-optimized TS

TS-6Re
B3LYP/6-31G(d) Energy = -5320.580726
B3LYP/6-31G(d) Free Energy = -5319.160152
Number of Imaginary Frequencies = 1 (-167.54)

B3LYP/6-31G(d) Geometry

C	0.10643	5.58853	2.35516
C	-0.83754	4.68687	1.78972
C	-0.22682	6.39043	3.42474
C	-2.13908	4.61686	2.38256
C	-0.53140	3.82579	0.67923
C	-2.45770	5.47144	3.47236
C	-3.08604	3.69557	1.86800
C	-1.52505	6.34322	3.98511
C	-1.44988	2.84144	0.33602
C	0.72307	3.98769	-0.11274
C	-2.76947	2.78857	0.87728
O	-1.12469	1.92937	-0.65009
C	-3.81495	1.84518	0.35692
C	1.58183	2.91222	-0.29869
C	1.04662	5.24287	-0.73961
C	2.30862	5.38103	-1.40236
C	0.15787	6.35409	-0.76738
C	3.18321	4.26799	-1.46705
C	2.65329	6.62064	-2.00563
C	2.83896	3.03080	-0.96380
C	3.78577	1.87513	-1.10770
O	1.25787	1.69127	0.25989
C	0.51333	7.53723	-1.37701
C	1.77889	7.68208	-1.99193
P	0.02082	0.77374	-0.36379
C	-4.33808	0.82320	1.18050
C	-4.35604	2.03686	-0.93942
C	4.54024	1.43323	0.00604
C	3.99523	1.27718	-2.37089
C	-5.40875	1.22260	-1.36126
C	-3.87055	3.13444	-1.88724
C	-5.97073	0.22343	-0.55608
C	-5.40348	0.04073	0.70711
C	-7.16852	-0.58871	-1.06814
C	-3.79775	0.53219	2.58158
C	4.96103	0.26553	-2.49306
C	3.24010	1.71424	-3.62848
C	5.73025	-0.18090	-1.41532
C	5.48458	0.41841	-0.17172
C	6.83637	-1.23736	-1.55487
C	4.40541	2.07318	1.38792
C	-3.32449	-0.92528	2.72927

C	-4.82886	0.88435	3.67230
C	-4.97897	4.16990	-2.16366
C	-3.30826	2.55445	-3.19895
C	3.98616	1.05491	2.46303
C	5.69879	2.80926	1.79082
C	2.49013	0.55366	-4.30936
C	4.18531	2.41681	-4.62427
O	-0.38273	-0.14206	0.77529
O	0.37351	0.16703	-1.68796
C	7.79758	-4.02357	-2.09946
C	7.73335	-3.46172	-0.66595
C	8.06670	-2.87007	-3.08537
C	6.59763	-2.42213	-0.57375
C	9.07610	-2.78812	-0.31572
C	6.93524	-1.82553	-2.98608
C	8.21656	-0.59847	-1.21439
C	9.41367	-2.20381	-2.74100
C	9.35038	-1.63987	-1.30804
C	-9.14702	-1.14593	-3.24188
C	-9.56314	-0.41296	-1.95004
C	-8.00081	-2.12994	-2.92964
C	-8.35660	0.36717	-1.38980
C	-10.03843	-1.44166	-0.90590
C	-6.79209	-1.35010	-2.37307
C	-7.67869	-1.63254	-0.04166
C	-8.47651	-3.15703	-1.88362
C	-8.88656	-2.41768	-0.59465
C	-1.32671	-5.13625	-0.97921
C	-1.29723	-3.72797	-0.93711
C	-2.48881	-3.01946	-0.68172
C	-3.68766	-3.69651	-0.50270
C	-3.69353	-5.09123	-0.57468
C	-2.52205	-5.81921	-0.80899
C	-0.08725	-2.95879	-1.14545
S	1.27807	-3.59041	-2.01494
C	2.39786	-2.31232	-1.34309
C	2.33738	-2.43674	0.19315
N	0.93300	-2.51042	0.63637
S	0.57718	-3.63901	1.91806
C	1.66658	-3.21177	3.28721
Cl	-5.19953	-5.95423	-0.35193
O	-0.81451	-3.37484	2.27017
O	1.00112	-4.94418	1.40381
C	1.52315	-2.00006	4.04103
C	2.41741	-1.82657	5.15505
C	3.37487	-2.83044	5.45754
C	3.47487	-3.97609	4.70365
C	2.61020	-4.16959	3.60541
C	0.58748	-0.96885	3.75999
C	0.54223	0.16750	4.53927

C	1.41145	0.33288	5.64108
C	2.32986	-0.64642	5.94002
H	1.10761	5.63099	1.94154
H	0.51632	7.06356	3.84406
H	-3.45502	5.41264	3.90223
H	-4.09139	3.69790	2.28101
H	-1.77800	6.98689	4.82330
H	-0.82034	6.26094	-0.31120
H	4.14638	4.39109	-1.95596
H	3.62137	6.70719	-2.49369
H	-0.18945	8.36607	-1.39015
H	2.04950	8.62318	-2.46290
H	-5.81815	1.39314	-2.35295
H	-3.05359	3.67300	-1.40103
H	-5.80073	-0.72300	1.36662
H	-2.92078	1.16603	2.73997
H	5.11566	-0.16677	-3.47530
H	2.48141	2.44165	-3.32888
H	6.07121	0.10971	0.68946
H	3.61483	2.82643	1.33716
H	-2.56035	-1.16479	1.98591
H	-2.88720	-1.08406	3.72242
H	-4.15018	-1.63891	2.62078
H	-5.13743	1.93434	3.61469
H	-5.73245	0.26963	3.58030
H	-4.40795	0.70879	4.66992
H	-5.35072	4.61169	-1.23213
H	-4.59559	4.98033	-2.79552
H	-5.83334	3.71986	-2.68312
H	-2.48725	1.86047	-2.99733
H	-4.07976	2.02143	-3.76817
H	-2.92529	3.36061	-3.83655
H	4.73138	0.25857	2.58180
H	3.87418	1.54763	3.43609
H	3.02441	0.59806	2.21018
H	6.54369	2.11708	1.88944
H	5.97244	3.56470	1.04586
H	5.56779	3.31467	2.75540
H	1.73239	0.14148	-3.63789
H	1.98033	0.91906	-5.20937
H	3.17023	-0.24807	-4.62376
H	4.69062	3.27438	-4.16560
H	4.96109	1.73326	-4.99061
H	3.62364	2.77960	-5.49344
H	6.85278	-4.52543	-2.35189
H	8.59050	-4.78028	-2.17591
H	7.53325	-4.27662	0.04297
H	8.10009	-3.26130	-4.11085
H	6.52051	-2.05017	0.45543
H	5.63540	-2.90072	-0.80786

H	9.88938	-3.52584	-0.35583
H	9.04759	-2.40064	0.71239
H	7.12197	-1.02012	-3.70840
H	5.97977	-2.28969	-3.26880
H	8.18935	-0.16894	-0.20503
H	8.40678	0.23490	-1.90408
H	9.63024	-1.39746	-3.45525
H	10.22991	-2.93443	-2.82661
H	10.30403	-1.15599	-1.05800
H	-8.82498	-0.41961	-4.00126
H	-10.00568	-1.68756	-3.66251
H	-10.37536	0.29263	-2.17127
H	-7.70001	-2.64997	-3.84912
H	-8.64299	0.90644	-0.47654
H	-8.03975	1.12681	-2.11493
H	-10.91003	-1.99369	-1.28429
H	-10.35840	-0.92858	0.01172
H	-5.96042	-2.03829	-2.16772
H	-6.42905	-0.64204	-3.12839
H	-7.96465	-1.12908	0.89168
H	-6.87504	-2.33753	0.21323
H	-7.67551	-3.87789	-1.66836
H	-9.32661	-3.73246	-2.27585
H	-9.21288	-3.14536	0.16033
H	-0.40581	-5.69162	-1.12268
H	-2.46601	-1.93609	-0.61184
H	-4.60203	-3.15087	-0.30125
H	-2.55329	-6.90251	-0.84112
H	-0.20214	-1.87948	-1.24646
H	2.04829	-1.32941	-1.66799
H	3.40769	-2.49162	-1.71530
H	2.82718	-1.56573	0.64094
H	2.85386	-3.34386	0.51358
H	0.46936	-1.56964	0.80256
H	4.03543	-2.67427	6.30697
H	4.20922	-4.73794	4.94640
H	2.66889	-5.07513	3.01270
H	-0.09455	-1.04689	2.92487
H	-0.17021	0.94814	4.29039
H	1.35490	1.23426	6.24463
H	3.00873	-0.53270	6.78152

TS-6Si

B3LYP/6-31G(d) Energy = -5320.579847
B3LYP/6-31G(d) Free Energy = -5319.157923
Number of Imaginary Frequencies = 1 (-183.59)

B3LYP/6-31G(d) Geometry

C	-0.55080	6.09311	1.81816

C	-1.36512	5.06451	1.26688
C	-1.07222	7.02717	2.68605
C	-2.73732	5.00994	1.67009
C	-0.86522	4.07053	0.35406
C	-3.25098	6.00100	2.54972
C	-3.55350	3.95434	1.19511
C	-2.43962	6.99358	3.04779
C	-1.67845	2.98645	0.04247
C	0.48942	4.20223	-0.25514
C	-3.05309	2.92362	0.42575
O	-1.19418	1.97973	-0.76534
C	-3.96124	1.80503	0.00756
C	1.41361	3.17119	-0.15094
C	0.86294	5.38961	-0.97913
C	2.21877	5.53591	-1.41423
C	-0.05822	6.41959	-1.31896
C	3.14196	4.49063	-1.16552
C	2.61079	6.71310	-2.10727
C	2.76815	3.29727	-0.58224
C	3.78134	2.20540	-0.40732
O	1.03910	1.99829	0.48236
C	0.34740	7.53992	-2.01049
C	1.69831	7.70011	-2.39823
P	0.01718	0.94813	-0.27988
C	-4.36117	1.66707	-1.34112
C	-4.50285	0.93100	0.98400
C	4.27181	1.88711	0.88233
C	4.32188	1.54927	-1.53700
C	-5.43024	-0.03849	0.58692
C	-4.12357	1.00262	2.46485
C	-5.85998	-0.18581	-0.73859
C	-5.29258	0.67536	-1.68242
C	-6.94749	-1.21301	-1.08757
C	-3.87067	2.60566	-2.44442
C	5.34426	0.60537	-1.35141
C	3.86341	1.84211	-2.96816
C	5.85924	0.28571	-0.09287
C	5.28786	0.93793	1.00742
C	7.02119	-0.69524	0.11721
C	3.77220	2.58725	2.14618
C	-5.03171	3.43666	-3.02720
C	-3.11076	1.85644	-3.55511
C	-3.40781	-0.27678	2.93249
C	-5.34197	1.31738	3.35440
C	3.13822	1.59608	3.13989
C	4.89151	3.40951	2.81525
C	3.28652	0.59739	-3.66771
C	4.99728	2.46981	-3.80354
O	-0.47565	0.00511	0.79856
O	0.59000	0.38002	-1.54461

C	9.87825	-1.51552	-0.27848
C	8.71842	-2.27694	-0.95015
C	9.38940	-0.92315	1.05741
C	7.54562	-1.30765	-1.20671
C	8.25275	-3.42164	-0.02882
C	8.21659	0.04255	0.79274
C	6.58714	-1.86792	1.04471
C	8.91712	-2.06264	1.98344
C	7.76272	-2.83134	1.30780
C	-7.92324	-3.69994	-2.44702
C	-8.37055	-2.29934	-2.90881
C	-7.64364	-3.66956	-0.93186
C	-7.26037	-1.27155	-2.60505
C	-9.65939	-1.89983	-2.16303
C	-6.53027	-2.64335	-0.63694
C	-8.26938	-0.84099	-0.35014
C	-8.92759	-3.26539	-0.17872
C	-9.38094	-1.86783	-0.64755
C	2.45522	-2.68914	-1.78205
C	1.22864	-3.35445	-1.98072
C	1.22907	-4.72622	-2.30193
C	2.42593	-5.41150	-2.45392
C	3.63002	-4.72372	-2.27154
C	3.65679	-3.36910	-1.93390
C	0.01468	-2.56410	-1.86984
S	-1.41615	-3.00670	-2.76869
C	-2.50986	-2.00912	-1.70223
C	-2.29178	-2.52509	-0.26942
N	-0.84358	-2.54963	0.01511
S	-0.25467	-3.87857	0.99313
C	-1.13540	-3.81917	2.56154
Cl	5.13995	-5.58927	-2.46510
O	-0.69465	-5.08171	0.28175
O	1.16020	-3.58222	1.19524
C	-0.81969	-2.87529	3.59519
C	-1.54550	-3.01322	4.83076
C	-2.52072	-4.03495	4.97119
C	-2.79341	-4.91201	3.94784
C	-2.08848	-4.80625	2.73090
C	0.13620	-1.82964	3.48968
C	0.36273	-0.97755	4.54859
C	-0.33971	-1.12166	5.76612
C	-1.27627	-2.11937	5.90082
H	0.50077	6.12962	1.55875
H	-0.42469	7.79530	3.10048
H	-4.29961	5.94846	2.83365
H	-4.60401	3.94282	1.47528
H	-2.84020	7.74179	3.72639
H	-1.09946	6.31140	-1.03952
H	4.17478	4.62449	-1.47707

H	3.64857	6.80936	-2.41801
H	-0.38015	8.30607	-2.26509
H	2.00688	8.59250	-2.93600
H	-5.84828	-0.68651	1.35264
H	-3.41109	1.82019	2.59310
H	-5.59643	0.60506	-2.72092
H	-3.16792	3.31486	-2.00060
H	5.75535	0.12765	-2.23404
H	3.05209	2.57219	-2.92092
H	5.66191	0.71823	2.00355
H	2.99011	3.29467	1.85902
H	-5.55027	3.99858	-2.24222
H	-4.65360	4.15384	-3.76561
H	-5.77279	2.80319	-3.52927
H	-2.23186	1.34567	-3.15053
H	-3.74875	1.11744	-4.05585
H	-2.76428	2.56260	-4.31923
H	-2.48299	-0.42087	2.36603
H	-3.14041	-0.19936	3.99300
H	-4.04221	-1.16505	2.81682
H	-5.83516	2.24654	3.04657
H	-6.09162	0.51777	3.31609
H	-5.03104	1.42925	4.40008
H	3.86688	0.85624	3.49320
H	2.75539	2.13208	4.01774
H	2.30496	1.06604	2.66889
H	5.71108	2.76977	3.16354
H	5.31429	4.14220	2.11869
H	4.50088	3.95264	3.68457
H	2.40154	0.24177	-3.13360
H	2.98716	0.84876	-4.69301
H	4.02039	-0.21586	-3.73060
H	5.38829	3.37985	-3.33391
H	5.83791	1.77653	-3.92830
H	4.63369	2.73399	-4.80399
H	10.23764	-0.71370	-0.93851
H	10.72635	-2.19300	-0.10706
H	9.05489	-2.68960	-1.91068
H	10.20764	-0.37079	1.53909
H	6.73689	-1.84525	-1.72121
H	7.87324	-0.50778	-1.88437
H	9.07896	-4.12471	0.14665
H	7.44590	-3.99158	-0.50990
H	7.89091	0.49462	1.73771
H	8.54224	0.86890	0.14619
H	5.74962	-2.40883	0.58314
H	6.21260	-1.47309	1.99733
H	8.58470	-1.65244	2.94742
H	9.75092	-2.74557	2.19813
H	7.42223	-3.64087	1.96719

H	-7.02026	-4.00866	-2.99244
H	-8.70187	-4.44081	-2.67484
H	-8.55838	-2.30993	-3.99062
H	-7.31535	-4.66240	-0.59553
H	-7.57799	-0.28205	-2.95896
H	-6.35206	-1.53276	-3.16635
H	-10.46314	-2.61471	-2.38720
H	-10.00398	-0.91410	-2.50482
H	-6.29822	-2.64915	0.43533
H	-5.60838	-2.93632	-1.16039
H	-8.58490	0.16342	-0.66306
H	-8.09020	-0.78982	0.73121
H	-8.74415	-3.25947	0.90492
H	-9.72066	-4.00298	-0.36365
H	-10.29271	-1.57588	-0.10948
H	2.45454	-1.63507	-1.52124
H	0.28865	-5.25627	-2.40741
H	2.43536	-6.46754	-2.69951
H	4.60121	-2.85706	-1.79085
H	0.16469	-1.48656	-1.75003
H	-3.54414	-2.15015	-2.02016
H	-2.25597	-0.95043	-1.78989
H	-2.69167	-3.53675	-0.17723
H	-2.79444	-1.86048	0.43870
H	-0.53479	-1.60115	0.38805
H	-3.05253	-4.11359	5.91629
H	-3.53723	-5.69341	4.06911
H	-2.27094	-5.51277	1.92963
H	0.68730	-1.68304	2.57155
H	1.08979	-0.17936	4.43722
H	-0.14155	-0.44077	6.58898
H	-1.82948	-2.24089	6.82876

TS-7Si

B3LYP/6-31G(d) Energy = -5320.573898
B3LYP/6-31G(d) Free Energy = -5319.153363
Number of Imaginary Frequencies = 1 (-167.14)

B3LYP/6-31G(d) Geometry

C	0.04752	5.22205	1.70100
C	-0.92941	4.27851	1.27775
C	-0.20001	6.08331	2.74788
C	-2.17597	4.23699	1.98295
C	-0.70509	3.34497	0.20795
C	-2.40619	5.14953	3.04797
C	-3.16056	3.29139	1.59445
C	-1.44180	6.05609	3.42620
C	-1.64172	2.34208	-0.00215
C	0.48867	3.44563	-0.68237
C	-2.92336	2.33610	0.62717

O	-1.37290	1.36317	-0.93496
C	-4.02778	1.41474	0.19338
C	1.36049	2.37177	-0.81577
C	0.73832	4.63961	-1.44542
C	1.94734	4.73612	-2.20622
C	-0.17815	5.72637	-1.51383
C	2.85904	3.65115	-2.19401
C	2.21234	5.91233	-2.95768
C	2.59094	2.47013	-1.53372
C	3.63689	1.39026	-1.51492
O	1.08298	1.19511	-0.15325
C	0.10016	6.84762	-2.26428
C	1.31174	6.95157	-2.98687
P	-0.20827	0.22768	-0.61681
C	-4.47548	0.36779	1.02668
C	-4.69846	1.66630	-1.02933
C	3.77675	0.49283	-2.59582
C	4.57313	1.35723	-0.45283
C	-5.80703	0.88697	-1.36558
C	-4.27649	2.77752	-1.99157
C	-6.29673	-0.13525	-0.54264
C	-5.60050	-0.37718	0.64296
C	-7.55323	-0.91505	-0.95283
C	-3.78199	0.01000	2.34050
C	5.63529	0.44941	-0.51036
C	4.49803	2.32624	0.72882
C	5.82458	-0.42817	-1.58757
C	4.86507	-0.39443	-2.60550
C	7.08148	-1.31098	-1.65097
C	2.82581	0.51692	-3.79329
C	-3.36303	-1.47103	2.38907
C	-4.65092	0.37549	3.55999
C	-5.39115	3.82528	-2.17928
C	-3.80947	2.20847	-3.34517
C	2.33669	-0.88020	-4.21210
C	3.47609	1.24616	-4.98727
C	5.71125	3.27654	0.75472
C	4.33570	1.59737	2.07508
O	-0.54002	-0.53073	0.65512
O	0.06608	-0.49063	-1.89476
C	9.74629	-2.06999	-0.51695
C	9.63396	-1.24130	-1.81273
C	8.52888	-3.00956	-0.40009
C	8.34135	-0.40101	-1.77391
C	9.59480	-2.19026	-3.02667
C	7.23352	-2.17256	-0.36354
C	7.08306	-2.27640	-2.86441
C	8.49027	-3.95700	-1.61473
C	8.37291	-3.12249	-2.90492
C	-8.96738	-3.43361	-1.74706

C	-8.61301	-2.34943	-2.78344
C	-9.21219	-2.76811	-0.37849
C	-7.33979	-1.60426	-2.33256
C	-9.78169	-1.34944	-2.89968
C	-7.94105	-2.01574	0.06762
C	-8.76332	0.05823	-1.07635
C	-10.38641	-1.77615	-0.49334
C	-10.03413	-0.68976	-1.52835
C	-1.20628	-3.36313	-1.04732
C	-0.56006	-4.09481	-0.02597
C	-1.29475	-5.03241	0.73260
C	-2.62606	-5.28633	0.44214
C	-3.23396	-4.57842	-0.60020
C	-2.54274	-3.60984	-1.33395
C	0.84881	-3.94958	0.25635
S	1.96452	-3.51429	-0.99930
C	3.25179	-2.92384	0.14614
C	2.59687	-1.83245	1.01631
N	1.28442	-2.27673	1.51653
S	1.19827	-2.86586	3.14620
C	1.96654	-1.64153	4.21913
Cl	-4.90734	-4.91141	-0.98152
O	-0.23046	-2.99099	3.42630
O	2.06515	-4.05534	3.14869
C	1.42601	-0.32719	4.40670
C	2.10868	0.51935	5.34987
C	3.24486	0.02999	6.04610
C	3.72419	-1.24153	5.83392
C	3.07999	-2.08720	4.90646
C	0.29935	0.19732	3.72078
C	-0.11928	1.49051	3.95009
C	0.54721	2.32199	4.87818
C	1.63725	1.84148	5.56547
H	1.00635	5.24918	1.19574
H	0.56659	6.78933	3.05635
H	-3.36217	5.11136	3.56527
H	-4.13415	3.32449	2.07689
H	-1.62891	6.74678	4.24407
H	-1.11675	5.66164	-0.97619
H	3.79990	3.75629	-2.72853
H	3.14089	5.96861	-3.52124
H	-0.62242	7.65832	-2.30597
H	1.52104	7.84381	-3.57066
H	-6.31557	1.10059	-2.30162
H	-3.42276	3.30333	-1.55616
H	-5.93238	-1.16818	1.30559
H	-2.86190	0.59829	2.39993
H	6.36116	0.45937	0.29846
H	3.60916	2.94893	0.59788
H	4.96935	-1.05461	-3.45857

H	1.93564	1.07988	-3.49929
H	-2.71954	-1.71387	1.53987
H	-2.79853	-1.67813	3.30541
H	-4.23139	-2.14104	2.37721
H	-4.90656	1.44135	3.56949
H	-5.59113	-0.18938	3.56135
H	-4.12175	0.14462	4.49270
H	-5.69627	4.25640	-1.21897
H	-5.04335	4.64168	-2.82401
H	-6.28239	3.39087	-2.64740
H	-2.98018	1.50857	-3.20611
H	-4.62148	1.68150	-3.86111
H	-3.46836	3.01793	-4.00227
H	1.80967	-1.36326	-3.38655
H	1.63041	-0.78616	-5.04537
H	3.15675	-1.52472	-4.55303
H	3.76722	2.26947	-4.72672
H	4.37614	0.71976	-5.32920
H	2.77675	1.29840	-5.83032
H	5.79867	3.83053	-0.18638
H	5.61150	4.00416	1.56930
H	6.64987	2.73077	0.90874
H	3.41808	1.00076	2.08708
H	4.27101	2.32075	2.89652
H	5.18327	0.93311	2.28492
H	9.79409	-1.40308	0.35537
H	10.67561	-2.65612	-0.52124
H	10.49753	-0.56800	-1.89647
H	8.60284	-3.59621	0.52562
H	8.25625	0.20954	-2.68292
H	8.37731	0.29872	-0.92925
H	10.51905	-2.78241	-3.07623
H	9.53654	-1.61027	-3.95805
H	6.36591	-2.84019	-0.26558
H	7.23731	-1.52925	0.52509
H	7.00040	-1.70397	-3.79732
H	6.20653	-2.93807	-2.81918
H	7.63831	-4.64630	-1.53016
H	9.39841	-4.57472	-1.64410
H	8.33125	-3.79145	-3.77469
H	-8.15056	-4.16501	-1.67149
H	-9.86256	-3.98631	-2.06511
H	-8.42907	-2.81707	-3.76022
H	-9.45101	-3.53737	0.36830
H	-7.06447	-0.85692	-3.08717
H	-6.49625	-2.30389	-2.26055
H	-10.68873	-1.86619	-3.24341
H	-9.54811	-0.58168	-3.65064
H	-8.11299	-1.56526	1.05462
H	-7.11341	-2.72843	0.18091

H	-8.52984	0.85634	-1.79219
H	-8.93408	0.54689	-0.10727
H	-10.58938	-1.31553	0.48358
H	-11.30159	-2.30535	-0.79386
H	-10.86317	0.02627	-1.61027
H	-0.67997	-2.57149	-1.57857
H	-0.80967	-5.56648	1.54418
H	-3.19261	-6.01597	1.00954
H	-3.05109	-3.04621	-2.10806
H	1.25372	-4.57135	1.04842
H	4.06417	-2.50415	-0.45039
H	3.62386	-3.75050	0.75674
H	2.43622	-0.92680	0.42916
H	3.26626	-1.58207	1.84551
H	0.50208	-1.59303	1.26285
H	3.73708	0.68886	6.75733
H	4.59400	-1.60421	6.37284
H	3.44517	-3.09274	4.73377
H	-0.23773	-0.39511	2.99236
H	-0.97041	1.87743	3.39967
H	0.19911	3.33879	5.03398
H	2.16308	2.46794	6.28179

TS-6Re

ωB97XD/6-31G(d) Energy = -5319.496638
ωB97XD/6-31G(d) Free Energy = -5318.043309
Number of Imaginary Frequencies = 1 (-105.18)

ωB97XD/6-31G(d) Geometry

C	0.43882	5.45738	1.78386
C	-0.58507	4.64473	1.22810
C	0.18999	6.25814	2.86933
C	-1.86813	4.65958	1.83964
C	-0.36568	3.77561	0.11241
C	-2.09901	5.51038	2.95203
C	-2.87824	3.78706	1.36231
C	-1.09534	6.29460	3.45759
C	-1.35511	2.88192	-0.23302
C	0.90889	3.78178	-0.65298
C	-2.63982	2.86146	0.37666
O	-1.10060	1.99273	-1.25013
C	-3.67870	1.86087	-0.01450
C	1.63893	2.61711	-0.78031
C	1.38499	4.97082	-1.29468
C	2.65598	4.95016	-1.92998
C	0.62672	6.17161	-1.34891
C	3.40589	3.74912	-1.93718
C	3.14711	6.12747	-2.55132
C	2.91765	2.58547	-1.40091

C	3.75319	1.34627	-1.39646
O	1.16207	1.45659	-0.22355
C	1.12176	7.29039	-1.96775
C	2.40134	7.27611	-2.56786
P	-0.16810	0.70622	-0.87210
C	-4.16783	0.94598	0.93744
C	-4.20208	1.84363	-1.32356
C	4.54409	1.06151	-0.26768
C	3.80744	0.51046	-2.52300
C	-5.19113	0.91922	-1.64430
C	-3.78060	2.83970	-2.39606
C	-5.72057	0.02394	-0.71403
C	-5.18881	0.06420	0.57055
C	-6.82799	-0.94314	-1.12973
C	-3.64671	0.86348	2.36666
C	4.65963	-0.59755	-2.49710
C	3.02487	0.83385	-3.78963
C	5.42839	-0.92454	-1.38205
C	5.34695	-0.07527	-0.27735
C	6.34895	-2.14338	-1.32922
C	4.53468	1.95422	0.96425
C	-3.19205	-0.55170	2.73560
C	-4.68788	1.37507	3.37184
C	-4.94717	3.77316	-2.75154
C	-3.22279	2.14200	-3.64285
C	3.71280	1.32215	2.09167
C	5.94848	2.31088	1.43960
C	2.37132	-0.38634	-4.44657
C	3.93590	1.55977	-4.79136
O	-0.76843	-0.04159	0.29077
O	0.17245	-0.02674	-2.12206
C	6.83178	-5.08514	-1.31285
C	6.92786	-4.25162	-0.02687
C	7.22607	-4.21235	-2.51327
C	5.97601	-3.05053	-0.12875
C	8.36846	-3.74816	0.15449
C	6.28010	-3.00468	-2.60799
C	7.81666	-1.67925	-1.15101
C	8.66985	-3.71834	-2.33595
C	8.76643	-2.88231	-1.05133
C	-8.53282	-2.09334	-3.27841
C	-9.11357	-1.12733	-2.23314
C	-7.38383	-2.89980	-2.65219
C	-8.01253	-0.16614	-1.75903
C	-9.64641	-1.92835	-1.03689
C	-6.28159	-1.93798	-2.18443
C	-7.39250	-1.75822	0.05425
C	-7.91181	-3.69586	-1.44939
C	-8.49279	-2.72424	-0.41076
C	-1.42477	-4.91875	0.38582

C	-1.36799	-3.59663	-0.08717
C	-2.50954	-2.77951	-0.02748
C	-3.70029	-3.28753	0.45947
C	-3.74299	-4.60766	0.89461
C	-2.61421	-5.43042	0.86915
C	-0.17298	-2.99761	-0.60536
S	1.18978	-3.83807	-1.19119
C	2.25613	-2.37649	-1.07135
C	2.31941	-1.94070	0.40838
N	0.98299	-1.95982	0.99502
S	0.77865	-2.64050	2.52952
C	1.66137	-1.57194	3.65592
Cl	-5.24085	-5.24491	1.50880
O	-0.64439	-2.56486	2.79659
O	1.46449	-3.92350	2.48880
C	1.27252	-0.21195	3.87691
C	2.04050	0.53357	4.81979
C	3.12081	-0.08800	5.49746
C	3.46318	-1.39021	5.24944
C	2.72550	-2.14179	4.31091
C	0.22612	0.45217	3.18753
C	-0.00367	1.78935	3.38639
C	0.75413	2.52909	4.31854
C	1.74262	1.90486	5.03321
H	1.43092	5.42912	1.34694
H	0.98830	6.86682	3.28353
H	-3.08640	5.51459	3.40649
H	-3.85797	3.82072	1.83034
H	-1.28047	6.93641	4.31361
H	-0.36198	6.19485	-0.90467
H	4.39698	3.75126	-2.38358
H	4.12517	6.09542	-3.02470
H	0.52180	8.19481	-2.00308
H	2.78261	8.17084	-3.05056
H	-5.57713	0.91669	-2.66002
H	-2.98454	3.47167	-1.99588
H	-5.57576	-0.60356	1.33334
H	-2.76659	1.50382	2.44465
H	4.70607	-1.22368	-3.38089
H	2.21121	1.51121	-3.51401
H	5.94033	-0.29440	0.60615
H	4.04395	2.89402	0.69492
H	-2.46993	-0.92856	2.00957
H	-2.70739	-0.55155	3.71766
H	-4.03168	-1.25550	2.78482
H	-5.00292	2.39986	3.14806
H	-5.58554	0.74550	3.36022
H	-4.27847	1.35658	4.38811
H	-5.31976	4.29234	-1.86205
H	-4.62557	4.52617	-3.47994

H	-5.78404	3.21760	-3.19060
H	-2.38654	1.48829	-3.38245
H	-3.99151	1.54186	-4.14424
H	-2.86495	2.88700	-4.36238
H	4.13583	0.35761	2.40236
H	3.69602	1.97770	2.96805
H	2.67728	1.16076	1.77742
H	6.48221	1.43707	1.83063
H	6.54601	2.73479	0.62589
H	5.89628	3.04869	2.24775
H	1.65633	-0.85406	-3.76712
H	1.81468	-0.06503	-5.33356
H	3.10755	-1.12820	-4.77813
H	4.35990	2.47230	-4.36095
H	4.76858	0.91389	-5.09574
H	3.37445	1.83721	-5.69035
H	5.80864	-5.46352	-1.44040
H	7.49305	-5.95889	-1.24827
H	6.63953	-4.86568	0.83472
H	7.14785	-4.79823	-3.43682
H	6.00640	-2.47515	0.80440
H	4.94425	-3.40967	-0.24532
H	9.05457	-4.59971	0.25032
H	8.44849	-3.16326	1.08046
H	6.55309	-2.39841	-3.48129
H	5.25162	-3.35726	-2.77087
H	7.90505	-1.06208	-0.24844
H	8.09530	-1.04065	-1.99933
H	8.97017	-3.11400	-3.20188
H	9.35656	-4.57327	-2.28423
H	9.79338	-2.52001	-0.92220
H	-8.16683	-1.53119	-4.14784
H	-9.31651	-2.77239	-3.63937
H	-9.92817	-0.54573	-2.68160
H	-6.96774	-3.58858	-3.39739
H	-8.41326	0.53961	-1.01955
H	-7.66393	0.43132	-2.60941
H	-10.44378	-2.60989	-1.36136
H	-10.08321	-1.24915	-0.29295
H	-5.44318	-2.50248	-1.75538
H	-5.88019	-1.38368	-3.04208
H	-7.79189	-1.07595	0.81652
H	-6.59999	-2.34429	0.53560
H	-7.10030	-4.28392	-1.00045
H	-8.68415	-4.40523	-1.77461
H	-8.85859	-3.28794	0.45588
H	-0.52766	-5.53008	0.40005
H	-2.44683	-1.73806	-0.33158
H	-4.57476	-2.65266	0.51777
H	-2.67399	-6.44635	1.24165

H	-0.27063	-1.97885	-0.97622
H	1.82867	-1.57662	-1.68246
H	3.24496	-2.62658	-1.45222
H	2.73980	-0.93115	0.44302
H	2.96469	-2.61815	0.97172
H	0.40521	-1.09796	0.86788
H	3.68876	0.49999	6.21384
H	4.29737	-1.85232	5.76680
H	2.98429	-3.17466	4.10603
H	-0.39564	-0.06689	2.47273
H	-0.77649	2.28434	2.80842
H	0.54983	3.58674	4.45519
H	2.33656	2.45698	5.75705

TS-6Si

ωB97XD/6-31G(d) Energy = -5319.489206
ωB97XD/6-31G(d) Free Energy = -5318.037816
Number of Imaginary Frequencies = 1 (-71.61)

ωB97XD/6-31G(d) Geometry

C	-0.50252	6.29224	1.67741
C	-1.29640	5.23624	1.15325
C	-1.04514	7.23810	2.50838
C	-2.66000	5.16388	1.54849
C	-0.77130	4.23265	0.27408
C	-3.19739	6.16675	2.39674
C	-3.45146	4.07302	1.11432
C	-2.41189	7.18643	2.86460
C	-1.56692	3.14675	-0.03497
C	0.61084	4.31903	-0.27049
C	-2.92513	3.04880	0.36987
O	-1.07427	2.14609	-0.83109
C	-3.76991	1.87126	0.00651
C	1.47440	3.25968	-0.09510
C	1.07568	5.46179	-0.99999
C	2.44439	5.52172	-1.38115
C	0.22303	6.53037	-1.38647
C	3.29995	4.43030	-1.08948
C	2.92481	6.66067	-2.07839
C	2.83606	3.28323	-0.49775
C	3.72431	2.10046	-0.28908
O	1.02642	2.14261	0.56463
C	0.71305	7.61088	-2.07386
C	2.08239	7.68708	-2.41466
P	0.06341	1.10407	-0.24796
C	-4.22205	1.69335	-1.31060
C	-4.17954	0.97346	1.01204
C	4.06811	1.69249	1.01502
C	4.25737	1.41326	-1.39449

C	-5.06791	-0.04686	0.68078
C	-3.69448	1.07409	2.45175
C	-5.55487	-0.23441	-0.61368
C	-5.10240	0.64502	-1.59383
C	-6.55368	-1.35680	-0.89138
C	-3.81336	2.62537	-2.44322
C	5.16526	0.37021	-1.17360
C	3.92002	1.78147	-2.83543
C	5.55230	-0.02487	0.10343
C	4.95999	0.63961	1.17836
C	6.60835	-1.09481	0.37764
C	3.54670	2.39070	2.26401
C	-5.03439	3.32441	-3.05669
C	-2.99245	1.89100	-3.51167
C	-3.03522	-0.22786	2.91661
C	-4.83501	1.48951	3.39027
C	2.73940	1.43106	3.14782
C	4.69167	3.04783	3.04743
C	3.30498	0.60987	-3.61018
C	5.15325	2.33882	-3.56041
O	-0.51786	0.19475	0.79547
O	0.72521	0.53644	-1.46268
C	9.42236	-2.09161	0.26069
C	8.30254	-2.73368	-0.57066
C	8.82490	-1.52514	1.55636
C	7.23892	-1.67526	-0.90609
C	7.66012	-3.87528	0.23178
C	7.76002	-0.47380	1.21188
C	5.99387	-2.26410	1.18633
C	8.17518	-2.66007	2.36399
C	7.06220	-3.31337	1.52928
C	-7.36417	-3.91411	-2.19381
C	-7.98444	-2.57021	-2.60382
C	-6.97323	-3.85989	-0.70977
C	-6.96902	-1.43895	-2.37530
C	-9.24100	-2.30850	-1.75973
C	-5.95442	-2.73031	-0.49764
C	-7.83650	-1.12297	-0.05378
C	-8.22337	-3.59139	0.14263
C	-8.85263	-2.25293	-0.27493
C	2.35872	-2.31616	-1.87699
C	1.17337	-2.95506	-2.28491
C	1.20641	-4.29479	-2.71101
C	2.41163	-4.96482	-2.78856
C	3.58195	-4.29491	-2.42207
C	3.56751	-2.98353	-1.95572
C	-0.02534	-2.17829	-2.21086
S	-1.48588	-2.56331	-2.99616
C	-2.50822	-1.54051	-1.90127
C	-2.39666	-2.12604	-0.48243

N	-0.99313	-2.28031	-0.12129
S	-0.51422	-3.70841	0.62867
C	-1.37911	-3.73039	2.19030
Cl	5.09938	-5.13476	-2.54835
O	-1.04625	-4.78726	-0.19223
O	0.91448	-3.57588	0.84456
C	-0.99528	-2.89371	3.28655
C	-1.77846	-2.99778	4.47509
C	-2.88665	-3.88229	4.51985
C	-3.22649	-4.65325	3.44122
C	-2.45754	-4.57893	2.26186
C	0.08228	-1.96820	3.26746
C	0.36185	-1.20305	4.37032
C	-0.40117	-1.32059	5.55172
C	-1.44930	-2.20017	5.60052
H	0.54974	6.34023	1.42129
H	-0.41677	8.03168	2.90157
H	-4.24500	6.10039	2.67952
H	-4.49589	4.02989	1.41293
H	-2.83013	7.94572	3.51849
H	-0.83159	6.48157	-1.13961
H	4.34464	4.49095	-1.38386
H	3.97600	6.69507	-2.35333
H	0.04130	8.41326	-2.36409
H	2.45878	8.55127	-2.95370
H	-5.39167	-0.71900	1.47141
H	-2.92380	1.84738	2.49856
H	-5.44708	0.53387	-2.61692
H	-3.17350	3.40898	-2.02890
H	5.59483	-0.12267	-2.04083
H	3.16293	2.56849	-2.81812
H	5.22562	0.34685	2.19061
H	2.87141	3.19408	1.96092
H	-5.60804	3.85514	-2.28975
H	-4.71647	4.05141	-3.81211
H	-5.70691	2.60998	-3.54560
H	-2.06272	1.50308	-3.08559
H	-3.55807	1.05938	-3.95052
H	-2.72647	2.57611	-4.32424
H	-2.17406	-0.45296	2.28385
H	-2.67209	-0.12344	3.94474
H	-3.72961	-1.07750	2.89902
H	-5.28024	2.44206	3.08364
H	-5.63297	0.73712	3.40061
H	-4.46478	1.60053	4.41547
H	3.36828	0.61635	3.52837
H	2.32788	1.96706	4.01132
H	1.90803	1.00005	2.58335
H	5.40163	2.30262	3.42465
H	5.24642	3.74886	2.41497

H	4.29775	3.59982	3.90838
H	2.35697	0.31999	-3.15080
H	3.10762	0.90946	-4.64609
H	3.97161	-0.26077	-3.63974
H	5.58340	3.19015	-3.02166
H	5.93717	1.57804	-3.65518
H	4.88671	2.67217	-4.56971
H	9.90657	-1.28988	-0.31242
H	10.19479	-2.83678	0.49227
H	8.71617	-3.12870	-1.50644
H	9.61515	-1.05322	2.15296
H	6.47229	-2.13649	-1.54155
H	7.69408	-0.86699	-1.49393
H	8.41248	-4.64122	0.46201
H	6.87593	-4.35992	-0.36239
H	7.36269	-0.04213	2.13789
H	8.20733	0.35310	0.64464
H	5.18126	-2.72529	0.60965
H	5.54123	-1.88187	2.10940
H	7.76052	-2.26452	3.30081
H	8.93037	-3.40933	2.63590
H	6.59721	-4.12395	2.10298
H	-6.47895	-4.12540	-2.80860
H	-8.07955	-4.72823	-2.36796
H	-8.25328	-2.59727	-3.66652
H	-6.51990	-4.81308	-0.41142
H	-7.40924	-0.48484	-2.69286
H	-6.08388	-1.61000	-3.00460
H	-9.98015	-3.10233	-1.92900
H	-9.70772	-1.36195	-2.06206
H	-5.62310	-2.71734	0.54810
H	-5.06441	-2.92426	-1.11121
H	-8.27310	-0.15491	-0.33173
H	-7.58020	-1.05993	1.01081
H	-7.95414	-3.56421	1.20695
H	-8.94773	-4.40606	0.01335
H	-9.74417	-2.05916	0.33343
H	2.31778	-1.29424	-1.50838
H	0.28306	-4.81075	-2.95397
H	2.45727	-5.99680	-3.11616
H	4.48212	-2.48819	-1.65502
H	0.09991	-1.13603	-1.89852
H	-3.53820	-1.56307	-2.25925
H	-2.15956	-0.50532	-1.92606
H	-2.89267	-3.09796	-0.44525
H	-2.89432	-1.44079	0.20949
H	-0.62149	-1.41249	0.33590
H	-3.46864	-3.93479	5.43628
H	-4.07507	-5.32782	3.48564
H	-2.70077	-5.20138	1.40802

H	0.68930	-1.85245	2.37979
H	1.18145	-0.49378	4.32857
H	-0.15826	-0.70816	6.41449
H	-2.05238	-2.29603	6.49945

TS-7Si

ωB97XD/6-31G(d) Energy = -5319.493206
ωB97XD/6-31G(d) Free Energy = -5318.041491
Number of Imaginary Frequencies = 1 (-77.87)

ωB97XD/6-31G(d) Geometry

C	0.10952	5.16566	1.50543
C	-0.87624	4.22245	1.11041
C	-0.11689	6.02636	2.54906
C	-2.09328	4.17013	1.84242
C	-0.67893	3.30322	0.03025
C	-2.30300	5.07996	2.91097
C	-3.06861	3.20015	1.49681
C	-1.34045	5.99345	3.25638
C	-1.60581	2.30455	-0.17002
C	0.50037	3.39935	-0.86714
C	-2.84119	2.25398	0.52939
O	-1.37758	1.37369	-1.14969
C	-3.91931	1.28605	0.16268
C	1.34838	2.32088	-1.00100
C	0.76886	4.58939	-1.61816
C	1.97348	4.67498	-2.36718
C	-0.13625	5.68334	-1.67262
C	2.87826	3.58513	-2.34557
C	2.25360	5.85164	-3.10842
C	2.58836	2.41694	-1.68926
C	3.61598	1.33764	-1.58293
O	1.04798	1.14432	-0.36879
C	0.15577	6.80319	-2.40799
C	1.36809	6.89666	-3.12828
P	-0.24371	0.21675	-0.87085
C	-4.20911	0.18779	0.98561
C	-4.71398	1.54849	-0.96736
C	3.75734	0.36629	-2.58393
C	4.49434	1.35324	-0.48150
C	-5.82421	0.74562	-1.20523
C	-4.40469	2.68232	-1.93490
C	-6.19369	-0.29737	-0.35433
C	-5.35051	-0.57331	0.71932
C	-7.48401	-1.06834	-0.62657
C	-3.31930	-0.17287	2.16615
C	5.49710	0.39158	-0.40923
C	4.34993	2.37589	0.63684
C	5.68120	-0.57581	-1.39961
C	4.79567	-0.56549	-2.47635

C	6.84904	-1.55661	-1.28761
C	2.86174	0.37238	-3.81452
C	-2.96777	-1.66270	2.20398
C	-3.92892	0.28376	3.49686
C	-5.57173	3.67160	-2.04684
C	-3.99586	2.13073	-3.30700
C	2.40117	-1.02229	-4.24453
C	3.56907	1.09698	-4.96927
C	5.69180	2.94723	1.10908
C	3.56312	1.78427	1.81292
O	-0.59413	-0.56905	0.36523
O	0.03666	-0.46028	-2.16294
C	9.34488	-2.40603	0.09597
C	9.38772	-1.71750	-1.27731
C	8.04642	-3.21815	0.22295
C	8.18201	-0.77534	-1.41433
C	9.33526	-2.78181	-2.38343
C	6.84051	-2.27683	0.08514
C	6.83220	-2.63764	-2.38936
C	7.99263	-4.28048	-0.88411
C	8.03313	-3.58681	-2.25325
C	-8.96817	-3.58588	-1.18828
C	-8.68687	-2.55910	-2.29552
C	-9.10546	-2.85921	0.15842
C	-7.38231	-1.81157	-1.98111
C	-9.84724	-1.55364	-2.36647
C	-7.80339	-2.10546	0.47048
C	-8.68228	-0.08698	-0.69757
C	-10.27192	-1.86342	0.08629
C	-9.98724	-0.83305	-1.01584
C	-1.36274	-3.23679	-1.05162
C	-0.62963	-3.91490	-0.05613
C	-1.29741	-4.72323	0.88438
C	-2.65761	-4.93267	0.77981
C	-3.35362	-4.29998	-0.25101
C	-2.72946	-3.43235	-1.14680
C	0.79240	-3.82939	0.03307
S	1.76824	-3.40104	-1.28808
C	3.19083	-2.85506	-0.31851
C	2.73316	-1.65369	0.53322
N	1.50603	-1.96876	1.24870
S	1.59399	-2.50764	2.82756
C	2.24431	-1.16219	3.79611
Cl	-5.05671	-4.59514	-0.40115
O	0.22609	-2.80441	3.21813
O	2.59296	-3.57424	2.81336
C	1.53988	0.07467	3.93129
C	2.16010	1.08203	4.72843
C	3.40546	0.81891	5.35436
C	4.04551	-0.38102	5.19545

C	3.45879	-1.38530	4.39824
C	0.30680	0.37651	3.29788
C	-0.24869	1.62361	3.42182
C	0.36789	2.62605	4.20032
C	1.54077	2.35242	4.85196
H	1.05614	5.19200	0.97691
H	0.65245	6.73611	2.83823
H	-3.24202	5.03284	3.45660
H	-4.02242	3.20396	2.01784
H	-1.51052	6.68456	4.07652
H	-1.07562	5.62093	-1.13451
H	3.83558	3.68566	-2.85092
H	3.18338	5.90323	-3.66933
H	-0.55438	7.62400	-2.44249
H	1.58818	7.79105	-3.70328
H	-6.43567	0.96118	-2.07773
H	-3.55054	3.24488	-1.54778
H	-5.58192	-1.39562	1.38757
H	-2.37336	0.35331	2.02133
H	6.17334	0.41506	0.44003
H	3.76747	3.21567	0.24677
H	4.91026	-1.29331	-3.27202
H	1.95489	0.92972	-3.56277
H	-2.49721	-1.95452	1.26347
H	-2.25180	-1.86183	3.00832
H	-3.84862	-2.29330	2.37737
H	-4.11705	1.36252	3.50377
H	-4.88307	-0.22369	3.68395
H	-3.25105	0.05193	4.32642
H	-5.84286	4.07072	-1.06364
H	-5.29817	4.51150	-2.69539
H	-6.46339	3.19903	-2.47470
H	-3.13129	1.46781	-3.21131
H	-4.81619	1.56645	-3.76689
H	-3.72953	2.94966	-3.98498
H	1.83560	-1.49545	-3.43926
H	1.72992	-0.93566	-5.10538
H	3.23654	-1.66660	-4.54545
H	3.83813	2.12148	-4.69291
H	4.48950	0.57169	-5.25258
H	2.91826	1.14247	-5.84942
H	6.28588	3.32044	0.26840
H	5.51809	3.77774	1.80187
H	6.29133	2.20182	1.64430
H	2.58213	1.41848	1.49564
H	3.40318	2.54211	2.58692
H	4.11171	0.95005	2.27034
H	9.39828	-1.65516	0.89546
H	10.21413	-3.06596	0.21433
H	10.31185	-1.13431	-1.36888

H	8.00998	-3.70493	1.20502
H	8.20547	-0.26231	-2.38458
H	8.22782	0.00381	-0.64312
H	10.20141	-3.45176	-2.30545
H	9.38462	-2.30282	-3.37003
H	5.91085	-2.84937	0.19777
H	6.85887	-1.54300	0.89933
H	6.86204	-2.16310	-3.37830
H	5.89840	-3.21572	-2.33853
H	7.07483	-4.87638	-0.78976
H	8.83857	-4.97311	-0.78645
H	7.98364	-4.33874	-3.04980
H	-8.15238	-4.31967	-1.14024
H	-9.88827	-4.14180	-1.41231
H	-8.58506	-3.07343	-3.25899
H	-9.29320	-3.59077	0.95384
H	-7.16463	-1.09453	-2.78273
H	-6.53946	-2.51322	-1.94566
H	-10.78214	-2.07357	-2.61443
H	-9.66230	-0.82289	-3.16505
H	-7.89279	-1.59939	1.44121
H	-6.98186	-2.82529	0.55762
H	-8.50280	0.67455	-1.46568
H	-8.76937	0.44392	0.25959
H	-10.39456	-1.35689	1.05270
H	-11.21041	-2.39371	-0.12334
H	-10.81072	-0.11028	-1.06796
H	-0.86966	-2.52265	-1.70989
H	-0.73704	-5.18482	1.69099
H	-3.18300	-5.56621	1.48442
H	-3.31299	-2.90445	-1.89195
H	1.28239	-4.33374	0.86083
H	3.96402	-2.54907	-1.02308
H	3.55282	-3.66943	0.31347
H	2.54354	-0.78979	-0.10664
H	3.54356	-1.38446	1.21870
H	0.67456	-1.36362	1.02119
H	3.85504	1.60255	5.95871
H	5.00146	-0.56771	5.67326
H	3.95454	-2.33932	4.25853
H	-0.20730	-0.35732	2.69098
H	-1.17810	1.84487	2.90963
H	-0.09290	3.60644	4.27098
H	2.02850	3.11089	5.45878

TS-8Re
B3LYP/6-31G(d) Energy = -4825.281089
B3LYP/6-31G(d) Free Energy = -4823.814468
Number of Imaginary Frequencies = 1 (-146.98)

B3LYP/6-31G(d) Geometry

C	-0.10568	5.73121	2.44731
C	-0.98417	4.79785	1.82907
C	-0.55271	6.58699	3.42982
C	-2.34109	4.75608	2.27934
C	-0.56260	3.88545	0.80060
C	-2.77793	5.66647	3.27947
C	-3.21972	3.80031	1.71553
C	-1.90549	6.56705	3.84476
C	-1.42636	2.86603	0.41310
C	0.76189	4.04520	0.13898
C	-2.79508	2.83618	0.82195
O	-1.00182	1.92008	-0.49769
C	-3.80248	1.85913	0.29231
C	1.66011	2.98746	0.10089
C	1.12045	5.28692	-0.49532
C	2.45013	5.44587	-0.99960
C	0.20780	6.36323	-0.68068
C	3.35588	4.36121	-0.90719
C	2.83084	6.67363	-1.60551
C	2.98679	3.12860	-0.40906
C	3.98089	2.00657	-0.40907
O	1.28510	1.77811	0.65836
C	0.60043	7.53452	-1.29038
C	1.92900	7.70232	-1.74635
P	0.18289	0.81059	-0.13878
C	-4.21556	1.91994	-1.06205
C	-4.45308	0.96468	1.17431
C	4.36394	1.39739	-1.62540
C	4.61035	1.61546	0.79646
C	-5.52519	0.19324	0.69986
C	-4.02771	0.79095	2.63510
C	-5.98171	0.26677	-0.61894
C	-5.28127	1.12008	-1.48124
C	-7.21366	-0.49454	-1.13040
C	-3.59003	2.87475	-2.07963
C	5.58659	0.61684	0.76039
C	4.31416	2.30822	2.12732
C	5.98299	-0.01244	-0.42755
C	5.34832	0.39831	-1.60229
C	7.10318	-1.06222	-0.40609
C	3.79870	1.82803	-2.98184
C	-4.61486	3.90952	-2.58629
C	-2.93531	2.11684	-3.24995
C	-3.36535	-0.58101	2.86660
C	-5.18817	1.02251	3.62116
C	3.13840	0.67523	-3.75927
C	4.88717	2.51280	-3.83406
C	5.55211	3.06301	2.65133

C	3.76671	1.33705	3.18766
O	-0.29650	-0.16104	0.92697
O	0.72894	0.29023	-1.42621
C	9.17645	-2.57605	1.13165
C	9.56800	-1.44741	0.15572
C	7.88738	-3.26181	0.63496
C	8.42932	-0.40923	0.08616
C	9.80747	-2.04266	-1.24561
C	6.74682	-2.22566	0.56447
C	7.37641	-1.68156	-1.80093
C	8.12699	-3.85508	-0.76704
C	8.51403	-2.72198	-1.73760
C	-9.08024	-1.14221	-3.37787
C	-9.50989	-0.21283	-2.22440
C	-8.06601	-2.17932	-2.85337
C	-8.27215	0.51746	-1.66506
C	-10.16244	-1.04880	-1.10665
C	-6.82585	-1.45093	-2.29567
C	-7.90301	-1.34174	-0.03039
C	-8.71850	-3.01280	-1.73300
C	-9.14175	-2.07793	-0.58257
C	2.59279	-2.53495	-1.80035
C	2.76177	-3.11637	-0.52517
C	3.39786	-4.37049	-0.40069
C	3.89002	-5.00910	-1.53041
C	3.73924	-4.41521	-2.79076
C	3.08937	-3.18546	-2.92496
C	2.26308	-2.37361	0.60938
S	2.91183	-2.59888	2.20949
C	1.43545	-1.92805	3.05219
C	0.24578	-2.77891	2.57788
N	0.23901	-2.79092	1.10921
S	-0.33548	-4.24202	0.32054
C	-2.04815	-4.45754	0.84451
O	-0.28018	-3.93623	-1.10455
O	0.50103	-5.30014	0.88896
C	-2.40251	-5.51668	1.71873
C	-3.75818	-5.64854	2.04518
C	-4.74293	-4.79571	1.55065
C	-4.34933	-3.76878	0.69012
C	-3.01968	-3.56827	0.31210
H	0.93541	5.75474	2.14657
H	0.14210	7.28217	3.89367
H	-3.81684	5.62629	3.59902
H	-4.26441	3.81346	2.01652
H	-2.24708	7.25362	4.61472
H	-0.81717	6.25158	-0.34787
H	4.36958	4.49813	-1.27535
H	3.84998	6.77638	-1.97124
H	-0.12076	8.33598	-1.42715

H	2.22764	8.63440	-2.21848
H	-6.02244	-0.46753	1.40141
H	-3.26622	1.54163	2.85632
H	-5.59675	1.19693	-2.51790
H	-2.79771	3.43763	-1.58192
H	6.07225	0.34110	1.69270
H	3.53735	3.05760	1.95270
H	5.63037	-0.05277	-2.54677
H	3.01391	2.56631	-2.80152
H	-5.05654	4.47123	-1.75524
H	-4.13024	4.62546	-3.26108
H	-5.43340	3.43457	-3.14029
H	-2.46883	2.82523	-3.94528
H	-2.15899	1.43668	-2.88855
H	-3.67263	1.53427	-3.81632
H	-2.47009	-0.67309	2.24310
H	-3.06774	-0.68426	3.91868
H	-4.04579	-1.40714	2.62839
H	-5.64892	2.00600	3.47349
H	-5.97715	0.26866	3.51328
H	-4.82449	0.97093	4.65458
H	3.83907	-0.14865	-3.94479
H	2.27284	0.29925	-3.20849
H	2.79077	1.03624	-4.73538
H	5.33662	3.36317	-3.30847
H	5.69638	1.81642	-4.08609
H	4.46052	2.88239	-4.77445
H	5.91535	3.78594	1.91250
H	5.30835	3.60933	3.57079
H	6.37692	2.37744	2.87965
H	2.83983	0.87550	2.83470
H	4.48461	0.54103	3.42000
H	3.54753	1.87166	4.12017
H	9.02179	-2.16669	2.13991
H	9.99063	-3.31036	1.20704
H	10.48340	-0.95436	0.50991
H	7.60361	-4.06222	1.33210
H	8.70233	0.40964	-0.59331
H	8.27830	0.04211	1.07494
H	10.62978	-2.77111	-1.21392
H	10.10842	-1.25109	-1.94590
H	5.82064	-2.70755	0.22421
H	6.54714	-1.83004	1.56817
H	7.64987	-0.89134	-2.51281
H	6.46253	-2.15530	-2.18420
H	7.21852	-4.36189	-1.12145
H	8.92368	-4.61131	-0.72971
H	8.67438	-3.13559	-2.74245
H	-8.63171	-0.55370	-4.19024
H	-9.95743	-1.65186	-3.80017

H	-10.22715	0.53068	-2.59715
H	-7.75594	-2.84035	-3.67371
H	-8.56517	1.19538	-0.85186
H	-7.82902	1.14324	-2.44903
H	-11.05642	-1.56234	-1.48694
H	-10.49324	-0.39403	-0.28854
H	-6.08893	-2.18375	-1.93823
H	-6.33622	-0.88462	-3.09754
H	-8.20208	-0.69469	0.80523
H	-7.19672	-2.07789	0.37755
H	-8.01093	-3.77047	-1.36615
H	-9.59206	-3.55477	-2.12099
H	-9.59500	-2.66807	0.22553
H	2.06486	-1.58799	-1.88411
H	3.47538	-4.84141	0.57360
H	4.37608	-5.97577	-1.43866
H	2.96172	-2.73739	-3.90536
H	1.88715	-1.37916	0.39507
H	1.58946	-2.01281	4.13065
H	1.28445	-0.88170	2.77678
H	-0.68610	-2.34259	2.95253
H	0.34670	-3.80394	2.94019
H	-0.15222	-1.88519	0.74820
C	-6.19156	-4.96759	1.93685
H	-5.09883	-3.09178	0.29085
C	-2.73003	-2.42245	-0.63433
C	-1.46308	-6.54258	2.32156
H	-4.04774	-6.45856	2.70967
H	-2.03563	-7.21670	2.96485
H	-0.96075	-7.13757	1.55542
H	-0.67178	-6.08819	2.92342
H	-3.65581	-1.88633	-0.85382
H	-2.03760	-1.68689	-0.21201
H	-2.29421	-2.77544	-1.57125
H	-6.52901	-4.14101	2.57481
H	-6.83991	-4.97598	1.05309
H	-6.35328	-5.90004	2.48585
H	4.11870	-4.92460	-3.67270

TS-8Si

B3LYP/6-31G(d) Energy = -4825.282327
B3LYP/6-31G(d) Free Energy = -4823.814916
Number of Imaginary Frequencies = 1 (-183.59)

B3LYP/6-31G(d) Geometry

C	-0.71946	6.14438	1.86830
C	-1.54384	5.07615	1.41618
C	-1.19089	7.07932	2.76347
C	-2.86910	4.98288	1.94923

C	-1.09683	4.07793	0.48088
C	-3.33273	5.97408	2.85589
C	-3.68879	3.89009	1.57404
C	-2.51536	7.00565	3.25512
C	-1.90314	2.96900	0.25487
C	0.20848	4.21846	-0.22610
C	-3.23085	2.86614	0.77079
O	-1.45772	1.96890	-0.58643
C	-4.13382	1.71271	0.44683
C	1.16090	3.21089	-0.14567
C	0.51045	5.38875	-1.00698
C	1.83319	5.54953	-1.53017
C	-0.45440	6.38706	-1.31851
C	2.79812	4.53965	-1.29247
C	2.15187	6.70942	-2.28690
C	2.48965	3.36221	-0.64228
C	3.55506	2.32444	-0.44479
O	0.84828	2.04301	0.52706
C	-0.12015	7.49096	-2.07174
C	1.19905	7.66520	-2.55214
P	-0.20173	0.96459	-0.16071
C	-4.69402	1.58794	-0.84402
C	-4.50042	0.78872	1.45777
C	4.07591	1.61606	-1.55573
C	4.12048	2.12282	0.83383
C	-5.40850	-0.22919	1.14475
C	-3.96962	0.87238	2.89111
C	-5.98670	-0.37349	-0.12383
C	-5.60079	0.54927	-1.10082
C	-7.02040	-1.48026	-0.37874
C	-4.40696	2.59260	-1.96091
C	5.20524	1.24694	0.97249
C	3.62983	2.86429	2.07753
C	5.76292	0.56160	-0.10919
C	5.16116	0.75569	-1.35907
C	7.00170	-0.33580	0.02176
C	3.51606	1.76917	-2.97185
C	-5.67592	3.38674	-2.33137
C	-3.78271	1.93236	-3.20395
C	-3.19886	-0.39356	3.30681
C	-5.10332	1.18375	3.88877
C	3.00439	0.43370	-3.54293
C	4.54584	2.41721	-3.91856
C	4.71954	3.79280	2.64929
C	3.10095	1.89585	3.15228
O	-0.61597	0.02904	0.95267
O	0.30850	0.38748	-1.44902
C	9.89712	-0.74476	0.68197
C	9.40823	-0.66991	-0.77763
C	8.77750	-1.33307	1.56325

C	8.15811	0.22978	-0.85590
C	9.05356	-2.08662	-1.27410
C	7.52567	-0.43509	1.47764
C	6.68836	-1.78086	-0.46291
C	8.43158	-2.75243	1.07247
C	7.94016	-2.67972	-0.38635
C	-8.62523	-3.78189	0.65971
C	-7.44307	-4.00147	-0.30633
C	-9.27961	-2.41534	0.37089
C	-6.40083	-2.88226	-0.10626
C	-7.95416	-3.97059	-1.75988
C	-8.23957	-1.29480	0.57395
C	-7.56011	-1.48106	-1.83214
C	-9.78910	-2.38629	-1.08322
C	-8.60131	-2.60039	-2.04220
C	2.33437	-2.98042	-1.57113
C	1.06166	-3.49519	-1.89290
C	0.95284	-4.80203	-2.40968
C	2.09446	-5.56592	-2.62001
C	3.35339	-5.04341	-2.30314
C	3.47212	-3.75430	-1.77736
C	-0.07789	-2.60251	-1.76455
S	-1.49397	-2.83177	-2.73531
C	-2.49657	-1.70642	-1.70747
C	-2.47678	-2.28363	-0.28336
N	-1.07780	-2.57420	0.12951
S	-1.06510	-3.94715	1.26060
C	0.67305	-4.24719	1.64423
O	-1.77339	-3.51653	2.46919
O	-1.61962	-5.04142	0.46094
C	1.25815	-5.49082	1.28820
C	2.60328	-5.68171	1.62491
C	3.36123	-4.72415	2.29732
C	2.72636	-3.54574	2.68814
C	1.38288	-3.28031	2.40386
H	0.30100	6.21226	1.51009
H	-0.53595	7.87899	3.09919
H	-4.34673	5.89059	3.24028
H	-4.70493	3.84627	1.95819
H	-2.87716	7.75396	3.95504
H	-1.47221	6.26584	-0.96669
H	3.81071	4.69159	-1.65766
H	3.16558	6.81827	-2.66565
H	-0.87961	8.23308	-2.30322
H	1.45145	8.54444	-3.13870
H	-5.68466	-0.92381	1.93326
H	-3.25894	1.70081	2.93949
H	-6.03289	0.48922	-2.09369
H	-3.67879	3.31698	-1.58730
H	5.63240	1.12492	1.96146

H	2.79270	3.50354	1.78646
H	5.56096	0.23548	-2.22558
H	2.65156	2.43565	-2.92248
H	-6.09587	3.89281	-1.45487
H	-5.44404	4.14844	-3.08563
H	-6.45470	2.73480	-2.74494
H	-3.57948	2.68757	-3.97270
H	-2.83448	1.44807	-2.95224
H	-4.45183	1.18428	-3.64722
H	-2.32673	-0.53742	2.66426
H	-2.84434	-0.29397	4.34035
H	-3.82043	-1.29526	3.25916
H	-5.63361	2.10560	3.62299
H	-5.84340	0.37513	3.92326
H	-4.69773	1.30547	4.90032
H	3.79916	-0.32084	-3.59894
H	2.18721	0.05121	-2.92613
H	2.62034	0.58302	-4.55980
H	4.88474	3.38908	-3.54194
H	5.43310	1.78425	-4.04274
H	4.10739	2.57319	-4.91166
H	5.06520	4.50895	1.89524
H	4.32922	4.35982	3.50317
H	5.59247	3.22763	2.99734
H	2.28587	1.28470	2.75362
H	3.89105	1.22764	3.51737
H	2.71734	2.45601	4.01370
H	10.17256	0.25687	1.03978
H	10.79964	-1.36798	0.75008
H	10.19798	-0.24471	-1.41135
H	9.11419	-1.37615	2.60767
H	7.82765	0.31548	-1.89853
H	8.39971	1.24713	-0.51990
H	9.94246	-2.73195	-1.24528
H	8.72141	-2.04776	-2.32105
H	6.73927	-0.83711	2.13123
H	7.77093	0.56667	1.85416
H	6.31725	-1.75376	-1.49570
H	5.88054	-2.19877	0.15535
H	7.65473	-3.19420	1.71296
H	9.31295	-3.40468	1.14453
H	7.68426	-3.68793	-0.74156
H	-8.27457	-3.82085	1.70040
H	-9.36319	-4.58741	0.54158
H	-6.97168	-4.97132	-0.09895
H	-10.11906	-2.25483	1.06067
H	-5.55078	-3.04071	-0.78576
H	-6.00015	-2.92666	0.91391
H	-8.68457	-4.77502	-1.92340
H	-7.12297	-4.14807	-2.45691

H	-8.69604	-0.31315	0.38767
H	-7.90126	-1.28972	1.61745
H	-6.73055	-1.61606	-2.54049
H	-8.01837	-0.50965	-2.06111
H	-10.27669	-1.42429	-1.29381
H	-10.54533	-3.16850	-1.23729
H	-8.95505	-2.56601	-3.08134
H	2.41842	-1.96757	-1.18782
H	-0.02776	-5.20735	-2.64104
H	2.00746	-6.56927	-3.02655
H	4.44930	-3.34857	-1.53680
H	0.14341	-1.55536	-1.53716
H	-2.05936	-0.70766	-1.75333
H	-3.51516	-1.67390	-2.09832
H	-3.05309	-3.20944	-0.25747
H	-2.91753	-1.55824	0.40481
H	-0.70290	-1.69269	0.55947
C	4.81860	-4.96181	2.60669
H	3.28228	-2.80653	3.25908
C	0.79330	-2.01208	2.97845
C	0.55385	-6.66804	0.64375
H	3.06550	-6.62923	1.36022
H	1.26511	-7.49185	0.53465
H	-0.28477	-7.01770	1.25180
H	0.14503	-6.42923	-0.33788
H	0.49457	-1.27730	2.22351
H	-0.09088	-2.22751	3.58304
H	1.53751	-1.52648	3.61541
H	5.45899	-4.52941	1.82634
H	5.10724	-4.49804	3.55561
H	5.04862	-6.03055	2.66326
H	4.24375	-5.64401	-2.46917

TS-9Si

B3LYP/6-31G(d) Energy = -4825.282903
B3LYP/6-31G(d) Free Energy = -4823.816098
Number of Imaginary Frequencies = 1 (-167.14)

B3LYP/6-31G(d) Geometry

C	-0.54808	5.06859	2.51542
C	-1.43316	4.10429	1.95828
C	-0.88918	5.77979	3.64507
C	-2.68397	3.87889	2.61797
C	-1.11205	3.32930	0.79094
C	-3.01311	4.64082	3.77109
C	-3.57696	2.91058	2.09282
C	-2.13788	5.57398	4.27746
C	-1.95217	2.27892	0.44211
C	0.07264	3.65063	-0.05783
C	-3.24074	2.09838	1.02918

O	-1.59472	1.44123	-0.59278
C	-4.26415	1.15570	0.46290
C	1.03143	2.68079	-0.31831
C	0.22264	4.94997	-0.65812
C	1.42095	5.24249	-1.38579
C	-0.78006	5.95816	-0.59757
C	2.41436	4.23991	-1.51565
C	1.59076	6.52545	-1.97222
C	2.24131	2.96405	-1.02153
C	3.34251	1.95342	-1.17043
O	0.85645	1.41573	0.20085
C	-0.59283	7.18719	-1.19119
C	0.60847	7.48349	-1.87665
P	-0.31059	0.40153	-0.43775
C	-4.67760	0.01223	1.18600
C	-4.91269	1.47909	-0.75095
C	3.57256	1.30846	-2.40564
C	4.22296	1.71957	-0.08648
C	-5.98063	0.68445	-1.18865
C	-4.52496	2.68928	-1.60142
C	-6.44629	-0.41770	-0.46752
C	-5.75657	-0.73897	0.70826
C	-7.67354	-1.23554	-0.89504
C	-3.98998	-0.43515	2.47590
C	5.30780	0.85671	-0.26453
C	4.05176	2.41488	1.26437
C	5.57796	0.21989	-1.48399
C	4.68426	0.45930	-2.53264
C	6.83995	-0.64291	-1.63698
C	2.68988	1.55235	-3.63083
C	-3.43222	-1.86567	2.35643
C	-4.92399	-0.30544	3.69502
C	-5.68628	3.69466	-1.73015
C	-3.99687	2.26376	-2.98502
C	2.19350	0.25139	-4.28701
C	3.41851	2.44088	-4.66002
C	5.27369	3.28452	1.61858
C	3.73458	1.41249	2.38860
O	-0.54730	-0.60879	0.66802
O	0.05086	-0.04873	-1.81454
C	8.24120	-3.25811	-2.06404
C	8.17152	-2.60220	-0.67140
C	8.23818	-2.15858	-3.14388
C	6.87824	-1.76841	-0.56218
C	9.39399	-1.68256	-0.47314
C	6.94902	-1.31819	-3.02844
C	8.10500	0.24813	-1.44888
C	9.46566	-1.24589	-2.95121
C	9.39637	-0.58778	-1.55934
C	-9.13399	-3.04124	-2.79135

C	-9.54580	-1.56827	-2.60006
C	-8.53116	-3.57408	-1.47694
C	-8.30926	-0.72897	-2.21563
C	-10.60352	-1.47193	-1.48281
C	-7.29519	-2.73049	-1.10240
C	-8.76753	-1.16027	0.21166
C	-9.58161	-3.47565	-0.35177
C	-10.00219	-2.00319	-0.16703
C	-1.53718	-5.02925	-0.34444
C	-0.86806	-3.95806	-0.97741
C	-1.61057	-2.95416	-1.63955
C	-2.99607	-3.05339	-1.69162
C	-3.64667	-4.13840	-1.09491
C	-2.91935	-5.12482	-0.41916
C	0.57357	-3.93201	-0.92794
S	1.48937	-3.23638	-2.22544
C	2.96713	-2.88007	-1.21751
C	2.48784	-1.99920	-0.04687
N	1.31132	-2.59741	0.60582
S	1.59281	-3.61726	1.98706
C	2.38569	-2.61797	3.26782
O	0.26100	-4.04316	2.41253
O	2.54090	-4.62133	1.48508
C	3.76853	-2.78270	3.54721
C	4.30852	-2.00788	4.58052
C	3.55343	-1.10137	5.32399
C	2.19769	-0.97710	5.02142
C	1.57793	-1.71285	4.00709
H	0.41567	5.23166	2.04622
H	-0.19043	6.50368	4.05624
H	-3.97190	4.46321	4.25298
H	-4.56001	2.80861	2.54573
H	-2.39805	6.14623	5.16390
H	-1.71121	5.74783	-0.08504
H	3.33825	4.48716	-2.03256
H	2.51273	6.73006	-2.51179
H	-1.37958	7.93497	-1.13627
H	0.74589	8.45908	-2.33507
H	-6.47154	0.96433	-2.11381
H	-3.71001	3.21552	-1.09861
H	-6.07445	-1.60024	1.28976
H	-3.13362	0.22386	2.64473
H	5.98295	0.70485	0.57337
H	3.19530	3.09003	1.18913
H	4.85715	-0.00326	-3.49788
H	1.79860	2.09025	-3.29694
H	-2.69857	-1.92623	1.54824
H	-2.93437	-2.15619	3.28951
H	-4.22513	-2.59916	2.16622
H	-4.39743	-0.58884	4.61465

H	-5.28787	0.72123	3.81638
H	-5.80083	-0.95763	3.60013
H	-6.03715	4.02343	-0.74530
H	-5.36248	4.58092	-2.28930
H	-6.54226	3.26270	-2.26216
H	-3.13262	1.60082	-2.88277
H	-4.76693	1.74198	-3.56674
H	-3.68556	3.14385	-3.56093
H	3.02040	-0.36795	-4.65785
H	1.59044	-0.32276	-3.57964
H	1.55916	0.49222	-5.14877
H	3.72590	3.39761	-4.22346
H	4.31962	1.94666	-5.04430
H	2.76363	2.65358	-5.51355
H	5.47674	4.02094	0.83314
H	5.09690	3.82717	2.55520
H	6.17949	2.68089	1.75184
H	4.54878	0.69119	2.53112
H	3.58739	1.93962	3.33954
H	2.81792	0.85812	2.16655
H	7.38555	-3.93295	-2.20768
H	9.14865	-3.87146	-2.15042
H	8.16445	-3.37966	0.10456
H	8.27376	-2.61939	-4.13996
H	6.80500	-1.33352	0.44230
H	6.00240	-2.42144	-0.68727
H	10.32056	-2.27073	-0.52602
H	9.36400	-1.22412	0.52534
H	6.94466	-0.55358	-3.81613
H	6.07439	-1.96026	-3.20544
H	8.06687	0.74627	-0.47193
H	8.10003	1.04365	-2.20614
H	9.48985	-0.47450	-3.73325
H	10.39082	-1.83042	-3.05009
H	10.26373	0.07078	-1.41750
H	-8.40085	-3.12671	-3.60564
H	-10.00569	-3.64407	-3.08157
H	-9.96294	-1.17758	-3.53781
H	-8.22719	-4.62190	-1.60713
H	-8.60296	0.32362	-2.10794
H	-7.57014	-0.77224	-3.02728
H	-11.49614	-2.05223	-1.75517
H	-10.92624	-0.42919	-1.35653
H	-6.83710	-3.12991	-0.18847
H	-6.53820	-2.80027	-1.89664
H	-9.05474	-0.11086	0.36252
H	-8.35758	-1.51242	1.16649
H	-9.16835	-3.87090	0.58690
H	-10.45740	-4.09169	-0.59878
H	-10.74736	-1.93078	0.63664

H	-0.96186	-5.77392	0.19731
H	-1.10155	-2.08526	-2.05081
H	-3.57431	-2.27118	-2.17343
H	-3.43393	-5.95438	0.05639
H	1.06464	-4.72852	-0.37880
H	3.42128	-3.80790	-0.86332
H	3.67237	-2.33168	-1.84558
H	2.19208	-1.01987	-0.42408
H	3.30697	-1.85332	0.66502
H	0.52428	-1.89657	0.73206
C	4.18673	-0.26322	6.40661
H	1.58786	-0.28265	5.59341
C	0.09909	-1.48454	3.79112
C	4.72508	-3.73427	2.85512
H	5.36407	-2.12774	4.81099
H	5.72658	-3.59948	3.27318
H	4.43077	-4.77776	2.98771
H	4.78317	-3.56518	1.77674
H	-0.13286	-1.12859	2.78146
H	-0.47395	-2.39973	3.95459
H	-0.25263	-0.72262	4.49204
H	4.47113	0.72255	6.01588
H	3.49500	-0.09505	7.23853
H	5.09229	-0.73394	6.80203
H	-4.72953	-4.20367	-1.13820

Distortion-interaction analysis

The reasons for the energy differences between **TS-4Re** and **TS-4Si** were further investigated using distortion-interaction analysis. The equation $\Delta\Delta E^{\ddagger} = \Delta\Delta E_{int} - \Delta\Delta E_{distort\mathbf{Cat}} - \Delta\Delta E_{distort\mathbf{Sub}}$ allows the relative energy difference between the two TS to be understood partially on the basis of the energy required to distort the structures of the catalyst and intermediate to the TS geometry. The energy required for this process is usually larger than the TS barrier but the interactions between the catalyst and intermediate, appearing as $\Delta\Delta E_{int}$ in the equation, offsets this energetically costly distortion process, shown as the two $\Delta\Delta E_{distort}$ terms. $\Delta\Delta E^{\ddagger}$ corresponds to the difference in M06-2X/6-31G(d,p) gas-phase energy between **TS-4Re** and **TS-4Si**. To determine the differences in catalyst and substrate distortion energies the catalyst and substrate portions of the two TS are separated and a single point energy taken in the gas-phase at the M06-2X/6-31G(d,p) level. The differences in energy of the distorted catalysts and substrates in **TS-4Re** and **TS-4Si** correspond to $\Delta\Delta E_{distort\mathbf{Cat}}$ and $\Delta\Delta E_{distort\mathbf{Sub}}$. This information can then be used to calculate $\Delta\Delta E_{int}$.

Distorted substrate **TS-4Re**
M06-2X/6-31G(d,p) energy = -2195.238013

C	3.24340	0.60438	0.69014
C	2.66749	0.60344	-0.59594
C	2.98888	-0.43317	-1.49561
C	3.88648	-1.42857	-1.13391
C	4.46348	-1.38870	0.13722
C	4.14775	-0.38164	1.05541
H	2.96028	1.36705	1.40718
C	1.74807	1.62774	-1.04791
H	2.52051	-0.46110	-2.47434
H	4.12690	-2.22804	-1.82386
Cl	5.59832	-2.63691	0.60165
H	4.59640	-0.38710	2.04175
S	1.69238	3.20957	-0.33278
N	-0.27487	1.13856	-0.73006
H	1.48720	1.62187	-2.10609
S	-0.47368	0.01847	0.58667
H	-0.43447	0.67599	-1.68252
O	0.07348	-1.24151	0.09153
O	0.10063	0.69153	1.75553
C	-4.93499	-0.37032	1.56763
C	-2.24783	-0.13053	0.86462
C	-2.69453	0.35559	2.07804
C	-4.05470	0.23443	2.43324
H	-5.98378	-0.46986	1.83422
H	-1.98700	0.81641	2.75710
H	-4.39270	0.61646	3.39088
C	-4.50734	-0.87921	0.31303
C	-3.12550	-0.76892	-0.07253
C	-2.73564	-1.27813	-1.34014
C	-3.66291	-1.86462	-2.17419
C	-5.01769	-1.98460	-1.79095
C	-5.42872	-1.49958	-0.57168

H	-1.71191	-1.20454	-1.67857
H	-3.34167	-2.23079	-3.14392
H	-5.73005	-2.45455	-2.46201
H	-6.46770	-1.57998	-0.26415
C	-0.90302	2.46164	-0.56602
H	-1.82791	2.51233	-1.14912
H	-1.13720	2.61369	0.48928
C	0.05387	3.56945	-1.05547
H	0.13682	3.55538	-2.14437
H	-0.27241	4.55356	-0.71778

Distorted substrate **TS-4Si**

M06-2X/6-31G(d,p) energy = -2195.238723

S	0.50207	0.06640	0.51859
N	0.25464	1.28572	-0.71230
S	-1.89392	3.18556	-0.44371
C	-0.23168	3.66527	-1.01994
H	-0.19463	3.64360	-2.11023
H	-0.01429	4.67826	-0.68066
C	0.73766	2.64570	-0.40151
H	1.73523	2.78887	-0.82495
H	0.76960	2.77545	0.68171
H	0.63089	0.99157	-1.67298
O	-0.00058	-1.16589	-0.08183
O	-0.10083	0.63342	1.72845
C	4.95354	-0.26488	1.54715
C	4.06985	0.40226	2.36211
C	2.71383	0.50165	1.98850
C	2.27527	-0.05761	0.80284
H	5.99877	-0.35493	1.83058
H	4.40071	0.84314	3.29664
H	2.00057	0.99384	2.63850
C	3.15864	-0.75574	-0.08629
C	4.53444	-0.85359	0.32568
C	5.46230	-1.54106	-0.50082
C	5.06320	-2.10474	-1.68928
C	3.71543	-1.99832	-2.09949
C	2.78350	-1.34509	-1.32340
H	6.49588	-1.60959	-0.17290
H	5.77952	-2.62671	-2.31618
H	3.40482	-2.43155	-3.04423
H	1.76313	-1.27762	-1.67243
C	-1.75967	1.56813	-1.09246
H	-1.51151	1.52436	-2.15764
C	-4.40595	-1.47373	0.19393
C	-4.05361	-0.47326	1.10476
C	-3.16637	0.51652	0.70733
C	-2.63668	0.51914	-0.59802
C	-2.98998	-0.51344	-1.48911
C	-3.88048	-1.50541	-1.09937

Cl	-5.52739	-2.72225	0.69268
H	-4.46300	-0.48346	2.10810
H	-2.85839	1.27854	1.41418
H	-2.57130	-0.52144	-2.49038
H	-4.16135	-2.29648	-1.78323

Distorted catalyst **TS-4Re**
M06-2X/6-31G(d,p) energy = -2580.624899

C	-0.57321	4.76843	2.65570
C	-1.90900	4.78648	3.11988
C	-2.79160	3.82441	2.68864
C	-2.38485	2.81551	1.77432
C	-1.04599	2.81980	1.26582
C	-0.15387	3.81506	1.75447
C	-3.27568	1.78744	1.37721
C	-2.88307	0.75098	0.55662
C	-1.55016	0.77773	0.04820
C	-0.65716	1.80570	0.32037
C	0.69168	1.82299	-0.31838
C	1.53422	0.72484	-0.19778
C	2.91335	0.75936	-0.56364
C	3.38273	1.90785	-1.16644
C	2.53462	3.00296	-1.47011
C	1.16620	2.96723	-1.04972
C	3.01735	4.13331	-2.18314
C	2.18299	5.17973	-2.50056
C	0.82217	5.13255	-2.11753
C	0.32853	4.05947	-1.40891
O	1.06301	-0.42865	0.40063
O	-1.17155	-0.22412	-0.82493
C	3.84743	-0.37339	-0.24919
C	-3.84864	-0.34541	0.21185
C	-4.22297	-1.29665	1.19071
C	-5.18814	-2.25797	0.85893
C	-5.79098	-2.31601	-0.39849
C	-5.39361	-1.37387	-1.35254
C	-4.44168	-0.38741	-1.07335
C	4.42061	-1.14233	-1.28886
C	5.35492	-2.13460	-0.95925
C	5.74119	-2.39490	0.35610
C	5.15275	-1.62930	1.36618
C	4.21746	-0.62655	1.09588
C	-4.12281	0.64727	-2.15238
C	-3.64871	-1.29719	2.60934
C	-6.88852	-3.33391	-0.68795
C	4.07546	-0.92930	-2.76314
C	6.80064	-3.44561	0.66616
C	3.66826	0.18375	2.27029
P	-0.05970	-1.36638	-0.36467

O	0.47210	-1.92363	-1.67274
O	-0.60113	-2.32234	0.65441
C	4.78387	0.98614	2.96894
C	2.90565	-0.70108	3.27419
C	3.59535	-2.22303	-3.44336
C	5.26127	-0.31579	-3.53410
C	6.33328	-4.47389	1.71185
C	8.12547	-2.78810	1.10011
C	-5.35871	1.50635	-2.48483
C	-3.53530	0.00160	-3.41952
C	-6.62203	-4.16659	-1.95453
C	-8.26872	-2.65188	-0.76607
C	-3.01335	-2.64509	2.99700
C	-4.72079	-0.88092	3.63649
H	0.13201	5.51084	3.01781
H	-2.22842	5.54848	3.82457
H	-3.81552	3.81001	3.05306
H	0.87572	3.81276	1.41907
H	-4.29377	1.80576	1.75604
H	4.43400	1.97476	-1.43136
H	4.06165	4.14820	-2.48422
H	2.56177	6.03532	-3.05183
H	0.15870	5.94900	-2.38765
H	-0.71788	4.03471	-1.12891
H	-5.49155	-2.97887	1.61467
H	-5.85815	-1.38627	-2.33509
H	5.80752	-2.71443	-1.76039
H	5.43941	-1.80525	2.39925
H	-3.36265	1.32488	-1.75646
H	-2.84999	-0.55295	2.64723
H	-6.91470	-4.02850	0.16241
H	3.24621	-0.21885	-2.81121
H	6.99751	-3.98969	-0.26794
H	2.95481	0.91258	1.87946
H	5.29830	1.64802	2.26481
H	4.36511	1.60363	3.77134
H	5.53606	0.32726	3.41626
H	2.08731	-1.23282	2.78273
H	3.56620	-1.43974	3.74196
H	2.48071	-0.08566	4.07496
H	2.73510	-2.64467	-2.92083
H	3.29312	-2.01897	-4.47640
H	4.38246	-2.98407	-3.48272
H	5.58613	0.63190	-3.09292
H	6.12427	-0.99098	-3.53640
H	4.98504	-0.12638	-4.57742
H	5.40472	-4.96541	1.40537
H	7.09472	-5.24757	1.85784
H	6.15226	-4.00292	2.68380
H	8.48855	-2.09115	0.33867

H	7.99685	-2.22598	2.03159
H	8.89958	-3.54500	1.26883
H	-5.75118	1.99864	-1.58947
H	-5.10095	2.28246	-3.21391
H	-6.16602	0.90265	-2.91356
H	-3.29677	0.76706	-4.16578
H	-2.61187	-0.53563	-3.18816
H	-4.24075	-0.69811	-3.88211
H	-5.66581	-4.69724	-1.89406
H	-7.41019	-4.91361	-2.09761
H	-6.59742	-3.53902	-2.85181
H	-8.48300	-2.09224	0.14927
H	-8.31186	-1.94778	-1.60428
H	-9.06325	-3.39289	-0.90838
H	-2.62724	-2.59174	4.02126
H	-2.17694	-2.87859	2.33487
H	-3.73979	-3.46555	2.96751
H	-5.14909	0.09844	3.40026
H	-5.54482	-1.60272	3.66724
H	-4.28749	-0.82745	4.64117

Distorted catalyst **TS-4Si**
M06-2X/6-31G(d,p) energy = -2580.625193

C	0.87485	4.99941	-2.27778
C	2.25912	5.06889	-2.56064
C	3.09457	4.06938	-2.12047
C	2.58845	2.96807	-1.37853
C	1.19579	2.91457	-1.05297
C	0.35849	3.95578	-1.54231
C	3.43296	1.90838	-0.96661
C	2.94637	0.78052	-0.33819
C	1.55153	0.73554	-0.03275
C	0.70061	1.80735	-0.27790
C	-0.69051	1.81280	0.25835
C	-1.55460	0.76007	-0.00954
C	-2.93859	0.78554	0.33682
C	-3.40458	1.89179	1.01704
C	-2.54882	2.93966	1.43722
C	-1.16417	2.89871	1.07689
C	-3.03746	4.01649	2.22539
C	-2.19260	5.00272	2.67735
C	-0.81539	4.94330	2.36089
C	-0.31585	3.92383	1.58106
O	-1.08256	-0.32662	-0.72765
O	1.08147	-0.37311	0.63904
C	-3.88595	-0.31646	-0.03427
C	3.88649	-0.33198	0.02111
C	4.22969	-0.56937	1.37336
C	5.17594	-1.55928	1.66868

C	5.80227	-2.31868	0.67821
C	5.44163	-2.07243	-0.64958
C	4.50305	-1.09458	-1.00287
C	-4.27685	-0.49053	-1.38207
C	-5.22957	-1.46752	-1.69081
C	-5.81784	-2.27331	-0.71594
C	-5.40974	-2.09087	0.60802
C	-4.45882	-1.13083	0.97472
C	4.19394	-0.89131	-2.48737
C	3.65881	0.25995	2.52400
C	6.88933	-3.32393	1.04187
C	-3.73572	0.38130	-2.51449
C	-6.90238	-3.27517	-1.09282
C	-4.10610	-0.98776	2.45729
P	-0.06388	-1.40009	0.00329
O	-0.67539	-2.09786	1.18078
O	0.52353	-2.23162	-1.12100
C	-3.51434	-2.28098	3.04690
C	-5.32108	-0.51109	3.27755
C	-4.85535	1.20841	-3.17570
C	-2.96386	-0.44905	-3.55675
C	-8.27831	-2.84006	-0.55243
C	-6.56781	-4.70964	-0.64957
C	3.51350	-2.12619	-3.10270
C	5.45071	-0.49090	-3.28375
C	8.28102	-2.80537	0.62814
C	6.63831	-4.72674	0.46118
C	4.76724	1.06290	3.23374
C	2.86414	-0.59701	3.52662
H	0.21075	5.77487	-2.64830
H	2.65442	5.90191	-3.13433
H	4.15740	4.09693	-2.34668
H	-0.70529	3.91475	-1.34253
H	4.49594	1.97602	-1.18207
H	-4.46005	1.94985	1.26776
H	-4.09455	4.03493	2.47758
H	-2.57481	5.81658	3.28633
H	-0.14283	5.70687	2.74079
H	0.74328	3.89135	1.35710
H	5.45542	-1.72545	2.70669
H	5.91941	-2.64192	-1.44246
H	-5.53893	-1.59408	-2.72566
H	-5.85623	-2.70174	1.38865
H	3.48197	-0.06870	-2.57385
H	2.96192	0.98808	2.10280
H	6.88748	-3.41647	2.13622
H	-3.02774	1.09469	-2.08619
H	-6.96653	-3.27934	-2.18898
H	-3.33174	-0.22327	2.54792
H	-2.58260	-2.53401	2.53640

H	-3.29147	-2.14104	4.11096
H	-4.21171	-3.12287	2.96695
H	-5.03724	-0.34947	4.32333
H	-5.72762	0.42816	2.88829
H	-6.13028	-1.24972	3.26402
H	-5.37851	1.82579	-2.43851
H	-4.43978	1.87307	-3.94139
H	-5.59947	0.56789	-3.66128
H	-2.13433	-0.97879	-3.08136
H	-3.61442	-1.18338	-4.04545
H	-2.55423	0.20428	-4.33584
H	-8.28108	-2.81416	0.54283
H	-9.06121	-3.53647	-0.87308
H	-8.54319	-1.83986	-0.90857
H	-5.60417	-5.03391	-1.05436
H	-6.52447	-4.78603	0.44307
H	-7.33458	-5.41163	-0.99479
H	2.56365	-2.32689	-2.60010
H	3.29963	-1.95503	-4.16320
H	4.15061	-3.01638	-3.03625
H	5.18880	-0.28191	-4.32670
H	5.92244	0.40516	-2.86734
H	6.20187	-1.28844	-3.28617
H	8.48381	-1.82635	1.07231
H	9.06694	-3.49731	0.95073
H	8.35320	-2.69861	-0.45977
H	5.67579	-5.13317	0.78957
H	6.63969	-4.71596	-0.63395
H	7.42048	-5.42235	0.78341
H	4.33516	1.70505	4.00890
H	5.30920	1.70020	2.52778
H	5.49769	0.40527	3.71765
H	2.01631	-1.08471	3.03883
H	3.49371	-1.36516	3.99040
H	2.46858	0.03191	4.33171

Distorted truncated substrate **TS-4Re**
M06-2X/6-31G(d,p) energy = -1504.671776

C	3.49923	-1.12454	0.50578
S	4.29372	-0.00488	-0.55809
N	1.52885	-0.67313	-0.08281
H	3.26619	-2.11201	0.16592
S	0.70484	0.30284	1.09889
H	1.17476	-1.68367	-0.09110
O	0.48999	-0.58823	2.23552
O	1.51356	1.51890	1.22630
C	-3.27257	1.75296	-0.66009
C	-0.86998	0.77428	0.36083
C	-1.01899	2.12422	0.10846

C	-2.23497	2.61905	-0.40867
H	-4.21329	2.12590	-1.05621
H	-0.19827	2.79758	0.32544
H	-2.34130	3.68197	-0.59886
C	-3.15055	0.36026	-0.41232
C	-1.92135	-0.16945	0.11566
C	-1.83066	-1.56934	0.33968
C	-2.89863	-2.39385	0.05851
C	-4.11042	-1.87277	-0.44816
C	-4.23039	-0.52253	-0.67897
H	-0.92265	-2.01425	0.72120
H	-2.79723	-3.46162	0.22358
H	-4.94045	-2.54033	-0.65804
H	-5.15383	-0.10677	-1.07258
C	1.72178	-0.06877	-1.41305
H	0.99587	-0.48106	-2.12090
H	1.57313	1.00996	-1.33646
C	3.14489	-0.36626	-1.93144
H	3.24370	-1.41828	-2.20763
H	3.39891	0.26893	-2.78054
H	3.24283	-0.82686	1.50104

Distorted truncated substrate **TS-4Si**
M06-2X/6-31G(d,p) energy = -1504.671333

S	-0.67088	0.11781	1.07558
N	-1.59562	-0.56901	-0.24207
S	-4.42040	-0.04237	-0.44475
C	-3.31710	-0.02810	-1.89654
H	-3.31906	-1.00841	-2.37568
H	-3.67584	0.71326	-2.61084
C	-1.92339	0.33615	-1.36131
H	-1.18524	0.21909	-2.15905
H	-1.92320	1.36623	-1.00054
H	-1.15958	-1.46730	-0.63442
O	-0.44130	-1.00239	1.98342
O	-1.43550	1.29807	1.48926
C	3.27380	1.84286	-0.48869
C	2.20345	2.64837	-0.17938
C	1.00017	2.06811	0.27193
C	0.89093	0.69531	0.39174
H	4.20846	2.28085	-0.82856
H	2.27712	3.72734	-0.26635
H	0.16126	2.69340	0.55255
C	1.97492	-0.18887	0.07320
C	3.19547	0.43057	-0.37253
C	4.31340	-0.38393	-0.69421
C	4.23945	-1.75274	-0.59236
C	3.03771	-2.36143	-0.16646
C	1.93305	-1.60630	0.16068
H	5.22838	0.09991	-1.02471

H	5.09817	-2.36812	-0.84234
H	2.97636	-3.44241	-0.09991
H	1.02884	-2.10675	0.47604
C	-3.44962	-1.22182	0.40464
H	-3.21300	-2.15550	-0.06137
H	-3.09195	-1.01019	1.39064

QTAIM analysis

The proposed thionium H-bond interaction was further analysed using Quantum Theory of Atoms In Molecules (QTAIM).[19] In this topological analysis of electron density, interacting nuclei are connected by bond paths upon which lie bond critical points (BCPs). QTAIM analysis shows a BCP between the thionium CH and the oxygen of the phosphate implying a CH···O bonding interaction. Further, the Laplacian of the electron density ($\nabla^2\rho(r)$) at this BCP is found to be positive (Laplacian = 0.7201201E^{-01}), indicative of a weak H-bonding contact. This analysis was performed using the Amsterdam Density Functional (ADF) software package with the following ADF settings; functional = M06-2X, basis set = DZP, numerical quality = good, QTAIM = Full.[20]

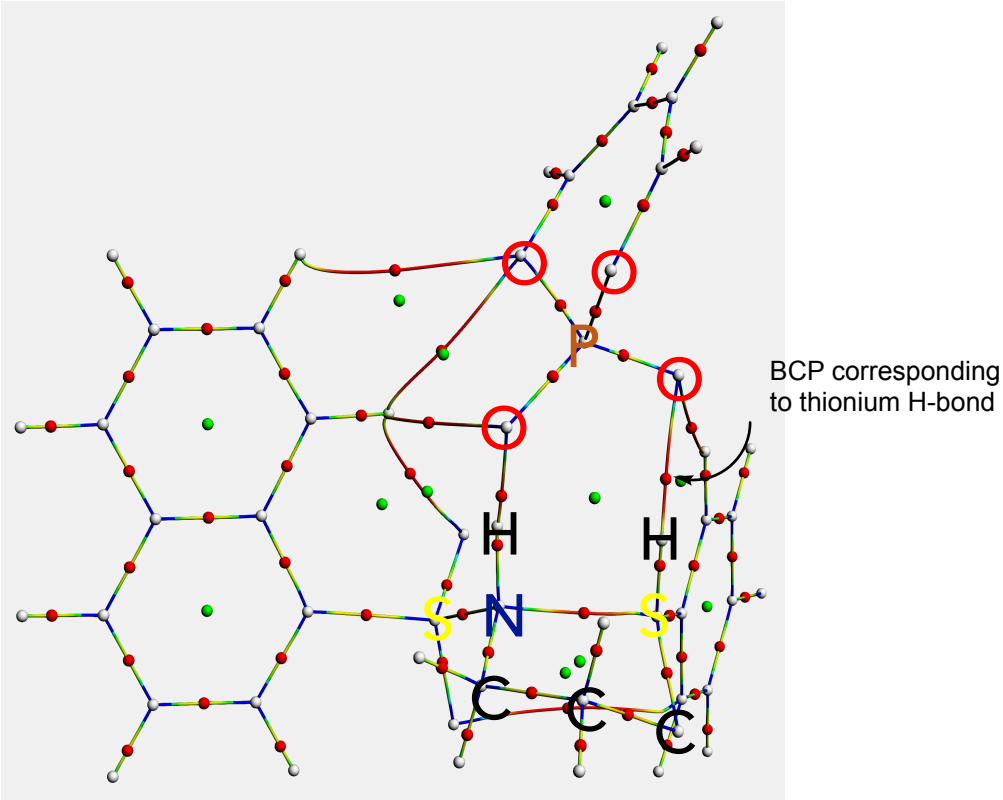


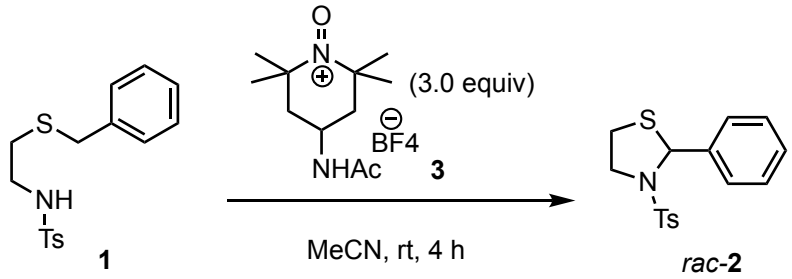
Figure S1. QTAIM plot showing atom critical points (shown in white, a few atoms have been added for clarity), ring critical points (in green) and bond critical points (in red).

Experimental Details

General Information

All commercial reagents were used as received; substrate **1** and product **2** was prepared according to reported procedures without modification.[21] Flash chromatography was carried out using 70-230 mesh silica gel and dry-packed columns. Thin layer chromatography was carried out using Merck TLC Silicagel 60 F254 aluminum sheets. Components were visualized by UV light (λ = 254 nm) and stained with phosphomolybdic dip. NMR spectra were recorded at 298 K on a Bruker Avance 400 Ultrashield apparatus. ^{1}H NMR spectroscopy chemical shifts are quoted in ppm relative to tetramethylsilane (TMS). $CDCl_3$ was used as internal standard for ^{13}C NMR spectra. Chemical shifts are given in ppm and coupling constants in Hz. High performance liquid chromatography (HPLC) was performed on Agilent Technologies chromatographs (1100 and 1200 Series), using Chiralpak AD-H columns. Specific optical rotation measurements were carried out on a Jasco P-2000 polarimeter.

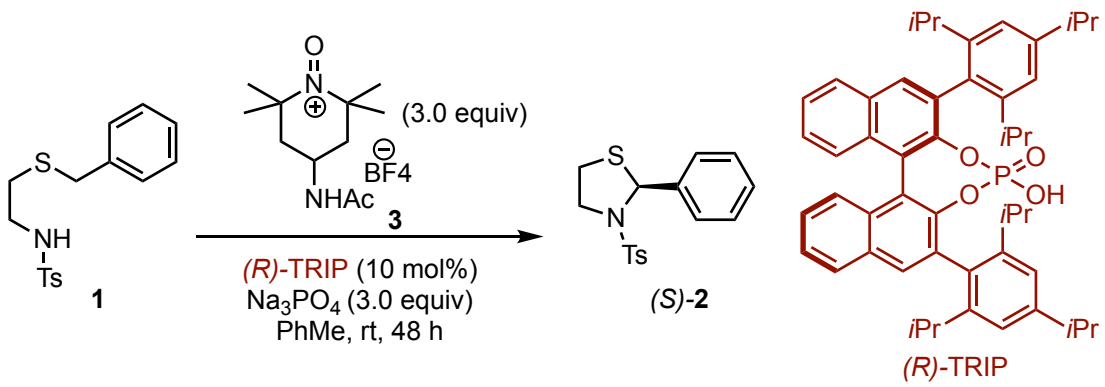
Synthesis of rac-2



Scheme S1. Synthesis of *rac*-**2**

Oxopiperidinium salt **3** (60 mg, 0.2 mmol, 2.0 equiv) was added to 1 mL MeCN solution (0.1 M) of the substrate **1** (32.1 mg, 0.1 mmol, 1.0 equiv) at room temperature. The mixture was stirred at room temperature for 4 h (the reaction was monitored by TLC until complete), then the solvent was removed under vacuum. The crude mixture was purified by flash column chromatography (SiO2, EtOAc/petroleum ether =1:5) to give the corresponding cyclization product *rac*-**2** (30 mg, 94% yield).

Synthesis of (*S*)-2



Scheme S2. Synthesis of *(S)*-**2**

A suspension of the substrate **1** (32.1 mg, 0.1 mmol, 1.0 equiv), Na_3PO_4 (49.2 mg, 0.3 mmol, 3.0 equiv), oxopiperidinium salt **3** (90 mg, 0.3 mmol, 3.0 equiv) and **(*R*)-TRIP** (7.5 mg, 10 mol %) in 1 mL toluene (0.1 M) was stirred vigorously at room temperature. After stirred at 48 h, the reaction mixture was directly subjected to flash column chromatography (SiO2, EtOAc/petroleum ether =1:5) to give the corresponding cyclization product *(S)*-**2** (18 mg, 57% ee, 56% yield).

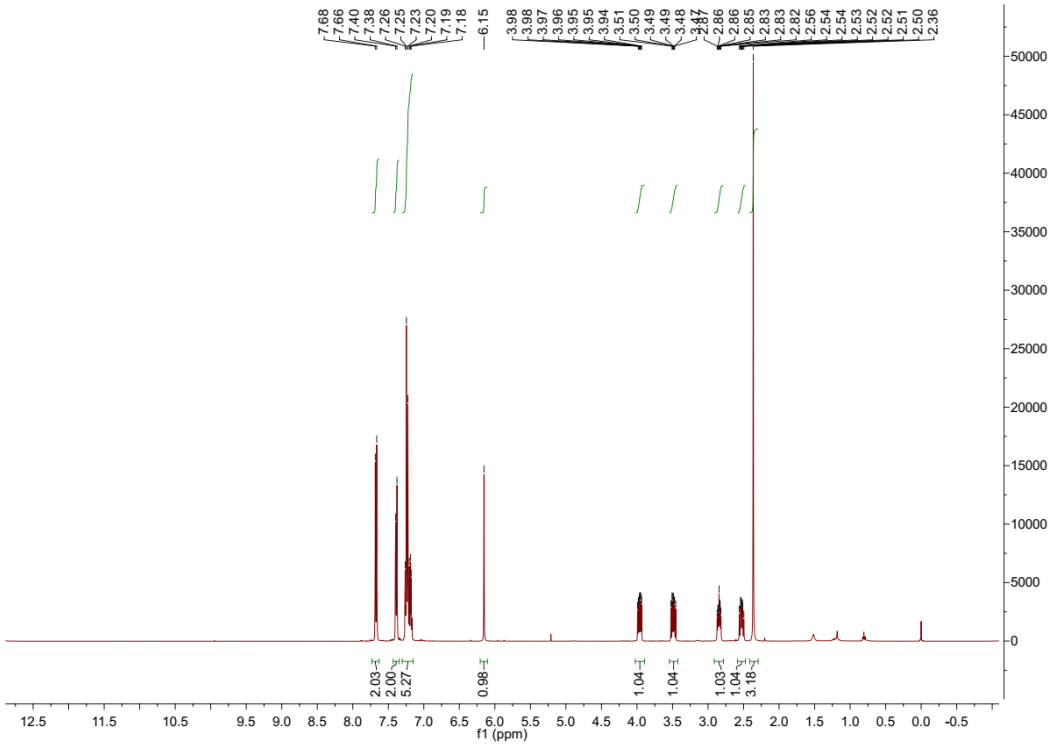
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 7.5 Hz, 2H), 7.29 – 7.14 (m, 5H), 6.15 (s, 1H), 3.96 (ddd, J = 12.3, 6.6, 4.0 Hz, 1H), 3.49 (ddd, J = 12.3, 8.4, 6.2 Hz, 1H), 2.85 (ddd, J = 10.6, 6.2, 4.0 Hz, 1H), 2.53 (ddd, J = 10.6, 8.4, 6.6 Hz, 1H), 2.36 (s, 3H).

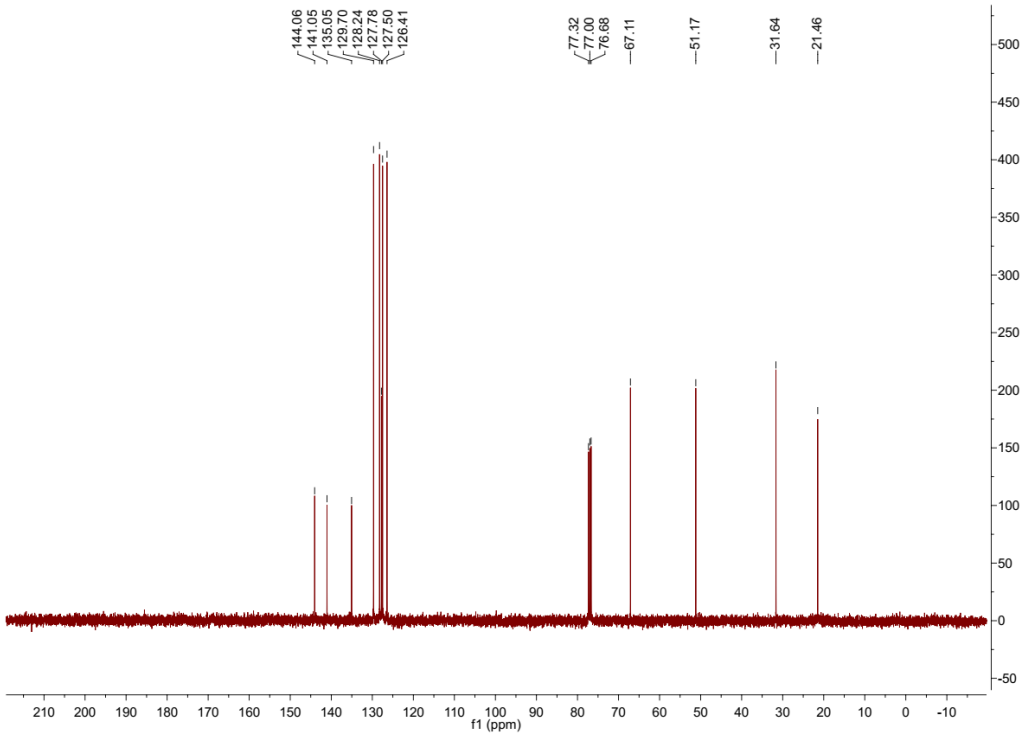
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.06, 141.05, 135.05, 129.70, 128.24, 127.78, 127.50, 126.41, 67.11, 51.17, 31.64, 21.46.

$[\alpha]_D^{22}$ -0.11 (c 1.2 in $CHCl_3$).

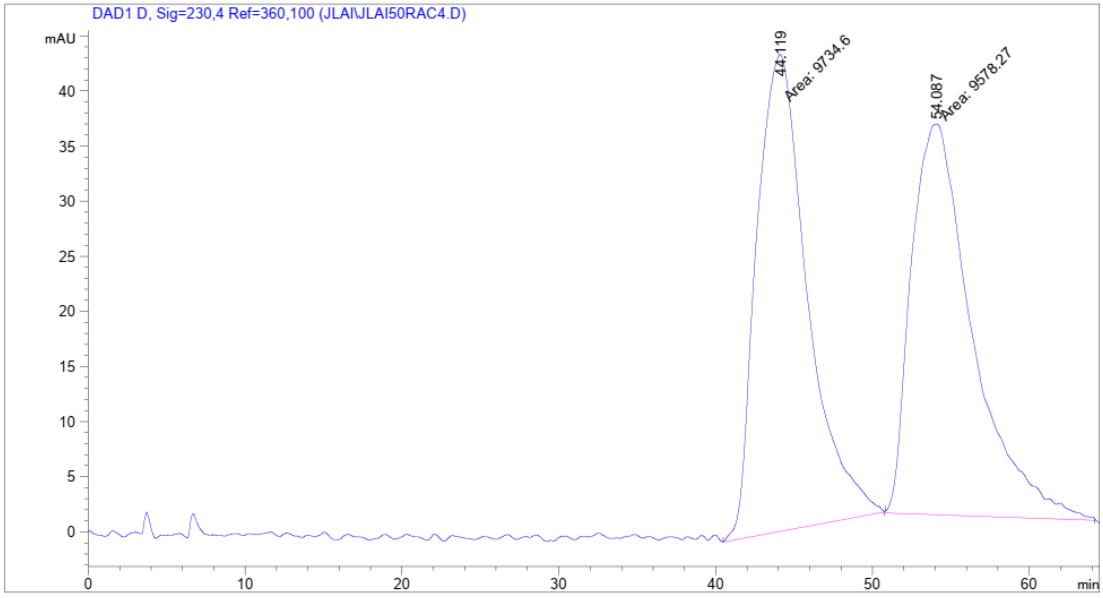
HPLC (Chiralpak AD-H column, 99:1 hexanes/isopropanol, 1.0 ml/min), tr = 45.17 min (major), 54.76 min (minor).

NMR spectra of (*S*)-2

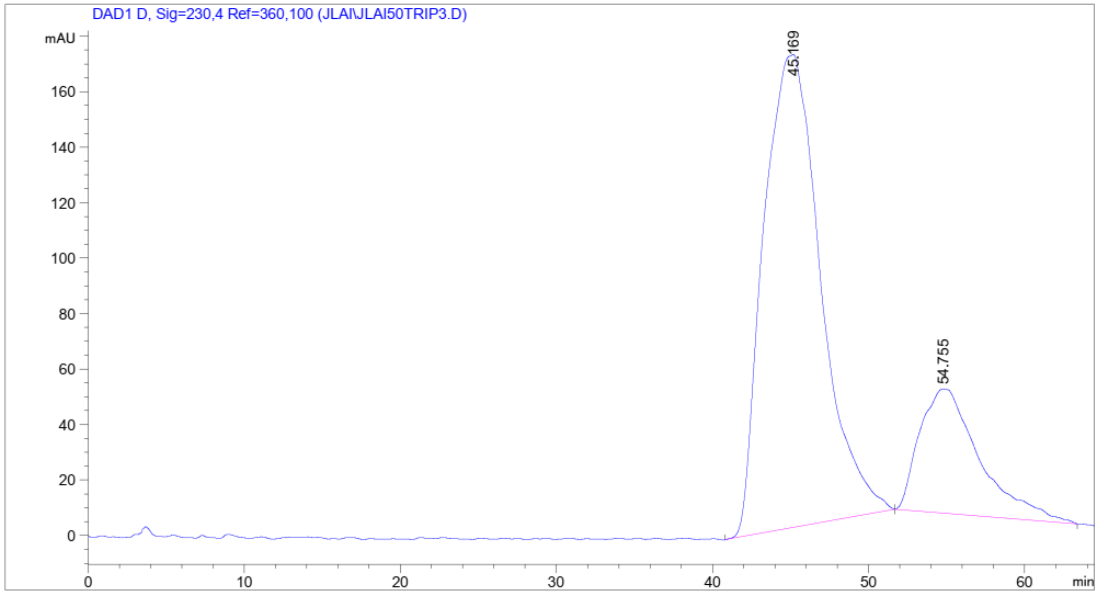




HPLC chromatogram of 2



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	44.119	MM	3.7485	9734.60449	43.28234	50.4047
2	54.087	MM	4.5058	9578.27344	35.42956	49.5953



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	45.169	BB	2.9776	4.33823e4	170.43498	78.4813
2	54.755	BB	3.1858	1.18949e4	44.73933	21.5187

Crystal Data

Experimental. Single colourless needle-shaped crystals of **(*S*)-2** recrystallised from a mixture of DCM and pentane by slow evaporation. A suitable crystal with dimensions 0.10 × 0.06 × 0.03 mm^3 was selected and mounted on a mylar loop in oil on a Bruker APEX-II CCD diffractometer.[22] The crystal was kept at a steady T = 90(2) K during data collection. The structure was solved with the **ShelXT** 2018/2 solution program[23] using Intrinsic Phasing methods and by using **Olex2** 1.5 as the graphical interface.[24] The model was refined with **XL** using full matrix least squares minimisation on $\boldsymbol{F^2}$.[25]

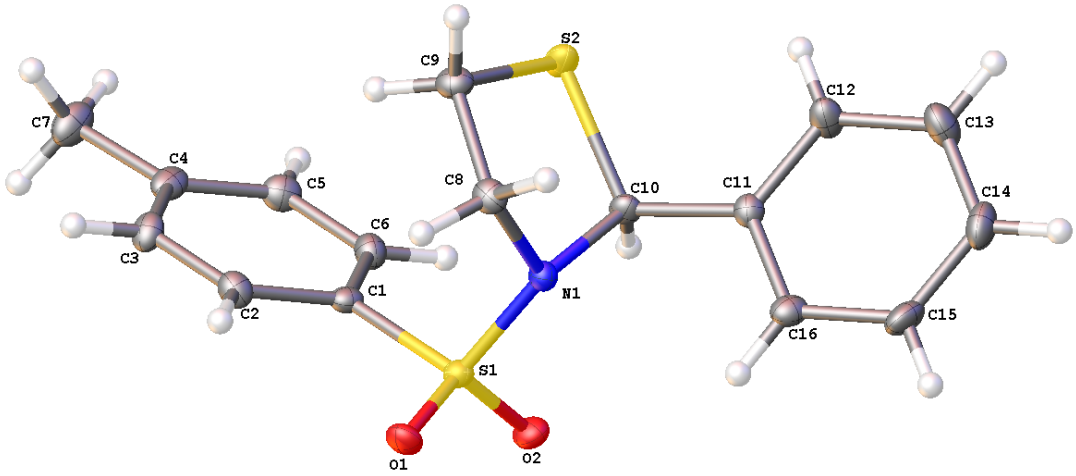


Figure S2. ORTEP X-ray structure of *(S)*-**2**.

Crystal Data. $C_{16}H_{17}NO_2S_2$, M_r = 319.42, orthorhombic, $P2_12_12_1$ (No. 19), a = 6.2635(5) Å, b = 11.4411(10) Å, c = 20.8675(18) Å, $\alpha = \beta = \gamma = 90^\circ$, V = 1495.4(2) Å^3, T = 90(2) K, Z = 4, Z' = 1, μ(CuK$_\alpha$) = 3.255, 40112 reflections measured, 2735 unique (R_{int} = 0.0616) which were used in all calculations. The final wR_2 was 0.0620 (all data) and R_1 was 0.0262 (I≥2 σ(I)).

Compound	**(S)-2**
Formula	$C_{16}H_{17}NO_2S_2$
$D_{calc.}$/ g cm^{-3}	1.419
μ/mm^{-1}	3.255
Formula Weight	319.42
Colour	colourless
Shape	needle-shaped
Size/mm^3	0.10×0.06×0.03
T/K	90(2)
Crystal System	orthorhombic
Flack Parameter	-0.010(7)
Hooft Parameter	-0.019(6)
Space Group	$P2_12_12_1$
a/Å	6.2635(5)
b/Å	11.4411(10)
c/Å	20.8675(18)
α/°	90
β/°	90
γ/°	90
V/Å^3	1495.4(2)
Z	4
Z'	1
Wavelength/Å	1.54178
Radiation type	CuK$_\alpha$
Θ_{min}/°	4.237
Θ_{max}/°	68.189
Measured Refl's.	40112
Indep't Refl's	2735
Refl's I≥2 σ(I)	2604
R_{int}	0.0616
Parameters	192
Restraints	0
Largest Peak	0.259
Deepest Hole	-0.256
GooF	1.057
wR_2 (all data)	0.0620
wR_2	0.0591
R_1 (all data)	0.0294
R_1	0.0262

Structure Quality Indicators

Reflections:	d min (Cu\a) 2Θ=136.4° 0.83	I/σ(I) 38.8	Rint 6.16%	Full 135.4° 99.9
Refinement:	Shift 0.001	Max Peak 0.3	Min Peak -0.3	GooF 1.057	Hooft -.019(6)

A colourless needle-shaped-shaped crystal with dimensions 0.10 × 0.06 × 0.03 mm^3 was mounted on a mylar loop in oil. Data were collected using a Bruker APEX-II CCD diffractometer operating at T = 90(2) K.

Data were measured using ϕ and ω scans of 1.0 ° per frame for between 20 and 60 s using CuK_α radiation (microfocus sealed X-ray tube, 45 kV, 0.60 mA). The total number of runs and images was based on the strategy calculation from the program APEX4. The maximum resolution that was achieved was Θ = 68.189° (0.83 Å).

The unit cell was refined (on 9906 reflections, 25% of the observed reflections) and data reduction carried out using **SAINT** (Bruker, V8.40B, 2016). Scaling and absorption corrections were performed using **SADABS-2016/2** (Bruker, 2016/2) was used for absorption correction. wR_2(int) was 0.0913 before and 0.0712 after correction.[26] The ratio of minimum to maximum transmission is 0.8821. The $\lambda/2$ correction factor is not present. The absorption coefficient μ of this material is 3.255 mm^{-1} at this wavelength (λ = 1.54178Å) and the minimum and maximum transmissions are 0.800 and 0.907. The final completeness is 99.90 % out to 68.189° in Θ.

The structure was solved and the space group $P2_12_12_1$ (# 19) determined by the **ShelXT** 2018/2 structure solution program[23] using Intrinsic Phasing methods and refined by full matrix least squares minimisation on F^2 using version 2018/3 of **XL**.[25] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

Table S6. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **(S)-2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
S1	647.3(9)	2457.4(5)	6731.1(3)	12.87(16)
S2	5059.5(10)	4553.6(6)	7137.0(3)	18.70(17)
O1	-1622(3)	2496.1(17)	6816.3(9)	17.4(4)
O2	1734(3)	1357.6(15)	6726.5(9)	18.2(4)
N1	1670(3)	3201.7(19)	7327.8(10)	12.8(5)
C1	1239(4)	3186(2)	6012.0(12)	13.6(6)
C2	-301(5)	3892(2)	5725.0(12)	16.8(6)
C3	186(5)	4450(2)	5154.6(12)	17.7(6)
C4	2190(5)	4324(2)	4867.7(13)	18.0(6)
C5	3702(5)	3634(2)	5170.7(13)	18.7(6)
C6	3241(5)	3058(2)	5739.6(13)	16.8(6)
C7	2669(5)	4910(3)	4237.8(14)	24.5(7)
C8	924(4)	4415(2)	7431.5(13)	16.0(6)
C9	2455(4)	5244(2)	7094.4(14)	16.9(6)
C10	3979(4)	3150(2)	7430.0(12)	13.6(6)
C11	4507(4)	2883(2)	8129.6(12)	13.7(6)
C12	6381(4)	3286(3)	8410.3(13)	19.9(6)
C13	6955(5)	2933(3)	9022.2(14)	24.0(7)
C14	5651(5)	2184(2)	9362.9(14)	24.0(7)
C15	3765(5)	1790(2)	9092.0(14)	21.9(7)
C16	3210(5)	2132(2)	8473.7(13)	17.1(6)

Table S7. Anisotropic Displacement Parameters ($\times 10^4$) for **(S)-2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	12.2(3)	11.9(3)	14.4(3)	0.3(3)	-0.2(2)	-1.2(3)
S2	12.0(3)	20.3(3)	23.8(3)	7.5(3)	-0.1(3)	-2.7(3)
O1	11.2(8)	20.2(10)	20.8(10)	0.1(9)	-0.3(7)	-3.7(8)
O2	19.5(10)	12.1(9)	23.0(10)	0.8(8)	-1.3(9)	0.5(8)
N1	12.1(11)	12.6(11)	13.5(11)	0.2(9)	-0.6(9)	0.8(9)
C1	15.5(14)	11.6(13)	13.7(13)	-1.9(11)	0.9(11)	-2.7(11)
C2	15.3(14)	18.4(13)	16.6(13)	-4.1(11)	-0.2(12)	2.6(11)
C3	22.6(15)	14.8(13)	15.8(13)	-0.7(10)	-0.1(12)	6.1(12)
C4	26.9(16)	13.5(14)	13.4(13)	-3.2(11)	1.2(12)	-1.3(12)
C5	19.4(14)	19.6(14)	17.2(14)	-3.8(12)	3.4(12)	0.4(11)
C6	17.4(14)	16.6(14)	16.5(14)	-1.6(11)	-2.2(12)	2.2(12)
C7	35.8(17)	20.8(15)	16.8(15)	0.5(12)	5.8(13)	3.4(13)
C8	14.4(13)	15.5(14)	18.1(14)	-3.1(11)	1.2(11)	3.3(11)
C9	16.5(13)	13.2(13)	20.9(14)	-2.2(12)	2.1(12)	0.7(11)
C10	9.5(13)	15.7(13)	15.7(13)	1.5(11)	1.6(11)	-0.9(10)
C11	14.1(13)	13.9(12)	13.1(13)	-1.4(10)	0.5(11)	2.6(10)
C12	14.8(13)	28.6(16)	16.2(15)	2.9(12)	0.7(12)	-1.1(12)
C13	19.3(15)	34.3(17)	18.4(15)	-2.2(13)	-4.2(13)	-0.5(13)
C14	33.3(17)	23.5(15)	15.1(14)	2.4(12)	-4.2(13)	6.8(14)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15	32.1(18)	15.2(14)	18.4(15)	4.7(12)	2.5(13)	-3.7(12)
C16	21.4(15)	13.3(13)	16.4(14)	-2.1(10)	1.6(12)	-1.2(11)

Table S8. Bond Lengths in Å for **(S)-2**.

Atom	Atom	Length/Å
S1	O1	1.4334(18)
S1	O2	1.4305(18)
S1	N1	1.639(2)
S1	C1	1.756(3)
S2	C9	1.815(3)
S2	C10	1.847(3)
N1	C8	1.481(3)
N1	C10	1.464(3)
C1	C2	1.394(4)
C1	C6	1.385(4)
C2	C3	1.385(4)
C3	C4	1.398(4)
C4	C5	1.386(4)
C4	C7	1.506(4)
C5	C6	1.388(4)
C8	C9	1.521(4)
C10	C11	1.528(3)
C11	C12	1.391(4)
C11	C16	1.383(4)
C12	C13	1.387(4)
C13	C14	1.380(4)
C14	C15	1.385(4)
C15	C16	1.392(4)

Table S9. Bond Angles in ° for **(S)-2**.

Atom	Atom	Atom	Angle/°
O1	S1	N1	106.09(11)
O1	S1	C1	107.50(12)
O2	S1	O1	119.99(12)
O2	S1	N1	106.04(11)
O2	S1	C1	108.13(12)
N1	S1	C1	108.68(12)
C9	S2	C10	93.76(12)
C8	N1	S1	118.37(18)
C10	N1	S1	118.42(18)
C10	N1	C8	109.2(2)
C2	C1	S1	119.7(2)
C6	C1	S1	119.5(2)
C6	C1	C2	120.8(2)
C3	C2	C1	118.9(3)

Atom	Atom	Atom	Angle/°
C2	C3	C4	121.2(3)
C3	C4	C7	120.4(2)
C5	C4	C3	118.5(2)
C5	C4	C7	121.0(3)
C4	C5	C6	121.2(3)
C1	C6	C5	119.3(3)
N1	C8	C9	108.6(2)
C8	C9	S2	105.80(17)
N1	C10	S2	106.19(18)
N1	C10	C11	111.2(2)
C11	C10	S2	114.27(18)
C12	C11	C10	121.2(2)
C16	C11	C10	119.6(2)
C16	C11	C12	118.9(2)
C13	C12	C11	120.6(3)
C14	C13	C12	120.1(3)
C13	C14	C15	119.7(3)
C14	C15	C16	120.0(3)
C11	C16	C15	120.6(3)

Table S10. Torsion Angles in ° for **(S)-2**.

Atom	Atom	Atom	Atom	Angle/°
S1	N1	C8	C9	-94.7(2)
S1	N1	C10	S2	104.45(18)
S1	N1	C10	C11	-130.7(2)
S1	C1	C2	C3	-179.3(2)
S1	C1	C6	C5	179.9(2)
S2	C10	C11	C12	-30.5(3)
S2	C10	C11	C16	156.0(2)
O1	S1	N1	C8	-54.4(2)
O1	S1	N1	C10	169.79(19)
O1	S1	C1	C2	14.8(2)
O1	S1	C1	C6	-165.7(2)
O2	S1	N1	C8	176.93(18)
O2	S1	N1	C10	41.2(2)
O2	S1	C1	C2	145.7(2)
O2	S1	C1	C6	-34.8(3)
N1	S1	C1	C2	-99.6(2)
N1	S1	C1	C6	79.9(2)
N1	C8	C9	S2	-32.3(2)
N1	C10	C11	C12	-150.7(2)
N1	C10	C11	C16	35.8(3)
C1	S1	N1	C8	60.9(2)
C1	S1	N1	C10	-74.9(2)
C1	C2	C3	C4	-0.5(4)
C2	C1	C6	C5	-0.6(4)
C2	C3	C4	C5	-0.7(4)
C2	C3	C4	C7	178.2(3)
C3	C4	C5	C6	1.3(4)
C4	C5	C6	C1	-0.6(4)
C6	C1	C2	C3	1.2(4)

Atom	Atom	Atom	Atom	Angle/°
C7	C4	C5	C6	-177.6(3)
C8	N1	C10	S2	-35.0(2)
C8	N1	C10	C11	89.8(3)
C9	S2	C10	N1	13.56(19)
C9	S2	C10	C11	-109.3(2)
C10	S2	C9	C8	10.47(19)
C10	N1	C8	C9	44.8(3)
C10	C11	C12	C13	-172.9(3)
C10	C11	C16	C15	174.0(2)
C11	C12	C13	C14	-0.8(4)
C12	C11	C16	C15	0.3(4)
C12	C13	C14	C15	-0.2(4)
C13	C14	C15	C16	1.2(4)
C14	C15	C16	C11	-1.3(4)
C16	C11	C12	C13	0.7(4)

Table S11. Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **(S)-2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H2	-1664.17	3988.96	5917.63	20
H3	-860.51	4927.35	4954.5	21
H5	5079.88	3553.16	4985.55	22
H6	4288.71	2580.98	5939.9	20
H7A	1895.25	4509.32	3893.59	37
H7B	4206.14	4872.08	4153.32	37
H7C	2216.1	5728.91	4256.55	37
H8A	884.16	4591.08	7895.88	19
H8B	-534.76	4511.56	7256.64	19
H9A	2477.79	6013.37	7311.77	20
H9B	2021.71	5360.6	6642.58	20
H10	4573.15	2507.86	7158.09	16
H12	7276.61	3809.51	8180.68	24
H13	8247.5	3206.21	9207.24	29
H14	6046.53	1940.07	9781.58	29
H15	2850.34	1286.51	9327.93	26
H16	1929.58	1847.36	8286.53	20

Out-of-sample predictions

The steps for ee prediction include: 1) locating the ground state of the targeted reaction variable by DFT, 2) acquiring the key molecular features necessary for prediction and 3) re-creating the statistical model and submitting the parameter values to the resulting mathematical equation.

DFT Calculations

All reaction components were optimized in the gas-phase with the M06-2X density functional[6] and the triple-ζ valence quality def2-TZVP basis set of Weigend and Ahlrichs,[27] as implemented in Gaussian 16 (C.01).[28] Parameters were acquired from these ground state structures. NBO charges were calculated using NBO6,[29] at the same level. Sterimol values were calculated using a modified version of Paton's Python script to accommodate non-terminal reference atoms.[30] The previously published iminium, nucleophile and catalyst descriptors,[31] was used to re-create the model in MATLAB®[32] using all the available data as the training set. More specifically, this comprehensive training model shown below now includes the data used as validation which corresponded to 10% of the data set and two out-of-sample prediction platforms as described in ref. 31. All the data required for re-constructing this model can be obtained from the accompanying excel spreadsheet in ref. 31. The resulting model was then used to predict the enantioselectivity outcome with thionium reactions. We also tested the prediction capability of the model shown in ref. 31 and the predictions only change by 0.02 kcal/mol on average. Therefore, the comprehensive training model and the model shown in ref. 31 have similar prediction capabilities.

$$\Delta\Delta G^{\ddagger} = -0.08 - 0.35\mathbf{NBO_S} + 0.02\mathbf{B1_L} + 0.19\mathbf{pol} + 0.69\mathbf{NBO_{Nu}} - 0.30\mathbf{L_{Nu}} - 0.77\mathbf{B5_{C5}} + 0.34\mathbf{L_{C6}} + 0.25\mathbf{PO_{as}}$$

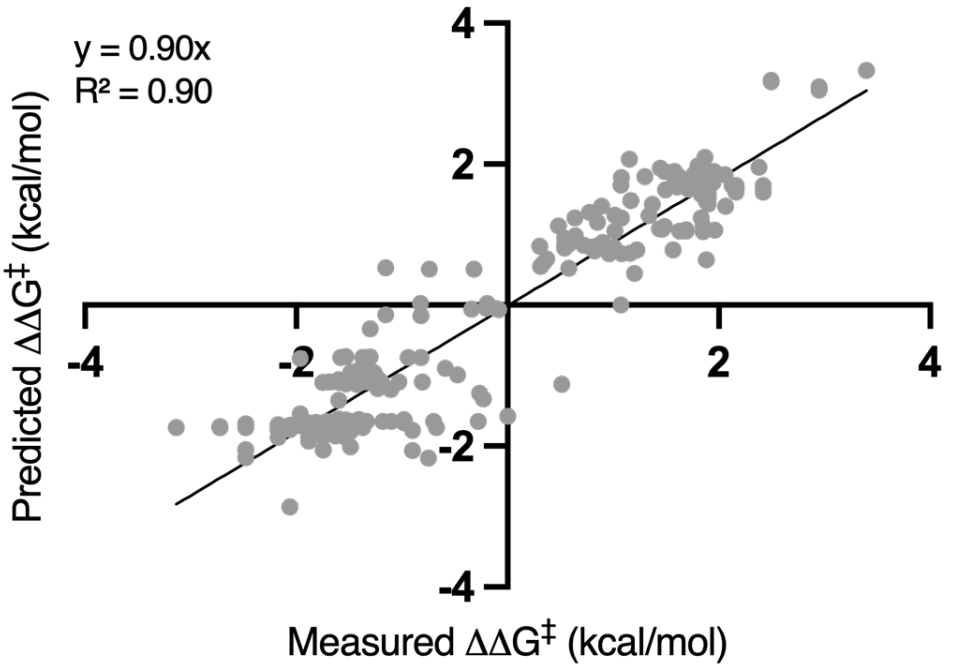


Figure S3. Re-built statistical model generated from all training dataset from ref. 31.

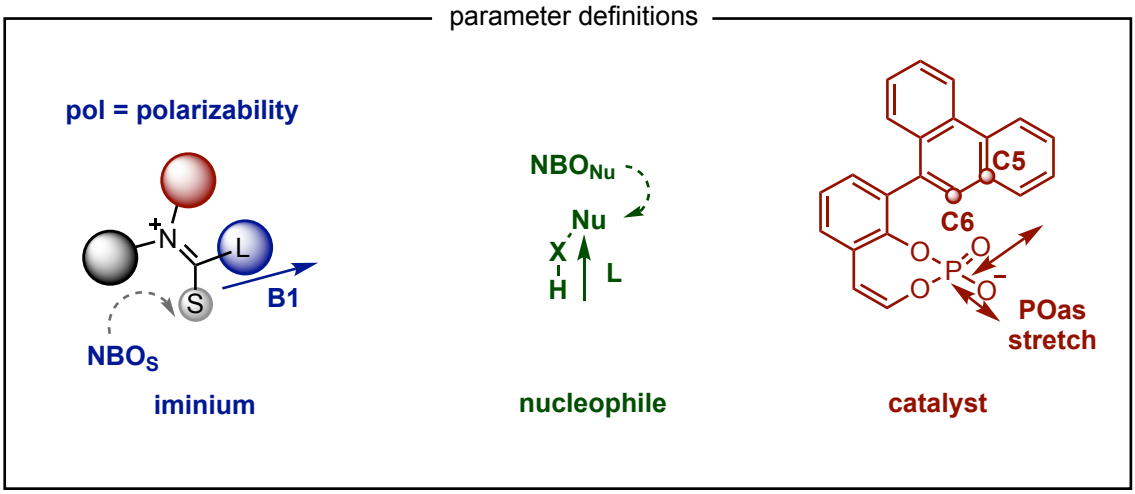


Figure S4. Key parameter definitions derived to describe electrophile (iminium or thionium), nucleophile and catalyst structure.

More details on the iminium parameters

From the ground state DFT optimized structures NBO charges and Sterimol values of the necessary substituent (SubL and SubS) in addition to polarizability were calculated and collected.

More details on the nucleophile parameters

Sterimol B5 value of the entire nucleophile unit and the NBO charge of the nucleophilic site were necessary for prediction.

More details on the model catalyst parameters

The vibration term POas (the asymmetric P–O stretching frequency) and Sterimol values from the C5 and C6 positions were calculated and collected from simple model phosphate structures.

Deploying the correlation

We evaluated the ability to transfer the mechanistic principles leading to enantioselective catalysis captured by a previously reported statistical model (iminium model as defined in ref. 31) to genuinely different structural motifs not contained in the training dataset. Treating the test reactions as virtual predictions the collected parameters were submitted to the equation in Figure S3. The ability to predict was determined by both enantioselectivity values and the average absolute $\Delta\Delta G^{\ddagger}$ error ($\Delta\Delta G^{\ddagger}$ error = absolute(model measured – experimentally measured/ no. of examples)).

Table S12. Reaction parameters and data. Note that the sign of the ee (either -ve or +ve) represents one of two electrophile orientations which result in opposite enantiomers when catalyzed by a (*R*)-CPA. In other words the sign of the ee can be used to predict the absolute stereochemistry.

Aromatic group thionium	*N*-substituent nucleophile	Temperature (°C)	Catalyst	measured ee	predicted ee	measured $\Delta\Delta G^{\ddagger}$	predicted $\Delta\Delta G^{\ddagger}$
Ph	1-naphth-SO_2-	0	AdDIP	-84	-90	-1.32	-1.61
4-MeC_6H_4	1-naphth-SO_2-	0	AdDIP	-82	-87	-1.26	-1.44
4-$tBuC_6H_4$	1-naphth-SO_2-	0	AdDIP	-88	-76	-1.49	-1.09
4-$SMeC_6H_4$	1-naphth-SO_2-	0	AdDIP	-72	-79	-0.98	-1.17
4-ClC_6H_4	1-naphth-SO_2-	0	AdDIP	-88	-88	-1.49	-1.52
4-BrC_6H_4	1-naphth-SO_2-	0	AdDIP	-84	-87	-1.32	-1.46
4-FC_6H_4	1-naphth-SO_2-	0	AdDIP	-86	-90	-1.40	-1.60
4-$CF_3C_6H_4$	1-naphth-SO_2-	0	AdDIP	-84	-89	-1.32	-1.56
3-MeC_6H_4	1-naphth-SO_2-	0	AdDIP	-90	-88	-1.60	-1.51
3-$OMeC_6H_4$	1-naphth-SO_2-	0	AdDIP	-74	-89	-1.03	-1.53
3-BrC_6H_4	1-naphth-SO_2-	0	AdDIP	-82	-90	-1.26	-1.59
4-FC_6H_4	1-naphth-SO_2-	0	AdDIP	-90	-91	-1.60	-1.68
4-$CF_3C_6H_4$	1-naphth-SO_2-	0	AdDIP	-90	-91	-1.60	-1.62
2-MeC_6H_4	1-naphth-SO_2-	0	AdDIP	-80	-89	-1.19	-1.52
Ph	4-MeC_6H_4-SO_2-	0	AdDIP	-76	-90	-1.08	-1.58
Ph	4-$OMeC_6H_4$-SO_2-	0	AdDIP	-76	-90	-1.08	-1.57
Ph	4-$NO_2C_6H_4$-SO_2-	0	AdDIP	-56	-90	-0.69	-1.60
Ph	4-ClC_6H_4-SO_2-	0	AdDIP	-74	-90	-1.03	-1.58
Ph	3,5-MeC_6H_3-SO_2-	0	AdDIP	-76	-93	-1.08	-1.82
Ph	2,4,6-MeC_6H_2-SO_2-	0	AdDIP	-62	-95	-0.79	-1.98
Ph	1-naphth-SO_2-	0	AdDIP	-84	-90	-1.32	-1.61
Ph	urea derivative	-30	TCYP	-70	-50	-0.84	-0.54

Table S13. Key electrophile and nucleophile parameters required for reaction prediction.

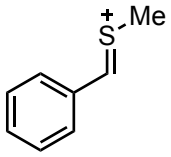
Aromatic group thionium	*N*-substituent nucleophile	NBO(S)	B1(L)	Polarizability	NBO(Nu)	LNu
Ph	1-naphth-SO_2-	0.248	1.7	121.46	-0.868	5.02
4-MeC_6H_4	1-naphth-SO_2-	0.246	1.89	141.83	-0.868	5.02
4-$tBuC_6H_4$	1-naphth-SO_2-	0.245	2.93	182.97	-0.868	5.02
4-$SMeC_6H_4$	1-naphth-SO_2-	0.242	1.8	187.59	-0.868	5.02
4-ClC_6H_4	1-naphth-SO_2-	0.248	1.74	146.7	-0.868	5.02
4-BrC_6H_4	1-naphth-SO_2-	0.248	1.83	158.56	-0.868	5.02
4-FC_6H_4	1-naphth-SO_2-	0.248	1.7	124.38	-0.868	5.02
4-$CF_3C_6H_4$	1-naphth-SO_2-	0.251	2.25	137.00	-0.868	5.02
3-MeC_6H_4	1-naphth-SO_2-	0.247	1.79	135.95	-0.868	5.02
3-$OMeC_6H_4$	1-naphth-SO_2-	0.248	1.78	142.17	-0.868	5.02
3-BrC_6H_4	1-naphth-SO_2-	0.25	1.75	144.44	-0.868	5.02
4-FC_6H_4	1-naphth-SO_2-	0.25	1.7	122.44	-0.868	5.02
4-$CF_3C_6H_4$	1-naphth-SO_2-	0.251	1.94	135.14	-0.868	5.02
2-MeC_6H_4	1-naphth-SO_2-	0.247	1.78	133.98	-0.868	5.02
Ph	4-MeC_6H_4-SO_2-	0.248	1.7	121.46	-0.867	4.93
Ph	4-$OMeC_6H_4$-SO_2-	0.248	1.7	121.46	-0.866	4.93
Ph	4-$NO_2C_6H_4$-SO_2-	0.248	1.7	121.46	-0.87	4.94
Ph	4-ClC_6H_4-SO_2-	0.248	1.7	121.46	-0.868	4.93
Ph	3,5-MeC_6H_3-SO_2-	0.248	1.7	121.46	-0.866	5.66
Ph	2,4,6-MeC_6H_2-SO_2-	0.248	1.7	121.46	-0.870	6.05
Ph	1-naphth-SO_2-	0.248	1.7	121.46	-0.868	5.02
Ph	urea derivative	0.248	1.7	121.46	-0.629	6.88

Table S14. Key catalyst parameters required for reaction prediction.

Catalyst	$B5_{C5}$	L_{C6}	nPOas
AdDIP	1.09	4.67	1388.72
TCYP	1.09	6.83	1382.90

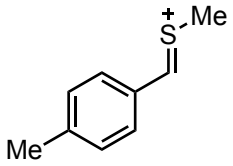
It should be noted that TCYP parameters are used to represent a reaction catalyzed by H_8-TCYP. This imputation strategy is justified by our previous work where in general only minor enantioselectivity differences were observed in changing the BINOL framework to the partially hydrogenated H8 BINOL.[31]

XYZ coordinates for truncated structures



M06-2X/def2TZVP geometry

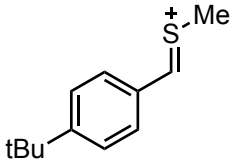
C	0.91776	-1.08700	-0.00001
C	2.27370	-1.30148	0.00000
C	3.15041	-0.21133	0.00001
C	2.67621	1.09648	0.00001
C	1.31650	1.32326	-0.00001
C	0.41844	0.23479	-0.00001
C	-0.96335	0.53031	-0.00001
S	-2.18604	-0.57923	-0.00000
C	-3.67074	0.44672	0.00001
H	0.23581	-1.92878	-0.00002
H	2.66575	-2.30898	0.00001
H	4.21814	-0.39064	0.00002
H	3.36806	1.92702	0.00001
H	0.92946	2.33492	-0.00001
H	-1.25261	1.57879	-0.00002
H	-4.50868	-0.24643	-0.00031
H	-3.69626	1.05594	-0.89970
H	-3.69656	1.05544	0.90005



M06-2X/def2TZVP geometry

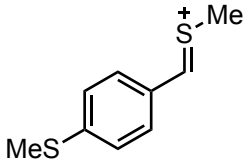
C	-0.07627	0.28706	-0.00011
C	0.79056	1.40212	-0.00019
C	2.15389	1.22261	-0.00046
C	2.69971	-0.06492	-0.00054
C	1.83565	-1.17894	-0.00053
C	0.47837	-1.01621	-0.00028
C	-1.46056	0.53086	0.00004
S	-2.64688	-0.62611	-0.00001
C	4.17601	-0.27857	0.00072
C	-4.16397	0.35156	0.00041
H	0.37239	2.40153	-0.00017
H	2.81286	2.08063	-0.00071
H	2.26192	-2.17418	-0.00080

H	-0.17026	-1.88404	-0.00033
H	-1.78959	1.56735	0.00023
H	4.46955	-0.87304	-0.86711
H	4.72350	0.66019	-0.01368
H	4.47040	-0.84530	0.88691
H	-4.97933	-0.36794	0.00001
H	-4.21094	0.95913	0.90028
H	-4.21087	0.96001	-0.89887



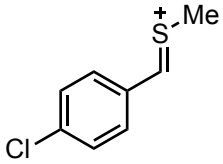
M06-2X/def2TZVP geometry

C	1.18991	0.34358	-0.00026
C	0.58513	-0.93722	-0.00039
C	-0.77609	-1.04864	-0.00033
C	-1.61145	0.09226	-0.00016
C	-1.00919	1.35667	-0.00018
C	0.36073	1.48549	-0.00021
C	2.58016	0.53776	-0.00008
S	3.72489	-0.66254	0.00014
C	-3.11580	-0.09326	0.00009
C	5.27541	0.26115	0.00021
H	1.19992	-1.82939	-0.00059
H	-1.22350	-2.03291	-0.00042
H	-1.61920	2.24737	-0.00017
H	0.81267	2.47030	-0.00018
H	2.94685	1.56153	-0.00009
H	5.34400	0.86751	-0.89906
H	5.34433	0.86701	0.89979
H	6.06523	-0.48628	-0.00012
C	-3.51171	-0.88806	1.25767
H	-3.05370	-1.87676	1.28067
H	-4.59387	-1.02222	1.26608
H	-3.22731	-0.35370	2.16521
C	-3.86906	1.23610	0.00010
H	-4.94037	1.03753	0.00030
H	-3.64513	1.82994	0.88798
H	-3.64542	1.82977	-0.88797
C	-3.51231	-0.88837	-1.25707
H	-3.22827	-0.35429	-2.16489
H	-3.05442	-1.87712	-1.28003
H	-4.59448	-1.02245	-1.26498



M06-2X/def2TZVP geometry

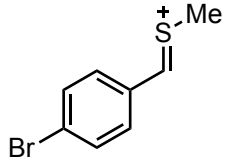
C	-0.87909	0.25299	-0.00018
C	0.04957	1.32394	-0.00022
C	1.39817	1.09544	-0.00020
C	1.88334	-0.22772	-0.00014
C	0.96198	-1.31065	-0.00022
C	-0.37666	-1.07848	-0.00023
C	-2.23998	0.55622	-0.00003
S	-3.48468	-0.55474	0.00022
S	3.53609	-0.65900	0.00011
C	-4.94874	0.50001	0.00007
H	-0.32082	2.34214	-0.00025
H	2.08101	1.93154	-0.00025
H	1.34248	-2.32402	-0.00028
H	-1.06343	-1.91629	-0.00033
H	-2.52586	1.60485	-0.00006
H	-4.96676	1.11070	0.89885
H	-4.96696	1.11009	-0.89912
H	-5.80080	-0.17558	0.00040
C	4.41133	0.90980	0.00029
H	4.18596	1.48047	0.89863
H	5.46671	0.64617	0.00058
H	4.18645	1.48041	-0.89821



M06-2X/def2TZVP geometry

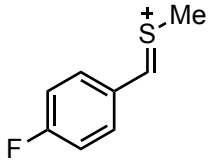
C	-0.47424	0.30583	-0.00028
C	0.09521	-0.98973	-0.00037
C	1.45441	-1.14588	-0.00029
C	2.27697	-0.00811	-0.00008
C	1.74163	1.28148	-0.00011
C	0.37679	1.43397	-0.00023
C	-1.86422	0.53012	-0.00008
S	-3.03223	-0.64254	0.00013
Cl	3.96294	-0.20994	0.00032
C	-4.56506	0.31010	0.00026
H	-0.54124	-1.86639	-0.00054
H	1.90641	-2.12777	-0.00040

H	2.40250	2.13661	-0.00002
H	-0.05341	2.42802	-0.00032
H	-2.20717	1.56205	-0.00003
H	-5.36798	-0.42330	0.00033
H	-4.62115	0.91691	0.90018
H	-4.62136	0.91699	-0.89959



M06-2X/def2TZVP geometry

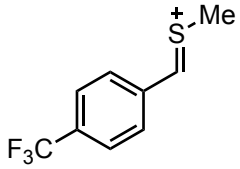
C	1.19978	0.32810	-0.00018
C	0.36813	1.47028	-0.00015
C	-0.99985	1.34062	-0.00007
C	-1.55767	0.06084	-0.00007
C	-0.75395	-1.08998	-0.00023
C	0.60838	-0.95723	-0.00028
C	2.59361	0.52813	-0.00003
S	3.74024	-0.66560	0.00015
Br	-3.40774	-0.12964	0.00011
C	5.29016	0.25878	0.00010
H	0.81494	2.45705	-0.00019
H	-1.64122	2.21038	0.00000
H	-1.21715	-2.06646	-0.00035
H	1.22954	-1.84483	-0.00041
H	2.95500	1.55375	-0.00002
H	6.07951	-0.48921	0.00036
H	5.35741	0.86472	0.89984
H	5.35762	0.86432	-0.89989



M06-2X/def2TZVP geometry

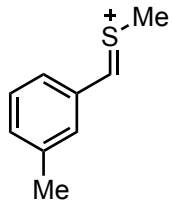
C	-0.02951	0.27914	-0.00018
C	0.51131	-1.03002	-0.00022
C	1.86635	-1.21634	-0.00014
C	2.69164	-0.08770	0.00002
C	2.20466	1.21498	0.00002
C	0.84323	1.39227	-0.00014
C	-1.41425	0.53195	-0.00008
S	-2.60805	-0.61431	0.00014
F	3.98944	-0.27141	0.00026

C	-4.11960	0.37205	0.00005
H	-0.14548	-1.89140	-0.00041
H	2.31612	-2.19944	-0.00021
H	2.89798	2.04424	0.00012
H	0.43043	2.39352	-0.00019
H	-1.73491	1.57106	-0.00009
H	-4.16233	0.98011	0.89984
H	-4.93819	-0.34387	0.00050
H	-4.16270	0.97944	-0.90017



M06-2X/def2TZVP geometry

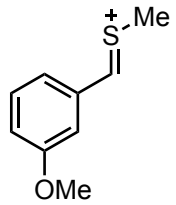
C	1.13939	0.33575	0.00050
C	0.55098	-0.94798	0.00065
C	-0.81517	-1.06844	0.00041
C	-1.60909	0.08351	0.00005
C	-1.05323	1.35372	-0.00002
C	0.32243	1.48151	0.00025
C	2.54394	0.53548	0.00031
S	3.67940	-0.65686	-0.00038
C	5.23889	0.25141	-0.00022
H	1.17007	-1.83664	0.00110
H	-1.28417	-2.04377	0.00051
H	-1.69017	2.22690	-0.00026
H	0.77567	2.46507	0.00027
H	2.90503	1.56150	0.00054
H	6.02013	-0.50514	-0.00031
H	5.30987	0.85610	0.90020
H	5.30993	0.85633	-0.90049
C	-3.11466	-0.10096	-0.00014
F	-3.75277	1.06208	-0.00012
F	-3.49057	-0.78730	-1.07689
F	-3.49084	-0.78751	1.07633



M06-2X/def2TZVP geometry

C	-0.03848	-0.54046	0.00003
C	-0.76095	0.67472	0.00004

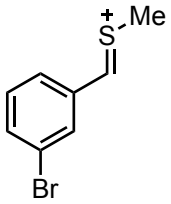
C	-2.13703	0.67539	0.00002
C	-2.79406	-0.56912	-0.00002
C	-2.10702	-1.77515	-0.00002
C	-0.72750	-1.76978	0.00001
C	1.37207	-0.58946	0.00001
S	2.38269	0.71837	-0.00003
C	4.02319	-0.03381	0.00002
H	-0.22835	1.61920	0.00008
C	-2.93480	1.94536	-0.00000
H	-2.65020	-2.70980	-0.00003
H	-0.17125	-2.69885	-0.00000
H	1.84104	-1.57069	-0.00001
H	4.72824	0.79412	-0.00058
H	4.15463	-0.62967	-0.89936
H	4.15498	-0.62867	0.90001
H	-3.87843	-0.58008	-0.00003
H	-3.57796	1.99158	-0.87965
H	-3.57838	1.99138	0.87934
H	-2.28993	2.82138	0.00025



M06-2X/def2TZVP geometry

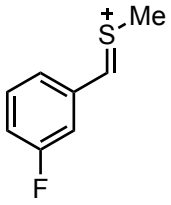
C	-0.25810	0.76811	0.00000
C	0.61764	-0.34274	-0.00013
C	1.97883	-0.12151	-0.00012
C	2.46600	1.20480	-0.00001
C	1.61224	2.28878	0.00008
C	0.24268	2.08222	0.00009
C	-1.66259	0.62719	0.00005
S	-2.48316	-0.80816	-0.00003
C	-4.21215	-0.29091	-0.00001
H	0.21875	-1.34751	-0.00031
O	2.91538	-1.07004	-0.00033
H	2.01424	3.29221	0.00015
H	-0.44222	2.92022	0.00017
H	-2.25968	1.53556	0.00015
H	-4.79597	-1.20829	-0.00023
H	-4.42475	0.28082	-0.89951
H	-4.42496	0.28046	0.89969
H	3.54058	1.33980	0.00001
C	2.50317	-2.42879	0.00030
H	1.92016	-2.65344	0.89620

H	1.92058	-2.65442	-0.89562
H	3.41433	-3.01748	0.00083



M06-2X/def2TZVP geometry

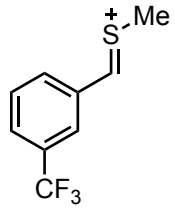
C	-1.00570	0.85521	-0.00002
C	0.02293	-0.11095	-0.00003
C	1.33296	0.30297	-0.00001
C	1.64117	1.66970	0.00004
C	0.63361	2.62469	0.00001
C	-0.68841	2.22749	-0.00003
C	-2.37717	0.50185	-0.00002
S	-2.97113	-1.03598	-0.00004
C	-4.75886	-0.79010	0.00007
H	-0.20746	-1.16899	-0.00005
Br	2.72183	-0.95891	0.00001
H	0.88969	3.67497	0.00003
H	-1.48302	2.96292	-0.00004
H	-3.10318	1.31160	-0.00003
H	-5.05576	-0.25791	-0.89991
H	-5.05574	-0.25848	0.90041
H	-5.19316	-1.78715	-0.00023
H	2.67950	1.97532	0.00007



M06-2X/def2TZVP geometry

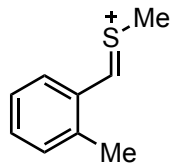
C	0.07716	0.49975	-0.00009
C	0.74787	-0.74097	-0.00010
C	2.11715	-0.73515	-0.00001
C	2.85183	0.45164	0.00008
C	2.19139	1.67074	0.00006
C	0.80920	1.70286	-0.00003
C	-1.33642	0.59929	-0.00008
S	-2.38368	-0.67260	0.00008
C	-4.00385	0.12222	0.00000
H	0.22051	-1.68653	-0.00019

F	2.77223	-1.88419	-0.00001
H	2.75896	2.59057	0.00011
H	0.28438	2.64955	-0.00004
H	-1.76841	1.59725	-0.00018
H	-4.11821	0.72021	-0.90039
H	-4.72942	-0.68785	0.00038
H	-4.11799	0.72087	0.89999
H	3.93297	0.39309	0.00015



M06-2X/def2TZVP geometry

C	-0.91329	0.25286	-0.00127
C	0.28896	-0.48301	-0.00277
C	1.49249	0.18390	-0.00262
C	1.52101	1.57602	-0.00095
C	0.33772	2.31407	0.00037
C	-0.87372	1.66269	0.00026
C	-2.12527	-0.48232	-0.00128
S	-3.64004	0.16489	0.00032
C	-4.71262	-1.28637	0.00121
H	0.26732	-1.56563	-0.00468
C	2.80356	-0.56992	-0.00001
H	0.37669	3.39428	0.00123
H	-1.79338	2.23525	0.00117
H	-2.05279	-1.56768	-0.00236
H	-5.72935	-0.90046	-0.00806
H	-4.53267	-1.87542	-0.89436
H	-4.54497	-1.86462	0.90618
H	2.47684	2.08706	-0.00141
F	3.50062	-0.29047	1.09905
F	2.60627	-1.88525	-0.04474
F	3.54423	-0.22300	-1.04990



M06-2X/def2TZVP geometry

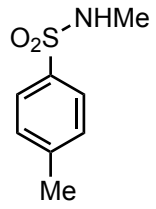
C	-0.33547	-0.04299	0.00023
C	-1.32665	0.98174	0.00016
C	-2.65576	0.58818	-0.00013

C	-3.00975	-0.75376	-0.00019
C	-2.03964	-1.76124	0.00003
C	-0.71727	-1.40784	0.00024
C	1.02468	0.32437	0.00015
S	2.31058	-0.71918	-0.00018
C	3.73380	0.39001	0.00001
H	-2.33204	-2.80167	0.00003
H	0.04453	-2.17820	0.00047
H	1.27225	1.38180	0.00022
H	3.72708	0.99980	-0.89957
H	3.72720	0.99945	0.89983
H	4.60983	-0.25442	-0.00017
H	-4.05825	-1.02436	-0.00037
H	-3.43050	1.34331	-0.00027
C	-0.98011	2.44217	-0.00001
H	-1.88622	3.04228	0.00054
H	-0.40246	2.71763	0.88412
H	-0.40356	2.71751	-0.88491

M06-2X/def2TZVP geometry

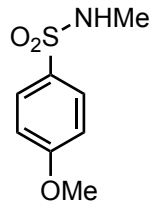
C	2.18389	-0.20174	2.15521
N	2.09834	-1.03307	0.95997
S	1.88072	-0.29338	-0.48350
C	0.33811	0.58105	-0.33036
O	2.90820	0.69264	-0.60416
C	0.40341	1.94578	-0.28155
C	-0.76486	2.71114	-0.08382
C	-1.96411	2.08611	0.08511
C	-2.06391	0.67297	0.04658
C	-0.90116	-0.11237	-0.18106
C	-3.31284	0.03264	0.22745
C	-3.41536	-1.32768	0.18351
C	-2.26747	-2.10777	-0.06094
C	-1.04470	-1.52248	-0.24240
O	1.74011	-1.33896	-1.44886
H	1.22731	0.25890	2.41919
H	2.52560	-0.82178	2.98124
H	2.92205	0.57733	1.97842
H	1.52154	-1.86065	1.04207
H	1.36414	2.42869	-0.39564
H	-0.69615	3.79021	-0.05805

H	-2.86699	2.66143	0.25153
H	-4.18766	0.64784	0.39997
H	-4.37424	-1.80913	0.32271
H	-2.35691	-3.18466	-0.12046
H	-0.19095	-2.13777	-0.48705



M06-2X/def2TZVP geometry

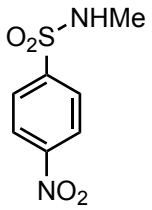
C	-2.07311	1.75350	1.20416
N	-2.30347	0.32720	1.01729
S	-1.69632	-0.39860	-0.31904
C	0.06165	-0.23062	-0.20774
O	-2.01551	-1.78579	-0.18550
O	-2.12603	0.37921	-1.43894
C	0.79614	-1.18400	0.48681
C	2.16540	-1.02557	0.60846
C	2.81612	0.07303	0.04571
C	2.05887	1.01260	-0.64734
C	0.68524	0.86749	-0.78040
C	4.30775	0.21283	0.16128
H	-2.69800	2.09893	2.02515
H	-1.02712	1.99043	1.42214
H	-2.18137	-0.25527	1.83565
H	0.29367	-2.04734	0.90376
H	2.74439	-1.76997	1.14217
H	2.55091	1.86681	-1.09638
H	0.09781	1.58475	-1.33861
H	4.80882	-0.45908	-0.53866
H	4.62869	1.22891	-0.06265
H	4.64921	-0.04496	1.16386
H	-2.37756	2.27119	0.29706



M06-2X/def2TZVP geometry

C	2.30438	1.76024	1.31408

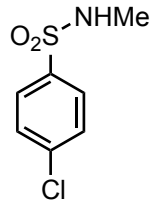
N	2.66153	0.38222	1.00579
S	2.07233	-0.28850	-0.36858
C	0.31537	-0.28802	-0.20264
O	2.39787	0.61024	-1.43228
C	-0.42499	0.76865	-0.70249
C	-1.80468	0.79315	-0.53904
C	-2.43379	-0.25377	0.12952
C	-1.68044	-1.32257	0.62630
C	-0.31350	-1.34020	0.46123
O	2.51657	-1.64758	-0.35445
H	1.24599	1.87904	1.56677
H	2.91288	2.09512	2.15158
H	2.53852	2.37663	0.44878
H	2.61665	-0.27150	1.77690
H	0.07743	1.56315	-1.23873
H	-2.37102	1.61957	-0.94172
H	-2.19945	-2.12887	1.12645
H	0.27579	-2.17442	0.81969
O	-3.76458	-0.32863	0.33909
C	-4.57624	0.71409	-0.15892
H	-5.59661	0.45736	0.11060
H	-4.30925	1.67164	0.29514
H	-4.49454	0.79089	-1.24590



M06-2X/def2TZVP geometry

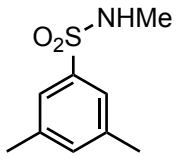
C	-2.63428	-1.62925	1.42349
N	-2.85110	-0.23055	1.07765
S	-2.30113	0.34381	-0.34374
C	-0.52812	0.22708	-0.25262
O	-2.72042	-0.57071	-1.35677
C	0.09793	-0.93835	-0.67451
C	1.47517	-1.04826	-0.56177
C	2.17750	0.01908	-0.03357
C	1.57020	1.19206	0.37891
C	0.19370	1.29410	0.26704
O	-2.63720	1.73119	-0.37029
H	-1.59066	-1.84865	1.66770
H	-3.26041	-1.87256	2.27901
H	-2.94648	-2.24317	0.58166

H	-2.75938	0.44732	1.82268
H	-0.49014	-1.73704	-1.10618
H	2.00452	-1.93397	-0.88043
H	2.17222	1.99921	0.76919
H	-0.32182	2.19992	0.55704
N	3.64768	-0.09511	0.08890
O	4.15640	-1.12852	-0.27584
O	4.24142	0.85163	0.54809



M06-2X/def2TZVP geometry

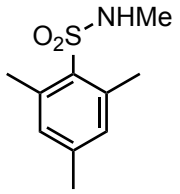
C	-2.38921	1.78980	1.19310
N	-2.62703	0.36201	1.02769
S	-2.04966	-0.38937	-0.30357
C	-0.28528	-0.24922	-0.21510
O	-2.38373	-1.77014	-0.14973
C	0.34584	0.84131	-0.79706
C	1.72181	0.97245	-0.69021
C	2.44269	0.00554	-0.00514
C	1.81658	-1.09284	0.56866
C	0.44173	-1.21904	0.46255
O	-2.47303	0.38175	-1.42953
H	-3.00811	2.14918	2.01246
H	-1.34131	2.02441	1.40376
H	-2.69625	2.29639	0.28073
H	-2.51828	-0.21219	1.85351
H	-0.23806	1.56733	-1.34737
H	2.23666	1.80991	-1.13978
H	2.40543	-1.83962	1.08249
H	-0.06837	-2.07676	0.88136
Cl	4.15889	0.16449	0.12762



M06-2X/def2TZVP geometry

C	-2.21967	1.04376	1.80225
N	-2.40699	-0.18743	1.04629
S	-1.78821	-0.28232	-0.46720

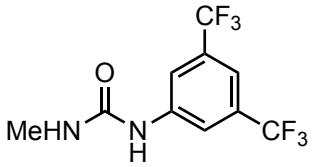
C	-0.03300	-0.12442	-0.27903
O	-2.06738	-1.60997	-0.91804
C	0.54568	1.12948	-0.34954
C	1.92010	1.26513	-0.15055
C	2.66552	0.12487	0.11416
C	2.08934	-1.14553	0.17842
C	0.72190	-1.26293	-0.01929
O	-2.24832	0.87342	-1.17177
H	-2.84859	1.00248	2.68918
H	-1.17976	1.20365	2.10342
H	-2.54738	1.87744	1.18495
H	-2.25595	-1.04907	1.55500
H	-0.06988	1.99084	-0.57937
C	2.56576	2.61980	-0.24187
C	2.94597	-2.35364	0.43723
H	0.23857	-2.23200	0.00029
H	3.73559	0.22085	0.26803
H	3.62043	2.57326	0.02450
H	2.48846	3.01489	-1.25619
H	2.07525	3.33149	0.42342
H	2.33971	-3.25149	0.54388
H	3.64535	-2.51351	-0.38519
H	3.53433	-2.22635	1.34700



M06-2X/def2TZVP geometry

C	2.05997	-0.72182	2.04246
N	2.31512	0.32683	1.06398
S	1.71566	0.13439	-0.45039
C	-0.05928	0.03994	-0.25697
O	2.04213	1.33300	-1.15717
C	-0.72223	-1.19971	-0.27284
C	-2.10506	-1.19904	-0.09188
C	-2.83335	-0.03862	0.10488
C	-2.14368	1.16589	0.13522
C	-0.76843	1.23884	-0.03990
O	2.19707	-1.12805	-0.91391
H	2.58922	-0.47183	2.95940
H	0.99499	-0.84614	2.26510
H	2.46032	-1.65806	1.65870
H	2.20447	1.27668	1.39214

H	-2.62459	-2.15003	-0.10596
H	-2.69419	2.08520	0.30026
C	-0.06965	-2.54522	-0.47493
H	-0.82334	-3.32347	-0.37099
H	0.38725	-2.62276	-1.45904
H	0.72326	-2.72994	0.24742
C	-0.14558	2.61196	0.00692
H	-0.89192	3.33355	0.33323
H	0.69808	2.66985	0.69396
H	0.23344	2.90555	-0.96961
C	-4.32661	-0.07197	0.26271
H	-4.81397	0.20537	-0.67438
H	-4.67317	-1.06699	0.53781
H	-4.65648	0.63392	1.02500



M06-2X/def2TZVP geometry

C	5.69681	-0.90317	-0.03496
N	4.35243	-1.44899	-0.03771
C	3.29522	-0.58512	0.05089
O	3.43062	0.60140	0.24762
H	5.79978	-0.22256	0.80636
H	6.40518	-1.72038	0.07916
H	5.91906	-0.35148	-0.95060
H	4.21045	-2.32810	-0.50562
N	2.06321	-1.21231	-0.07812
H	2.06249	-2.21869	-0.04990
C	-1.80262	0.42839	0.01119
C	-0.69576	1.25773	-0.02976
C	0.60034	0.76428	-0.05384
C	0.80328	-0.61506	-0.03518
C	-0.30613	-1.46171	0.00552
C	-1.58521	-0.94065	0.02828
H	-2.80366	0.83291	0.03266
C	-0.87092	2.75380	-0.02170
H	1.44407	1.43570	-0.07953
H	-0.16726	-2.53627	0.02547
C	-2.75260	-1.88888	0.01976
F	-0.15299	3.33822	-0.98657
F	-2.14542	3.11216	-0.20009
F	-0.46883	3.28633	1.13836
F	-3.03878	-2.30100	-1.22316

F	-2.50410	-2.98899	0.74135
F	-3.85865	-1.32793	0.51128

AdDIP

M06-2X/def2TZVP geometry

C	-4.79499	-1.70830	-1.32122
C	-4.48594	-0.85630	-0.25934
C	-3.13876	-0.51211	-0.07030
C	-2.13817	-1.02016	-0.89868
C	-2.49155	-1.85818	-1.95332
C	-3.81713	-2.19967	-2.17012
H	-5.83270	-1.98089	-1.47695
H	-1.70844	-2.24491	-2.59551
H	-4.08652	-2.84951	-2.99318
C	-5.56846	-0.41907	0.62354
H	-6.49326	-0.97018	0.49603
C	-5.64212	0.53542	1.56213
H	-6.57610	0.63476	2.10699
O	-2.76235	0.28083	0.96461
O	-4.74400	1.43050	1.98356
P	-3.38860	1.80880	1.10945
O	-3.82091	2.24205	-0.23295
O	-2.50962	2.55510	2.01338
C	-0.70058	-0.70126	-0.64839
C	0.11903	-1.64480	-0.00377
C	-0.15951	0.51503	-1.06935
C	1.46445	-1.35945	0.17254
C	1.20185	0.75818	-0.87477
C	2.03558	-0.16256	-0.26001
H	2.08754	-2.09037	0.67281
H	1.59769	1.70544	-1.21539
C	-0.47480	-2.91289	0.58343
H	-1.31651	-3.20944	-0.04425
C	0.49722	-4.08959	0.63291
H	1.28344	-3.93305	1.37506
H	-0.03732	-4.99793	0.91776
H	0.97275	-4.25852	-0.33520
C	-1.02395	-2.61366	1.98270
H	-1.74072	-1.79246	1.95917
H	-1.51070	-3.49699	2.40327
H	-0.20559	-2.32134	2.64606
C	-1.00875	1.56247	-1.76083
H	-2.05879	1.32959	-1.58752
C	-0.76034	1.52661	-3.27088
H	0.28477	1.75872	-3.49658

H	-0.98455	0.53928	-3.68097
H	-1.39144	2.26076	-3.77613
C	-0.78858	2.96558	-1.19656
H	-1.54560	3.63796	-1.60192
H	-0.89995	2.97147	-0.11106
H	0.19845	3.35847	-1.45920
C	3.52095	0.08361	-0.02555
C	3.82769	0.03392	1.48662
C	4.35221	-1.01001	-0.72964
C	3.99343	1.44767	-0.55499
H	3.50160	-0.92457	1.89765
H	3.24624	0.81128	1.99111
C	5.32453	0.22645	1.74991
H	4.14501	-0.97485	-1.80401
H	4.03843	-1.99563	-0.37646
C	5.84857	-0.81663	-0.46721
H	3.42508	2.24614	-0.06876
H	3.79316	1.51383	-1.62900
C	5.49140	1.65031	-0.29604
H	5.51128	0.17892	2.82620
C	6.11306	-0.88085	1.04137
C	5.76557	1.58986	1.20986
H	6.40958	-1.60824	-0.97210
C	6.28821	0.54916	-1.00290
H	5.79229	2.62726	-0.68406
H	5.81161	-1.85868	1.42997
H	7.18364	-0.76525	1.23969
H	5.21937	2.38776	1.72136
H	6.83197	1.74595	1.40355
H	7.36034	0.69351	-0.83319
H	6.11736	0.59906	-2.08264

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