

THEORETICAL STUDY OF THE ASYMMETRIC CONJUGATE ALKENYLATION OF ENONES CATALYZED BY BINAPHTHOLS

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Nacional de Rosario, Suipacha 531, Rosario (2000), Argentina

Supplementary Information

List of contents:

- Activation energies including zero-point energy (ZPE) corrections, activation enthalpies, activation free energies and activation free energies in solution for all the reactions of enone **1b** (Tables S1 and S2). Page S2.
- Cartesian coordinates, absolute energies including ZPE (in hartrees) and number of imaginary frequencies of all the stationary points reported in the paper; free energies in solution of selected structures; values of imaginary frequencies of all transition structures. Optimized geometries of key structures not included in the paper. Energies of the frontier molecular orbitals of the reactants not included in the paper (in eV). Pages S3-S59.

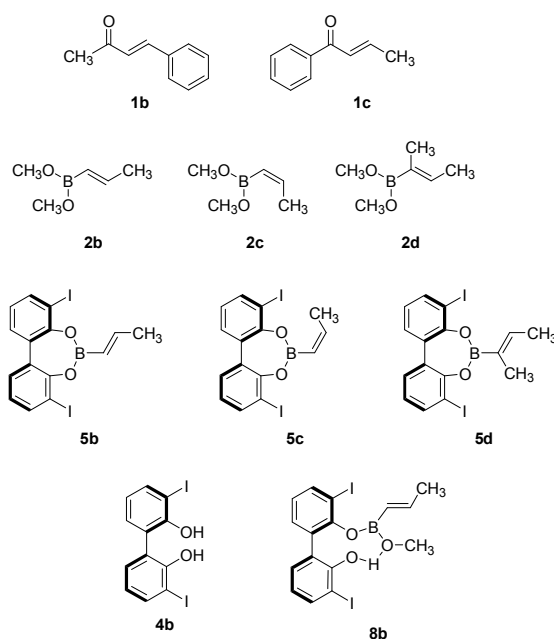


Table S1. B3LYP/631LAN Activation Energies including Zero-point Energy (ZPE) Corrections, Activation Enthalpies, Activation Free Energies and Activation Free Energies in Solution (in kcal mol⁻¹) for the TSs of the Conjugate Addition of Alkenylboronates **2b**, **5b** and **8b** to Enone **1b**

TS 1b+	$\Delta E_0^\ddagger$ (kcal mol ⁻¹)	$\Delta S^\ddagger$ (kcal mol ⁻¹)	$\Delta G^\ddagger$ (kcal mol ⁻¹)	$\Delta G_{\text{DCM}}^\ddagger$ (kcal mol ⁻¹)
2b-endo	29.80	28.75	45.64	30.29
2b-exo	28.10	27.13	43.62	29.43
5b-Re-endo	18.57	17.75	34.37	20.62
5b-Re-exo	13.89	13.05	29.61	16.04
5b-Si-endo	18.93	18.14	34.64	22.25
5b-Si-exo	16.51	15.69	32.17	20.30
8b-Re-exo	22.72	21.69	39.29	24.30
8b-Si-exo	25.00	23.93	41.81	26.39

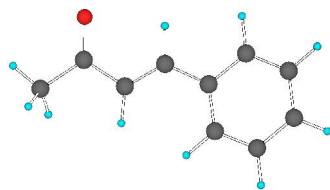
Table S2. B3LYP/631LAN Activation Energies including Zero-point Energy (ZPE) Corrections, Activation Enthalpies, Activation Free Energies and Activation Free Energies in solution (in kcal mol⁻¹) for the Transition Structures of the Hetero Diels-Alder Reactions of Enone **1b** with Alkenylboronates **2b** and **5b**

DATS 1b+	$\Delta E_0^\ddagger$ (kcal mol ⁻¹)	$\Delta S^\ddagger$ (kcal mol ⁻¹)	$\Delta G^\ddagger$ (kcal mol ⁻¹)	$\Delta G_{\text{DCM}}^\ddagger$ (kcal mol ⁻¹)
2b-Aa-endo	31.64	30.76	46.61	31.88
2b-Aa-exo	30.55	29.59	45.97	32.27
2b-Ba-endo	39.62	38.50	55.46	37.89
2b-Ba-exo	41.60	40.52	57.41	41.10
2b-Ab-endo	28.64	27.83	43.53	29.76
2b-Ab-exo	29.44	28.59	44.52	29.45
5b-Aa-Re-exo	34.59	33.96	49.02	37.88
5b-Aa-Si-exo	32.85	32.15	47.87	37.00
5b-Ba-Re-endo	27.58	26.51	43.34	28.74
5b-Ba-Re-exo	30.04	28.95	46.41	31.56
5b-B-Si-endo (CBTS)	29.29	28.03	45.34	30.02
5b-Ba-Si-exo	30.30	29.25	46.65	33.06
5b-Ab-Re-endo	30.45	29.82	45.11	35.39
5b-Ab-Re-exo	30.24	29.57	45.48	34.58
5b-Ab-Si-endo	30.70	30.03	45.86	34.67
5b-Ab-Si-exo	29.59	28.94	44.40	34.42

Gaussian Calculations¹

Reactants

Enone 1b



B3LYP/6-31G* Geometry

O 0	2.624420	-2.506287	0.000000
C 0	2.624420	-1.282608	0.000000
C 0	3.921753	-0.491013	0.000000
C 0	1.368958	-0.488220	0.000000
C 0	0.168106	-1.099884	0.000000
C 0	-1.160278	-0.489288	0.000000
C 0	-2.288177	-1.330765	-0.000092
C 0	-1.370697	0.903793	0.000076
C 0	-3.578583	-0.805222	-0.000092
C 0	-2.658157	1.428986	0.000061
C 0	-3.768066	0.577240	0.000000
H 0	3.974319	0.160721	0.881744
H 0	4.772659	-1.174622	0.000000
H 0	3.974319	0.160721	-0.881744
H 0	1.463516	0.595474	0.000000
H 0	0.192871	-2.189500	0.000000
H 0	-2.141846	-2.408173	-0.000153
H 0	-0.519684	1.578476	0.000153
H 0	-4.434814	-1.474121	-0.000153
H 0	-2.800339	2.506302	0.000107
H 0	-4.772659	0.991211	0.000000

B3LYP/6-31G* Energy = -462.127525

B3LYP/6-31G* Free energy in solution = -462.301586

Number of Imaginary Frequencies = 0

B3LYP/631LAN Geometry

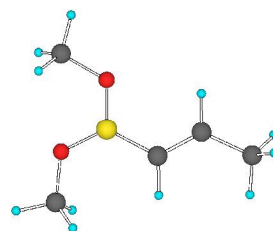
O 0	2.624619	-2.506607	0.000000
C 0	2.624985	-1.282806	0.000000
C 0	3.922760	-0.491318	0.000000
C 0	1.369461	-0.488052	0.000000
C 0	0.168243	-1.099991	0.000000
C 0	-1.160477	-0.489456	0.000000
C 0	-2.288666	-1.331177	-0.000061
C 0	-1.370987	0.903976	0.000076
C 0	-3.579437	-0.805557	-0.000076
C 0	-2.658829	1.429291	0.000061
C 0	-3.769012	0.577271	0.000000
H 0	3.975555	0.160416	0.881821
H 0	4.773651	-1.175034	0.000000
H 0	3.975540	0.160416	-0.881821
H 0	1.464218	0.595612	0.000000
H 0	0.193268	-2.189575	0.000000
H 0	-2.142258	-2.408585	-0.000122
H 0	-0.520004	1.578690	0.000137
H 0	-4.435700	-1.474411	-0.000137
H 0	-2.801056	2.506607	0.000122
H 0	-4.773636	0.991226	-0.000015

B3LYP/631LAN Energy = -462.11824

B3LYP/631LAN Free energy in solution = -462.292315

Number of Imaginary Frequencies = 0

B-1-propenyldimethylboronate 2b



B3LYP/6-31G* Geometry

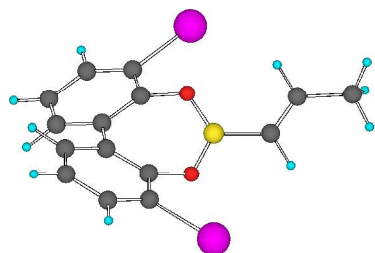
C 0	1.203598	0.590347	-0.000549
C 0	1.203598	1.933685	-0.000549
B 0	-0.109787	-0.253098	-0.000549
O 0	-0.149673	-1.625992	-0.000427
O 0	-1.307465	0.409775	-0.000671
C 0	2.416855	2.815842	-0.000595
C 0	1.019287	-2.428024	0.000214
C 0	-2.537445	-0.302002	-0.000549
H 0	2.176575	0.093063	-0.000595
H 0	0.241852	2.448654	-0.000534
H 0	2.424026	3.475174	-0.879684
H 0	2.424057	3.475235	0.878448
H 0	3.344162	2.233124	-0.000580
H 0	0.703140	-3.475235	0.001144
H 0	1.633102	-2.248900	-0.891342
H 0	1.633255	-2.247360	0.891357
H 0	-2.628693	-0.941956	0.884705
H 0	-3.344162	0.436554	0.004639
H 0	-2.633148	-0.934067	-0.891052

B3LYP/6-31G* Energy = -372.368467

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.02, Gaussian, Inc., Wallingford CT, 2004.

B3LYP/6-31G* Free energy in solution = -372.520707
 Number of Imaginary Frequencies = 0

B-1-propenylboronate 5b

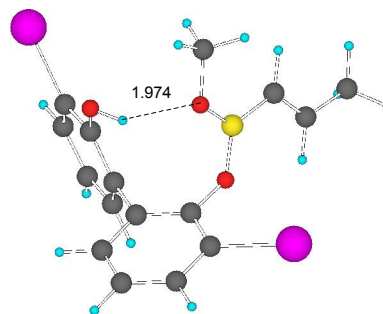


B3LYP/631LAN Geometry

C 0	-0.130905	2.090790	-0.280975
C 0	-1.164078	2.847336	0.132294
B 0	-0.115341	0.551300	-0.209732
O 0	-1.186295	-0.139100	0.333862
O 0	1.001572	-0.106522	-0.690842
C 0	-1.213379	4.344879	0.112595
C 0	1.512619	-1.263962	-0.176910
C 0	-1.610886	-1.370926	-0.082016
C 0	0.715652	-2.397842	0.081436
C 0	2.891174	-1.309158	0.077332
C 0	-0.730911	-2.461075	-0.257202
C 0	-2.983063	-1.548004	-0.313904
C 0	1.336121	-3.527191	0.643127
C 0	3.490906	-2.447479	0.609344
C 0	-1.263565	-3.673569	-0.727951
C 0	-3.493958	-2.766785	-0.752853
I 0	4.106873	0.396744	-0.346222
I 0	-4.351074	0.063049	0.010529
C 0	2.701523	-3.558609	0.903885
C 0	-2.622391	-3.831406	-0.974777
H 0	0.757477	2.593018	-0.666962
H 0	-2.052490	2.348312	0.519073
H 0	-0.294067	4.779083	-0.293213
H 0	-1.368378	4.743134	1.124939
H 0	-2.061386	4.698227	-0.490219
H 0	0.724304	-4.388290	0.891373
H 0	4.557571	-2.460236	0.803619
H 0	-0.586563	-4.500641	-0.914688
H 0	-4.557571	-2.877182	-0.931107
H 0	3.153732	-4.443848	1.340988
H 0	-3.005630	-4.779083	-1.340988

B3LYP/631LAN Energy = -776.129391
 B3LYP/631LAN Free energy in solution = -776.352759
 Number of Imaginary Frequencies = 0

B-1-propenylboronate 8b



B3LYP/631LAN Geometry

C 0	0.933792	-1.001648	-1.858231
C 0	1.273972	0.278214	-1.364044
C 0	0.441208	-1.112579	-3.166900
C 0	1.074982	1.401062	-2.174896
C 0	0.265411	0.010361	-3.970917
I 0	-0.059006	-3.044983	-3.936981
C 0	0.572510	1.275772	-3.468567
O 0	1.097351	-2.125534	-1.116500
C 0	-2.544067	-0.082413	1.085907
C 0	-3.069200	1.155411	1.109711
B 0	-1.016037	-0.337128	1.116318
O 0	-0.418457	-1.573593	1.162567
O 0	-0.167130	0.756119	1.093643
C 0	-4.529526	1.491470	1.080933
C 0	1.195374	0.660217	1.149368
C 0	1.869583	0.855820	2.362335
I 0	0.760086	1.245071	4.150238
C 0	-1.173080	-2.786575	1.192535
C 0	3.260483	0.808746	2.426819
C 0	3.994125	0.562714	1.266220
C 0	3.333755	0.376800	0.053986
C 0	1.935471	0.426697	-0.027481
H 0	1.335953	2.379486	-1.781921
H 0	-0.117722	-0.101746	-4.979630
H 0	0.428040	2.154724	-4.089630
H 0	1.001144	-1.894379	-0.171448
H 0	-3.240143	-0.922043	1.041946
H 0	-2.387772	2.005676	1.154633
H 0	-4.766891	2.123444	0.214050
H 0	-4.814590	2.069092	1.970993
H 0	-5.155228	0.594055	1.035828
H 0	-1.676102	-2.955643	0.235123
H 0	-1.911835	-2.767471	1.999771
H 0	-0.470200	-3.603058	1.372498
H 0	3.765411	0.960938	3.374435
H 0	5.078445	0.523788	1.311386
H 0	3.899582	0.193298	-0.854400

B3LYP/631LAN Energy = -891.806526
 B3LYP/631LAN Free energy in solution = -892.079382
 Number of Imaginary Frequencies = 0

Methanol

B3LYP/6-31G* Geometry

C 0	-0.587585	-0.008179	0.000000
O 0	0.826645	-0.117325	0.000000
H 0	-0.820175	1.060226	-0.000015
H 0	-1.048645	-0.458130	0.893127

H 0 -1.048630 -0.458145 -0.893127
H 0 1.048645 -1.060211 0.000015

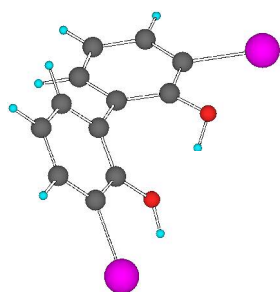
B3LYP/6-31G* Energy = -115.662929
B3LYP/6-31G* Free energy in solution = -115.717203
Number of Imaginary Frequencies = 0

B3LYP/631LAN Geometry

C 0 -0.588287 -0.008224 0.000000
O 0 0.825409 -0.117920 0.000000
H 0 -0.820663 1.060287 0.000000
H 0 -1.049652 -0.457900 0.893204
H 0 -1.049652 -0.457916 -0.893204
H 0 1.049637 -1.060272 0.000015

B3LYP/631LAN Energy = -115.660732
B3LYP/631LAN Free energy in solution = -115.714979
Number of Imaginary Frequencies = 0

3,3'-diiodo-1,1'-biphenyl-2,2'-diol (4b)



B3LYP/631LAN Geometry

O 0 1.341019 -1.843414 -1.526367
C 0 1.341019 -0.488693 -1.526367
C 0 0.407883 0.279327 -0.783264
C 0 2.343765 0.179688 -2.247864
C 0 -0.601974 -0.323318 0.136353
C 0 0.495575 1.680481 -0.837555
C 0 2.426758 1.568054 -2.271027
I 0 3.781769 -0.965057 -3.340897
C 0 -1.486343 -1.356339 -0.244766
C 0 -0.719498 0.182190 1.440262
C 0 1.486267 2.324356 -1.570740
O 0 -1.360153 -1.842316 -1.520508
C 0 -2.437637 -1.836685 0.663132
C 0 -1.671341 -0.297211 2.336655
C 0 -2.541016 -1.315063 1.949600
I 0 -3.781784 -3.408875 0.066208
H 0 0.413651 -2.152039 -1.526367
H 0 -0.238937 2.266800 -0.293274
H 0 3.209045 2.055008 -2.842819
H 0 -0.029861 0.959900 1.752197
H 0 1.529572 3.408890 -1.600891
H 0 -2.027542 -2.535400 -1.680206
H 0 -1.731552 0.110855 3.340912
H 0 -3.282928 -1.702255 2.638641

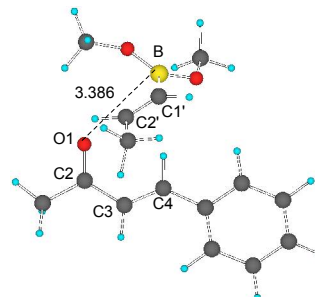
B3LYP/631LAN Energy = -635.112066
B3LYP/631LAN Free energy in solution = -635.291074
Number of Imaginary Frequencies = 0

Study of the reaction mechanism and rationalization of the stereoselectivity

TSs of Conjugate Additions to Enone 1b

Conjugate Addition of 2b to 1b

Complex 1b-2b-*endo*



B3LYP/6-31G* Geometry

O 0 2.265335 -2.478958 -1.647568
B 0 1.086136 -2.446747 -0.962800
C 0 3.501633 -2.938446 -1.124588
C 0 0.789841 -2.998367 0.471664
O 0 0.001831 -1.908630 -1.623154
C 0 1.578964 -2.902588 1.553696
C 0 0.145386 -1.406189 -2.948532
C 0 1.224457 -3.377396 2.934250
H 0 3.362778 -3.784393 -0.442184
H 0 4.005173 -2.123795 -0.594727
H 0 4.121964 -3.256958 -1.968613
H 0 -0.198700 -3.443405 0.620361
H 0 2.548920 -2.413712 1.464752
H 0 0.399994 -2.209854 -3.648926
H 0 0.928314 -0.642380 -3.002594
H 0 -0.813232 -0.966370 -3.238342
H 0 1.965424 -4.097534 3.308624
H 0 1.216705 -2.542603 3.648911
H 0 0.239410 -3.855713 2.956955
O 0 2.957184 0.031800 0.385651
C 0 2.753036 1.146652 0.855942
C 0 3.896713 1.984300 1.404602
C 0 1.404068 1.752700 0.925446
C 0 0.320923 1.094940 0.461426
C 0 -1.072540 1.534836 0.452164
C 0 -1.499222 2.777115 0.961700
C 0 -2.037537 0.666687 -0.094864
C 0 -2.842056 3.135696 0.924179
C 0 -3.382965 1.028427 -0.130768
C 0 -3.789627 2.262726 0.378021
H 0 3.962067 2.940994 0.870605
H 0 3.726334 2.220779 2.462830
H 0 4.838379 1.442383 1.298691
H 0 1.329269 2.744797 1.365662
H 0 0.497391 0.109116 0.037430
H 0 -0.775100 3.464386 1.389709
H 0 -1.715073 -0.293243 -0.491104
H 0 -3.155045 4.097549 1.321625
H 0 -4.114029 0.346008 -0.555862
H 0 -4.838394 2.546341 0.351196

B3LYP/6-31G* Energy = -834.498775
 B3LYP/6-31G* Free energy in solution = -834.817513
 Number of Imaginary Frequencies = 0

TS 1b+2b-endo

B3LYP/6-31G* Geometry

O 0	0.057846	-2.758362	0.878937
B 0	0.057846	-1.332047	0.878937
C 0	-1.146835	-3.469376	0.878937
C 0	-0.504333	-0.763184	-0.633911
O 0	1.378372	-0.792618	1.013840
O 0	-0.868042	-0.855667	2.004272
C 0	-1.748978	-0.891449	-1.171478
C 0	2.173400	-1.253098	2.086044
C 0	-1.489243	0.292206	2.069305
C 0	-2.068405	-1.159119	-2.606934
C 0	-2.438904	0.406952	3.231812
C 0	-1.364044	1.289444	1.125351
C 0	-0.445984	1.194962	0.033646
C 0	-0.553589	2.101181	-1.130753
C 0	-1.779480	2.634460	-1.567322
C 0	0.615417	2.454437	-1.825745
C 0	-1.829865	3.506729	-2.651367
C 0	0.566483	3.328476	-2.910736
C 0	-0.656235	3.858673	-3.325363
H 0	-1.788773	-3.189941	0.021637
H 0	-1.728897	-3.305389	1.797455
H 0	-0.920456	-4.538879	0.794434
H 0	0.318222	-0.834625	-1.352310
H 0	-2.612381	-0.709488	-0.525803
H 0	2.289093	-2.343918	2.061951
H 0	1.745132	-0.975769	3.061874
H 0	3.163437	-0.789795	2.000732
H 0	-2.804291	-1.967392	-2.710098
H 0	-2.525131	-0.265106	-3.061371
H 0	-1.175491	-1.418610	-3.183000
H 0	-1.881470	0.318008	4.171722
H 0	-2.973709	1.360077	3.229996
H 0	-3.163452	-0.415436	3.212570
H 0	-2.077667	2.106140	1.154785
H 0	0.578659	0.932877	0.290726
H 0	-2.696900	2.354813	-1.056519
H 0	1.567535	2.041351	-1.502182
H 0	-2.784943	3.911850	-2.974960
H 0	1.482010	3.595764	-3.431213
H 0	-0.697525	4.538879	-4.171738

B3LYP/6-31G* Energy = -834.448501
 B3LYP/6-31G* Free energy in solution = -834.774024
 Number of Imaginary Frequencies = 1 (-350.32)

Product 1b+2b-endo

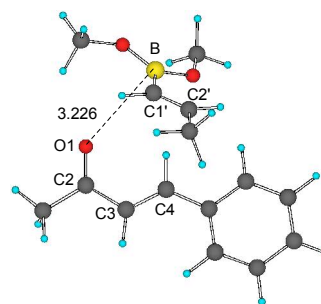
B3LYP/6-31G* Geometry

O 0	3.382156	-1.163925	1.361511
B 0	2.441040	-0.197784	1.151520
C 0	3.220795	-2.126358	2.398285
C 0	-2.335510	-1.445892	1.472809
O 0	2.602554	0.714157	0.147247
O 0	1.320206	-0.159653	1.948792

C 0	-2.776627	-1.192596	2.707336
C 0	3.769592	0.685532	-0.668854
C 0	0.362961	0.847153	1.903580
C 0	-3.789063	-2.023178	3.444046
C 0	0.805740	2.134338	2.535110
C 0	-0.850708	0.613037	1.395172
C 0	-1.289261	-0.658646	0.706345
C 0	-1.733521	-0.331696	-0.726013
C 0	-3.082855	-0.221512	-1.080780
C 0	-0.762375	-0.091705	-1.709137
C 0	-3.454666	0.104553	-2.387756
C 0	-1.129959	0.232590	-3.013779
C 0	-2.480515	0.328812	-3.359909
H 0	2.349014	-2.764084	2.213608
H 0	3.096634	-1.643936	3.373917
H 0	4.122025	-2.744919	2.412750
H 0	-2.730530	-2.313644	0.940643
H 0	-2.376404	-0.331635	3.242691
H 0	3.905700	-0.295959	-1.135361
H 0	4.666138	0.918365	-0.083084
H 0	3.641510	1.442627	-1.446777
H 0	-3.371216	-2.424423	4.377625
H 0	-4.666138	-1.425110	3.727112
H 0	-4.136551	-2.867828	2.838974
H 0	1.651840	2.560074	1.981812
H 0	-0.005035	2.867828	2.544846
H 0	1.137955	1.964478	3.567276
H 0	-1.577774	1.420135	1.439285
H 0	-0.405457	-1.306091	0.621155
H 0	-3.848511	-0.392914	-0.328934
H 0	0.290070	-0.140060	-1.438309
H 0	-4.508545	0.182251	-2.643753
H 0	-0.361862	0.411407	-3.762268
H 0	-2.768707	0.579071	-4.377625

B3LYP/6-31G* Energy = -834.530069
 B3LYP/6-31G* Free energy in solution = -834.851191
 Number of Imaginary Frequencies = 0

Complex 1b-2b-exo



B3LYP/6-31G* Geometry

O 0	0.446350	1.938461	-3.225403
B 0	0.958115	1.999435	-1.959747
C 0	-0.718903	2.652100	-3.615906
C 0	0.467224	2.970627	-0.840363
O 0	2.015381	1.162918	-1.671036
C 0	1.172287	3.228195	0.272873
C 0	2.537200	0.300003	-2.676437
C 0	0.766357	4.160553	1.376892
H 0	-0.622116	3.725754	-3.412064

H 0	-1.598602	2.258728	-3.097275
H 0	-0.843750	2.512573	-4.693954
H 0	-0.487991	3.486923	-0.955215
H 0	2.131821	2.726547	0.408615
H 0	2.988968	0.873917	-3.493698
H 0	1.754410	-0.339966	-3.097061
H 0	3.304779	-0.323898	-2.209183
H 0	0.703888	3.630203	2.337479
H 0	1.508194	4.959930	1.513458
H 0	-0.205475	4.625046	1.178207
O 0	-1.814300	0.483170	-1.309845
C 0	-2.263748	-0.309555	-0.488907
C 0	-3.752319	-0.611084	-0.427078
C 0	-1.408936	-1.022049	0.488358
C 0	-0.077332	-0.808900	0.530029
C 0	0.909470	-1.414337	1.422089
C 0	0.590332	-2.382355	2.394424
C 0	2.251587	-1.004929	1.299606
C 0	1.578262	-2.918228	3.213287
C 0	3.239990	-1.542221	2.122025
C 0	2.907104	-2.500290	3.080872
H 0	-4.280746	-0.032104	-1.186874
H 0	-3.933853	-1.681335	-0.589661
H 0	-4.152740	-0.366577	0.565231
H 0	-1.902939	-1.713257	1.167847
H 0	0.322235	-0.093200	-0.184800
H 0	-0.436661	-2.717682	2.507309
H 0	2.503387	-0.257065	0.551605
H 0	1.315430	-3.664856	3.958008
H 0	4.270172	-1.213455	2.014359
H 0	3.676224	-2.921432	3.722794

B3LYP/6-31G* Energy = -834.501226
 B3LYP/6-31G* Free energy in solution = -834.819639
 Number of Imaginary Frequencies = 0

TS 1b+2b-*exo*

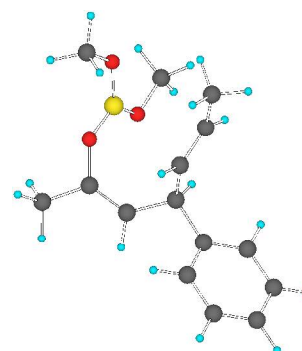
B3LYP/6-31G* Geometry

O 0	0.022842	-2.909348	0.640518
B 0	0.022842	-1.484421	0.640518
C 0	-1.173172	-3.641846	0.640518
C 0	-0.717865	-0.826736	-0.742615
O 0	1.345215	-0.942184	0.710281
O 0	-0.850403	-1.036530	1.845596
C 0	-0.015793	-0.817383	-1.915833
C 0	2.229065	-1.465210	1.680573
C 0	-1.591110	0.032990	1.914108
C 0	-0.560654	-1.024323	-3.286804
C 0	-2.560135	0.049133	3.065674
C 0	-1.549591	1.040161	0.971054
C 0	-0.574570	1.049530	-0.080093
C 0	-0.738007	2.038559	-1.181473
C 0	-1.998276	2.365189	-1.708069
C 0	0.394135	2.682480	-1.705750
C 0	-2.122910	3.314682	-2.720840
C 0	0.270386	3.637772	-2.713913
C 0	-0.989349	3.957230	-3.224731
H 0	-1.711288	-3.562332	-0.319916
H 0	-1.858292	-3.324310	1.440338
H 0	-0.930954	-4.699814	0.797989
H 0	-1.794434	-0.997406	-0.845734

H 0	1.052582	-0.603683	-1.851500
H 0	2.332626	-2.552979	1.586105
H 0	1.889542	-1.240600	2.703262
H 0	3.211000	-0.999741	1.533890
H 0	-0.441605	-0.103149	-3.878769
H 0	0.002900	-1.803879	-3.817917
H 0	-1.620041	-1.296951	-3.276535
H 0	-2.009384	-0.005402	4.011932
H 0	-3.175186	0.952637	3.068634
H 0	-3.211014	-0.832230	3.024231
H 0	-2.341614	1.781326	0.970871
H 0	0.458389	0.887878	0.217697
H 0	-2.882965	1.862366	-1.326630
H 0	1.375977	2.436798	-1.308212
H 0	-3.105835	3.553848	-3.118088
H 0	1.157196	4.133774	-3.099243
H 0	-1.087418	4.699814	-4.011948

B3LYP/6-31G* Energy = -834.451217
 B3LYP/6-31G* Free energy in solution = -834.775399
 Number of Imaginary Frequencies = 1 (-337.13)

Product 1b+2b-*exo* (7b)



B3LYP/6-31G* Geometry

O 0	-4.275558	-0.608017	-0.690200
B 0	-3.274063	0.195267	-0.220779
C 0	-4.692810	-0.526352	-2.047607
C 0	-0.515289	-0.900269	-1.278229
O 0	-2.898758	0.129807	1.090454
O 0	-2.697678	1.112869	-1.070526
C 0	-1.058441	-2.079651	-0.963333
C 0	-3.540039	-0.784592	1.970978
C 0	-1.638184	1.943085	-0.757553
C 0	-1.590927	-3.080200	-1.949112
C 0	-2.014572	3.391541	-0.881622
C 0	-0.411972	1.507553	-0.443314
C 0	0.076202	0.078247	-0.277588
C 0	1.603302	0.009232	-0.367050
C 0	2.298782	0.630234	-1.413910
C 0	2.336563	-0.713104	0.581726
C 0	3.687271	0.531525	-1.508896
C 0	3.725876	-0.812210	0.492676
C 0	4.407028	-0.190002	-0.554581
H 0	-3.866272	-0.750992	-2.730606
H 0	-5.078781	0.471298	-2.285858
H 0	-5.488998	-1.262283	-2.190262
H 0	-0.432358	-0.609421	-2.326400
H 0	-1.128372	-2.360504	0.089294
H 0	-3.298981	-1.821579	1.708618

H 0	-4.628998	-0.667480	1.947662
H 0	-3.175461	-0.576660	2.980698
H 0	-1.074005	-4.045120	-1.856583
H 0	-2.657928	-3.274841	-1.776382
H 0	-1.470383	-2.731567	-2.980698
H 0	-2.798859	3.649185	-0.157913
H 0	-1.154968	4.045120	-0.711731
H 0	-2.420746	3.596558	-1.880264
H 0	0.323532	2.280000	-0.235214
H 0	-0.210754	-0.266098	0.725967
H 0	1.746277	1.199554	-2.157730
H 0	1.812454	-1.201859	1.400208
H 0	4.207748	1.020996	-2.328384
H 0	4.275940	-1.373093	1.244156
H 0	5.489014	-0.264389	-0.625366

B3LYP/6-31G* Energy = -834.527203
 B3LYP/6-31G* Free energy in solution = -834.851817
 Number of Imaginary Frequencies = 0

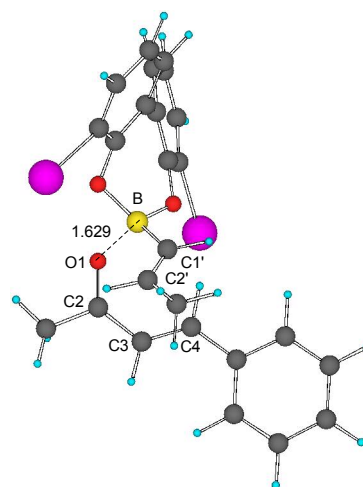
B3LYP/631LAN Geometry

O 0	-0.107925	-2.787277	2.121033
B 0	-0.107925	-1.420303	2.121033
C 0	-1.331802	-3.510880	2.121033
O 0	1.071716	-0.733337	2.149384
O 0	-1.310822	-0.751068	2.160706
C 0	2.306656	-1.437424	2.162552
C 0	-1.469284	0.619827	2.099258
C 0	-2.149887	1.154480	3.326920
C 0	-1.114868	1.370193	1.048340
C 0	-0.414917	0.944122	-0.231293
C 0	-0.855988	-0.410889	-0.758957
C 0	-0.611603	1.987793	-1.334412
C 0	-0.028229	-1.392700	-1.128632
C 0	-1.882919	2.498016	-1.633713
C 0	0.477783	2.427612	-2.096161
C 0	-0.452300	-2.712662	-1.707520
C 0	-2.059296	3.421417	-2.665085
C 0	0.306839	3.353439	-3.126892
C 0	-0.963959	3.853821	-3.415817
H 0	-1.933563	-3.272614	1.237030
H 0	-1.925659	-3.288834	3.015076
H 0	-1.083252	-4.575806	2.111481
H 0	2.476456	-1.956482	1.211578
H 0	2.338318	-2.177887	2.969360
H 0	3.101456	-0.702072	2.315491
H 0	-1.530243	0.982040	4.216721
H 0	-2.346848	2.226379	3.241592
H 0	-3.101456	0.633804	3.493820
H 0	-1.314789	2.434433	1.139709
H 0	0.663010	0.880600	-0.025955
H 0	-1.932465	-0.542587	-0.876541
H 0	1.046967	-1.244034	-1.012039
H 0	-2.739975	2.171356	-1.049530
H 0	1.470900	2.041153	-1.877548
H 0	-0.013077	-2.871582	-2.701889
H 0	-0.116638	-3.546280	-1.076035
H 0	-1.541504	-2.776794	-1.806671
H 0	-3.053284	3.805283	-2.880905
H 0	1.167633	3.686005	-3.701553
H 0	-1.099503	4.575821	-4.216736

B3LYP/631LAN Energy = -834.512354
 B3LYP/631LAN Free energy in solution = -834.837086
 Number of Imaginary Frequencies = 0

Conjugate Addition of 5b to 1b

Complex 1b-5b-Re-endo



B3LYP/631LAN Geometry

O 0	2.063232	0.442261	0.486343
B 0	2.613876	-0.908173	0.454483
C 0	2.727402	1.568909	0.153458
C 0	1.476776	-1.952637	0.036179
O 0	3.893692	-1.016479	-0.225586
C 0	3.477264	1.683029	-1.047760
C 0	2.598648	2.715500	0.957840
C 0	1.518845	-3.284576	0.173981
C 0	3.921661	-0.748764	-1.545975
C 0	3.645355	0.560684	-2.007904
C 0	3.191025	3.932144	0.633041
C 0	4.083389	2.912445	-1.352234
I 0	1.420425	2.640976	2.753235
C 0	0.469940	-4.254288	-0.293442
C 0	3.948212	4.027618	-0.532593
C 0	4.290482	-1.728256	-2.481934
C 0	3.645523	0.808945	-3.388931
C 0	4.312271	-1.461945	-3.848953
C 0	3.962631	-0.190308	-4.304504
I 0	4.902756	-3.667252	-1.806503
H 0	0.589783	-1.538895	-0.455246
H 0	2.387833	-3.741791	0.652435
H 0	3.068970	4.789413	1.285797
H 0	4.689148	2.979080	-2.250595
H 0	0.889221	-4.964279	-1.019806
H 0	0.077011	-4.856186	0.538803
H 0	-0.371826	-3.738342	-0.768448
H 0	4.432816	4.964279	-0.792100
H 0	3.389221	1.803055	-3.743149
H 0	4.591293	-2.240311	-4.550751
H 0	3.952606	0.018829	-5.370300
O 0	3.164246	-1.223022	1.954956
C 0	2.706894	-1.553955	3.079819
C 0	0.306961	-0.985535	2.805679
C 0	3.735443	-1.977982	4.099686
C 0	1.325684	-1.572479	3.490723

C 0	-1.100204	-0.981674	3.175522
C 0	-1.982315	-0.188965	2.413422
C 0	-1.625244	-1.734512	4.246979
C 0	-3.340729	-0.141418	2.715485
C 0	-2.981628	-1.688049	4.545029
C 0	-3.842911	-0.890152	3.781815
H 0	0.555344	-0.421768	1.913422
H 0	3.494324	-2.972610	4.493622
H 0	4.728241	-1.990097	3.648483
H 0	3.727005	-1.283707	4.949326
H 0	1.142242	-2.058731	4.444885
H 0	-1.585526	0.395233	1.587952
H 0	-0.970871	-2.366700	4.839294
H 0	-4.006317	0.477203	2.120697
H 0	-3.373947	-2.275436	5.370300
H 0	-4.902771	-0.857086	4.018585

B3LYP/631LAN Energy = -1238.239199

B3LYP/631LAN Free energy in solution = -1238.632311

Number of Imaginary Frequencies = 0

TS 1b+5b-Re-endo

B3LYP/631LAN Geometry

O 0	1.628571	0.757751	0.717834
B 0	1.534180	-0.706573	0.711517
C 0	2.813812	1.403015	0.681107
C 0	-0.074509	-0.972809	0.244141
O 0	2.466049	-1.358810	-0.193466
C 0	3.683762	1.262695	-0.427689
C 0	3.167191	2.302521	1.699753
O 0	1.858765	-1.297470	2.026810
C 0	-0.693329	-2.187973	0.108521
C 0	2.764893	-0.881943	-1.412918
C 0	3.333084	0.405762	-1.589432
C 0	4.354340	3.029068	1.664627
C 0	4.885605	1.986984	-0.441727
I 0	1.835266	2.604584	3.353897
C 0	1.028519	-1.450668	3.038513
C 0	-0.837524	-0.291351	1.921219
C 0	-1.728226	-2.539978	-0.898529
C 0	5.224533	2.859314	0.588181
C 0	2.604004	-1.697525	-2.546800
C 0	3.636505	0.841278	-2.888443
C 0	1.637756	-2.181213	4.200867
C 0	-0.279907	-1.045883	3.017242
C 0	-2.311676	-0.137650	1.803421
C 0	2.929535	-1.261581	-3.827942
C 0	3.433273	0.027908	-3.999466
I 0	1.900131	-3.711166	-2.299683
C 0	-2.830215	1.047821	1.256700
C 0	-3.212326	-1.128296	2.232819
C 0	-4.206818	1.245941	1.153580
C 0	-4.588058	-0.931030	2.131668
C 0	-5.089722	0.257446	1.592087
H 0	-0.384750	-0.228989	-0.495712
H 0	-0.483704	-2.953690	0.858688
H 0	4.600098	3.711166	2.470947
H 0	5.568787	1.846558	-1.273880
H 0	-0.311783	0.632431	1.683533
H 0	-1.512772	-3.512634	-1.357605
H 0	-2.702789	-2.639359	-0.391769

H 0	-1.819504	-1.783707	-1.682587
H 0	6.162643	3.405823	0.558472
H 0	4.034683	1.842865	-3.020996
H 0	0.909225	-2.359192	4.995697
H 0	2.059509	-3.136948	3.869385
H 0	2.465652	-1.588837	4.608231
H 0	-0.932114	-1.377747	3.817322
H 0	2.787003	-1.916824	-4.680344
H 0	3.672287	0.388519	-4.995712
H 0	-2.144073	1.821900	0.921936
H 0	-2.830780	-2.057236	2.648636
H 0	-4.589005	2.172821	0.735107
H 0	-5.270828	-1.704544	2.472809
H 0	-6.162659	0.409531	1.513458

B3LYP/631LAN Energy = -1238.218039

B3LYP/631LAN Free energy in solution = -1238.612211

Number of Imaginary Frequencies = 1 (-315.45)

Product 1b+5b-Re-endo

B3LYP/631LAN Geometry

O 0	-1.001480	-1.443481	-0.276489
B 0	0.121506	-0.959488	-0.915482
C 0	-1.217484	-2.765488	0.019500
C 0	-0.052505	3.689500	0.170502
O 0	1.333496	-1.620483	-0.898483
C 0	-0.230500	-3.582489	0.612503
C 0	-2.488480	-3.294495	-0.244492
O 0	0.091492	0.211502	-1.588486
C 0	0.246506	4.395493	-0.923492
C 0	1.841492	-2.157486	0.253494
C 0	1.104492	-3.076492	1.028503
C 0	-2.788483	-4.627487	0.028503
C 0	-0.547485	-4.929489	0.856506
I 0	-4.024490	-2.058487	-1.064484
C 0	-1.034485	0.976500	-1.894485
C 0	-0.812485	2.373489	0.222504
C 0	1.030502	5.676498	-0.927490
C 0	-1.803482	-5.450485	0.571503
C 0	3.137497	-1.793488	0.642502
C 0	1.687500	-3.560486	2.212494
C 0	-1.637482	0.616500	-3.218491
C 0	-1.422485	1.980500	-1.103485
C 0	-1.898483	2.395493	1.305496
C 0	3.706497	-2.306488	1.805496
C 0	2.968506	-3.185486	2.598495
I 0	4.265503	-0.430511	-0.551483
C 0	-2.144485	1.255493	2.080505
C 0	-2.687485	3.533493	1.518494
C 0	-3.148483	1.252502	3.049500
C 0	-3.695480	3.533493	2.485504
C 0	-3.927490	2.392502	3.256500
H 0	0.279495	4.055496	1.143494
H 0	-0.078506	4.025497	-1.895493
H 0	-3.776489	-5.016495	-0.189484
H 0	0.220505	-5.576492	1.267502
H 0	-0.089508	1.598495	0.510498
H 0	1.947495	5.578491	-1.524490
H 0	0.452500	6.497498	-1.375488
H 0	1.317505	5.978500	0.085495
H 0	-2.019485	-6.497482	0.767502

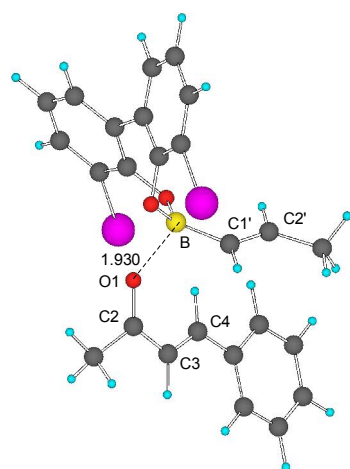
H 0	1.111496	-4.231491	2.841492
H 0	-2.463486	1.288498	-3.467484
H 0	-0.882492	0.678497	-4.012482
H 0	-2.022491	-0.411500	-3.207489
H 0	-2.271484	2.571503	-1.438492
H 0	4.709503	-2.012482	2.095505
H 0	3.396500	-3.571487	3.519500
H 0	-1.549484	0.360489	1.916504
H 0	-2.504486	4.427490	0.927505
H 0	-3.322479	0.358490	3.643494
H 0	-4.295486	4.426498	2.638504
H 0	-4.709488	2.392502	4.012497

B3LYP/631LAN Energy = -1238.277133

B3LYP/631LAN Free energy in solution = -1238.667887

Number of Imaginary Frequencies = 0

TS for the formation of complex 1b-5b-Re-exo



B3LYP/631LAN Geometry

O 0	1.269211	-1.749222	0.841064
B 0	0.133300	-2.295135	0.210236
C 0	2.282730	-2.475357	1.377686
C 0	-0.701370	-1.299500	-0.670624
O 0	0.187073	-3.664642	-0.190048
C 0	2.919144	-3.523865	0.668076
C 0	2.784042	-2.118073	2.639450
C 0	-0.248871	-0.107437	-1.089417
C 0	1.154068	-4.022659	-1.066605
C 0	2.517776	-3.924957	-0.705185
C 0	3.858200	-2.783203	3.224060
C 0	3.991028	-4.194153	1.279541
I 0	1.910721	-0.487732	3.723618
C 0	-0.964890	0.830902	-2.019211
C 0	4.459839	-3.837250	2.538895
C 0	0.819626	-4.547653	-2.324448
C 0	3.494110	-4.293198	-1.644135
C 0	1.799271	-4.932724	-3.236343
C 0	3.144882	-4.787155	-2.897278
I 0	-1.239914	-4.795364	-2.854309
H 0	-1.671158	-1.634613	-1.045547
H 0	0.731064	0.227524	-0.743286
H 0	4.213623	-2.486557	4.204391
H 0	4.449387	-5.024979	0.752411
H 0	-1.933090	0.426865	-2.333954
H 0	-1.138611	1.805267	-1.540771

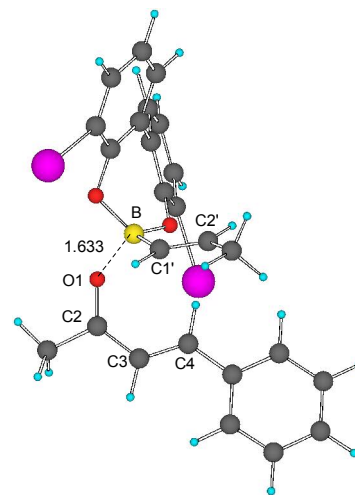
H 0	-0.367706	1.028732	-2.920181
H 0	5.286728	-4.377182	2.990875
H 0	4.541931	-4.178955	-1.383560
H 0	1.515244	-5.330460	-4.204391
H 0	3.915375	-5.063248	-3.611374
O 0	-1.025787	-2.719437	1.693954
C 0	-2.058929	-2.365173	2.285767
C 0	-1.734300	0.077179	2.131424
C 0	-2.907349	-3.435318	2.939423
C 0	-2.522934	-0.987579	2.412979
C 0	-2.082581	1.490067	2.243103
C 0	-1.083923	2.445297	1.969193
C 0	-3.365906	1.947525	2.605133
C 0	-1.354095	3.809311	2.056854
C 0	-3.634583	3.308838	2.692169
C 0	-2.630066	4.244720	2.419342
H 0	-0.719727	-0.128204	1.807800
H 0	-2.443939	-4.413132	2.801453
H 0	-3.032196	-3.228226	4.009308
H 0	-3.910431	-3.440308	2.493393
H 0	-3.528946	-0.858887	2.804000
H 0	-0.091202	2.103027	1.689911
H 0	-4.157500	1.234300	2.814056
H 0	-0.570587	4.530731	1.843323
H 0	-4.629150	3.645600	2.971176
H 0	-2.844543	5.307663	2.488480

B3LYP/631LAN Energy = -1238.242246

B3LYP/631LAN Free energy in solution = -1238.631532

Number of Imaginary Frequencies = 1 (-105.47)

Complex 1b-5b-Re-exo



B3LYP/631LAN Geometry

O 0	0.559891	-0.497208	-0.778625
B 0	1.122482	0.300873	0.298676
C 0	1.279907	-1.160629	-1.709961
C 0	0.232056	0.272003	1.618759
O 0	2.544373	0.095413	0.518585
C 0	2.355545	-2.023987	-1.369415
C 0	0.901810	-1.084137	-3.062225
C 0	-0.689758	-0.658493	1.905426
C 0	2.938019	-1.131744	0.913071
C 0	2.811600	-2.229782	0.029739
C 0	1.550049	-1.799332	-4.064880

C 0	3.009720	-2.725769	-2.394318
I 0	-0.756454	0.151900	-3.644394
C 0	-1.447556	-0.784317	3.197876
C 0	2.620712	-2.623932	-3.725510
C 0	3.529449	-1.340836	2.168732
C 0	3.215164	-3.501755	0.463211
C 0	3.947815	-2.604279	2.578659
C 0	3.771378	-3.693741	1.724609
I 0	3.832214	0.322205	3.486160
O 0	1.226440	1.833847	-0.253769
C 0	0.480026	2.843811	-0.342926
C 0	-1.752884	1.771515	-0.309692
C 0	1.181686	4.153870	-0.604553
C 0	-0.955627	2.872330	-0.226959
C 0	-3.205551	1.744095	-0.222458
C 0	-3.861053	0.524628	-0.487900
C 0	-3.986420	2.869171	0.115509
C 0	-5.249207	0.433060	-0.427795
C 0	-5.371536	2.775208	0.177353
C 0	-6.007126	1.557922	-0.096069
H 0	0.459824	1.004578	2.398941
H 0	-0.918030	-1.414139	1.150436
H 0	1.228149	-1.706238	-5.096237
H 0	3.856064	-3.352310	-2.130112
H 0	-1.168106	0.002655	3.906754
H 0	-2.533066	-0.727585	3.031784
H 0	-1.256973	-1.755219	3.676147
H 0	3.149323	-3.175323	-4.497620
H 0	3.081161	-4.350540	-0.200989
H 0	4.396225	-2.738815	3.556961
H 0	4.074265	-4.686447	2.045105
H 0	-1.280426	0.817474	-0.508194
H 0	2.262497	4.008072	-0.598800
H 0	0.870422	4.558243	-1.575806
H 0	0.902954	4.892746	0.156418
H 0	-1.387878	3.864838	-0.135651
H 0	-3.266663	-0.345963	-0.749863
H 0	-3.506241	3.816544	0.340805
H 0	-5.738983	-0.513016	-0.639023
H 0	-5.961105	3.648544	0.441208
H 0	-7.090363	1.489273	-0.047089

B3LYP/6311LAN Energy = -1238.24306

B3LYP/6311LAN Free energy in solution = -1238.635786

Number of Imaginary Frequencies = 0

TS 1b+5b-Re-exo

B3LYP/6311LAN Geometry

O 0	-1.165222	-0.378128	-0.550507
B 0	-0.563568	-0.364227	0.784805
C 0	-2.446503	-0.750778	-0.757324
C 0	0.765289	0.642685	0.710175
O 0	-1.468857	0.070724	1.839279
C 0	-3.516861	-0.023392	-0.182037
C 0	-2.746216	-1.812424	-1.624847
O 0	-0.148590	-1.726563	1.226410
C 0	0.682129	1.824112	0.016937
C 0	-2.260376	1.143234	1.674561
C 0	-3.270157	1.162140	0.677597
C 0	-4.057251	-2.181885	-1.913055
C 0	-4.833267	-0.414337	-0.469116

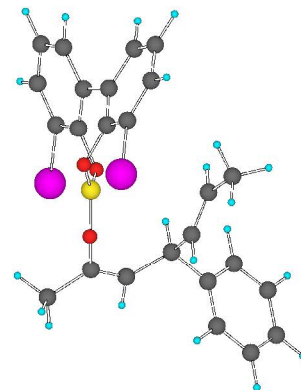
I 0	-1.143250	-2.887802	-2.561234
C 0	1.053772	-2.236710	1.110291
C 0	1.779100	-0.537033	-0.515274
C 0	1.360153	3.103378	0.358536
C 0	-5.107605	-1.479996	-1.321457
C 0	-2.155518	2.247833	2.539337
C 0	-4.086914	2.295975	0.557373
C 0	1.273315	-3.474411	1.931213
C 0	2.042984	-1.654419	0.351608
C 0	2.938828	0.159332	-1.137192
C 0	-2.984177	3.360855	2.418243
C 0	-3.947433	3.388260	1.409500
I 0	-0.720291	2.209549	4.133713
C 0	2.849900	0.587418	-2.471939
C 0	4.135239	0.384476	-0.436798
C 0	3.932571	1.206146	-3.096313
C 0	5.215729	1.009094	-1.058304
C 0	5.119370	1.418503	-2.390930
H 0	1.367400	0.676010	1.621307
H 0	0.109955	1.817764	-0.912277
H 0	-4.255585	-3.011169	-2.583084
H 0	-5.651108	0.123138	0.001526
H 0	0.936400	-0.648911	-1.190765
H 0	1.809204	3.083420	1.354935
H 0	2.150482	3.304962	-0.382935
H 0	0.658646	3.945557	0.297043
H 0	-6.134476	-1.769669	-1.524536
H 0	-4.837555	2.317017	-0.227188
H 0	1.052400	-3.271179	2.985489
H 0	0.580490	-4.258179	1.603271
H 0	2.296326	-3.847000	1.837250
H 0	3.062592	-2.002106	0.474304
H 0	-2.875946	4.197845	3.099564
H 0	-4.587952	4.258179	1.296204
H 0	1.929169	0.417160	-3.024979
H 0	4.214783	0.075180	0.601868
H 0	3.850479	1.518738	-4.133713
H 0	6.134476	1.176300	-0.502594
H 0	5.963486	1.901321	-2.875626

B3LYP/6311LAN Energy= -1238.225495

B3LYP/6311LAN Free energy in solution= -1238.619507

Number of Imaginary Frequencies= 1 (-289.60)

Product 1b+5b-Re-exo (6b)



B3LYP/6311LAN Geometry

O 0	2.571167	0.987961	-0.388947
B 0	2.863770	-0.004852	0.523087

H 0	-0.135513	4.361496	-1.515991
H 0	1.990494	4.859497	-1.770996
H 0	2.750488	0.771500	-0.643997
H 0	4.413483	5.261505	-1.944000
H 0	5.184494	1.177505	-0.822998
H 0	6.027496	3.428497	-1.474000

B3LYP/631LAN Energy = -1238.252067
 B3LYP/631LAN Free energy in solution = -1238.634871
 Number of Imaginary Frequencies = 0

TS 1b+5b-Si-endo

B3LYP/631LAN Geometry

O 0	1.685806	1.684250	1.554657
B 0	0.859970	0.566559	1.142044
C 0	3.028091	1.553986	1.467346
C 0	-0.721619	1.061371	1.407089
O 0	1.000748	0.185852	-0.271957
O 0	1.251343	-0.619308	1.951859
C 0	3.650696	1.455856	0.203415
C 0	3.830032	1.572830	2.617950
C 0	-1.150925	1.510788	2.627228
C 0	0.472702	-1.589325	2.371384
C 0	-1.528900	-0.744095	1.199081
C 0	1.606644	0.903320	-1.232239
C 0	2.860764	1.552780	-1.052155
C 0	5.047424	1.327194	0.146042
C 0	5.216600	1.468796	2.548355
I 0	2.909897	1.785706	4.545273
C 0	-2.132996	2.599335	2.872192
C 0	1.167023	-2.567535	3.275925
C 0	-0.867889	-1.663391	2.087524
C 0	-3.011063	-0.638672	1.233414
C 0	1.030975	0.951904	-2.518188
C 0	3.410156	2.275970	-2.123383
C 0	5.825333	1.331909	1.300217
C 0	-3.746658	-0.849045	2.413925
C 0	-3.709183	-0.323853	0.056030
C 0	1.601898	1.652237	-3.575760
C 0	2.796906	2.338623	-3.369370
I 0	-0.771240	-0.143692	-2.927750
C 0	-5.137131	-0.767563	2.410004
C 0	-5.101624	-0.241608	0.051682
C 0	-5.819839	-0.465622	1.227264
H 0	-1.151260	1.588486	0.550751
H 0	-0.782028	0.998428	3.518417
H 0	-1.121765	-0.684616	0.189316
H 0	5.523788	1.209869	-0.822571
H 0	5.812363	1.482193	3.454514
H 0	-3.035919	2.185700	3.349655
H 0	-2.425369	3.110229	1.950974
H 0	-1.722153	3.334503	3.577957
H 0	1.982925	-3.055756	2.730057
H 0	0.482239	-3.334503	3.646164
H 0	1.620529	-2.040665	4.123398
H 0	-1.465363	-2.376480	2.644241
H 0	4.342453	2.807526	-1.959412
H 0	6.904541	1.228195	1.233780
H 0	-3.223434	-1.074203	3.339417
H 0	-3.151108	-0.149445	-0.859436
H 0	1.116302	1.666687	-4.545273

H 0	3.244064	2.910645	-4.176910
H 0	-5.690506	-0.937027	3.329773
H 0	-5.624542	-0.004257	-0.870651
H 0	-6.904541	-0.401825	1.225600

B3LYP/631LAN Energy = -1238.217472
 B3LYP/631LAN Free energy in solution = -1238.609617
 Number of Imaginary Frequencies = 1 (-313.96)

Product 1b+5b-Si-endo

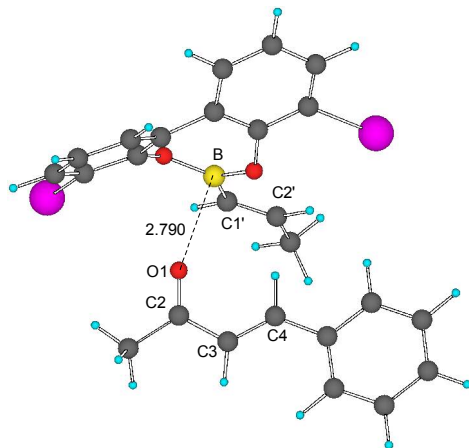
B3LYP/631LAN Geometry

O 0	2.063995	-0.267502	-0.737991
B 0	0.994003	-0.482498	0.108002
C 0	3.261993	-0.903488	-0.557983
C 0	-2.189987	3.477509	-0.457993
O 0	0.632004	-1.742477	0.537994
O 0	0.308014	0.619507	0.485992
C 0	3.352997	-2.308487	-0.479980
C 0	4.422989	-0.121490	-0.477982
C 0	-1.954987	4.277496	0.584991
C 0	-0.806992	0.703506	1.317993
C 0	-2.095993	1.960495	-0.478989
C 0	0.895996	-2.897476	-0.153000
C 0	2.175003	-3.194489	-0.669983
C 0	4.619995	-2.878479	-0.268005
C 0	5.671997	-0.709488	-0.293991
I 0	4.287003	2.002502	-0.635986
C 0	-2.034988	5.777496	0.550003
C 0	-0.616989	0.136505	2.694000
C 0	-1.892990	1.355500	0.890991
C 0	-3.327988	1.336502	-1.145981
C 0	-0.148987	-3.819489	-0.302994
C 0	2.338989	-4.403488	-1.367981
C 0	5.765000	-2.096481	-0.177002
C 0	-4.618988	1.799500	-0.860992
C 0	-3.184982	0.262497	-2.033981
C 0	0.043015	-5.021484	-0.979980
C 0	1.294998	-5.307480	-1.521988
I 0	-2.079987	-3.396484	0.502991
C 0	-5.737991	1.204498	-1.446991
C 0	-4.299988	-0.333496	-2.623993
C 0	-5.581985	0.135498	-2.331985
H 0	-2.468994	3.923508	-1.413986
H 0	-1.667984	3.832504	1.539000
H 0	-1.226990	1.697510	-1.095993
H 0	4.696000	-3.956482	-0.160995
H 0	6.559998	-0.089493	-0.231003
H 0	-2.764984	6.156509	1.278992
H 0	-2.325989	6.143509	-0.440994
H 0	-1.069992	6.232498	0.808990
H 0	-0.446991	-0.944489	2.658997
H 0	-1.497986	0.328506	3.311996
H 0	0.254013	0.595505	3.179993
H 0	-2.718994	1.450500	1.591003
H 0	3.306000	-4.620483	-1.808990
H 0	6.731995	-2.561478	-0.011002
H 0	-4.745987	2.639496	-0.182007
H 0	-2.188995	-0.111496	-2.262985
H 0	-0.778992	-5.719482	-1.090988
H 0	1.449997	-6.232483	-2.069992
H 0	-6.731995	1.580505	-1.215988

H 0 -4.166992 -1.164490 -3.311981
H 0 -6.451996 -0.325500 -2.791992

B3LYP/631LAN Energy = -1238.277448
B3LYP/631LAN Free energy in solution = -1238.668712
Number of Imaginary Frequencies = 0

Complex 1b-5b-Si-exo



B3LYP/631LAN Geometry

O 0	2.064194	1.767410	1.591293
B 0	0.729980	1.845718	1.238510
C 0	3.001877	1.006287	0.964737
C 0	-0.301865	2.079971	2.362869
O 0	0.320877	1.823990	-0.089844
C 0	3.168304	1.008850	-0.435226
C 0	3.848557	0.221848	1.761108
C 0	-1.604202	2.333466	2.147919
C 0	1.060959	2.268906	-1.145874
C 0	2.420715	1.930786	-1.332077
C 0	4.131592	0.148315	-0.989578
C 0	4.818726	-0.599960	1.195221
I 0	3.657410	0.275909	3.889206
C 0	-2.639755	2.551224	3.210419
C 0	0.421097	3.075424	-2.100464
C 0	3.091721	2.474258	-2.441696
C 0	4.945969	-0.648422	-0.192886
C 0	1.096268	3.578995	-3.208633
C 0	2.448227	3.283554	-3.370605
I 0	-1.651596	3.568268	-1.881683
H 0	0.050903	2.027374	3.394058
H 0	-1.961380	2.391144	1.119492
H 0	4.229843	0.101500	-2.069336
H 0	5.457703	-1.204193	1.829605
H 0	-3.444427	1.806778	3.131287
H 0	-3.117050	3.534607	3.097122
H 0	-2.210831	2.489090	4.215958
H 0	4.149292	2.263672	-2.561172
H 0	5.681152	-1.305817	-0.647675
H 0	0.575867	4.204239	-3.925446
H 0	2.995667	3.689667	-4.215958
O 0	0.644913	-0.938797	1.382248
C 0	0.219482	-2.087814	1.335907
C 0	-1.540588	-1.588043	-0.319031
C 0	0.848923	-3.187042	2.174026
C 0	-0.919098	-2.484497	0.475388
C 0	-2.670883	-1.816391	-1.218460

C 0	-3.291641	-3.071716	-1.378616
C 0	-3.165894	-0.729309	-1.963516
C 0	-4.363861	-3.228836	-2.250290
C 0	-4.240372	-0.887115	-2.837204
C 0	-4.843216	-2.137329	-2.983658
H 0	-1.154465	-0.569550	-0.289398
H 0	1.660004	-2.774918	2.776855
H 0	1.238235	-3.984268	1.527283
H 0	0.098343	-3.646515	2.830002
H 0	-1.227127	-3.527023	0.513840
H 0	-2.931976	-3.928909	-0.817078
H 0	-2.698395	0.245500	-1.851471
H 0	-4.830063	-4.204239	-2.360855
H 0	-4.605118	-0.034195	-3.402969
H 0	-5.681168	-2.264191	-3.663818

B3LYP/631LAN Energy = -1238.251768
B3LYP/631LAN Free energy in solution = -1238.634681
Number of Imaginary Frequencies = 0

TS 1b+5b-Si-exo

B3LYP/631LAN Geometry

O 0	-1.567261	-0.501343	1.300659
B 0	-0.773743	0.003189	0.198181
C 0	-2.657913	0.216675	1.649292
C 0	0.681717	-0.805573	0.259781
O 0	-1.398666	-0.160446	-1.117432
O 0	-0.530090	1.465897	0.429108
C 0	-3.739975	0.338562	0.749023
C 0	-2.749573	0.821671	2.911148
C 0	0.775925	-2.085327	-0.227173
C 0	0.589233	2.107483	0.202835
C 0	1.552002	0.266510	-1.131958
C 0	-2.638245	-0.603577	-1.382507
C 0	-3.769150	-0.412125	-0.536346
C 0	-4.840759	1.125519	1.126419
C 0	-3.862381	1.568710	3.286850
I 0	-1.138107	0.593170	4.307816
C 0	1.608475	-3.184738	0.326172
C 0	0.648132	3.475861	0.818375
C 0	1.645477	1.547287	-0.476944
C 0	2.827148	-0.351044	-1.601074
C 0	-2.854431	-1.255264	-2.615356
C 0	-5.007217	-0.941254	-0.943390
C 0	-4.906326	1.734680	2.376007
C 0	3.998138	-0.301804	-0.826508
C 0	2.876587	-0.980835	-2.854584
C 0	-4.092941	-1.744675	-3.011658
C 0	-5.181992	-1.597565	-2.155060
I 0	-1.221558	-1.500565	-3.993729
C 0	5.186432	-0.858368	-1.297485
C 0	4.067245	-1.530914	-3.329803
C 0	5.225967	-1.471466	-2.552643
H 0	1.258102	-0.609177	1.168213
H 0	0.233582	-2.315262	-1.145935
H 0	0.728714	0.141342	-1.831436
H 0	-5.652588	1.266815	0.419708
H 0	-3.907089	2.028168	4.268204
H 0	2.400772	-3.443054	-0.394531
H 0	1.006897	-4.094910	0.455536
H 0	2.071213	-2.920670	1.280777

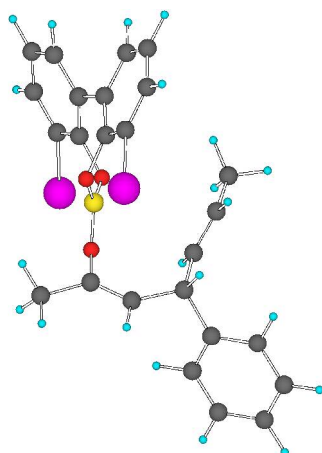
H 0	-0.163100	4.094910	0.418030
H 0	1.601913	3.969437	0.616196
H 0	0.493881	3.406494	1.901398
H 0	2.607910	2.044540	-0.432175
H 0	-5.851837	-0.841675	-0.269287
H 0	-5.768097	2.338500	2.645477
H 0	3.973419	0.168259	0.152954
H 0	1.976135	-1.026337	-3.460922
H 0	-4.202591	-2.243271	-3.968384
H 0	-6.153381	-1.996109	-2.432037
H 0	6.082962	-0.813004	-0.685074
H 0	4.089722	-2.003860	-4.307816
H 0	6.153381	-1.901474	-2.920853

B3LYP/631LAN Energy = -1238.221327

B3LYP/631LAN Free energy in solution = -1238.612721

Number of Imaginary Frequencies = 1 (-274.27)

Product 1b+5b-Si-exo



B3LYP/631LAN Geometry

O 0	2.033829	-0.058853	1.280319
B 0	1.727875	-0.749756	0.126312
C 0	3.289612	0.398010	1.565353
C 0	-1.282242	0.041077	0.089127
O 0	2.280700	-0.452698	-1.103592
O 0	0.886551	-1.798996	0.273727
C 0	4.022964	1.183578	0.653702
C 0	3.833511	0.093491	2.821304
C 0	-0.979400	1.321671	-0.151215
C 0	0.268372	-2.495056	-0.760849
C 0	-1.791672	-0.925903	-0.961960
C 0	2.686859	0.797852	-1.486100
C 0	3.472000	1.627319	-0.654938
C 0	5.315842	1.592636	1.024719
C 0	5.105469	0.532822	3.179825
I 0	2.704636	-1.061569	4.218475
C 0	-0.542023	2.316116	0.887421
C 0	1.042511	-3.710175	-1.179886
C 0	-0.918961	-2.132309	-1.254578
C 0	-3.218185	-1.361145	-0.598419
C 0	2.337631	1.238312	-2.771408
C 0	3.797119	2.913193	-1.121460
C 0	5.853195	1.276900	2.267624
C 0	-3.450562	-2.415192	0.294830
C 0	-4.319870	-0.674957	-1.124649
C 0	2.697357	2.505676	-3.224014

C 0	3.415405	3.353958	-2.383148
I 0	1.259079	-0.039368	-4.101257
C 0	-4.751404	-2.773865	0.652512
C 0	-5.622009	-1.032898	-0.772598
C 0	-5.842331	-2.084717	0.119080
H 0	-1.218475	-0.342606	1.106262
H 0	-1.058900	1.697037	-1.173431
H 0	-1.861267	-0.366455	-1.907120
H 0	5.909698	2.155792	0.312195
H 0	5.511108	0.285095	4.154480
H 0	-1.255783	3.148331	0.961288
H 0	0.430740	2.756683	0.631912
H 0	-0.453568	1.852280	1.874847
H 0	2.010895	-3.417557	-1.605774
H 0	0.496246	-4.289581	-1.928711
H 0	1.246400	-4.353485	-0.314758
H 0	-1.328796	-2.793854	-2.015045
H 0	4.353897	3.576614	-0.467911
H 0	6.855438	1.603851	2.527969
H 0	-2.604813	-2.961014	0.705276
H 0	-4.154449	0.149521	-1.814972
H 0	2.409851	2.828217	-4.218460
H 0	3.678100	4.353500	-2.716324
H 0	-4.912308	-3.594833	1.346817
H 0	-6.464157	-0.491318	-1.196136
H 0	-6.855438	-2.366058	0.394150

B3LYP/631LAN Energy = -1238.27579

B3LYP/631LAN Free energy in solution = -1238.668085

Number of Imaginary Frequencies = 0

Study of competitive pathways

Conjugate Addition of 8b to 1b

TS 1b+8b-Re-exo

B3LYP/631LAN Geometry

O 0	1.919434	0.520157	-0.111694
B 0	1.640381	-0.081375	1.195007
C 0	3.147354	0.529160	-0.686234
C 0	0.063507	-0.671570	1.160202
O 0	2.627151	-1.093704	1.494614
C 0	3.528839	-0.523743	-1.552643
C 0	4.042740	1.601776	-0.522202
O 0	1.701462	0.917740	2.325073
C 0	-0.411224	-1.379242	0.084702
C 0	2.490036	-2.840912	-1.329742
C 0	2.568878	-1.590805	-1.990784
C 0	5.310989	1.596069	-1.100052
C 0	4.807037	-0.521652	-2.124756
I 0	3.454483	3.376663	0.532288
C 0	0.709473	1.640961	2.782669
C 0	-0.752274	1.109314	0.873840
C 0	-1.386612	-2.500031	0.123306
C 0	5.705338	0.515167	-1.886230
C 0	1.710464	-3.856491	-1.911545
C 0	1.832169	-1.389877	-3.164398
C 0	1.004257	2.333847	4.082153
C 0	-0.514633	1.710541	2.159790
C 0	-2.159912	1.028946	0.391205
C 0	0.996307	-3.649765	-3.089264

C 0	1.042664	-2.401230	-3.711502
I 0	1.614990	-5.770721	-0.953690
C 0	-2.440400	1.273682	-0.962784
C 0	-3.227112	0.736008	1.256149
C 0	-3.751724	1.244339	-1.436813
C 0	-4.537659	0.699722	0.781937
C 0	-4.804672	0.957550	-0.565277
O 0	3.160263	-3.087357	-0.188644
C 0	2.669052	-1.696594	2.776810
H 0	-0.332825	-0.994598	2.128235
H 0	-0.087738	-1.065750	-0.908310
H 0	5.981583	2.433914	-0.942688
H 0	5.084900	-1.345306	-2.776016
H 0	-0.046249	1.361176	0.087402
H 0	-1.638900	-2.803192	1.143295
H 0	-2.309921	-2.200287	-0.397247
H 0	-0.992081	-3.366013	-0.424500
H 0	6.695251	0.501312	-2.332870
H 0	1.906082	-0.427292	-3.663071
H 0	1.313843	1.605057	4.840668
H 0	1.842789	3.025986	3.941544
H 0	0.140549	2.893860	4.449112
H 0	-1.345612	2.151245	2.699203
H 0	0.405563	-4.454590	-3.514084
H 0	0.485138	-2.230362	-4.627869
H 0	-1.623093	1.501938	-1.642715
H 0	-3.026062	0.528168	2.303696
H 0	-3.951019	1.448196	-2.485306
H 0	-5.351929	0.470581	1.464081
H 0	-5.826645	0.932953	-0.933289
H 0	3.159164	-2.262314	0.364182
H 0	1.742294	-2.243881	3.002884
H 0	2.838318	-0.947098	3.557571
H 0	3.497070	-2.411911	2.785629

B3LYP/631LAN Energy= -1353.888567

B3LYP/631LAN Free energy in solution= -1354.332977

Number of Imaginary Frequencies= 1 (-301.97)

TS 1b+8b-Si-exo

B3LYP/631LAN Geometry

O 0	-1.186203	-0.983215	-2.782959
B 0	-0.701721	-0.008835	-1.839188
C 0	-0.876511	-0.833832	-4.159088
C 0	-1.019135	1.581833	-2.322922
O 0	-1.286530	-0.254089	-0.517838
O 0	0.806976	-0.100220	-1.810486
C 0	-2.281296	2.114182	-2.317230
C 0	1.640732	0.860107	-1.496445
C 0	-0.152374	2.382141	-0.742615
C 0	-1.795349	-1.427811	-0.079102
C 0	-1.035843	-2.623900	-0.000137
C 0	-2.837692	3.075821	-3.307587
C 0	3.083008	0.535049	-1.759155
C 0	1.225555	2.091400	-1.038483
C 0	-0.537796	3.807648	-0.540924
C 0	-3.120178	-1.478485	0.401855
C 0	0.439468	-2.710770	-0.262573
C 0	-1.650009	-3.804900	0.441406
C 0	0.014191	4.844711	-1.310852
C 0	-1.467651	4.134109	0.459610

C 0	-3.713303	-2.652725	0.855362
I 0	-4.313309	0.305800	0.532059
C 0	0.923400	-3.183609	-1.504074
C 0	1.338104	-2.487869	0.784515
C 0	-2.977997	-3.835587	0.852432
C 0	-0.345900	6.171524	-1.079025
C 0	-1.823181	5.461807	0.696533
C 0	2.289352	-3.474900	-1.627090
C 0	2.699463	-2.756210	0.637451
C 0	-1.262878	6.484665	-0.072037
O 0	0.093613	-3.377960	-2.551849
C 0	3.174164	-3.271881	-0.570114
I 0	3.034576	-4.227692	-3.488739
H 0	-1.442200	-0.002014	-4.601318
H 0	-1.160126	-1.756073	-4.674484
H 0	0.195557	-0.663696	-4.320679
H 0	-0.393448	1.912903	-3.158554
H 0	-2.934800	1.859482	-1.483826
H 0	-0.655319	1.706802	-0.056335
H 0	-2.997253	4.050400	-2.818985
H 0	-3.824783	2.746841	-3.659454
H 0	-2.179016	3.223114	-4.168549
H 0	3.218735	0.229462	-2.803085
H 0	3.382385	-0.316574	-1.138077
H 0	3.734955	1.384415	-1.539993
H 0	1.950424	2.897491	-1.011566
H 0	-1.050552	-4.709900	0.474655
H 0	0.722641	4.607529	-2.099960
H 0	-1.905640	3.339249	1.058502
H 0	-4.739441	-2.642776	1.205811
H 0	0.952911	-2.126480	1.733994
H 0	-3.432266	-4.761703	1.191696
H 0	0.089691	6.962219	-1.683914
H 0	-2.535919	5.697174	1.482117
H 0	3.385254	-2.591858	1.463669
H 0	-1.540176	7.519226	0.110535
H 0	-0.597061	-2.672012	-2.522476
H 0	4.226227	-3.507584	-0.691360

B3LYP/631LAN Energy = -1353.884918

B3LYP/631LAN Free energy in solution = -1354.329645

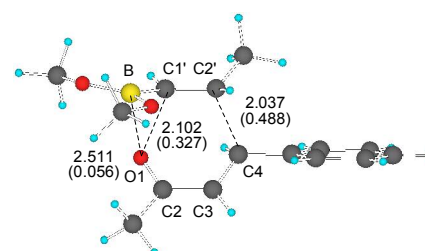
Number of Imaginary Frequencies = 1 (-316.65)

TSs of Hetero Diels-Alder Reactions

Hetero Diels-Alder Reaction between 1b and 2b

TSs leading to regioisomers 9

DATSAa 1b+2b-endo



B3LYP/6-31G* Geometry

C 0	1.603958	-0.280487	-1.121979
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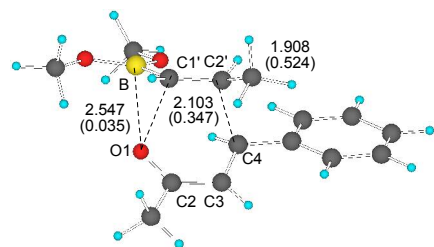
C O	0.211000	-0.327500	-0.888977
B O	2.666962	-0.926483	-0.175980
O O	3.976959	-1.153488	-0.497986
O O	2.223984	-1.331482	1.056992
C O	4.570969	-0.620500	-1.672958
C O	3.121979	-1.910461	1.995956
C O	-0.697983	-0.511490	-2.096985
H O	1.901978	-0.019485	-2.135986
H O	-0.093979	-0.882462	-0.003998
H O	4.426971	0.463486	-1.721985
H O	4.153992	-1.081482	-2.577972
H O	5.640945	-0.843475	-1.632980
H O	3.952957	-1.233490	2.225967
H O	3.540970	-2.848465	1.615967
H O	2.556992	-2.111496	2.909973
H O	-0.612000	-1.534485	-2.485977
H O	-0.419983	0.171478	-2.909973
H O	-1.748978	-0.341476	-1.851959
C O	-0.313980	1.520477	-0.211000
C O	0.529984	1.861465	0.876953
C O	-1.782959	1.479477	0.012009
C O	1.910950	1.873459	0.688950
C O	-2.334000	0.848465	1.140976
C O	-2.657959	2.089478	-0.900986
O O	2.390976	1.552475	-0.459000
C O	2.874954	2.132477	1.826965
C O	-4.035980	2.089478	-0.685974
C O	-3.711000	0.841461	1.354980
C O	-4.567963	1.465469	0.443970
H O	-0.011978	1.948471	-1.164978
H O	0.119995	1.962463	1.876953
H O	-1.674973	0.353485	1.847961
H O	-2.248978	2.579453	-1.781982
H O	3.641937	2.848465	1.514969
H O	2.362961	2.526459	2.711960
H O	3.388977	1.204468	2.106995
H O	-4.693985	2.576477	-1.400986
H O	-4.116974	0.346481	2.232971
H O	-5.640945	1.459488	0.611954

B3LYP/6-31G* Energy = -834.445577

B3LYP/6-31G* Free energy in solution = -834.771493

Number of Imaginary Frequencies = 1 (-509.44)

DATSAa 1b+2b-exo



B3LYP/6-31G* Geometry

C O	-2.453583	-1.983109	-0.314743
C O	-1.143707	-2.362213	-0.593689
O O	-2.779282	-0.739639	-0.340698
C O	-3.500702	-2.978516	0.142624
C O	-0.193161	-1.329926	-0.833664
C O	1.231033	-1.644135	-1.136063

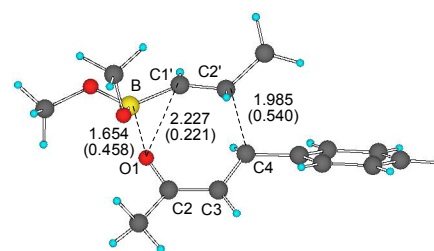
C O	1.874329	-2.805496	-0.677017
C O	1.974548	-0.738770	-1.912231
C O	3.208496	-3.058090	-0.995453
C O	3.307251	-0.989380	-2.232620
C O	3.930145	-2.152847	-1.775711
H O	-0.836731	-3.392654	-0.445847
H O	-4.416779	-2.861069	-0.446716
H O	-3.151962	-4.011780	0.047974
H O	-3.767258	-2.794144	1.191391
H O	-0.575943	-0.505264	-1.429672
H O	1.329483	-3.519226	-0.066055
H O	1.492020	0.170029	-2.264542
H O	3.685349	-3.964981	-0.632751
H O	3.859406	-0.277588	-2.840668
H O	4.969238	-2.351563	-2.024109
C O	-0.177032	-0.196976	0.790421
C O	-1.463531	0.394012	0.845825
C O	0.289612	-1.053421	1.952759
B O	-1.860260	1.617752	-0.048828
O O	-0.946167	2.012543	-0.990250
O O	-3.034561	2.305817	0.040512
C O	-1.256363	3.063538	-1.900375
C O	-4.094940	1.902084	0.899109
H O	0.587723	0.453247	0.367783
H O	-2.095734	0.122665	1.688202
H O	-0.467636	-1.798889	2.220840
H O	0.475830	-0.435349	2.840683
H O	1.220718	-1.579666	1.718842
H O	-0.412567	3.161591	-2.588791
H O	-1.402802	4.011795	-1.371307
H O	-2.166077	2.840439	-2.467896
H O	-4.328979	0.844116	0.751831
H O	-4.969238	2.509583	0.648575
H O	-3.839600	2.079147	1.951981

B3LYP/6-31G* Energy = -834.447301

B3LYP/6-31G* Free energy in solution = -834.770864

Number of Imaginary Frequencies = 1 (-521.75)

DATSBa 1b+2b-endo



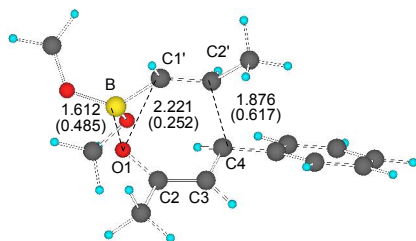
B3LYP/6-31G* Geometry

C O	0.898148	-1.649048	-1.477585
C O	0.898148	-0.277939	-1.477585
O O	-0.258942	-2.289688	-1.477585
C O	2.149673	-2.478760	-1.408478
C O	-0.334259	0.468597	-1.400772
C O	-0.241623	1.954041	-1.372986
C O	0.711472	2.622681	-0.585175
C O	-1.115921	2.721970	-2.158112
C O	0.795547	4.013123	-0.596542
C O	-1.027359	4.113647	-2.176971
C O	-0.071304	4.763916	-1.395523

H 0	1.842682	0.247025	-1.381516
H 0	2.167404	-3.196808	-2.236908
H 0	3.048203	-1.856522	-1.461533
H 0	2.149643	-3.047180	-0.473419
H 0	-1.119980	0.109726	-2.061035
H 0	1.384644	2.047577	0.044983
H 0	-1.861557	2.219666	-2.769623
H 0	1.538300	4.513138	0.019226
H 0	-1.705719	4.688934	-2.801086
H 0	-0.002930	5.848221	-1.405258
B 0	-0.905823	-2.737000	-0.022919
O 0	-1.773239	-3.831421	-0.210327
C 0	-1.689911	-1.347610	-0.055054
O 0	0.197388	-2.865189	0.881363
C 0	-1.238144	-0.056992	0.286469
C 0	-1.211197	-5.098907	-0.478546
C 0	-0.129456	-3.122330	2.228622
C 0	-2.293091	1.007416	0.566116
H 0	-2.624054	-1.362762	-0.627625
H 0	-0.379898	-0.021790	0.958282
H 0	-0.421768	-5.364624	0.238480
H 0	-0.778229	-5.138519	-1.488785
H 0	-2.008286	-5.848221	-0.414307
H 0	-0.698242	-4.055771	2.346848
H 0	-0.731476	-2.309280	2.667542
H 0	0.801331	-3.206467	2.801086
H 0	-1.847885	2.000778	0.661041
H 0	-2.809692	0.782242	1.506775
H 0	-3.048218	1.042100	-0.227432

B3LYP/6-31G* Energy = -834.43286
 B3LYP/6-31G* Free energy in solution = -834.761913
 Number of Imaginary Frequencies = 1 (-405.56)

DATSBa 1b+2b-*exo*



B3LYP/6-31G* Geometry

C 0	1.491500	-2.172974	-0.135712
C 0	1.491500	-0.803955	-0.135712
O 0	0.405411	-2.920441	-0.135712
C 0	2.759200	-2.979996	-0.006348
C 0	0.269135	-0.026779	-0.205185
C 0	0.391022	1.465210	-0.216019
C 0	1.377197	2.155060	0.507065
C 0	-0.514709	2.212875	-0.985840
C 0	1.463440	3.545898	0.449356
C 0	-0.429184	3.602676	-1.047409
C 0	0.562180	4.274628	-0.329208
H 0	2.443069	-0.300598	-0.007095
H 0	2.838760	-3.693588	-0.834076
H 0	3.645721	-2.339935	-0.005600
H 0	2.739731	-3.566177	0.920273
H 0	-0.406830	-0.384308	-0.979553

H 0	2.080261	1.601700	1.123230
H 0	-1.285492	1.692215	-1.549789
H 0	2.235626	4.061203	1.014404
H 0	-1.133728	4.160400	-1.658478
H 0	0.631256	5.358078	-0.374756
B 0	-1.196762	-2.749893	-0.194611
O 0	-1.660904	-2.022964	-1.330490
C 0	-0.931183	-0.444931	1.174744
C 0	-1.082031	-1.855515	1.123444
O 0	-1.635437	-4.094894	-0.044739
C 0	-1.633331	-2.658691	-2.596024
C 0	-3.006058	-4.281723	0.214188
C 0	-0.557510	0.195618	2.504639
H 0	-1.744293	0.064392	0.651428
H 0	-0.765488	-2.406052	2.014938
H 0	-1.885284	-3.722961	-2.519440
H 0	-0.640381	-2.574966	-3.062744
H 0	-2.362442	-2.164490	-3.248474
H 0	-3.645737	-3.865051	-0.579330
H 0	-3.317047	-3.817902	1.166229
H 0	-3.200333	-5.358078	0.283463
H 0	0.373917	-0.228577	2.896591
H 0	-1.343582	0.017914	3.248474
H 0	-0.427475	1.277145	2.412155

B3LYP/6-31G* Energy = -834.429693
 B3LYP/6-31G* Free energy in solution = -834.7568
 Number of Imaginary Frequencies = 1 (-382.86)

TSs leading to regioisomers 10

DATSAb 1b+2b-*endo*

B3LYP/6-31G* Geometry

O 0	2.426300	-0.793030	-2.002213
C 0	2.419769	0.494797	-2.013657
C 0	1.762070	1.189011	-1.001678
C 0	3.024261	1.192276	-3.210739
C 0	1.118607	0.433838	-0.000809
C 0	0.323151	1.059021	1.079117
C 0	-0.396332	2.251923	0.888779
C 0	0.277390	0.452606	2.346359
C 0	-1.123200	2.821884	1.932068
C 0	-0.447861	1.022079	3.391907
C 0	-1.151520	2.211044	3.188507
H 0	1.606995	2.259705	-1.088120
H 0	4.015854	0.781693	-3.429688
H 0	3.112700	2.271866	-3.053162
H 0	2.396851	1.019333	-4.094803
H 0	1.647583	-0.466919	0.296585
H 0	-0.394806	2.728806	-0.087067
H 0	0.827484	-0.471252	2.511185
H 0	-1.673248	3.743881	1.763138
H 0	-0.461258	0.539474	4.365692
H 0	-1.718994	2.657089	4.000809
C 0	0.685181	-1.624786	-1.928436
C 0	-0.185211	-0.920074	-1.053268
C 0	1.192047	-2.995422	-1.574814
B 0	-1.238510	0.051666	-1.657578
O 0	-2.467987	0.337753	-1.119690
O 0	-0.905167	0.681854	-2.831604
C 0	-2.972580	-0.299866	0.044022

C 0	-1.814682	1.570114	-3.467087
H 0	0.568024	-1.431808	-2.990326
H 0	-0.425369	-1.452942	-0.132767
H 0	2.066193	-3.257935	-2.176025
H 0	0.408844	-3.743896	-1.755569
H 0	1.468109	-3.049789	-0.515700
H 0	-4.015869	0.007889	0.162048
H 0	-2.413849	-0.001480	0.937363
H 0	-2.938538	-1.392441	-0.049866
H 0	-2.739807	1.056580	-3.753876
H 0	-1.324524	1.955917	-4.365677
H 0	-2.080063	2.408722	-2.812866

B3LYP/6-31G* Energy = -834.450347
 B3LYP/6-31G* Free energy in solution = -834.774864
 Number of Imaginary Frequencies = 1 (-521.31)

DATSAb 1b+2b-*exo*

B3LYP/6-31G* Geometry

C 0	-2.276215	-1.593445	0.807022
C 0	-0.925018	-1.178177	0.822083
C 0	-2.800415	-2.606155	1.790695
B 0	-0.157410	-1.169250	-0.537506
O 0	-0.835602	-0.723282	-1.644150
O 0	1.135864	-1.585495	-0.716110
C 0	-0.218918	-0.724792	-2.925858
C 0	1.950180	-2.077545	0.336000
H 0	-2.787262	-1.558990	-0.149887
H 0	-0.373383	-1.450089	1.723251
H 0	-3.892593	-2.611862	1.819351
H 0	-2.417664	-2.408264	2.798965
H 0	-2.460693	-3.612335	1.506302
H 0	0.086960	-1.735184	-3.220154
H 0	0.667557	-0.080475	-2.940262
H 0	-0.953094	-0.347168	-3.643234
H 0	2.879425	-2.443909	-0.110077
H 0	1.466522	-2.905396	0.869324
H 0	2.192322	-1.285110	1.053207
O 0	-3.460205	-0.094345	1.433670
C 0	-2.972931	0.551086	2.427078
C 0	-1.685944	1.088730	2.337524
C 0	-3.784241	0.624313	3.705353
C 0	-0.984650	0.937729	1.123611
C 0	0.400300	1.445557	0.973480
C 0	1.332062	1.389984	2.025085
C 0	0.804184	2.021622	-0.242798
C 0	2.089569	2.539429	-0.399109
C 0	2.618042	1.903961	1.868759
C 0	3.001541	2.482895	0.656036
H 0	-1.195786	1.483566	3.222534
H 0	-3.321426	1.282150	4.447876
H 0	-3.900360	-0.374329	4.144058
H 0	-4.791336	0.995773	3.485260
H 0	-1.592163	0.992340	0.225525
H 0	1.044464	0.935684	2.969513
H 0	0.095703	2.066757	-1.065491
H 0	2.378372	2.988571	-1.345749
H 0	3.323151	1.853180	2.694519
H 0	4.004105	2.884369	0.535202

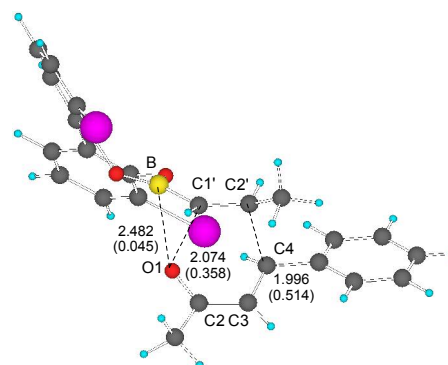
B3LYP/6-31G* Energy = -834.449071

B3LYP/6-31G* Free energy in solution = -834.775355
 Number of Imaginary Frequencies = 1 (-490.84)

Hetero Diels-Alder Reaction between 1b and 5b

TSs leading to regioisomers 9

DATSAa 1b+5b-*Re-exo*



B3LYP/631LAN Geometry

C 0	-2.226730	-0.124954	-0.302994
C 0	-2.226730	1.297806	-0.302994
C 0	-3.498688	-0.898500	-0.302994
C 0	-0.992386	1.943390	-0.317215
C 0	-4.699478	-0.389847	0.222672
C 0	-3.513184	-2.196640	-0.841843
O 0	0.082153	1.237076	-0.350266
C 0	-0.856293	3.444382	-0.171524
C 0	-4.683975	-2.953018	-0.871796
C 0	-5.872162	-1.143890	0.193359
C 0	-5.870468	-2.428360	-0.355164
H 0	-1.457794	-0.552475	-0.940979
H 0	-3.136032	1.869171	-0.146271
H 0	-4.718536	0.602982	0.662231
H 0	-2.592560	-2.611862	-1.244171
H 0	-1.823380	3.951859	-0.246658
H 0	-0.404007	3.692078	0.797409
H 0	-0.188919	3.838715	-0.945602
H 0	-4.669708	-3.951859	-1.299942
H 0	-6.789093	-0.727554	0.602249
H 0	-6.784622	-3.015366	-0.376907
C 0	-1.208649	-0.735916	1.301971
C 0	-2.114716	-0.496948	2.500198
C 0	0.030685	-0.045029	1.278870
B 0	1.389938	-0.561249	0.751709
O 0	1.453262	-1.582825	-0.171616
O 0	2.523544	0.023392	1.289551
C 0	2.489380	-1.791489	-1.045746
C 0	3.644165	-0.669968	1.641129
C 0	3.845779	-1.741180	-0.652481
C 0	2.174728	-2.103775	-2.376938
C 0	4.168106	-0.467667	2.926056
C 0	4.284439	-1.559540	0.756378
C 0	4.831390	-1.921997	-1.637802
C 0	3.168777	-2.304428	-3.332031
I 0	0.146561	-2.305145	-3.011154
C 0	5.302689	-1.149353	3.358231
C 0	5.410507	-2.260132	1.221405
I 0	3.212128	0.899400	4.262314
C 0	4.506592	-2.195358	-2.960709

B3LYP/631LAN Energy = -1238.192506
B3LYP/631LAN Free energy in solution = -1238.584707
Number of Imaginary Frequencies = 1 (-524.17)

C 0	-1.353394	0.744598	0.085770
C 0	-1.353394	2.173538	0.085770
C 0	-2.645203	-0.003067	0.085770
C 0	-0.124939	2.819794	0.128998
C 0	-3.802002	0.478928	-0.550369
C 0	-2.722275	-1.236069	0.754227
O 0	0.957047	2.123749	0.212479
C 0	0.016602	4.317307	-0.038910
C 0	-3.913971	-1.958969	0.796188
C 0	-4.994492	-0.243500	-0.511810
C 0	-5.055878	-1.465256	0.162140
H 0	-0.621811	0.317795	0.769440
H 0	-2.259323	2.738998	-0.105988
H 0	-3.770493	1.425980	-1.081345
H 0	-1.836945	-1.625916	1.249542
H 0	-0.954880	4.821625	-0.028656
H 0	0.525040	4.544235	-0.984085
H 0	0.638077	4.730011	0.763200
H 0	-3.950516	-2.906800	1.326782
H 0	-5.877563	0.149277	-1.008957
H 0	-5.985626	-2.026932	0.192535
C 0	-0.349533	0.150803	-1.468567
C 0	0.950974	0.715103	-1.358337
C 0	-1.152145	0.488708	-2.715759
B 0	2.090912	0.203827	-0.448441
O 0	3.368027	0.715347	-0.612381
O 0	1.815155	-0.782837	0.473663
C 0	4.076600	1.200836	0.450531
C 0	2.743149	-1.546387	1.127625
C 0	4.296800	0.427475	1.609085

B3LYP/631LAN Energy = -1238.195284
B3LYP/631LAN Free energy in solution = -1238.586107
Number of Imaginary Frequencies = 1 (-510.81)

C 0	0.711853	1.611420	-0.536667
C 0	-0.488708	2.404465	-0.735672
O 0	0.607193	0.358521	-0.465530
C 0	2.035294	2.296234	-0.39923
C 0	-1.715942	1.827087	-0.809006
C 0	-3.001846	2.481644	-0.987961
C 0	-3.147659	3.875565	-1.151840
C 0	-4.160446	1.678329	-0.993942
C 0	-4.407227	4.439316	-1.313919
C 0	-5.421814	2.245560	-1.155731
C 0	-5.547943	3.626907	-1.316025
H 0	-0.353287	3.478607	-0.810547
H 0	1.950912	3.379089	-0.508896
H 0	2.451294	2.046448	0.585358
H 0	2.741013	1.886459	-1.128403
H 0	-1.747574	0.743134	-0.714478
H 0	-2.271683	4.517075	-1.153854
H 0	-4.057602	0.604004	-0.864975
H 0	-4.505890	5.513733	-1.439514

H 0	-6.304276	1.612366	-1.156342
H 0	-6.530594	4.072800	-1.442627
B 0	1.762589	-0.807083	-0.136124
O 0	2.769394	-0.522736	-1.151031
O 0	1.016678	-2.023010	-0.291840
C 0	3.363403	-0.248718	1.873672
C 0	2.168304	-0.613434	1.387802
C 0	3.361221	-1.427826	-1.953613
C 0	0.411118	-2.344238	-1.451630
C 0	3.721085	-0.143936	3.331207
C 0	2.642410	-2.436813	-2.649185
C 0	4.746017	-1.326645	-2.192581
C 0	-0.974396	-2.573685	-1.486755
C 0	1.158400	-2.526917	-2.637939
C 0	3.355896	-3.352051	-3.440979
C 0	5.431976	-2.224915	-3.003952
I 0	5.870117	0.297531	-1.350403
C 0	-1.632889	-2.935364	-2.658951
C 0	0.477966	-2.863144	-3.819580
I 0	-2.119644	-2.401154	0.320267
C 0	4.732010	-3.263702	-3.614900
C 0	-0.898895	-3.064346	-3.838058
H 0	4.170578	-0.025833	1.175797
H 0	1.385727	-0.849487	2.116364
H 0	2.865433	-0.374878	3.975449
H 0	4.080765	0.863281	3.585983
H 0	4.536407	-0.835037	3.587219
H 0	2.806229	-4.154449	-3.922943
H 0	6.501205	-2.118744	-3.149521
H 0	-2.703918	-3.106567	-2.653900
H 0	1.045944	-2.959366	-4.739807
H 0	5.258392	-3.989716	-4.227448
H 0	-1.402786	-3.324295	-4.764496

B3LYP/631LAN Energy = -1238.250026
 B3LYP/631LAN Free energy in solution = -1238.642683
 Number of Imaginary Frequencies = 0

DATSba 1b+5b-Re-endo

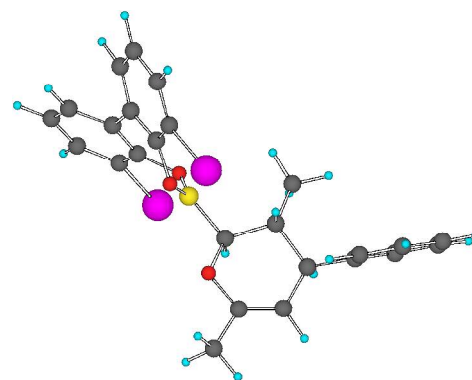
B3LYP/631LAN Geometry

C 0	0.417984	0.726746	-2.692474
C 0	-0.932037	0.849442	-2.820511
O 0	0.912400	-0.310379	-2.006912
C 0	1.409882	1.712936	-3.237198
C 0	-1.850693	-0.081314	-2.176483
B 0	1.105072	-0.198395	-0.469162
C 0	-3.308243	0.141541	-2.412857
O 0	1.463211	1.175003	-0.152695
O 0	2.017900	-1.210815	-0.022995
C 0	-1.604950	0.061493	-0.282761
C 0	-0.394897	-0.656448	-0.159744
C 0	-3.882767	1.422852	-2.346786
C 0	-4.134186	-0.948792	-2.726746
C 0	2.256744	1.525162	0.880524
C 0	3.326096	-1.113892	-0.355300
C 0	-2.830215	-0.522781	0.414398
C 0	-5.240051	1.606430	-2.602554
C 0	-5.491592	-0.764786	-2.991486
C 0	3.544205	0.958435	1.071960
C 0	1.845703	2.545776	1.756012
C 0	3.936523	-2.104340	-1.138748

C 0	4.113190	-0.048843	0.138977
C 0	-6.048630	0.513397	-2.928940
C 0	4.323090	1.398041	2.153717
C 0	2.638062	2.984482	2.813019
I 0	-0.049393	3.511597	1.459473
C 0	5.288651	-2.044205	-1.466995
C 0	5.470200	0.009354	-0.214706
I 0	2.778870	-3.769943	-1.827377
C 0	3.884064	2.394562	3.019333
C 0	6.055252	-0.971481	-1.010223
H 0	-1.334732	1.727341	-3.313370
H 0	0.919754	2.473618	-3.851929
H 0	1.935898	2.200256	-2.409958
H 0	2.159180	1.191254	-3.843704
H 0	-1.576202	-1.125702	-2.312592
H 0	-1.514175	1.142685	-0.182602
H 0	-0.522125	-1.742554	-0.083450
H 0	-3.263748	2.277817	-2.087814
H 0	-3.703995	-1.946045	-2.777832
H 0	-2.957642	-1.586075	0.181824
H 0	-3.742538	0.005936	0.129028
H 0	-2.712662	-0.427094	1.499908
H 0	-5.668686	2.603287	-2.547333
H 0	-6.112305	-1.619583	-3.245346
H 0	-7.106277	0.658707	-3.130463
H 0	5.289932	0.932144	2.317993
H 0	2.282883	3.769943	3.470871
H 0	5.735672	-2.819748	-2.079117
H 0	6.067108	0.846329	0.135086
H 0	4.504517	2.712814	3.851929
H 0	7.106277	-0.905960	-1.276428

B3LYP/631LAN Energy = -1238.20368
 B3LYP/631LAN Free energy in solution = -1238.599274
 Number of Imaginary Frequencies = 1 (-333.00)

Product DATSba 1b+5b-Re-endo



B3LYP/631LAN Geometry

C 0	1.683487	-2.095490	1.653488
C 0	2.427490	-2.895493	0.875488
O 0	0.604492	-1.387497	1.197495
C 0	1.906494	-1.849487	3.116486
C 0	2.218491	-3.044495	-0.615509
B 0	-0.956497	-0.661500	-0.523514
C 0	3.542496	-3.032486	-1.372498
O 0	-0.710495	0.651489	-0.224518
O 0	-2.075500	-1.078491	-1.206497
C 0	1.252487	-1.937500	-1.124496

C 0	0.105484	-1.766495	-0.100510
C 0	4.476486	-2.004486	-1.172500
C 0	3.855484	-4.042496	-2.290497
C 0	-1.130493	1.735489	-0.951492
C 0	-3.318497	-0.509506	-1.110504
C 0	0.722488	-2.243500	-2.531494
C 0	5.681488	-1.984497	-1.875504
C 0	5.061493	-4.028488	-2.995500
C 0	-2.440491	1.857498	-1.462494
C 0	-0.197510	2.759491	-1.169495
C 0	-4.409500	-1.374496	-0.943497
C 0	-3.527496	0.882492	-1.178497
C 0	5.978485	-2.997498	-2.791504
C 0	-2.737488	2.989487	-2.242493
C 0	-0.525497	3.885498	-1.920502
I 0	1.767487	2.614487	-0.349518
C 0	-5.705490	-0.882492	-0.811508
C 0	-4.840500	1.357498	-1.010498
I 0	-4.097488	-3.486496	-0.876495
C 0	-1.801498	3.990494	-2.471497
C 0	-5.915497	0.495500	-0.831497
H 0	3.250488	-3.438492	1.330490
H 0	2.789490	-2.386490	3.473480
H 0	2.045486	-0.777496	3.304489
H 0	1.035492	-2.167496	3.701492
H 0	1.741486	-4.016495	-0.822510
H 0	1.808487	-0.991500	-1.149490
H 0	-0.402496	-2.738495	0.002487
H 0	4.256485	-1.221497	-0.451508
H 0	3.147491	-4.852493	-2.452500
H 0	0.075485	-3.129486	-2.527496
H 0	1.551483	-2.433487	-3.219498
H 0	0.136490	-1.411500	-2.939500
H 0	6.390488	-1.178497	-1.705505
H 0	5.283493	-4.824493	-3.701492
H 0	6.918488	-2.983490	-3.336502
H 0	-3.724487	3.070496	-2.686493
H 0	0.212494	4.664490	-2.081497
H 0	-6.535492	-1.567490	-0.679520
H 0	-5.009491	2.429489	-1.006500
H 0	-2.060500	4.852493	-3.079498
H 0	-6.918488	0.892487	-0.703506

B3LYP/631LAN Energy = -1238.249758

B3LYP/631LAN Free energy in solution = -1238.646424

Number of Imaginary Frequencies = 0

DATSBa 1b+5b-Re-exo

B3LYP/631LAN Geometry

C 0	-0.602921	-1.835571	1.729355
C 0	-1.610718	-2.341568	0.966446
O 0	0.481949	-1.229645	1.250015
C 0	-0.545380	-1.999527	3.224365
C 0	-1.684921	-2.181625	-0.485794
B 0	1.039307	-0.801468	-0.106857
C 0	-2.893829	-2.761902	-1.161697
O 0	2.395981	-0.408295	0.200241
O 0	0.246902	0.204529	-0.787140
C 0	-0.239868	-2.825027	-1.378296
C 0	0.885178	-2.273941	-0.704056
C 0	-3.480759	-3.970200	-0.753540

C 0	-3.468231	-2.070053	-2.239975
C 0	3.187164	0.002258	-0.814209
C 0	0.503311	1.533752	-0.725525
C 0	-0.261047	-4.334152	-1.595825
C 0	-4.616760	-4.463959	-1.394928
C 0	-4.605621	-2.560425	-2.880692
C 0	2.898743	1.202393	-1.506454
C 0	4.341949	-0.715652	-1.164749
C 0	-0.525726	2.431320	-0.393860
C 0	1.768021	2.066360	-1.083054
C 0	-5.183929	-3.760086	-2.459610
C 0	3.744690	1.605377	-2.550629
C 0	5.186020	-0.294022	-2.189316
I 0	4.849564	-2.497910	-0.084396
C 0	-0.334000	3.810562	-0.389893
C 0	1.949631	3.457794	-1.059158
I 0	-2.475067	1.692123	0.107590
C 0	4.874512	0.868576	-2.894700
C 0	0.918091	4.326385	-0.719498
H 0	-2.385605	-2.903336	1.474548
H 0	-0.482971	-1.018066	3.708038
H 0	-1.427277	-2.522812	3.602997
H 0	0.354645	-2.556900	3.510223
H 0	-1.543564	-1.142868	-0.776413
H 0	-0.471909	-2.252991	-2.281998
H 0	1.572662	-2.993103	-0.249527
H 0	-3.045135	-4.531052	0.068588
H 0	-3.027542	-1.130264	-2.564346
H 0	-1.167725	-4.654984	-2.114349
H 0	-0.204971	-4.869049	-0.641052
H 0	0.599380	-4.640305	-2.201965
H 0	-5.058960	-5.399368	-1.062897
H 0	-5.042557	-2.003174	-3.704819
H 0	-6.070068	-4.143921	-2.957581
H 0	3.501694	2.508041	-3.103317
H 0	6.070068	-0.870178	-2.439377
H 0	-1.150803	4.472229	-0.123459
H 0	2.931122	3.856003	-1.297700
H 0	5.515854	1.195526	-3.708023
H 0	1.085205	5.399384	-0.703400

B3LYP/631LAN Energy = -1238.199752

B3LYP/631LAN Free energy in solution = -1238.594779

Number of Imaginary Frequencies = 1 (-294.88)

DATSBa 1b+5b-Si-exo

B3LYP/631LAN Geometry

C 0	-0.278671	-1.269455	1.324890
C 0	-1.410095	-1.201965	0.570892
O 0	0.685272	-0.355698	1.308456
C 0	-0.038834	-2.338379	2.357162
C 0	-1.654419	-0.161652	-0.426361
B 0	1.059784	0.969528	0.600723
C 0	-2.962402	-0.264908	-1.158890
O 0	1.314392	0.761383	-0.810196
C 0	-1.549393	1.540176	0.238403
C 0	-0.340302	1.609772	0.986832
O 0	2.152893	1.533203	1.345947
C 0	-4.154831	-0.624344	-0.508194
C 0	-3.005569	-0.015549	-2.539215
C 0	2.443481	1.119766	-1.458740

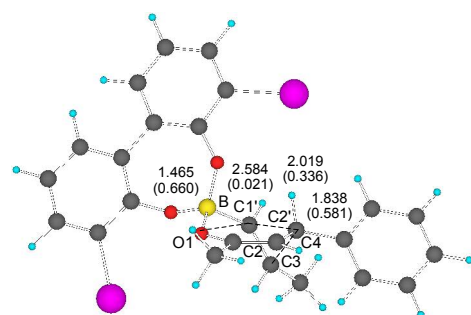
C O	3.235657	0.737595	1.521576
C O	-2.822769	2.014664	0.930664
C O	-5.350204	-0.736710	-1.217270
C O	-4.199570	-0.132034	-3.251053
C O	3.749268	0.908890	-0.939362
C O	2.332291	1.677948	-2.746109
C O	3.620941	0.321060	2.803802
C O	4.012711	0.342468	0.409439
C O	-5.376785	-0.491562	-2.592209
C O	4.854828	1.263748	-1.730743
C O	3.438049	2.005783	-3.523331
I O	0.394638	2.083038	-3.574982
C O	4.725800	-0.502991	3.002045
C O	5.105743	-0.513107	0.619446
I O	2.503021	0.978729	4.510117
C O	4.715027	1.794418	-3.007462
C O	5.459518	-0.936737	1.896942
H O	-2.179031	-1.943253	0.754578
H O	0.896484	-2.867188	2.141190
H O	-0.856720	-3.063507	2.377960
H O	0.070694	-1.886215	3.349960
H O	-0.818588	-0.056915	-1.116989
H O	-1.407303	1.971619	-0.758026
H O	-0.439545	1.840958	2.051758
H O	-4.149231	-0.812332	0.561829
H O	-2.091049	0.256424	-3.058289
H O	-2.718323	3.063507	1.231934
H O	-3.691956	1.941376	0.273148
H O	-3.025024	1.426636	1.833054
H O	-6.261581	-1.016159	-0.695526
H O	-4.208038	0.054169	-4.321594
H O	-6.307953	-0.580994	-3.145004
H O	5.848236	1.136734	-1.312500
H O	3.303482	2.434586	-4.510117
H O	5.002106	-0.813812	4.003600
H O	5.679520	-0.853149	-0.237350
H O	5.590225	2.061310	-3.592224
H O	6.307953	-1.600052	2.038330

B3LYP/631LAN Energy = -1238.199347

B3LYP/631LAN Free energy in solution = -1238.59239

Number of Imaginary Frequencies = 1 (-312.34)

CBTS 1b+5b-Si-endo²



2. We could not find the transition structure **DATSba 1b+5b-Si-endo** corresponding to the [4+3] *endo* attack of **5b** to the *Si* face of the enone since all calculations merged in a transition structure that seems to correspond to the [4+3] cycloboration pathway (**CBTS 1b+5b-Si-endo**).

B3LYP/631LAN Geometry

C O	-1.989319	-1.096313	-0.577408
C O	-1.964844	-1.080536	0.773727
O O	-0.910461	-1.218262	-1.364319
C O	-3.271835	-1.068405	-1.362915
C O	-0.731537	-1.127090	1.619034
B O	0.450439	-0.857681	-0.959167
C O	-0.942413	-1.326584	3.102036
O O	0.512878	0.604126	-0.763184
C O	0.221649	-2.615814	1.114532
C O	0.873398	-1.563004	0.473495
O O	1.412506	-1.381882	-1.902893
C O	-1.904205	-2.233124	3.573303
C O	-0.203308	-0.578430	4.026611
C O	1.466980	1.425354	-1.228531
C O	1.294220	-0.991013	-3.195236
C O	0.878815	-3.432877	2.202972
C O	-2.138367	-2.366180	4.940567
C O	-0.433212	-0.718353	5.395798
C O	1.989900	1.353363	-2.550598
C O	1.925140	2.468292	-0.398500
C O	0.996170	-1.924332	-4.197861
C O	1.532227	0.354980	-3.554581
C O	-1.409103	-1.602936	5.855377
C O	2.957626	2.291336	-2.943954
C O	2.865952	3.403275	-0.815720
I O	1.141617	2.660522	1.580505
C O	0.891434	-1.549057	-5.534058
C O	1.401932	0.723190	-4.903442
I O	0.699860	-3.974792	-3.675873
C O	3.394119	3.306900	-2.101089
C O	1.086807	-0.212875	-5.883500
H O	-2.903671	-1.007156	1.310318
H O	-3.228088	-0.267914	-2.113174
H O	-4.145370	-0.913239	-0.717422
H O	-3.396240	-2.015793	-1.910065
H O	-0.153580	-0.197433	1.506592
H O	-0.528946	-3.145462	0.531631
H O	1.741516	-1.158218	1.003632
H O	-2.477173	-2.824800	2.864044
H O	0.545258	0.126129	3.671982
H O	0.145767	-3.954361	2.825867
H O	1.510315	-4.189651	1.716934
H O	1.515854	-2.819778	2.848618
H O	-2.894394	-3.063187	5.292297
H O	0.140213	-0.123047	6.101257
H O	-1.595932	-1.703995	6.921219
H O	3.383377	2.205826	-3.939163
H O	3.189255	4.189651	-0.141922
H O	0.651672	-2.287796	-6.291656
H O	1.542496	1.763657	-5.180405
H O	4.145386	4.016357	-2.435852
H O	0.987396	0.093353	-6.921219

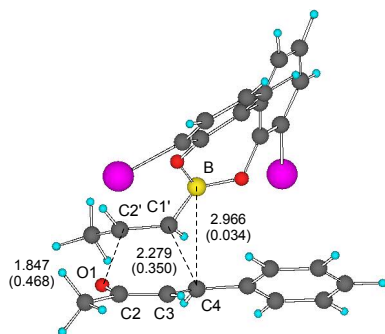
B3LYP/631LAN Energy = -1238.200958

B3LYP/631LAN Free energy in solution = -1238.597242

Number of Imaginary Frequencies = 1 (-62.29)

TSs leading to regioisomers 10

DATSAb 1b+5b-Re-endo



B3LYP/631LAN Geometry

B 0	0.046524	-0.213440	0.765823
O 0	0.046524	1.177460	0.765823
O 0	-1.145630	-0.931259	0.765823
C 0	1.346954	-1.008667	0.796860
C 0	-0.940903	1.986359	0.283432
C 0	-2.248383	-0.593628	1.486862
C 0	2.604294	-0.440567	1.155273
C 0	-2.316544	1.756226	0.518112
C 0	-0.556305	3.125687	-0.442520
C 0	-2.835541	-1.574448	2.300888
C 0	-2.824417	0.691635	1.423264
C 0	3.466553	-1.135757	2.179993
C 0	-3.246475	2.623367	-0.081543
C 0	-1.494095	3.989929	-1.001480
I 0	1.513031	3.600647	-0.684464
C 0	-3.965759	-1.301254	3.066422
C 0	-3.946884	0.957230	2.226807
I 0	-1.983505	-3.533539	2.390259
C 0	-2.851273	3.720993	-0.836777
C 0	-4.515915	-0.020325	3.035248
H 0	1.226500	-2.060150	1.059311
H 0	2.633728	0.645813	1.201767
H 0	3.028503	-1.009628	3.177902
H 0	3.523911	-2.208939	1.969650
H 0	4.479477	-0.725555	2.187729
H 0	-4.303818	2.416824	0.047592
H 0	-1.166000	4.855850	-1.565384
H 0	-4.400757	-2.074219	3.690247
H 0	-4.365692	1.958221	2.223770
H 0	-3.593674	4.370621	-1.290604
H 0	-5.382339	0.212662	3.647003
O 0	3.837067	-0.566544	-0.214233
C 0	3.485855	-0.027969	-1.336838
C 0	2.308685	-0.431335	-1.960037
C 0	4.364731	1.072922	-1.879303
C 0	1.586273	-1.507111	-1.413803
C 0	0.297729	-1.971603	-1.954315
C 0	-0.586014	-1.113876	-2.634811
C 0	-0.063614	-3.322174	-1.809509
C 0	-1.255554	-3.807449	-2.342957
C 0	-1.778061	-1.597473	-3.167603
C 0	-2.116409	-2.946411	-3.026566
H 0	1.915451	0.143448	-2.792114
H 0	5.382324	0.692886	-2.030563
H 0	4.434418	1.893372	-1.155212
H 0	3.992188	1.466202	-2.829712
H 0	2.190369	-2.275925	-0.945313
H 0	-0.341187	-0.060486	-2.738251
H 0	0.603683	-3.994614	-1.275955

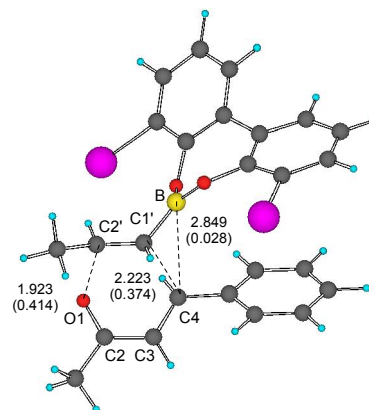
H 0 -1.513992 -4.855835 -2.222397
H 0 -2.448151 -0.920135 -3.690262
H 0 -3.048264 -3.321442 -3.440979

B3LYP/631LAN Energy = -1238.199113

B3LYP/631LAN Free energy in solution = -1238.588669

Number of Imaginary Frequencies = 1 (-488.16)

DATSAb 1b+5b-*Re-endo*



B3LYP/631LAN Geometry

O 0	-3.807922	0.601440	1.544739
C 0	-3.807922	1.887451	1.544739
C 0	-2.595932	2.580383	1.544739
C 0	-5.141144	2.598145	1.454681
C 0	-1.402512	1.839264	1.607422
C 0	-0.076309	2.491302	1.587540
C 0	0.965439	1.960815	2.369919
C 0	0.174515	3.656143	0.841064
C 0	2.210144	2.586578	2.422180
C 0	1.419327	4.278961	0.890442
C 0	2.440674	3.748947	1.683807
H 0	-2.580109	3.653152	1.379364
H 0	-5.038010	3.678680	1.594955
H 0	-5.607834	2.414139	0.478729
H 0	-5.825073	2.206131	2.215561
H 0	-1.453583	0.916962	2.176895
H 0	0.786407	1.058000	2.946976
H 0	-0.607300	4.065353	0.207900
H 0	2.999420	2.166382	3.039642
H 0	1.596252	5.175430	0.302673
H 0	3.411240	4.236237	1.720779
C 0	-2.798477	-0.221725	0.129852
C 0	-3.938919	-0.300674	-0.855743
C 0	-1.637329	0.534546	-0.176651
B 0	-0.250778	-0.116196	-0.115540
O 0	0.089600	-0.928696	0.957306
O 0	0.625931	0.124298	-1.160843
C 0	0.963150	-1.978226	0.931671
C 0	1.982208	0.222824	-1.076645
C 0	2.222351	-1.915390	0.294846
C 0	0.587311	-3.151794	1.603928
C 0	2.603058	1.256760	-1.793671
C 0	2.771118	-0.684158	-0.337830
C 0	3.016632	-3.076157	0.291794
C 0	1.405029	-4.278519	1.614700
I 0	-1.268860	-3.239822	2.661850
C 0	3.978851	1.457565	-1.731476

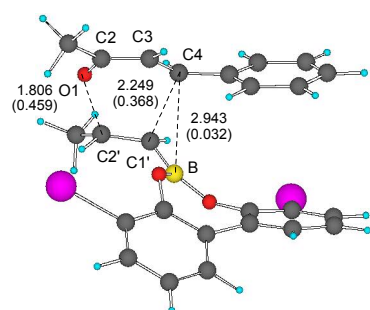
C 0	4.154190	-0.442352	-0.260925
O 0	1.431473	2.540527	-3.039658
C 0	2.621994	-4.242035	0.937241
C 0	4.754425	0.612411	-0.938950
H 0	-2.650635	-1.113831	0.730682
H 0	-4.842850	-0.700974	-0.390442
H 0	-3.659622	-0.959534	-1.689117
H 0	-4.160385	0.685425	-1.279449
H 0	-1.763123	1.295410	-0.947418
H 0	3.958954	-3.058075	-0.245331
H 0	1.087631	-5.175446	2.134308
H 0	4.435944	2.269333	-2.286148
H 0	4.763397	-1.097061	0.353500
H 0	3.257492	-5.122208	0.913818
H 0	5.825089	0.775116	-0.858398

B3LYP/631LAN Energy = -1238.19944

B3LYP/631LAN Free energy in solution = -1238.589965

Number of Imaginary Frequencies = 1 (-477.66)

DATSAb 1b+5b-Si-endo



B3LYP/631LAN Geometry

C 0	2.273926	1.530518	-1.279419
C 0	2.273926	2.957596	-1.279419
B 0	0.979965	0.714615	-1.279419
C 0	3.209671	3.697266	-2.201828
O 0	0.916977	-0.421417	-2.080643
O 0	-0.102386	1.116241	-0.508500
C 0	0.333298	-1.603485	-1.742294
C 0	-1.413086	0.803940	-0.731445
C 0	-0.943771	-1.679626	-1.145920
C 0	1.031113	-2.785202	-2.034836
C 0	-2.360382	1.832581	-0.609116
C 0	-1.850586	-0.504440	-1.036270
C 0	-1.408310	-2.943054	-0.739777
C 0	0.535095	-4.030304	-1.659378
O 0	2.875839	-2.691605	-3.110687
C 0	-3.720276	1.601974	-0.797760
C 0	-3.225677	-0.708786	-1.249207
O 0	-1.744568	3.823746	-0.131866
C 0	-0.680771	-4.103302	-0.980133
C 0	-4.152359	0.319595	-1.128265
H 0	3.108505	1.077408	-1.815628
H 0	1.308212	3.434265	-1.135880
H 0	2.852692	3.615234	-3.236115
H 0	4.215881	3.266769	-2.157730
H 0	3.269836	4.755432	-1.935500
H 0	-2.361084	-3.007523	-0.224182
H 0	1.096817	-4.929749	-1.885056
H 0	-4.428757	2.416870	-0.701523

H 0	-3.564087	-1.698151	-1.537521
H 0	-1.063675	-5.065918	-0.654388
H 0	-5.207367	0.129135	-1.300827
O 0	2.964218	3.678589	0.289841
C 0	2.436356	3.239578	1.384460
C 0	2.430389	1.873000	1.645218
C 0	1.771912	4.245392	2.293427
C 0	3.089493	1.010529	0.751328
C 0	3.095398	-0.452881	0.942215
C 0	2.002213	-1.136154	1.506653
C 0	4.242126	-1.191177	0.604309
C 0	4.308609	-2.562012	0.846893
C 0	2.065125	-2.507492	1.741470
C 0	3.220734	-3.224518	1.418411
H 0	1.839737	1.479706	2.465927
H 0	0.896622	4.682022	1.797379
H 0	2.464737	5.065903	2.512192
H 0	1.449844	3.792709	3.236115
H 0	3.980927	1.417923	0.286591
H 0	1.096176	-0.588058	1.748550
H 0	5.092072	-0.677994	0.161026
H 0	5.207367	-3.113510	0.585205
H 0	1.208694	-3.019852	2.170975
H 0	3.268967	-4.294067	1.604248

B3LYP/631LAN Energy = -1238.198701

B3LYP/631LAN Free energy in solution = -1238.589829

Number of Imaginary Frequencies = 1 (-499.18)

DATSAb 1b+5b-Si-exo

B3LYP/631LAN Geometry

O 0	-3.156693	-0.446579	-1.469223
C 0	-3.156693	0.841064	-1.469223
C 0	-1.944641	1.532684	-1.469223
C 0	-4.490448	1.550308	-1.384308
C 0	-0.751633	0.792877	-1.555679
C 0	0.576981	1.434158	-1.507385
C 0	1.622070	0.921295	-2.295273
C 0	0.833466	2.561157	-0.706924
C 0	2.877914	1.526520	-2.299408
C 0	2.089066	3.163284	-0.707260
C 0	3.115372	2.650360	-1.505829
H 0	-1.926453	2.603470	-1.290878
H 0	-4.384293	2.634125	-1.493118
H 0	-4.977539	1.338028	-0.424515
H 0	-5.158997	1.181015	-2.170212
H 0	-0.811783	-0.115768	-2.146408
H 0	1.440018	0.049225	-2.918427
H 0	0.046982	2.954086	-0.068970
H 0	3.670486	1.119324	-2.921341
H 0	2.271240	4.030258	-0.077972
H 0	4.094986	3.120651	-1.503342
C 0	-2.167404	-1.263977	-0.055222
C 0	-3.294434	-1.292191	0.948486
C 0	-0.976349	-0.541580	0.222809
B 0	0.379120	-1.240402	0.120178
O 0	0.515945	-2.377792	-0.668365
O 0	1.450394	-0.727554	0.834198
C 0	1.647263	-2.749634	-1.334167
C 0	2.429214	-1.476578	1.414886
C 0	2.920807	-2.769333	-0.724411

C 0	1.514633	-3.158493	-2.670746
C 0	2.753860	-1.206345	2.753281
C 0	3.132324	-2.483994	0.719635
C 0	4.025894	-3.130676	-1.514236
C 0	2.619904	-3.542236	-3.426163
I 0	-0.417816	-3.203995	-3.585831
C 0	3.737686	-1.929000	3.422333
C 0	4.102386	-3.220245	1.421875
I 0	1.723206	0.339417	3.811798
C 0	3.886246	-3.511124	-2.844238
C 0	4.406921	-2.951630	2.751404
H 0	-2.048828	-2.174820	-0.634445
H 0	-4.214844	-1.681046	0.506134
H 0	-3.018127	-1.938919	1.792160
H 0	-3.485855	-0.291962	1.353546
H 0	-1.053452	0.241379	0.976913
H 0	5.015060	-3.097733	-1.069504
H 0	2.493027	-3.849854	-4.458130
H 0	3.966736	-1.705170	4.458145
H 0	4.612106	-4.030258	0.910568
H 0	4.759293	-3.784073	-3.429459
H 0	5.159012	-3.538940	3.269669

B3LYP/631LAN Energy = -1238.20048

B3LYP/631LAN Free energy in solution = -1238.590217

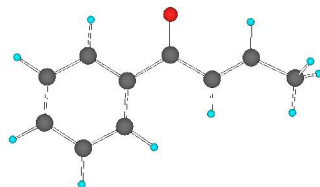
Number of Imaginary Frequencies = 1 (-478.60)

Jaguar Calculations

Study of the effect of substitution on the enone and on the alkenylboronate

Reactants

Enone 1c



HOMO energy= -6.640

LUMO energy= -1.761

B3LYP/6-31G* Geometry

C1	-0.05053088	0.04472057	0.08543709
O2	-0.00700211	0.08768063	1.31261026
C3	2.22596762	0.94566822	-0.15114848
C4	1.11963514	0.46022911	-0.73355095
H5	1.08061421	0.35404127	-1.81356233
H6	2.22060452	1.02606769	0.93559268
C7	-3.69063011	-1.38240764	-1.72475382
C8	-2.69138263	-0.85687906	-2.54413733
C9	-1.50048867	-0.39169321	-1.98646059
C10	-1.29657282	-0.44275437	-0.59919273
C11	-2.31394202	-0.96766314	0.2147787
C12	-3.49878809	-1.43644831	-0.34124253
H13	-4.61683716	-1.74725791	-2.16163352
H14	-2.83874172	-0.8075269	-3.619764
H15	-0.74302977	0.0210148	-2.64447177
H16	-2.14528338	-0.9947333	1.28641023
H17	-4.27547529	-1.84391656	0.30074413
C18	3.46337585	1.38342388	-0.86765522
H19	3.377612	1.26186488	-1.9522774
H20	3.6839909	2.43803477	-0.65309671
H21	4.33483542	0.81035302	-0.52244875

B3LYP/6-31G* Energy = -462.1238189

Number of Imaginary Frequencies = 0

B3LYP/lacvp* Geometry

C1	-0.05088089	0.04591369	0.08565877
O2	-0.0078833	0.08965273	1.313325
C3	2.22626315	0.94587108	-0.15112134
C4	1.11959416	0.46100703	-0.73366442
H5	1.0802634	0.3548908	-1.81368115
H6	2.22065445	1.0263001	0.93555273
C7	-3.69057756	-1.38361315	-1.72512675
C8	-2.6914174	-0.85740051	-2.54452872
C9	-1.50046266	-0.3916816	-1.98659614
C10	-1.29647124	-0.4426878	-0.59909813
C11	-2.3138554	-0.96813201	0.2149132
C12	-3.4986822	-1.43766273	-0.34132863

H13	-4.61651929	-1.74887629	-2.16202282
H14	-2.83879823	-0.80782221	-3.6200782
H15	-0.74321677	0.02166381	-2.64444453
H16	-2.14545415	-0.99501094	1.28656401
H17	-4.27509365	-1.84554633	0.30062813
C18	3.46409055	1.3824534	-0.86784819
H19	3.37738284	1.26292456	-1.95268602
H20	3.68693893	2.43633761	-0.65174575
H21	4.3347208	0.80712756	-0.52423924

B3LYP/lacvp* Energy = -462.1145782

Number of Imaginary Frequencies = 0

B-1-propenyldimethylboronate 2b

B3LYP/6-31G* Geometry

B1	1.7665833	0.03459037	2.92424352
C2	2.9883048	-0.77122333	2.38109989
O3	0.80071526	-0.48500999	3.75121135
O4	1.63928138	1.34720632	2.55798502
C5	3.905724	-0.23636904	1.55884848
H6	3.1258997	-1.81761806	2.6648236
H7	3.7868058	0.80683022	1.26259769
C8	0.54719017	2.13268833	3.01663088
H9	0.68162417	3.14444965	2.62263065
H10	-0.4094053	1.7321545	2.66098612
H11	0.51547013	2.17331984	4.11139883
C12	0.81501985	-1.82924904	4.20242509
H13	-0.04613513	-1.96690001	4.86317011
H14	0.73103832	-2.53592267	3.36727727
H15	1.72801645	-2.05863832	4.76594152
C16	5.10360896	-0.94244807	0.99610395
H17	6.03299322	-0.43350131	1.28749271
H18	5.16057067	-1.98224209	1.33567235
H19	5.08266486	-0.93956218	-0.10261713

B3LYP/6-31G* Energy = -372.3685281

Number of Imaginary Frequencies = 0

B-1-propenylboronate 5b

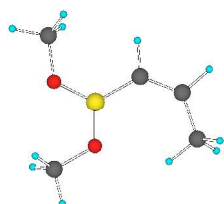
B3LYP/lacvp* Geometry

B1	11.2590649	-0.20825493	-0.30599455
C2	12.757169	-0.17712536	-0.66622235
C3	13.5979398	0.79424726	-0.26632028
H4	13.1600535	-1.00423136	-1.25319739
H5	13.1966758	1.61867667	0.32370086
C6	9.23360508	2.64467196	0.38452708
C7	9.42695129	1.25498435	0.38745286
I8	10.8960839	3.966034	0.54354453
O9	10.7107242	0.79170958	0.4802966
C10	7.03626646	0.97785261	0.18783402
C11	8.30856669	0.39643774	0.32447545
C12	7.38801047	-1.77598078	1.12435934
C13	8.40528269	-1.08363705	0.44502579
C14	9.40812305	-3.24025563	-0.07376629

C15	9.44583351	-1.83894157	-0.13321391
H16	10.9515389	-4.38857149	-0.98484149
C17	8.37405573	-3.90525957	0.57979358
C18	7.36600167	-3.16381842	1.19299058
H19	8.36391828	-4.98909379	0.61948248
C20	7.96022266	3.1980529	0.27751914
C21	6.85695546	2.35534803	0.16447493
H22	7.83471296	4.27535478	0.27108815
O23	10.5038743	-1.26508286	-0.7797143
C24	15.066411	0.8558117	-0.55850848
H25	15.3175258	1.78235138	-1.09343166
H26	15.6492577	0.87027349	0.37306655
H27	15.3993975	0.00524937	-1.16202706
H28	6.5681999	-3.67158902	1.72736937
H29	6.61014281	-1.20489746	1.62096682
H30	6.17500019	0.32643034	0.08267576
H31	5.86153022	2.775883	0.0545938

B3LYP/lacvp* Energy = -776.1314699
Number of Imaginary Frequencies = 0

***B*-1-propenyldimethylboronate 2c**



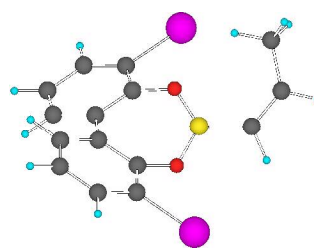
HOMO energy= -6.665
LUMO energy= -0.277

B3LYP/6-31G* Geometry

B1	1.7756755	0.02628403	2.96754358
C2	3.05945043	-0.71231943	2.46711125
O3	0.75679084	-0.61547481	3.6307339
O4	1.61249566	1.37073517	2.75721355
C5	4.13922746	-0.2019657	1.84405427
C6	0.44414091	2.04320181	3.2117492
H7	0.55147289	3.09857767	2.9457943
H8	-0.45705147	1.63993104	2.73605348
H9	0.32889385	1.95275028	4.29773254
C10	0.76512963	-1.99900613	3.93563236
H11	-0.15934702	-2.22398126	4.47587189
H12	0.79696037	-2.61331173	3.02703745
H13	1.61688566	-2.26859501	4.57246097
C14	4.40304446	1.22526919	1.46220124
H15	5.32976976	1.5788731	1.93646743
H16	4.56606833	1.30382723	0.37781479
H17	3.58357692	1.88502152	1.74647549
H18	4.94351939	-0.89111829	1.57181604
H19	3.10070958	-1.78974666	2.64123046

B3LYP/6-31G* Energy = -372.3650976
Number of Imaginary Frequencies = 0

***B*-1-propenylboronate 5c**



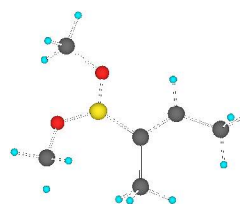
HOMO-3 energy= -7.002
LUMO energy= -1.342

B3LYP/lacvp* Geometry

B1	1.04922441	-0.19232203	-0.46391214
C2	2.55251581	-0.15289108	-0.82218503
C3	3.55775792	0.51862614	-0.2273383
H4	2.83547917	-0.82290922	-1.63576195
C5	-1.21192073	2.48357431	0.19938404
C6	-0.88836842	1.11945559	0.25703154
I7	0.32005646	3.95962092	0.14130776
O8	0.44052607	0.78409485	0.30093832
C9	-3.25002717	0.6104109	0.2433897
C10	-1.9201036	0.15835228	0.29954479
C11	-2.55394481	-2.08787991	1.18191321
C12	-1.67058369	-1.30191562	0.42330491
C13	-0.51103819	-3.34744918	-0.20228232
C14	-0.61421869	-1.94947908	-0.24887946
H15	1.0485962	-4.33791643	-1.25796697
C16	-1.41670276	-4.10986936	0.53135024
C17	-2.43383088	-3.47147961	1.2388377
H18	-1.3189806	-5.18971215	0.55996081
C19	-2.53780101	2.90866329	0.16719339
C20	-3.56082411	1.96319948	0.18293679
H21	-2.76633599	3.96773843	0.1177235
O22	0.32394142	-1.26364933	-0.96843549
H23	4.56712054	0.37102213	-0.61917536
C24	3.48742966	1.43661487	0.95607805
H25	3.8616145	2.43429961	0.68822276
H26	2.47513919	1.54300804	1.3464694
H27	4.14217645	1.06661268	1.75780055
H28	-4.59703307	2.28567398	0.13796083
H29	-4.04908799	-0.12346885	0.22790126
H30	-3.34075382	-1.59502173	1.74417856
H31	-3.12880576	-4.05667337	1.83405792

B3LYP/lacvp* Energy = -776.1260262
Number of Imaginary Frequencies = 0

***B*-1-propenyldimethylboronate 2d**



HOMO energy= -6.295

LUMO energy= 0.163

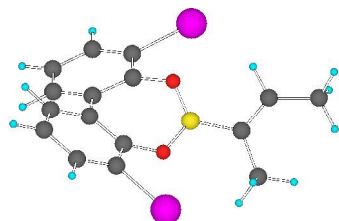
B3LYP/6-31G* Geometry

B1	1.6273894	0.09056536	2.69890015
C2	2.78958736	-0.72488431	2.01823866
O3	0.68443348	-0.40199526	3.56780372
O4	1.546423	1.42736217	2.41097049
C5	3.9427674	-0.06303108	1.79131355
H6	3.97578449	0.98767154	2.07960669
C7	0.58363926	2.26039493	3.04346114
H8	0.82168536	3.29492571	2.77937442
H9	-0.42914089	2.02628434	2.69509698
H10	0.60540515	2.14839031	4.13324745
C11	0.70966841	-1.68549148	4.1662768
H12	0.08049369	-1.64612806	5.06111075
H13	0.3051941	-2.44825418	3.49067541
H14	1.7230316	-1.97840666	4.46400375
C15	5.21945467	-0.5733663	1.1846305
H16	6.04767416	-0.48341629	1.9017441
H17	5.16698235	-1.61840493	0.86845426
H18	5.50151861	0.03326319	0.31290883
C19	2.59138719	-2.18014179	1.62778143
H20	3.26844417	-2.49119921	0.82622426
H21	2.7554565	-2.86604318	2.46984518
H22	1.56943565	-2.361176	1.27289116

B3LYP/6-31G* Energy = -411.6497319

Number of Imaginary Frequencies = 0

B-1-propenylboronate 5d



HOMO-1 energy= -6.361

LUMO energy= -1.308

B3LYP/lacvp* Geometry

B1	0.59143462	-11.3139227	-0.16876221
C2	2.06333862	-11.1179895	-0.62212444
C3	2.77871765	-10.1380277	-0.02585095
H4	2.26223712	-9.52372197	0.70970726
C5	-1.56144107	-8.60639346	0.63016572
C6	-1.30506362	-9.98536847	0.59090192
I7	0.02808901	-7.21321822	0.88403953
O8	-0.0070098	-10.4051652	0.69563473
C9	-3.6768164	-10.3629815	0.31894181
C10	-2.38263918	-10.888142	0.4729624
C11	-3.21306206	-13.1109323	1.21565192
C12	-2.21669652	-12.3627573	0.56444949
C13	-1.10326004	-14.4586795	0.03525788
C14	-1.12941665	-13.0561764	-0.00676532

I15	0.49612026	-15.5383939	-0.86121298
C16	-2.11575471	-15.1805586	0.66245535
C17	-3.17005283	-14.4987752	1.26601174
H18	-2.07307791	-16.264015	0.68792224
C19	-2.85677187	-8.10884225	0.50829655
C20	-3.91765831	-8.99475952	0.33526357
H21	-3.03118841	-7.03871005	0.53634111
O22	-0.09386744	-12.4208464	-0.63619503
C23	4.21825557	-9.7671361	-0.22939087
H24	4.29938978	-8.71355797	-0.53147425
H25	4.7713877	-9.85823283	0.71601516
H26	4.72841654	-10.376731	-0.97891636
C27	2.62700782	-12.0585662	-1.66756602
H28	3.62651409	-11.7696919	-2.00440906
H29	2.68304798	-13.0845218	-1.28480902
H30	1.97633759	-12.1000027	-2.54942633
H31	-4.92758996	-8.61436236	0.2123735
H32	-4.50380386	-11.050072	0.17157551
H33	-3.95165349	-15.0529703	1.77757358
H34	-4.02559905	-12.5826942	1.70354157

B3LYP/lacvp* Energy = -815.4158295

Number of Imaginary Frequencies = 0

Methanol

B3LYP/6-31G* Geometry

C	-3.52982282	-3.31988339	8.21690075
H2	-4.1485947	-2.66375708	8.83531364
H3	-4.19974536	-3.96192344	7.62367324
H4	-2.93694078	-3.96189727	8.88717101
O5	-2.72235789	-2.47745102	7.40988526
H6	-2.16802109	-3.04515696	6.85417213

B3LYP/6-31G* Energy = -115.6629837

Number of Imaginary Frequencies = 0

B3LYP/lacvp* Geometry

C1	-3.5294107	-3.31951029	8.21673746
H2	-4.14782356	-2.66304434	8.83524036
H3	-4.20008301	-3.96157929	7.62418508
H4	-2.93674451	-3.96155422	8.88732983
O5	-2.72278642	-2.47790957	7.4099611
H6	-2.16675693	-3.04372192	6.85431545

B3LYP/lacvp* Energy = -115.6607701

Number of Imaginary Frequencies = 0

3,3'-diiodo-1,1'-biphenyl-2,2'-diol (4b)

B3LYP/lacvp* Geometry

C1	-0.22791961	2.97003744	3.46123906
C2	0.51986922	1.78821859	3.59507747
I3	-0.13858102	4.05895804	1.63306949
O4	1.30632221	1.40544104	2.5595965
C5	-0.36276683	1.56877208	5.84408282

C6	0.47186399	1.08230984	4.82427604
C7	2.03811112	-0.12113628	6.3456207
C8	1.33604851	-0.0965901	5.13120346
C9	2.24988315	-2.30986317	4.6718138
C10	1.45827746	-1.2211211	4.28555785
H11	2.4229991	-4.01471639	3.38150458
C12	2.92936521	-2.31409125	5.88679773
C13	2.82037115	-1.20785079	6.72628773
H14	3.53919633	-3.16527997	6.16921025
C15	-1.02966226	3.44704834	4.4934454
C16	-1.10624627	2.73309932	5.68938722
H17	-1.60018425	4.35986446	4.3590268
O18	0.7709872	-1.184584	3.0996819
H19	1.2961739	0.42929965	2.50861931
H20	0.91397735	-2.01312176	2.60502835
H21	-1.74678194	3.08552294	6.49256833
H22	-0.42433752	1.01144375	6.7745171
H23	1.97228636	0.74693432	6.99393976
H24	3.35540362	-1.19266414	7.67115125

B3LYP/lacvp* Energy = -635.1139868
Number of Imaginary Frequencies = 0

TSs of Conjugate Additions to Enone 1c

Conjugate Addition of 2b to 1c

Complex 1c-2b-endo

B3LYP/6-31G* Geometry

C1	-0.41727301	0.39128295	-0.40831562
O2	-0.29556269	0.2169111	0.80425194
B3	2.17482518	-0.22737685	3.09684524
C4	3.28108104	-1.11879453	2.43709572
C5	1.78741462	1.47059729	-0.63532533
C6	0.63767846	1.06972519	-1.2009268
O7	1.15448812	-0.62891704	3.91475451
O8	2.29363756	1.11871892	2.85782907
H9	0.46817661	1.25321392	-2.25803178
H10	1.93536357	1.27831272	0.42706783
H11	4.23084403	-0.614936	2.23446034
C12	3.1734871	-2.38801334	2.01280941
C13	-4.05773552	-1.03304087	-2.22828306
C14	-3.06098172	-0.49874503	-3.04440209
C15	-1.87362183	-0.02794992	-2.48413193
C16	-1.66656498	-0.08737348	-1.09762392
C17	-2.6775026	-0.63143149	-0.28850312
C18	-3.86225103	-1.09852911	-0.84604275
H19	-4.98307573	-1.39808409	-2.66663927
H20	-3.20612188	-0.44820845	-4.1202183
H21	-1.11240046	0.37596703	-3.14294361
H22	-2.50417822	-0.6744376	0.78170436
H23	-4.63591913	-1.51420543	-0.20574382
C24	1.30927196	2.02820069	3.34210174
H25	1.69427775	3.04060914	3.18679026
H26	0.37357945	1.90233305	2.78811636
H27	1.11331986	1.87409211	4.40845653

C28	0.91383075	-1.9538953	4.34601582
H29	0.28160803	-2.48590143	3.62413058
H30	1.84422699	-2.51612818	4.48559988
H31	0.38020495	-1.90548151	5.30115885
C32	2.89537572	2.16845315	-1.35802935
H33	2.67182256	2.3193093	-2.41947735
H34	3.09574347	3.14788972	-0.90236057
H35	3.82964753	1.59666706	-1.27598182
H36	2.23464267	-2.92589227	2.15219267
C37	4.24753689	-3.1666291	1.30718836
H38	4.49281358	-4.08897416	1.85239997
H39	3.91788196	-3.47689137	0.30574683
H40	5.16515398	-2.57856237	1.1988003

B3LYP/6-31G* Energy = -834.4925636
Number of Imaginary Frequencies = 0

TS 1c+2b-endo

B3LYP/6-31G* Geometry

C1	-0.07088781	0.13295391	-0.02261042
O2	-0.06401028	-0.07331859	1.26478899
B3	1.12565966	-0.08525833	2.21536712
C4	2.57705554	-0.53100214	1.42776664
C5	2.26941945	0.84798185	-0.05457191
C6	1.06451107	0.5134664	-0.72383956
O7	0.73723421	-1.06338281	3.18530231
O8	1.41308005	1.24027765	2.71522114
H9	1.08510854	0.3521561	-1.79736201
H10	2.18473354	1.52829767	0.79180821
H11	3.43279513	-0.12412325	1.97845733
C12	2.83843182	-1.6806388	0.74676963
C13	-3.8049986	-0.78368281	-1.9237889
C14	-2.86552019	0.00762016	-2.58824268
C15	-1.65158477	0.31189808	-1.97801912
C16	-1.35683854	-0.17567195	-0.69455891
C17	-2.31340502	-0.95868103	-0.02856316
C18	-3.52555833	-1.26288531	-0.64239043
H19	-4.75330641	-1.01918547	-2.40022772
H20	-3.08383822	0.39668363	-3.5793256
H21	-0.94000547	0.95325195	-2.48987676
H22	-2.08738331	-1.32134981	0.96851544
H23	-4.25581285	-1.87459022	-0.11908413
C24	0.38055598	1.91621369	3.40265152
H25	0.80789835	2.81021528	3.87243666
H26	-0.42519529	2.23307743	2.72322148
H27	-0.0685544	1.28888795	4.18510475
C28	1.56484885	-1.28327694	4.29777568
H29	0.99999485	-1.85639103	5.04308875
H30	2.46285118	-1.86882696	4.03409706
H31	1.90269797	-0.34481673	4.7620815
C32	3.53525175	1.00698407	-0.86064919
H33	3.63796326	0.23748967	-1.63268974
H34	3.5115931	1.98510469	-1.36218507
H35	4.42430712	0.99039505	-0.22380704
H36	2.04975938	-2.09329073	0.11153113
C37	4.12330996	-2.44304277	0.74343462

H38	3.95770925	-3.47706797	1.07835113
H39	4.53352053	-2.51801557	-0.27541543
H40	4.87477431	-1.98380217	1.39290492

B3LYP/6-31G* Energy = -834.4446857

Number of Imaginary Frequencies = 1 (-348.96)

Product 1c+2b-endo

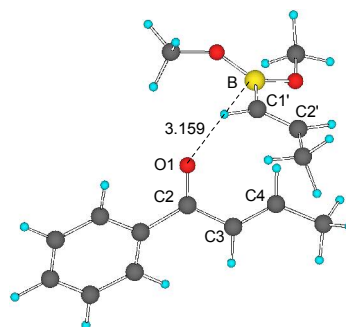
B3LYP/6-31G* Geometry

C1	0.14331126	-0.35183945	0.40898332
O2	0.04256517	-0.59708526	1.76432034
B3	0.34604864	0.27884258	2.78995213
C4	3.66960567	-1.16384397	-0.16034341
C5	2.68589347	-0.2136497	0.49854079
C6	1.34200488	-0.20557744	-0.18170209
O7	0.73986782	-0.32413338	3.94698479
O8	0.25992014	1.64330321	2.74330135
H9	1.35893417	-0.08107388	-1.26092194
H10	2.55234236	-0.55168198	1.53618628
H11	4.70620238	-1.03279964	0.15872893
C12	3.3923998	-2.12159703	-1.04837886
C13	-3.64447706	-0.52983538	-1.62380565
C14	-2.54464122	0.0609141	-2.24982097
C15	-1.31734373	0.13124125	-1.59750889
C16	-1.15750187	-0.3945514	-0.30343327
C17	-2.27435737	-0.97611447	0.3198171
C18	-3.50235556	-1.04573588	-0.33635441
H19	-4.60315308	-0.58032084	-2.13336807
H20	-2.64582674	0.47974374	-3.24784458
H21	-0.48240948	0.6187442	-2.09158254
H22	-2.16682408	-1.38432375	1.31885151
H23	-4.35082644	-1.50675816	0.16301742
C24	-0.41702364	2.39689506	1.74429579
H25	-0.68759086	3.35898931	2.18970793
H26	0.23282563	2.573804	0.88117196
H27	-1.3270848	1.89385452	1.40221784
C28	0.96600736	0.42603986	5.13227572
H29	0.85062022	-0.25394859	5.98137617
H30	1.98439296	0.83331413	5.14196484
H31	0.25918767	1.25662722	5.22948201
C32	3.28348933	1.2137089	0.55783941
H33	3.39318554	1.63597034	-0.44807958
H34	2.64117805	1.87756282	1.14544497
H35	4.27538443	1.20013791	1.02587349
H36	2.35884931	-2.27315144	-1.3607894
C37	4.40840286	-3.0456164	-1.65816117
H38	4.17572886	-4.09561986	-1.43365629
H39	4.42321116	-2.95638521	-2.75330391
H40	5.41814548	-2.83619767	-1.28806545

B3LYP/6-31G* Energy = -834.5247121

Number of Imaginary Frequencies = 0

Complex 1c-2b-exo



B3LYP/6-31G* Geometry

C1	-0.19069753	-0.14428641	-0.24079572
O2	0.06632557	-0.38097832	0.93961469
B3	2.06510439	0.30841689	3.28720878
C4	2.86642936	-0.93347858	2.78212605
C5	1.64640993	1.48567521	-0.49748638
C6	0.62410175	0.80422754	-1.03872244
O7	0.92467256	0.25406967	4.04127969
O8	2.56467207	1.55776441	2.99784983
H9	0.39933486	0.92392359	-2.09505859
H10	1.86562413	1.34014857	0.55959507
C11	4.10446625	-0.84983029	2.27020032
H12	2.42248804	-1.92924181	2.84918057
H13	4.56864652	0.13511049	2.19445899
C14	-3.51903822	-2.23382938	-2.00936041
C15	-2.97050761	-1.1424759	-2.68292322
C16	-1.88758913	-0.45434521	-2.13647091
C17	-1.3448155	-0.84437228	-0.90273711
C18	-1.91413573	-1.93764992	-0.23014867
C19	-2.98724868	-2.63053835	-0.77928135
H20	-4.35957113	-2.77275695	-2.43930171
H21	-3.38693515	-0.82431829	-3.6351363
H22	-1.48727066	0.40076898	-2.67149273
H23	-1.49189668	-2.22631943	0.72724593
H24	-3.41213454	-3.47983677	-0.25022169
C25	1.90407039	2.72254174	3.47629187
H26	2.44211116	3.59088058	3.0832491
H27	0.86183802	2.75702165	3.1400644
H28	1.91223859	2.76218505	4.57186797
C29	0.23652872	-0.95970789	4.30046487
H30	-0.58149098	-0.73506326	4.99216675
H31	-0.18023996	-1.36878443	3.37423025
H32	0.89143528	-1.70664466	4.76673667
C33	4.93510184	-2.00084397	1.78069674
H34	5.88194558	-2.07064772	2.33471822
H35	4.40645363	-2.95474133	1.88420986
H36	5.20525074	-1.87191532	0.72290185
C37	2.52267395	2.440579	-1.24428115
H38	2.24086511	2.52728961	-2.29936331
H39	2.48073254	3.44021501	-0.78945968
H40	3.57323666	2.12348175	-1.18852772

B3LYP/6-31G* Energy = -834.4958416

Number of Imaginary Frequencies = 0

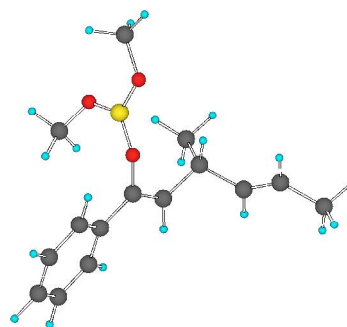
TS 1c+2b-exo

B3LYP/6-31G* Geometry

C1	0.00162745	0.00125816	0.00937376
O2	-0.00126321	0.02167323	1.31065871
B3	1.22318657	0.00187035	2.24944124
C4	2.54603602	-0.56090726	1.37941833
C5	2.29366759	0.83349685	-0.08146368
C6	1.14130319	0.31427645	-0.72411924
O7	0.83170189	-0.96853976	3.23192066
O8	1.54365948	1.32375134	2.72464757
H9	1.20887864	-0.01260834	-1.75713081
H10	2.13618157	1.59288115	0.67988
C11	3.82044326	-0.32648544	1.81284663
H12	2.39059792	-1.51792143	0.87115837
H13	4.01332647	0.63007988	2.30270674
C14	-3.63177501	-1.40211005	-1.7774163
C15	-2.71944328	-0.67552483	-2.54560443
C16	-1.5393873	-0.20959005	-1.9725037
C17	-1.25342638	-0.46790376	-0.62211454
C18	-2.18342354	-1.18631078	0.14657051
C19	-3.36100751	-1.65335596	-0.43075315
H20	-4.55273036	-1.7658226	-2.22595495
H21	-2.9323283	-0.46489225	-3.590347
H22	-0.84758828	0.37797364	-2.56918933
H23	-1.95992656	-1.37448958	1.19143217
H24	-4.06998071	-2.21590948	0.17093066
C25	0.53451347	2.03445325	3.41282426
H26	0.99404574	2.90244379	3.90068114
H27	-0.24857731	2.39468167	2.72908049
H28	0.04891202	1.41684492	4.18112336
C29	1.62207269	-1.10842632	4.38171665
H30	1.20195807	-1.9154822	4.99381471
H31	2.66574403	-1.37401872	4.13502422
H32	1.6549609	-0.19098166	4.98860008
C33	4.99928541	-1.23111249	1.64452739
H34	5.4803492	-1.43547088	2.6109101
H35	4.72222099	-2.18433681	1.18384906
H36	5.76970164	-0.7530508	1.01936466
C37	3.54207861	1.00911699	-0.9157835
H38	3.82117116	0.08543074	-1.43432764
H39	3.34554485	1.77041884	-1.68361676
H40	4.39294576	1.34837305	-0.32037371

B3LYP/6-31G* Energy = -834.4520727

Number of Imaginary Frequencies = 1 (-306.36)

Product 1c+2b-exo

B3LYP/6-31G* Geometry

C1	0.26764378	-0.41585552	0.51393065
O2	0.24122704	-0.53320595	1.89049577
B3	0.37989581	0.47299327	2.82600909
C4	3.8139695	-0.79476829	-0.24620515
C5	2.78029038	0.01407583	0.50686028
C6	1.42323919	-0.18026353	-0.13089248
O7	0.84239555	0.05271086	4.03870283
O8	0.08473165	1.79776848	2.65827113
H9	1.39965323	-0.16915908	-1.21744372
H10	2.73796821	-0.35405438	1.53843492
C11	4.527505	-1.80307631	0.25932489
H12	3.96872985	-0.50621301	-1.28953075
H13	4.36533309	-2.09102177	1.29975281
C14	-3.51415794	-1.28852226	-1.3438032
C15	-2.50541301	-0.65929132	-2.0773001
C16	-1.28172529	-0.36513032	-1.48358837
C17	-1.03316706	-0.69908586	-0.14027671
C18	-2.05929869	-1.32287124	0.58911325
C19	-3.28404214	-1.61702129	-0.00866353
H20	-4.47030754	-1.51438327	-1.80859692
H21	-2.67653829	-0.3867279	-3.11565962
H22	-0.52024719	0.14555546	-2.06593098
H23	-1.88245769	-1.58856444	1.62561645
H24	-4.06011597	-2.10690773	0.57409152
C25	-0.64886007	2.36053213	1.57724604
H26	-1.03686866	3.32557034	1.91685408
H27	-0.00436223	2.5213794	0.7070492
H28	-1.48811603	1.72314488	1.28127928
C29	0.91396126	0.95831074	5.13154693
H30	1.31158559	0.40308025	5.98514702
H31	1.57593229	1.80358544	4.91056772
H32	-0.074295	1.35650421	5.39049819
C33	5.55375652	-2.59941331	-0.49563826
H34	5.28889255	-3.66530787	-0.52183558
H35	5.65325014	-2.25009558	-1.52927352
H36	6.54124014	-2.53371222	-0.0185873
C37	3.17757372	1.50966325	0.54287907
H38	3.2082587	1.93345936	-0.46855934
H39	2.4582029	2.08803708	1.13272257
H40	4.17076192	1.63266461	0.98972295

B3LYP/6-31G* Energy = -834.5255391

Number of Imaginary Frequencies = 0

B3LYP/lacvp* Geometry

C1	0.26383576	-0.41615961	0.51334228
O2	0.23729447	-0.5419295	1.88906945
B3	0.38807751	0.46421248	2.82389347
C4	3.80686664	-0.78812447	-0.23450514
C5	2.77382576	0.03114361	0.50879789
C6	1.41773442	-0.1669634	-0.13022068
O7	0.86131627	0.04214684	4.03137269
O8	0.09374894	1.78939879	2.65646547
H9	1.39426479	-0.14796237	-1.21666188
H10	2.72951967	-0.32592378	1.54436629
C11	4.51538289	-1.79473874	0.28228468
H12	3.96515082	-0.50983758	-1.27998859
H13	4.34941586	-2.07256876	1.32482073
C14	-3.51441018	-1.29835677	-1.34940899
C15	-2.50991717	-0.65739282	-2.07912752
C16	-1.28754007	-0.35929341	-1.48375163
C17	-1.03572356	-0.7017573	-0.14282783
C18	-2.05810436	-1.33660382	0.58306805
C19	-3.28174266	-1.63410647	-0.01613128
H20	-4.4692201	-1.5272674	-1.81535078
H21	-2.68324607	-0.37880016	-3.11545934
H22	-0.53075246	0.16183242	-2.06257655
H23	-1.8791523	-1.60734897	1.61787751
H24	-4.05472675	-2.13209148	0.56375943
C25	-0.65011938	2.35115403	1.58306717
H26	-1.04280888	3.31254646	1.9279256
H27	-0.01204595	2.51950431	0.70949564
H28	-1.48693495	1.70961107	1.28892106
C29	0.95388607	0.94035806	5.12772389
H30	1.25093129	0.35654149	6.00388251
H31	1.70534944	1.71721674	4.94264572
H32	-0.00565741	1.43104643	5.3294605
C33	5.5406162	-2.60203787	-0.46304059
H34	5.27149127	-3.66711568	-0.48007374
H35	5.64397854	-2.26251498	-1.49960511
H36	6.52720116	-2.53576498	0.0159699
C37	3.17431491	1.52641533	0.52793549
H38	3.20552433	1.93853749	-0.48839668
H39	2.45625839	2.11275881	1.11149475
H40	4.16802543	1.65248015	0.97293939

B3LYP/lacvp* Energy = -834.5106627

Number of Imaginary Frequencies = 0

Conjugate Addition of 5b to 1c

Complex 1c-5b-Re-endo

B3LYP/lacvp* Geometry

C1	-0.39830196	-0.28642884	-0.55060093
O2	-0.05603589	0.20332551	0.52654573
B3	1.9904642	0.89005049	2.48811609
C4	2.83923759	1.7919948	1.56839215
C5	1.57441902	-1.76085	-0.72082396
C6	0.4589834	-1.25809439	-1.27338107
C7	3.30873416	-2.14350232	3.84247865

C8	2.2332419	-1.26973626	3.61869302
I9	4.94729304	-2.18110048	2.4794153
C10	1.20079649	-2.11793615	5.62797347
C11	1.13454595	-1.27574608	4.50423025
C12	-1.33443959	-1.02498096	4.67591924
C13	-0.10051735	-0.47346823	4.2887907
C14	-1.28302796	1.57949457	3.74983922
C15	-0.09146731	0.84002814	3.77213502
I16	-1.28039541	3.598895	3.07025211
C17	-2.48879378	1.02533172	4.16972744
C18	-2.51433668	-0.29335614	4.61832973
H19	-3.39902995	1.61430046	4.1348924
C20	3.33719229	-2.99329903	4.94422959
C21	2.27848824	-2.966794	5.84976283
H22	4.18182849	-3.65577633	5.09978624
O23	1.04427906	1.45073375	3.32706694
O24	2.30045251	-0.46294865	2.52279366
H25	0.17747723	-1.5523596	-2.28061217
H26	1.83411394	-1.44038237	0.28702247
H27	3.61310294	1.31955844	0.96042611
C28	2.71015649	3.12860885	1.50871955
C29	-4.17885053	0.96088914	-2.19378274
C30	-3.54047774	-0.15529298	-2.73615145
C31	-2.31167798	-0.57486273	-2.22700345
C32	-1.709625	0.11449908	-1.16274617
C33	-2.36837803	1.2283939	-0.61710458
C34	-3.58944912	1.65199112	-1.13124346
H35	-5.1339456	1.29013683	-2.59575632
H36	-4.0000492	-0.70159658	-3.55573759
H37	-1.84084569	-1.45516436	-2.6525073
H38	-1.89968721	1.74823524	0.21225352
H39	-4.08409983	2.52068477	-0.70429501
C40	2.49526079	-2.73463812	-1.38484008
H41	2.16719749	-2.99273974	-2.39729332
H42	3.51347716	-2.32619005	-1.43992705
H43	2.57083851	-3.65884185	-0.79561654
H44	1.94104317	3.60482955	2.11764417
C45	3.54192168	4.05084517	0.66836186
H46	4.06911397	4.78409856	1.2949867
H47	4.28510405	3.50507436	0.07752979
H48	2.90957189	4.63015047	-0.01894266
H49	2.29988399	-3.60503506	6.72849703
H50	0.38883411	-2.08984706	6.34738793
H51	-1.36127492	-2.05452041	5.01771758
H52	-3.45443504	-0.74528878	4.92159088

B3LYP/lacvp* Energy = -1238.249987

Number of Imaginary Frequencies = 0

TS 1c+5b-Re-endo

B3LYP/lacvp* Geometry

C1	-0.01578414	0.13840777	-0.20508957
O2	0.07852629	0.32112843	1.09141709
B3	1.31880542	0.37632177	1.92860727
C4	2.66053755	0.9411707	1.10314978
C5	2.38924375	-0.29887379	-0.43852966

C6	1.09677696	-0.07971351	-0.997569
C7	2.85879011	-2.37405113	3.81816671
C8	1.84583943	-1.41695941	3.60731083
I9	4.01343115	-3.08111607	2.15961204
C10	1.39553736	-1.5331437	5.99373335
C11	1.07870022	-1.00615645	4.73189128
C12	-1.20327983	-0.24187383	5.43191121
C13	-0.06112222	-0.05567596	4.63704148
C14	-1.01273499	2.04664609	3.88507638
C15	0.01470885	1.0930175	3.81701341
I16	-0.85075776	3.84364553	2.73963692
C17	-2.12814663	1.86200989	4.69775878
C18	-2.22790255	0.69925593	5.46184906
H19	-2.91196549	2.61164409	4.72875356
C20	3.14305618	-2.90095374	5.07305338
C21	2.40771735	-2.46783748	6.17431219
H22	3.93498199	-3.63294705	5.19038534
O23	1.08682752	1.30149621	3.01927997
O24	1.59793303	-1.00329746	2.35363025
H25	1.01463052	0.10358901	-2.06411867
H26	2.45866799	-1.07455082	0.32339475
H27	3.59514027	0.56490325	1.53079543
C28	2.75667226	2.17327729	0.51792091
C29	-3.98028287	0.57806415	-1.78021688
C30	-2.98647831	-0.02461124	-2.55569619
C31	-1.6984649	-0.17109958	-2.04890692
C32	-1.38063003	0.28870985	-0.75920248
C33	-2.3909207	0.87729244	0.01891422
C34	-3.67825793	1.02442553	-0.49221565
H35	-4.98658115	0.6907275	-2.17591467
H36	-3.21862521	-0.39053934	-3.55246391
H37	-0.94344948	-0.67063425	-2.64831275
H38	-2.15477738	1.21774798	1.02029418
H39	-4.44852083	1.48820973	0.11823011
C40	3.58922769	-0.25831357	-1.3559546
H41	3.55686459	0.58801897	-2.04985196
H42	4.526431	-0.22369936	-0.7932748
H43	3.60115045	-1.18139987	-1.95251829
H44	1.86410392	2.58477959	0.04064799
C45	3.98105376	3.01689866	0.42497705
H46	3.80296651	3.98860829	0.90839202
H47	4.84653367	2.54485462	0.89887369
H48	4.22296312	3.24228719	-0.625098
H49	2.63093944	-2.85415032	7.16465946
H50	0.83524113	-1.1811972	6.85432835
H51	-1.28677772	-1.14561725	6.02813788
H52	-3.10566617	0.53393879	6.08047803

B3LYP/lacvp* Energy = -1238.219309

Number of Imaginary Frequencies = 1 (-315.30)

Product 1c+5b-Re-endo

B3LYP/lacvp* Geometry

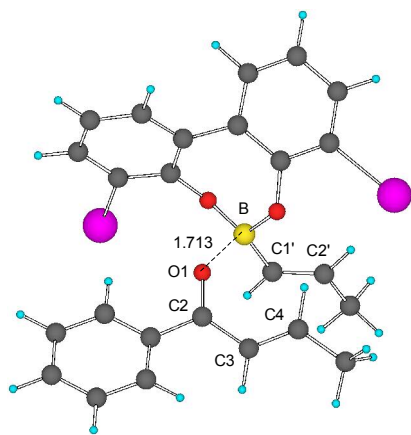
C1	1.12456777	0.88144544	-0.03975763
O2	1.17342811	1.29193706	1.29190013
B3	0.99956168	0.4911993	2.37353617

C4	4.09735483	2.63471527	-1.16397513
C5	3.58577316	1.44622162	-0.36969303
C6	2.21673841	1.00280567	-0.80744689
C7	1.62969585	-3.00347019	2.76993554
C8	1.02802705	-1.80684089	3.18689968
I9	2.11605273	-3.3073278	0.72224099
C10	0.99828085	-2.66426432	5.44397588
C11	0.6710442	-1.63670646	4.54175687
C12	-1.03493878	-0.63330091	6.06117662
C13	-0.07292804	-0.45385382	5.05191825
C14	-0.48716801	1.94246995	5.18921761
C15	0.1756966	0.85726321	4.59945166
I16	-0.08789274	3.92310809	4.52469265
C17	-1.41486968	1.74304616	6.20859028
C18	-1.69590958	0.44611375	6.63574821
H19	-1.92207038	2.59216295	6.65403355
C20	1.9197421	-4.01882385	3.6785112
C21	1.61207835	-3.83856315	5.02556776
H22	2.3904468	-4.9342032	3.33697041
O23	1.07735403	1.11838716	3.60180173
O24	0.77538834	-0.85859067	2.22927825
H25	2.10596873	0.75969177	-1.8614222
H26	3.5356559	1.74172306	0.68730975
H27	5.15060862	2.87046866	-0.99352729
C28	3.40731775	3.38774703	-2.02472139
C29	-2.75784979	-0.2435979	-1.50341951
C30	-1.60537287	-0.77713187	-2.08563661
C31	-0.34592785	-0.43092778	-1.60163498
C32	-0.21149847	0.46667633	-0.52872621
C33	-1.37699698	0.99050604	0.05500556
C34	-2.63640325	0.63951645	-0.42967914
H35	-3.73974845	-0.51921009	-1.87909465
H36	-1.68788087	-1.47934654	-2.91151354
H37	0.54075824	-0.87967566	-2.03847148
H38	-1.2933268	1.69614447	0.87651502
H39	-3.52507276	1.06326361	0.03140273
C40	4.59303392	0.27424607	-0.47727812
H41	4.67192795	-0.07731898	-1.5131914
H42	5.59233268	0.5912213	-0.15426219
H43	4.28080755	-0.57017125	0.14574406
H44	2.3521572	3.17086852	-2.19349381
C45	3.97541695	4.54751453	-2.79430854
H46	3.43919718	5.47928209	-2.56717714
H47	5.03545011	4.7023542	-2.56469027
H48	3.88358531	4.3903543	-3.87824903
H49	1.85586652	-4.61444978	5.74553372
H50	0.77541112	-2.52227555	6.49641612
H51	-1.27318105	-1.64155655	6.38407276
H52	-2.43614922	0.28198341	7.41353831

B3LYP/lacvp* Energy = -1238.281494

Number of Imaginary Frequencies = 0

Complex 1c-5b-Re-exo



B3LYP/lacvp* Geometry

C1	0.06695714	-0.07475554	-0.10313083
O2	0.20442638	0.09331721	1.13935875
B3	1.47736661	0.29245254	2.26755932
C4	2.55222837	1.25077042	1.6036695
C5	2.27226731	-1.08467321	-0.63158357
C6	1.13932347	-0.45780273	-1.01095386
C7	2.79403714	-2.76111604	3.88287731
C8	1.79922152	-1.79136228	3.64002214
I9	4.34953946	-3.08783345	2.45017362
C10	0.79324019	-2.46500196	5.74469272
C11	0.73886714	-1.67845037	4.57978945
C12	-1.69714303	-1.22096131	4.90048845
C13	-0.4487324	-0.79545327	4.41394574
C14	-1.45539593	1.36688393	3.95779178
C15	-0.34666081	0.50706514	3.87540618
I16	-1.26189252	3.38632274	3.28819897
C17	-2.67258893	0.94348717	4.4840789
C18	-2.79747224	-0.37073167	4.93383938
H19	-3.5136877	1.62725955	4.5337631
C20	2.80867681	-3.55090542	5.0263216
C21	1.804641	-3.38682756	5.97731327
H22	3.6011197	-4.27597042	5.17729507
O23	0.80366072	0.96165306	3.34036423
O24	1.89012485	-1.0752354	2.50212104
H25	0.98702617	-0.22452815	-2.06067737
H26	2.40372249	-1.36712979	0.40842187
C27	3.87486473	1.04363405	1.54327121
H28	2.18256682	2.21602214	1.24184103
H29	4.27864841	0.10182185	1.9184284
C30	-3.87910387	0.59767162	-1.63442462
C31	-2.94795482	-0.0911939	-2.41524021
C32	-1.66075609	-0.31042621	-1.93363035
C33	-1.28993394	0.15344958	-0.65759903
C34	-2.24205046	0.8287886	0.12691731
C35	-3.52361381	1.05505383	-0.36292988
H36	-4.88172727	0.77420196	-2.01537892
H37	-3.22648255	-0.46065647	-3.39816504
H38	-0.95650194	-0.867636	-2.54248061
H39	-1.96023153	1.17678851	1.11340211
H40	-4.24606463	1.58948547	0.24748767
C41	4.89128287	2.02019453	1.01707726

H42	5.48264909	1.5848311	0.19810888
H43	4.41752571	2.93605628	0.64630438
H44	5.61060967	2.30226342	1.79888523
C45	3.36511531	-1.46819459	-1.57213406
H46	3.15381868	-1.17907376	-2.60646234
H47	4.30385236	-0.99318272	-1.25677633
H48	3.54227623	-2.55128565	-1.5319022
H49	-3.75084156	-0.72352611	5.31732245
H50	-1.80027909	-2.24055369	5.25851684
H51	0.01967709	-2.32810871	6.49346773
H52	1.81678172	-3.97267262	6.89188543

B3LYP/lacvp* Energy = -1238.241966

Number of Imaginary Frequencies = 0

TS 1c-5b-Re-exo

B3LYP/lacvp* Geometry

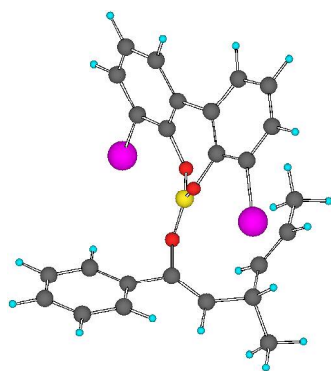
C1	-0.05182843	-0.09597938	-0.05306356
O2	0.00654027	-0.09184318	1.25655627
B3	1.25229832	0.03730039	2.10430474
C4	2.42871055	0.79198013	1.20887014
C5	2.35927341	-0.52884436	-0.25316392
C6	1.09213249	-0.21080573	-0.82862667
C7	2.68079595	-2.85213357	3.95337867
C8	1.71567176	-1.85183141	3.71142667
I9	4.01454823	-3.43475741	2.38089323
C10	0.97658604	-2.18290767	6.00203155
C11	0.81288009	-1.53441299	4.76526349
C12	-1.51869506	-0.81077286	5.32482323
C13	-0.31330466	-0.56742519	4.64499468
C14	-1.19877691	1.60307276	4.00826128
C15	-0.17443169	0.64622551	3.93363086
I16	-0.94624472	3.48403681	3.0289255
C17	-2.37281264	1.36177817	4.71688782
C18	-2.53793285	0.13564698	5.3610129
H19	-3.15182424	2.11607371	4.75671895
C20	2.80525583	-3.50074604	5.17528548
C21	1.94880631	-3.15087033	6.21710685
H22	3.56695841	-4.26020862	5.31548928
O23	0.94828984	0.90240394	3.2260484
O24	1.67817915	-1.31089851	2.48396552
H25	1.05518453	0.1148197	-1.86309848
H26	2.38614186	-1.37072948	0.43304232
C27	3.74848046	0.75114525	1.57977418
H28	2.10706556	1.73153711	0.74991971
H29	4.12078474	-0.17049709	2.03127246
C30	-3.95448207	0.55290532	-1.70782571
C31	-2.9304501	0.05032842	-2.5151235
C32	-1.66349701	-0.16816747	-1.98169474
C33	-1.39668989	0.11909331	-0.63147098
C34	-2.43713141	0.6063252	0.17681216
C35	-3.70319481	0.82539132	-0.36138833
H36	-4.94355103	0.72335896	-2.12504417
H37	-3.12226564	-0.18042412	-3.55972151
H38	-0.8843009	-0.58782702	-2.61116677
H39	-2.23940326	0.81542601	1.22194253

H40	-4.49617684	1.21165242	0.27334773
C41	4.75166507	1.83678417	1.3892613
H42	5.60005885	1.48444949	0.78285383
H43	4.31961861	2.72382295	0.91704514
H44	5.17798762	2.12867317	2.36019579
C45	3.56350648	-0.44862926	-1.16867224
H46	3.66113581	0.53907017	-1.63245958
H47	4.49409788	-0.68869811	-0.64821722
H48	3.43431012	-1.18127174	-1.97693311
H49	-3.46205441	-0.07525849	5.89210607
H50	-1.65631919	-1.76360292	5.82670147
H51	0.32389124	-1.89728627	6.82105389
H52	2.04706455	-3.62699669	7.18841677

B3LYP/lacvp* Energy= -1238.223707

Number of Imaginary Frequencies= 1 (-269.31)

Product 1c+5b-Re-exo



B3LYP/lacvp* Geometry

C1	0.77532788	0.06706616	-0.18953189
O2	0.7981567	0.7563249	1.01898731
B3	0.87538358	0.18688933	2.24506046
C4	3.60705315	0.88653441	0.70408661
C5	3.35604921	-0.03938353	-0.46261668
C6	1.90286853	-0.22337572	-0.85487194
C7	1.90583879	-3.09106723	3.27649334
C8	1.23245888	-1.87888575	3.49320605
I9	2.19842327	-3.83378077	1.30437152
C10	1.49476616	-2.22192995	5.86996413
C11	0.976995	-1.45131129	4.81500216
C12	-0.71236742	-0.32500916	6.26615285
C13	0.14163124	-0.26676674	5.15099919
C14	-0.53958344	2.05042452	4.84446578
C15	0.19878191	0.93658252	4.4210933
I16	-0.42406486	3.87873502	3.76318759
C17	-1.35746068	1.97927621	5.96941467
C18	-1.45066742	0.78003318	6.67419151
H19	-1.92605025	2.84835516	6.28278012
C20	2.38515504	-3.85215021	4.34043705
C21	2.1921796	-3.4019397	5.64444273
H22	2.91061946	-4.78121628	4.14877246
O23	0.98561977	1.06410715	3.30903929
O24	0.80634533	-1.18156439	2.39365637
H25	1.76078325	-0.68139236	-1.83118138

H26	3.74369682	-1.03545746	-0.19425772
C27	4.28451668	0.56434111	1.81055033
H28	3.23505456	1.90525494	0.58935238
H29	4.65697531	-0.45635394	1.92258254
C30	-3.20734678	-0.64589344	-1.64534704
C31	-2.15472924	-1.46603796	-2.05767251
C32	-0.86448511	-1.2466124	-1.58215982
C33	-0.59556456	-0.19397836	-0.69106141
C34	-1.66450747	0.6171602	-0.27393141
C35	-2.9557227	0.39394572	-0.7498921
H36	-4.21539204	-0.82266952	-2.01184789
H37	-2.34224003	-2.2919004	-2.73941551
H38	-0.06361048	-1.91657613	-1.87982101
H39	-1.47526199	1.43347366	0.41596075
H40	-3.76750508	1.03716992	-0.41928253
C41	4.58119975	1.51003659	2.94138625
H42	5.66322487	1.60838464	3.10646278
H43	4.17356802	2.50744291	2.74542343
H44	4.14717233	1.15118673	3.8841186
C45	4.1577067	0.44627877	-1.69568537
H46	3.83399051	1.44833638	-2.00145721
H47	5.22731808	0.4886784	-1.4648887
H48	4.01578508	-0.22762264	-2.54967174
H49	-2.105802	0.71069351	7.53786578
H50	-0.804749	-1.26117435	6.80718798
H51	1.35105285	-1.8712975	6.88699626
H52	2.58436881	-3.97403719	6.48027736

B3LYP/lacvp* Energy = -1238.279911

Number of Imaginary Frequencies = 0

Complex 1c-5b-Si-endo

B3LYP/lacvp* Geometry

C1	0.24186405	0.2368261	-0.16179588
C2	2.80935322	-0.80398388	1.64256016
C3	2.3704418	1.4652203	-0.46395293
C4	1.29408534	0.8257978	-0.96996901
C5	2.90938638	-1.9233336	0.91230005
C6	-3.48338437	-0.93037433	-1.91814475
C7	-2.65513137	-0.03916274	-2.60436634
C8	-1.43801583	0.34813136	-2.05122401
C9	-1.0394308	-0.14901834	-0.79718412
C10	-1.88904242	-1.03419605	-0.10639589
C11	-3.09841122	-1.42603686	-0.66911698
C12	0.67387655	3.05335522	3.75286651
C13	1.10776104	1.71693179	3.82629006
C14	0.39441899	1.72210704	6.15073888
C15	0.97848753	1.04242784	5.06956607
C16	2.01719692	-0.72212525	6.50871036
C17	1.43753958	-0.35556743	5.28495784
C18	1.43606831	-2.69795746	4.65649759
C19	1.19406652	-1.3573659	4.31390967
C20	1.98718828	-3.04933244	5.88620569
C21	2.30174257	-2.05075574	6.80708107
C22	0.11356331	3.71823575	4.83979695
C23	-0.03167546	3.04154682	6.0488272

C24	3.46711055	2.03771858	-1.29683341
O25	0.33010614	-0.008082	1.07334283
O26	1.72100724	1.15719355	2.7611414
O27	0.67084633	-1.02735476	3.11482369
C28	4.18427509	-2.54852736	0.41875303
B29	1.46463891	-0.17564463	2.23902744
I30	0.88048493	4.152079	1.92836118
I31	0.8939862	-4.26211287	3.30787196
H32	1.19170917	0.72696992	-2.04616422
H33	2.44908925	1.60714482	0.60934914
H34	3.7459063	-0.2958263	1.89635344
H35	-4.43061965	-1.23582627	-2.35513928
H36	-2.96030562	0.35703219	-3.56874651
H37	-0.816186	1.05932549	-2.58503671
H38	-1.57827463	-1.40683555	0.8643104
H39	-3.74332135	-2.11774675	-0.13456243
H40	2.17376194	-4.09224389	6.12016524
H41	-0.21242884	4.74783115	4.73948234
H42	3.30583008	1.88637216	-2.36863813
H43	3.57634107	3.11228645	-1.09873232
H44	4.42343447	1.57545963	-1.01571651
H45	2.75632193	-2.31526644	7.75778583
H46	2.24754766	0.05322399	7.23369114
H47	0.25960143	1.18656818	7.08552516
H48	-0.48372029	3.54143464	6.90079617
H49	1.99834551	-2.46369992	0.64536752
H50	4.19447638	-2.63264924	-0.67797229
H51	4.29653146	-3.57010358	0.80833795
H52	5.06205537	-1.96909828	0.72601266

B3LYP/lacvp* Energy = -1238.239057

Number of Imaginary Frequencies = 0

TS 1c+5b-Si-endo

B3LYP/lacvp* Geometry

C1	-0.04283825	0.27789993	0.01293633
C2	2.62549957	-0.52431877	1.30673425
C3	2.33504953	0.87733319	-0.078793
C4	1.07597895	0.6409905	-0.70945389
C5	2.86146388	-1.6126339	0.51164088
C6	-3.91641662	-0.28210554	-1.73566962
C7	-2.96274041	0.49641441	-2.39596218
C8	-1.70294336	0.68359262	-1.8337243
C9	-1.37558036	0.08875998	-0.60369597
C10	-2.34542436	-0.68096962	0.05953445
C11	-3.60420636	-0.86712094	-0.50668345
C12	0.17243197	2.89508758	3.63770381
C13	0.76229177	1.62867379	3.7826615
C14	-0.21358114	1.51594928	6.00204496
C15	0.58886753	0.93857826	5.00661561
C16	1.80430661	-0.59234441	6.55429562
C17	1.27659042	-0.35087004	5.27715219
C18	1.9002622	-2.61549571	4.67658939
C19	1.35796058	-1.3741721	4.29770629
C20	2.39966348	-2.84700485	5.95447627
C21	2.36441601	-1.81905081	6.89581319

C22	-0.60580866	3.46508602	4.6422747
C23	-0.80831479	2.76156497	5.82825807
C24	3.55818463	1.03400438	-0.95345387
O25	0.01209116	-0.01467376	1.29296889
O26	1.55224368	1.11912631	2.80930289
O27	0.85144518	-1.22048434	3.06336047
C28	4.15905768	-2.32493807	0.34609792
B29	1.22116959	-0.14828367	2.1522017
I30	0.48789452	4.02265854	1.85097256
I31	1.91343311	-4.22899253	3.27207691
H32	1.0387594	0.5724136	-1.79200761
H33	2.32143353	1.56335826	0.76703965
H34	3.50543663	-0.16432846	1.84976057
H35	-4.90126361	-0.42418116	-2.17355471
H36	-3.20607071	0.96864626	-3.34417643
H37	-0.98047423	1.31938197	-2.33713727
H38	-2.09651467	-1.12665	1.01664322
H39	-4.34525378	-1.46800576	0.01390636
H40	2.8149287	-3.81611396	6.21025987
H41	-1.05324212	4.44246152	4.49648037
H42	3.60029229	0.28571841	-1.75181382
H43	3.52212039	2.0258263	-1.42542696
H44	4.48294893	0.98368899	-0.37139493
H45	2.76971942	-1.98072903	7.89068238
H46	1.77670378	0.20812566	7.28794272
H47	-0.37920093	0.96535522	6.92345408
H48	-1.43005715	3.18720852	6.61097147
H49	2.04004415	-1.98291436	-0.10634039
H50	4.47037445	-2.32920055	-0.7097115
H51	4.04279073	-3.37855629	0.63732466
H52	4.95409292	-1.88371013	0.95401801

B3LYP/lacvp* Energy = -1238.219759

Number of Imaginary Frequencies = 1 (-301.76)

Product 1c+5b-Si-endo

B3LYP/lacvp* Geometry

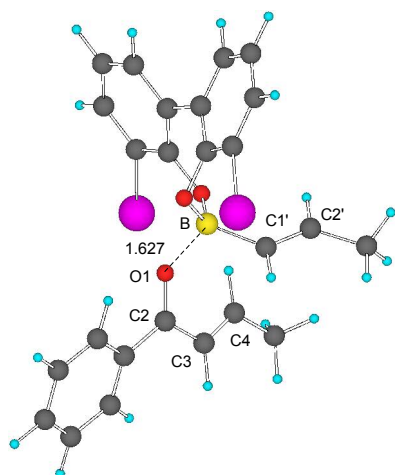
C1	0.7016688	-0.50655609	0.09894173
C2	4.18388205	-1.31779339	-0.76635266
C3	3.24877234	-0.52259901	0.12602258
C4	1.89113645	-0.31742329	-0.48973556
C5	3.86467737	-1.99282391	-1.87379676
C6	-3.13813458	0.0500372	-1.7503448
C7	-2.01522091	0.71326093	-2.25198724
C8	-0.77242705	0.54616309	-1.64919553
C9	-0.61950389	-0.29811942	-0.53486917
C10	-1.75634223	-0.95466681	-0.03595878
C11	-3.00171504	-0.78178282	-0.63971025
C12	-0.20652653	3.0495423	3.24805205
C13	0.43778641	1.84637424	3.57183925
C14	0.30448852	2.45801895	5.90466487
C15	0.73202202	1.55119567	4.92010467
C16	2.41543124	0.46832206	6.41382304
C17	1.50618445	0.35618455	5.34798531
C18	2.00343064	-2.0264482	5.26753975
C19	1.32764505	-0.90978378	4.75749454

C20	2.8787509	-1.897476	6.34334413
C21	3.09243118	-0.64069473	6.90819032
C22	-0.59978805	3.94299515	4.2419725
C23	-0.35231383	3.63753108	5.57806936
C24	3.89072823	0.84291982	0.48075741
O25	0.64003103	-1.05268738	1.38090554
O26	0.80244643	1.01877767	2.53819212
O27	0.48121119	-1.09041036	3.69467914
C28	4.84241441	-2.75532875	-2.72356559
B29	0.63962014	-0.34938707	2.53827303
I30	-0.60590305	3.5580557	1.22459801
I31	1.70295965	-3.94272648	4.39660242
H32	1.88474582	0.03920021	-1.51578806
H33	3.12869192	-1.08076957	1.06534844
H34	5.22647161	-1.31698173	-0.43969168
H35	-4.10970711	0.18769397	-2.217837
H36	-2.11076097	1.37610226	-3.10847527
H37	0.08175248	1.09717596	-2.0304915
H38	-1.65773492	-1.61489615	0.8195436
H39	-3.86774326	-1.30252188	-0.23901439
H40	3.39856347	-2.76902702	6.72655826
H41	-1.10376083	4.8645822	3.97151176
H42	4.01827805	1.45759282	-0.41787631
H43	3.26147694	1.39462137	1.18580862
H44	4.87964438	0.70030679	0.9340955
H45	3.79244053	-0.53077941	7.73145012
H46	2.59824677	1.44695856	6.84597977
H47	0.48279468	2.21446016	6.94712299
H48	-0.67569654	4.31901624	6.35962875
H49	2.82559911	-2.01531486	-2.20330319
H50	4.85846297	-2.37304058	-3.75385885
H51	4.57097655	-3.81802584	-2.78869375
H52	5.86017297	-2.68963148	-2.32339928

B3LYP/lacvp* Energy = -1238.280962

Number of Imaginary Frequencies = 0

Complex 1c-5b-Si-exo



B3LYP/lacvp* Geometry

C1	0.22021635	-0.09593489	-0.16289836
O2	0.25212071	-0.13268946	1.10123611

B3	1.38659169	-0.06449022	2.26493151
C4	2.74100042	-0.70659063	1.72057563
C5	2.22535875	1.29854638	-0.5526361
C6	1.27248812	0.44867671	-0.99777365
H7	1.27459712	0.14215102	-2.03941871
H8	2.18545889	1.65415187	0.47106799
C9	3.97642192	-0.2376025	1.95003527
H10	2.66716992	-1.67107839	1.20759499
H11	4.08535115	0.71301397	2.47681246
C12	-3.26624138	-1.85573765	-1.90966703
C13	-2.47423832	-0.99974304	-2.67879118
C14	-1.3354746	-0.42096833	-2.12653898
C15	-0.98072732	-0.68901047	-0.79196538
C16	-1.79417364	-1.54002156	-0.02033505
C17	-2.92476939	-2.12372024	-0.58094436
H18	-4.15163972	-2.3116718	-2.34522234
H19	-2.74694096	-0.78077613	-3.70730037
H20	-0.74121442	0.26037892	-2.72677633
H21	-1.51593574	-1.73696405	1.00993386
H22	-3.54149967	-2.78885956	0.01677644
C23	0.24805025	3.19755237	3.39693955
C24	0.83474219	1.94060315	3.63098357
I25	0.34631345	4.09212051	1.45557181
O26	1.52853119	1.33219633	2.64154033
C27	0.08062793	2.13444756	5.93426959
C28	0.75807905	1.40590094	4.94482412
C29	1.98680527	-0.0525515	6.57336407
C30	1.37328016	0.10613229	5.32129129
C31	1.71023584	-2.2629155	4.92210196
C32	1.26471465	-1.01341499	4.46275833
I33	1.4650686	-3.99055474	3.69195951
C34	2.29625187	-2.41121526	6.1764591
C35	2.44870757	-1.29449086	6.99843881
H36	2.63850141	-3.38695652	6.50524832
C37	-0.40667438	3.91490527	4.39469937
C38	-0.49400778	3.37351564	5.67495472
H39	-0.84972834	4.8791416	4.17050201
O40	0.68784821	-0.8810083	3.24984835
C41	5.26031461	-0.92219956	1.56560588
H42	5.88390951	-0.28290974	0.92304971
H43	5.86799102	-1.15302299	2.45191011
H44	5.07132902	-1.86100691	1.03297446
C45	3.32445465	1.83494867	-1.40596356
H46	3.28162442	1.46283691	-2.43430611
H47	3.29655162	2.93262187	-1.4199571
H48	4.29367699	1.55742158	-0.97003094
H49	-1.01649821	3.91329834	6.45961761
H50	-0.00755943	1.69972579	6.92545418
H51	2.10598013	0.81572825	7.21491725
H52	2.92581919	-1.4001669	7.96890188

B3LYP/lacvp* Energy = -1238.243171

Number of Imaginary Frequencies = 0

TS 1c+5b-Si-exo

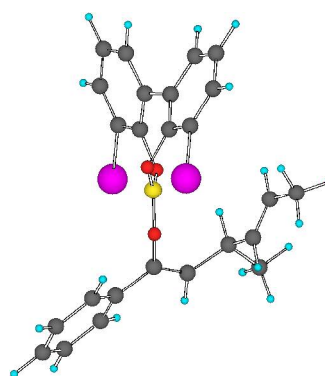
B3LYP/lacvp* Geometry

C1	0.00480368	-0.05734424	-0.05145348
O2	-0.01125371	-0.05291737	1.25897224
B3	1.18179817	-0.00614232	2.1726791
C4	2.54701662	-0.45910528	1.34460295
C5	2.26989853	0.87083955	-0.11219532
C6	1.14079934	0.29476743	-0.76349135
H7	1.2321374	-0.02169569	-1.79758465
H8	2.06484201	1.67094369	0.59298026
C9	3.79790064	-0.12946016	1.79954111
H10	2.47578378	-1.42766442	0.84273353
H11	3.9136404	0.83536441	2.29732371
C12	-3.58888536	-1.49020461	-1.88788599
C13	-2.67220019	-0.7516992	-2.64046904
C14	-1.50401108	-0.27942008	-2.04908287
C15	-1.23289298	-0.54436577	-0.69601132
C16	-2.16665047	-1.27545299	0.05664943
C17	-3.33339688	-1.74783857	-0.53905046
H18	-4.50205381	-1.85686998	-2.35005968
H19	-2.87393963	-0.53486556	-3.68624391
H20	-0.81247489	0.32122841	-2.63275647
H21	-1.95925627	-1.46877649	1.10371012
H22	-4.04635704	-2.31812472	0.05048073
C23	-0.13357673	3.04082463	3.39767059
C24	0.58892716	1.86304403	3.64425949
I25	0.00405644	3.99864516	1.49316991
O26	1.40220186	1.34115618	2.69582698
C27	-0.30493776	1.87639185	5.9016624
C28	0.51839318	1.28308932	4.93384169
C29	1.93775107	0.00993991	6.54804075
C30	1.32803584	0.08946391	5.28746158
C31	2.12371051	-2.15694411	4.83446684
C32	1.44267315	-1.00740427	4.39535124
I33	2.22627964	-3.87171524	3.56395446
C34	2.71114854	-2.22711586	6.09471798
C35	2.62643095	-1.13024059	6.95184229
H36	3.23185174	-3.12775097	6.40285324
C37	-0.93691286	3.62678293	4.37229611
C38	-1.02874134	3.03312296	5.63002083
H39	-1.49032073	4.53278514	4.14899587
O40	0.84703362	-0.99384512	3.19034884
C41	5.03609728	-0.94722735	1.64731669
H42	5.80126204	-0.39589157	1.07899297
H43	5.47987638	-1.15263468	2.63187426
H44	4.84127276	-1.90117926	1.14923661
C45	3.51348261	1.08000877	-0.94967953
H46	3.84589657	0.15193867	-1.42771442
H47	3.27693502	1.79592486	-1.7488261
H48	4.34159132	1.49258932	-0.36790644
H49	-1.66762428	3.47289472	6.39077525
H50	-0.38544768	1.40668757	6.87778656
H51	1.87211876	0.86508611	7.21424858
H52	3.09543346	-1.1709129	7.9310149

B3LYP/lacvp* Energy = -1238.227548

Number of Imaginary Frequencies = 1 (-273.51)

Product 1c+5b-Si-exo



B3LYP/lacvp* Geometry

C1	0.50586963	-0.21398645	-0.1451416
O2	0.636393	-0.77845922	1.11489143
B3	0.74747291	-0.17896101	2.32007586
C4	3.59833504	-0.2552293	0.44993239
C5	2.82433416	0.910854	-0.13274901
C6	1.48605854	0.50029382	-0.71975152
H7	1.30054301	0.80978932	-1.74489514
H8	2.64783495	1.63742497	0.67170727
C9	4.23670534	-0.24423723	1.62446281
H10	3.65934062	-1.14395098	-0.18097369
H11	4.17041936	0.6489404	2.25001985
C12	-3.15320957	-1.39408537	-2.06943375
C13	-2.48362352	-0.24186791	-2.48722469
C14	-1.30527846	0.15322366	-1.85945138
C15	-0.76336509	-0.60255571	-0.80600958
C16	-1.45370953	-1.75135293	-0.38374247
C17	-2.63379081	-2.14348454	-1.01355693
H18	-4.07581136	-1.69868494	-2.55685252
H19	-2.88855038	0.361017	-3.29616556
H20	-0.81517819	1.07020804	-2.17245337
H21	-1.05370283	-2.33965315	0.43524081
H22	-3.14839906	-3.03976936	-0.67614297
C23	-0.13739887	3.14411421	3.29323475
C24	0.52043154	1.92696655	3.52685188
I25	-0.51100372	3.81265271	1.30913894
O26	0.89773196	1.18779898	2.43423622
C27	0.35050928	2.34737975	5.89744758
C28	0.80782658	1.5291339	4.85007188
C29	2.46962722	0.35940739	6.29851945
C30	1.59560022	0.31520921	5.19811145
C31	2.11351829	-2.05453855	4.97893156
C32	1.45587014	-0.90750765	4.51147134
I33	1.8389177	-3.91786303	3.99055522
C34	2.94929819	-1.99414534	6.0918749
C35	3.13937373	-0.77521152	6.74161131
H36	3.45537874	-2.88869391	6.43896844
C37	-0.5565581	3.95111708	4.34874732
C38	-0.32135778	3.5395888	5.65861326
H39	-1.07065438	4.88428457	4.14655286
O40	0.66215982	-1.02889333	3.40634012
C41	5.07274977	-1.37122814	2.16402651
H42	6.11667099	-1.05742532	2.30590463
H43	4.70817428	-1.7075677	3.14345318

H44	5.06763611	-2.23311557	1.48800627
C45	3.66946369	1.61089608	-1.21947028
H46	3.90160638	0.92184665	-2.0411709
H47	3.13091531	2.4693399	-1.63986178
H48	4.61547549	1.96818531	-0.80106341
H49	-0.66615103	4.1485392	6.4892749
H50	0.51690218	2.02308374	6.91956577
H51	2.62851297	1.30700102	6.80297726
H52	3.81111262	-0.71578982	7.59314922

B3LYP/lacvp* Energy = -1238.280228
Number of Imaginary Frequencies = 0

Conjugate Addition of 2c to 1c

Complex 1c-2c-endo

B3LYP/6-31G* Geometry

C1	-0.42716978	0.54863861	-0.32813271
O2	-0.29226045	0.24430094	0.85774952
B3	2.19417214	-0.5578436	2.99206609
C4	3.11330986	-1.55115852	2.19164135
C5	1.72118556	1.75203464	-0.46003846
C6	0.54435655	1.42926614	-1.02009219
O7	1.23594007	-0.90752833	3.90320529
O8	2.43358632	0.77963744	2.80965337
H9	0.2849598	1.822259	-1.99952721
H10	1.95822775	1.33916119	0.52013004
H11	4.18951798	-1.37707878	2.27143112
C12	2.73222448	-2.54146629	1.36879544
C13	-3.85869228	-1.0272406	-2.39984696
C14	-2.83103468	-0.44271309	-3.14035584
C15	-1.71369557	0.0839917	-2.49291261
C16	-1.6087032	0.02562493	-1.09508147
C17	-2.64455232	-0.57576054	-0.36244866
C18	-3.76261443	-1.09303491	-1.00709516
H19	-4.73105096	-1.4331884	-2.9057745
H20	-2.89758505	-0.3984603	-4.22417557
H21	-0.91773978	0.51969489	-3.08813512
H22	-2.54549278	-0.62362427	0.71720891
H23	-4.56050923	-1.54953451	-0.42707421
C24	1.61756137	1.7549732	3.45451851
H25	2.1046512	2.72641055	3.32523697
H26	0.62476015	1.77871695	2.99366031
H27	1.50860315	1.54188562	4.52297536
C28	0.96847907	-2.22939765	4.33621503
H29	0.0085043	-2.56570728	3.92826233
H30	1.75193867	-2.9285342	4.0258334
H31	0.89943932	-2.22710322	5.42992019
C32	2.74913941	2.63735306	-1.0891241
H33	2.43099786	3.01503399	-2.06633838
H34	2.96906164	3.49509245	-0.43893567
H35	3.69791121	2.09830809	-1.21494511
H36	3.50141591	-3.12906148	0.86110451
C37	1.32035415	-2.92908038	1.02302951
H38	1.08361411	-3.93856441	1.38977001
H39	0.58650065	-2.22597904	1.42569873

H40	1.18772753	-2.95788756	-0.06677442
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B3LYP/6-31G* Energy = -834.4900802
Number of Imaginary Frequencies = 0

TS 1c+2c-endo

B3LYP/6-31G* Geometry

C1	-0.07872567	0.15739384	-0.03048415
O2	-0.06851738	-0.11174098	1.24114344
B3	1.13731406	-0.17712251	2.20516179
C4	2.57133288	-0.52187818	1.38524815
C5	2.26988845	0.84973391	-0.02367876
C6	1.06861294	0.54334921	-0.71723907
O7	0.73113788	-1.23382717	3.08936216
O8	1.37858902	1.1148366	2.79876415
H9	1.08439288	0.45452071	-1.79892349
H10	2.16500023	1.52481009	0.82521207
H11	3.44222384	-0.06167265	1.85933322
C12	2.8473267	-1.7145614	0.7565507
C13	-3.82648166	-0.60425339	-1.97089514
C14	-2.87471072	0.20367544	-2.59708538
C15	-1.65658036	0.45955338	-1.97338598
C16	-1.37092808	-0.09327314	-0.71458678
C17	-2.33996924	-0.89146088	-0.08571749
C18	-3.55601119	-1.14788721	-0.7135258
H19	-4.77759806	-0.80275259	-2.45831122
H20	-3.08637384	0.64257634	-3.56857218
H21	-0.93434628	1.11258445	-2.45483717
H22	-2.12083234	-1.30290962	0.89386927
H23	-4.29612679	-1.77248373	-0.22012793
C24	0.32853033	1.70782767	3.53423726
H25	0.73495825	2.56279115	4.08764136
H26	-0.47661838	2.07140999	2.87773761
H27	-0.11639653	1.00450004	4.25150843
C28	1.56667231	-1.55311017	4.17235208
H29	1.0245865	-2.23358597	4.83999379
H30	2.48908947	-2.06440745	3.84571665
H31	1.86501009	-0.66406514	4.74811832
C32	3.53230558	1.05877796	-0.82967885
H33	3.65569387	0.30138086	-1.61037123
H34	3.4816577	2.04104938	-1.32011055
H35	4.42220383	1.0569014	-0.19400814
H36	3.8770235	-2.07518523	0.70336798
C37	1.8082667	-2.53440668	0.08748001
H38	2.19113262	-3.48146873	-0.30110287
H39	0.97401123	-2.72023807	0.77642721
H40	1.37011615	-1.95454343	-0.74939467

B3LYP/6-31G* Energy = -834.4467966
Number of Imaginary Frequencies = 1 (-346.99)

Product 1c+2c-endo

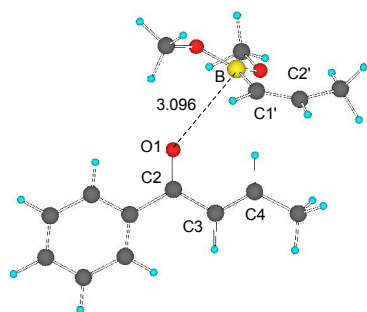
B3LYP/6-31G* Geometry

C1	0.06716648	-0.19192043	0.22899228
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O2	0.09845603	-0.74229582	1.4916418
B3	0.4243561	-0.15456624	2.69625316
C4	3.20442464	-1.22483107	0.37745771
C5	2.58656601	0.16442349	0.21888475
C6	1.19952946	0.18517307	-0.38950364
O7	0.71310932	-1.04249899	3.69024746
O8	0.45791261	1.18365773	2.97766767
H9	1.1160073	0.5304636	-1.41574977
H10	2.50998717	0.57508943	1.23531653
H11	3.71920743	-1.37169084	1.32689089
C12	3.23432518	-2.24423859	-0.48794234
C13	-3.87067038	-0.209531	-1.50428104
C14	-2.86427299	0.57724254	-2.06896003
C15	-1.58934305	0.59618826	-1.51109208
C16	-1.28587525	-0.18013224	-0.37848221
C17	-2.30997883	-0.95948194	0.18571244
C18	-3.58647111	-0.97482358	-0.37390207
H19	-4.86697867	-0.21956312	-1.93853179
H20	-3.07632037	1.18892094	-2.94223857
H21	-0.8300635	1.23683371	-1.94931899
H22	-2.09141666	-1.56274646	1.05996692
H23	-4.36119556	-1.59008115	0.07675602
C24	-0.04422102	2.23102208	2.15923192
H25	-0.23729845	3.08849373	2.81110681
H26	0.68826028	2.52026836	1.39818821
H27	-0.9763739	1.94752794	1.65939753
C28	0.96868148	-0.59534437	5.01366227
H29	0.95803215	-1.47468557	5.66375207
H30	1.95079809	-0.11230258	5.0840299
H31	0.20950308	0.11730081	5.35485755
C32	3.53856045	1.09770295	-0.56024911
H33	3.66194731	0.75179823	-1.59279175
H34	3.15190055	2.12418368	-0.58638209
H35	4.53050978	1.11813282	-0.09666802
H36	3.76085493	-3.1432278	-0.16406828
C37	2.63527525	-2.33751809	-1.86290746
H38	3.40490467	-2.59880268	-2.60216996
H39	1.87921309	-3.13339898	-1.90292915
H40	2.15512869	-1.41102765	-2.18284704

B3LYP/6-31G* Energy = -834.517004
Number of Imaginary Frequencies = 0

Complex 1c-2c-exo



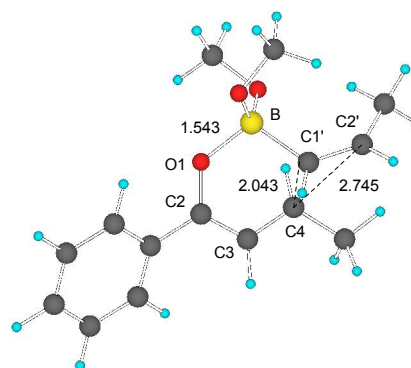
B3LYP/6-31G* Geometry

C1	-0.14981805	-0.29969188	-0.23821554
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O2	0.01243805	-0.43406942	0.97495731
B3	1.96747757	0.27567153	3.26814293
C4	3.02240595	-0.75117377	2.73286223
C5	1.86732405	1.09110763	-0.5575437
C6	0.85015086	0.39224918	-1.08574556
O7	0.87920488	-0.07726419	4.01914324
O8	2.13341904	1.61714092	3.01232505
H9	0.75590424	0.31294023	-2.1654722
H10	1.94197048	1.16152438	0.52614432
C11	4.31590109	-0.53908747	2.43024141
C12	-3.74202495	-1.93927769	-1.96125015
C13	-2.9661848	-1.06242255	-2.71979175
C14	-1.79288855	-0.52671329	-2.18901182
C15	-1.3853758	-0.85747841	-0.88741125
C16	-2.18259267	-1.73049832	-0.1303177
C17	-3.34730105	-2.27202024	-0.66264384
H18	-4.65371896	-2.35956506	-2.37828205
H19	-3.27609917	-0.79234536	-3.72580111
H20	-1.21375467	0.16749069	-2.78902538
H21	-1.86495956	-1.96716097	0.87986571
H22	-3.95107814	-2.9519689	-0.0672148
C23	1.15756983	2.55311827	3.46035814
H24	1.46343752	3.5405704	3.10225491
H25	0.16720896	2.30969906	3.06150421
H26	1.09560611	2.56927903	4.55431842
C27	0.50755376	-1.42438612	4.25677639
H28	-0.29525001	-1.42105897	5.00053009
H29	0.13638937	-1.88713862	3.33552623
H30	1.34441532	-2.01638415	4.64761983
C31	2.91810709	1.79582486	-1.35476847
H32	2.77322418	1.67449726	-2.43338377
H33	2.92662624	2.86938423	-1.12250551
H34	3.91534362	1.41750109	-1.09221222
C35	5.08612692	0.74736086	2.52821292
H36	5.96046697	0.62298254	3.18275561
H37	5.48141321	1.03413993	1.54268861
H38	4.4707875	1.5654298	2.90449751
H39	4.9084784	-1.38773666	2.07746602
H40	2.67750616	-1.77867647	2.60128379

B3LYP/6-31G* Energy = -834.4925431
Number of Imaginary Frequencies = 0

TS 1c+2c-exo



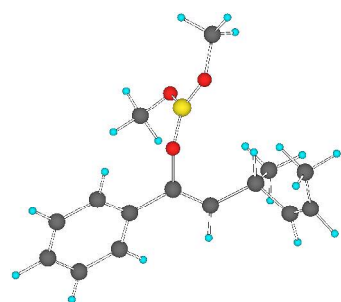
B3LYP/6-31G* Geometry

C1	0.00701338	-0.0707672	0.06050776
O2	0.01172631	-0.08420486	1.3605507
B3	1.23798587	-0.0141085	2.2950951
C4	2.57916544	-0.52973959	1.41689884
C5	2.27260282	0.85441529	-0.05406591
C6	1.12627035	0.3024605	-0.67807002
O7	0.908618	-0.99336814	3.29011765
O8	1.4479285	1.33812244	2.75261947
H9	1.18939035	-0.00689723	-1.71681144
H10	2.10865421	1.61100212	0.70858183
C11	3.88554975	-0.36587943	1.80139776
C12	-3.59641077	-1.5451993	-1.73119012
C13	-2.71276126	-0.77372019	-2.48905154
C14	-1.54140477	-0.28768928	-1.91481345
C15	-1.23533956	-0.57032899	-0.57371194
C16	-2.13653561	-1.33487524	0.18470351
C17	-3.30542619	-1.82191874	-0.39370003
H18	-4.5110682	-1.92379312	-2.18030179
H19	-2.94162701	-0.54337867	-3.52622687
H20	-0.87351294	0.3351861	-2.5027306
H21	-1.89913877	-1.54116596	1.22302156
H22	-3.99232818	-2.41912853	0.20012763
C23	0.38746438	1.95701122	3.45506982
H24	0.76684715	2.8796046	3.90982592
H25	-0.44577109	2.21583763	2.78545081
H26	-0.00854619	1.30974774	4.24930499
C27	1.74833401	-1.12750982	4.40464354
H28	1.31646234	-1.88027063	5.07479461
H29	2.75992392	-1.46736032	4.11779834
H30	1.86356735	-0.18637808	4.96387204
C31	3.49585228	1.06180979	-0.9183279
H32	3.7547948	0.15895893	-1.48104937
H33	3.27361988	1.85320693	-1.64816238
H34	4.36593115	1.38102752	-0.34129346
C35	4.4741819	0.82877984	2.48358306
H36	4.97147926	0.5172533	3.41328169
H37	5.26281025	1.2824228	1.86335927
H38	3.71455186	1.57285386	2.72429659
H39	4.60236024	-1.16183461	1.5788068
H40	2.38965927	-1.47918394	0.90829925

B3LYP/6-31G* Energy = -834.4494774

Number of Imaginary Frequencies = 1 (-347.19)

Product 1c+2c-*exo*



B3LYP/6-31G* Geometry

C1	0.28368661	-0.30265392	0.3819511
O2	0.3251397	-0.53277984	1.74430784
B3	0.53668866	0.40893608	2.73358304
C4	3.79112013	-0.26539886	-0.34798692
C5	2.69509664	0.53021013	0.33134599
C6	1.3587804	0.16757427	-0.27460225
O7	1.26043934	-0.0378001	3.80097158
O8	0.06741621	1.69262528	2.73741908
H9	1.28953666	0.25518182	-1.35561436
H10	2.6836531	0.27578815	1.39413697
C11	4.51401453	-1.26435723	0.17041474
C12	-3.40027664	-1.59723995	-1.42472392
C13	-2.53205667	-0.76298608	-2.13269429
C14	-1.34208395	-0.33185554	-1.55436181
C15	-0.98605632	-0.73034061	-0.25367828
C16	-1.87329332	-1.56040898	0.45181185
C17	-3.06461782	-1.99126949	-0.1302487
H18	-4.33068959	-1.93044547	-1.87701333
H19	-2.78809203	-0.43745803	-3.13780273
H20	-0.69494569	0.33710378	-2.1133361
H21	-1.61345795	-1.87477465	1.4565988
H22	-3.73172412	-2.63923533	0.43273615
C23	-0.88527916	2.21258157	1.81720755
H24	-1.38302537	3.05615967	2.30455114
H25	-0.39259477	2.56633439	0.90560302
H26	-1.63562662	1.46389222	1.54335056
C27	1.43763134	0.77892028	4.95169935
H28	1.95166993	0.17457132	5.7041126
H29	2.04636703	1.66078199	4.72122629
H30	0.47696246	1.11843743	5.35490316
C31	2.97078688	2.0458535	0.20745735
H32	2.95832646	2.36452261	-0.84239134
H33	2.21186528	2.62272424	0.74746712
H34	3.9543554	2.29460273	0.62199766
C35	4.41518644	-1.86457553	1.54528468
H36	4.22824603	-2.94469987	1.4768674
H37	5.36137611	-1.74684602	2.09177785
H38	3.6157807	-1.43027461	2.15103747
H39	5.26982468	-1.71710822	-0.47330136
H40	3.99057129	0.02833028	-1.3807031

B3LYP/6-31G* Energy = -834.523457

Number of Imaginary Frequencies = 0

Conjugate Addition of 5c to 1c

Complex 1c-5c-*Re-endo*

B3LYP/lacvp* Geometry

C1	0.08003864	0.08595248	-0.48150783
O2	0.11841714	0.37328789	0.74723816
B3	1.25226662	0.65340998	1.94342027
C4	2.50834569	1.47830539	1.40161568
C5	2.37926478	-0.7974531	-0.78899542
C6	1.23319194	-0.28924771	-1.28600881
C7	2.97701316	-1.86727595	3.86667544

C8	1.80379883	-1.15339757	3.55910619
I9	4.45604495	-2.21743281	2.36198708
C10	1.11681902	-1.48052725	5.86689834
C11	0.84102408	-0.98076294	4.58456117
C12	-1.61008614	-0.79800213	4.99499672
C13	-0.46316379	-0.30812696	4.35135722
C14	-1.77672889	1.58907686	3.61482793
C15	-0.5625476	0.87965707	3.58587287
I16	-1.91199823	3.50992219	2.68857731
C17	-2.89837689	1.10406556	4.28232103
C18	-2.81998998	-0.11403206	4.95469704
H19	-3.82272576	1.6721449	4.27622403
C20	3.22412638	-2.37799978	5.13740345
C21	2.28817149	-2.17370586	6.14856528
H22	4.14270615	-2.91933797	5.33715917
O23	0.49583628	1.38891168	2.91905524
O24	1.58435641	-0.727934	2.2987986
H25	1.13500588	-0.14966516	-2.35832219
H26	2.45849255	-0.99348551	0.27602187
H27	3.47477778	1.05915765	1.69580983
C28	2.56981065	2.61480012	0.69103978
C29	-3.79305401	0.31586991	-2.30062228
C30	-2.76139793	-0.35368562	-2.96292104
C31	-1.49694876	-0.42913644	-2.38686196
C32	-1.24939043	0.16227702	-1.13359086
C33	-2.30176498	0.81581941	-0.46724621
C34	-3.56060683	0.89823997	-1.05193158
H35	-4.77811306	0.37973867	-2.75565642
H36	-2.94358449	-0.82023396	-3.92693303
H37	-0.71358821	-0.97381001	-2.90305014
H38	-2.11612594	1.26242809	0.50238927
H39	-4.36110838	1.41778181	-0.5329698
C40	3.5580219	-1.16543625	-1.62588786
H41	3.3997062	-0.96606973	-2.69038573
H42	4.43851491	-0.60270856	-1.28728837
H43	3.80497407	-2.22728636	-1.4930667
H44	3.55357708	3.03366695	0.46176215
C45	1.4197637	3.40890196	0.13932708
H46	1.4839533	4.45784696	0.45946262
H47	1.44210812	3.42029147	-0.96135002
H48	0.4523729	3.02144613	0.46476507
H49	2.47944445	-2.54839868	7.15008801
H50	0.3958713	-1.3033178	6.65917739
H51	-1.54173217	-1.73661801	5.53705039
H52	-3.69602371	-0.51502263	5.45673372

B3LYP/lacvp* Energy = -1238.236721

Number of Imaginary Frequencies = 0

TS 1c+5c-Re-endo

B3LYP/lacvp* Geometry

C1	0.04856488	0.11816238	-0.41509549
O2	-0.01798896	0.29328838	0.87887953
B3	1.11950851	0.44652076	1.8634449
C4	2.49374013	1.0778955	1.18081737
C5	2.49492395	-0.1318669	-0.3804

C6	1.26294922	0.0083922	-1.08148662
C7	2.84864905	-2.09687244	3.82558544
C8	1.73791446	-1.26547887	3.58298644
I9	4.06207738	-2.77618802	2.19684284
C10	1.30391557	-1.32536487	5.977753
C11	0.93231066	-0.89914997	4.69337837
C12	-1.44076002	-0.44583301	5.31780109
C13	-0.32099662	-0.1164413	4.53998521
C14	-1.54732855	1.79771229	3.70706461
C15	-0.38818612	1.00495414	3.67925464
I16	-1.64980689	3.59056699	2.54869618
C17	-2.64372278	1.47271745	4.50223835
C18	-2.59454589	0.33073316	5.29915057
H19	-3.52759616	2.10194162	4.49448707
C20	3.19130723	-2.52988415	5.10282141
C21	2.41782161	-2.12969102	6.1903043
H22	4.05742674	-3.16696446	5.24683267
O23	0.66769329	1.34948497	2.90590202
O24	1.42121799	-0.92235845	2.32193
H25	1.28154526	0.16645939	-2.1547595
H26	2.52032457	-0.91913539	0.37191963
H27	3.39997196	0.71489066	1.67224462
C28	2.64286612	2.32921344	0.61608937
C29	-3.73218497	0.25405269	-2.43271207
C30	-2.61453436	-0.27084333	-3.08652899
C31	-1.38451484	-0.32001559	-2.43695609
C32	-1.25184811	0.16015523	-1.12231952
C33	-2.38545182	0.66892213	-0.46739026
C34	-3.61359574	0.72011676	-1.12205311
H35	-4.69242743	0.29164729	-2.94093767
H36	-2.70470432	-0.65132666	-4.10052219
H37	-0.53051672	-0.75859155	-2.94456388
H38	-2.29038151	1.02572277	0.5514985
H39	-4.4804221	1.12451455	-0.60624115
C40	3.77986206	-0.02088577	-1.17208202
H41	3.78198294	0.84436592	-1.8429071
H42	4.65301611	0.03489137	-0.51613142
H43	3.89005331	-0.92306554	-1.78961562
H44	3.63161339	2.79215182	0.61741463
C45	1.56729673	3.05167297	-0.09736633
H46	1.87591664	4.03893536	-0.44996079
H47	1.24851154	2.4406782	-0.96803
H48	0.67070907	3.14427812	0.52745139
H49	2.68744285	-2.44494764	7.19419039
H50	0.70384302	-1.00410095	6.82378324
H51	-1.40061644	-1.33440379	5.94095748
H52	-3.45322574	0.05511453	5.90496755

B3LYP/lacvp* Energy = -1238.220494

Number of Imaginary Frequencies = 1 (-297.74)

Product 1c+5c-Re-endo

B3LYP/lacvp* Geometry

C1	0.72846524	1.13192657	-0.04328544
O2	0.7211303	1.48195298	1.30726987
B3	0.67500798	0.59800685	2.3359321

H43	4.26893713	-0.73922816	-1.38959899
H44	3.55062397	-2.29604743	-1.76895276
C45	4.39706708	0.70867195	3.28230928
H46	5.29854614	0.14519428	3.00381704
H47	4.71664015	1.48155598	3.9954674
H48	3.72161932	0.02884948	3.80664292
H49	1.97182838	-4.33660012	6.59398119
H50	0.14779031	-2.68181481	6.38280177
H51	-1.7558904	-2.53739423	5.22962765
H52	-3.70890697	-1.02911315	5.40462911

B3LYP/lacvp* Energy = -1238.236177

Number of Imaginary Frequencies = 0

TS 1c+5c-*Re-exo*

B3LYP/lacvp* Geometry

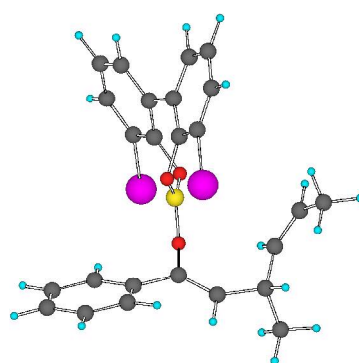
C1	0.04482141	-0.07850864	-0.00309839
O2	0.07020782	-0.06788102	1.30590184
B3	1.30351594	0.07961884	2.17199801
C4	2.38279397	1.02118882	1.33025475
C5	2.50420479	-0.2411528	-0.19886157
C6	1.20657704	-0.07185969	-0.7647569
C7	2.47131839	-3.17653157	3.63748244
C8	1.64944126	-2.0304947	3.53459048
I9	3.76326894	-3.70731531	2.01139719
C10	0.74941157	-2.64762239	5.70403656
C11	0.70257588	-1.80424446	4.5773095
C12	-1.61851101	-1.07547611	5.15703715
C13	-0.3823241	-0.78024826	4.55368046
C14	-1.23239536	1.45527086	4.1144437
C15	-0.20833921	0.50286049	3.98856645
I16	-0.94605664	3.407844	3.2988199
C17	-2.43317206	1.15861028	4.75223423
C18	-2.62864432	-0.12502167	5.26125523
H19	-3.20975239	1.91186363	4.83559507
C20	2.4666675	-4.01735303	4.74268056
C21	1.61154181	-3.72998349	5.80437712
H22	3.12686898	-4.87709266	4.77745073
O23	0.93956023	0.82748222	3.35553315
O24	1.81351415	-1.26708584	2.44182313
H25	1.13430984	0.26209486	-1.79512229
H26	2.64896972	-1.08931807	0.46417952
C27	3.68295954	1.28379705	1.69379886
H28	1.88438781	1.88520807	0.88446833
C29	-3.86177685	0.21163442	-1.73879587
C30	-2.78937512	-0.23989611	-2.51203783
C31	-1.51899444	-0.33913549	-1.95208716
C32	-1.3010719	0.01601387	-0.60976447
C33	-2.38863965	0.45203857	0.1650521
C34	-3.65735243	0.55378497	-0.40031737
H35	-4.85377348	0.28916013	-2.17671502
H36	-2.94575688	-0.52409903	-3.54934638
H37	-0.69782875	-0.72063529	-2.55185512
H38	-2.22556579	0.71362468	1.20465677
H39	-4.48959167	0.90152724	0.2058171
H40	4.09004497	2.27399626	1.47285847

C41	3.68143174	0.03600115	-1.11054687
H42	3.61122245	1.02185712	-1.58192753
H43	4.6380422	-0.04144405	-0.58864147
H44	3.67930634	-0.7158044	-1.91208228
C45	4.63879887	0.35720462	2.36174502
H46	5.57431193	0.27700379	1.78848946
H47	4.92213031	0.78054259	3.33758361
H48	4.22418564	-0.63683506	2.52070351
H49	1.61588486	-4.35012134	6.69601009
H50	0.08542509	-2.42752507	6.53314513
H51	-1.79339636	-2.0767337	5.53690769
H52	-3.57338224	-0.38155074	5.73264419

B3LYP/lacvp* Energy= -1238.217445

Number of Imaginary Frequencies= 1 (-307.67)

Product 1c+5c-*Re-exo*



B3LYP/lacvp* Geometry

C1	1.03151509	0.1609021	-0.15044727
O2	0.89289513	0.76839757	1.09398541
B3	0.77530809	0.11666774	2.27743259
C4	3.75613247	0.88931416	1.15054777
C5	3.58701563	0.61060246	-0.32589046
C6	2.21734446	0.14131021	-0.77526663
C7	1.66879274	-3.2419295	3.10644626
C8	1.00623548	-2.03754229	3.38683432
I9	2.00661542	-3.8515658	1.09762574
C10	1.18149784	-2.5468834	5.74092359
C11	0.70920469	-1.69895967	4.7247183
C12	-1.02276173	-0.66192952	6.18769776
C13	-0.12989773	-0.53213736	5.1095187
C14	-0.80030824	1.80166594	4.93519888
C15	-0.04620733	0.71751793	4.46497258
I16	-0.65052212	3.69707559	3.98094
C17	-1.65714138	1.6578362	6.02352297
C18	-1.77435172	0.4148218	6.64356841
H19	-2.236488	2.50540857	6.37374403
C20	2.10145591	-4.08034936	4.13130573
C21	1.8720975	-3.7181567	5.45656996
H22	2.61905694	-5.00334624	3.8933464
O23	0.7811567	0.92588659	3.39593704
O24	0.63654362	-1.25316744	2.32622709
H25	2.20019157	-0.2402493	-1.79388385
H26	4.28175812	-0.19149204	-0.60926873

C27	4.50539738	0.20288573	2.02417716
H28	3.24309883	1.77835538	1.51325113
C29	-2.6573577	-1.20250109	-1.88559933
C30	-1.44567669	-1.77955606	-2.27298071
C31	-0.24854598	-1.35120814	-1.70518029
C32	-0.23677503	-0.32611247	-0.74325802
C33	-1.46204486	0.24124977	-0.3559244
C34	-2.65931676	-0.19248608	-0.92344811
H35	-3.59149074	-1.54387669	-2.32434939
H36	-1.43486406	-2.58013717	-3.008486
H37	0.68186085	-1.83570627	-1.98509083
H38	-1.47142351	1.03902183	0.38045369
H39	-3.59617416	0.26390845	-0.61357745
H40	4.54482995	0.58275907	3.04639732
C41	3.99178711	1.86120012	-1.14776734
H42	3.34690111	2.71163344	-0.89840376
H43	5.02940192	2.14151463	-0.93512943
H44	3.89888658	1.67324109	-2.22413503
C45	5.31796211	-1.04049396	1.78656247
H46	6.37663937	-0.86335721	2.02241872
H47	4.98178548	-1.85457841	2.44233359
H48	5.25827768	-1.40377619	0.75699042
H49	2.22920061	-4.35284228	6.26243256
H50	1.00711994	-2.26565257	6.77454111
H51	-1.13457102	-1.63223896	6.66052789
H52	-2.45855953	0.28926133	7.47786363

B3LYP/lacvp* Energy = -1238.276187
Number of Imaginary Frequencies = 0

Complex 1c-5c-Si-endo

B3LYP/lacvp* Geometry

C1	0.11927073	0.2051806	-0.11586355
O2	0.23646548	-0.10008219	1.10617828
B3	1.39757308	-0.29728144	2.22050827
C4	2.74992796	-0.89923747	1.60223392
C5	2.30554716	1.32011386	-0.46188028
C6	1.17612838	0.75337078	-0.94219268
H7	1.03352115	0.68476048	-2.01615425
H8	2.42393065	1.44933636	0.60840553
H9	3.66200676	-0.43862189	1.99349952
C10	2.94200059	-1.89889677	0.72574066
C11	-3.73712889	-0.63719792	-1.77326785
C12	-2.86650963	0.20977277	-2.46312908
C13	-1.60760481	0.4908376	-1.94050827
C14	-1.20707656	-0.07053296	-0.71449092
C15	-2.09899735	-0.90835507	-0.01861032
C16	-3.35141809	-1.19385573	-0.55035441
H17	-4.71760594	-0.85978424	-2.18639148
H18	-3.17093184	0.65468766	-3.406304
H19	-0.95217343	1.17011075	-2.47559662
H20	-1.78927809	-1.32736272	0.93308188
H21	-4.02958052	-1.84959052	-0.01165224
C22	0.54125177	2.94267973	3.63948684
C23	0.99525892	1.61781074	3.76649293
I24	0.85177577	4.02533033	1.82080898

O25	1.67259056	1.03321643	2.75347844
C26	0.15627091	1.65638268	6.0498166
C27	0.81743761	0.97313909	5.01767744
C28	1.89310037	-0.69030778	6.53755619
C29	1.32878876	-0.39480471	5.28832526
C30	1.47606691	-2.74724153	4.73005138
C31	1.16551997	-1.4335521	4.33956358
I32	1.06307695	-4.38443444	3.42695599
C33	2.01489503	-3.02931247	5.98344068
C34	2.24603786	-1.99035141	6.88336191
H35	2.25599715	-4.0525578	6.25175855
C36	-0.0984995	3.61370051	4.67801761
C37	-0.30036974	2.95997807	5.89122918
H38	-0.43968888	4.63382889	4.53736752
O39	0.64882204	-1.16713127	3.12028726
C40	3.40361971	1.84529902	-1.32403968
H41	3.20440857	1.70911954	-2.39151572
H42	3.56751773	2.91259504	-1.12351015
H43	4.34447949	1.33709482	-1.07303143
H44	3.96693024	-2.18022128	0.46950571
C45	1.88662301	-2.69358202	0.00818465
H46	2.12662586	-3.7639232	0.02548558
H47	0.89716636	-2.56762258	0.4532736
H48	1.83131558	-2.40208778	-1.05307941
H49	2.68966846	-2.2011106	7.85249865
H50	2.05817654	0.11966765	7.2422623
H51	-0.01048928	1.1385376	6.98948807
H52	-0.8141222	3.46731262	6.70293178

B3LYP/lacvp* Energy = -1238.235961
Number of Imaginary Frequencies = 0

TS 1c+5c-Si-endo

B3LYP/lacvp* Geometry

C1	-0.10406385	0.27012386	0.03376954
O2	-0.020209	-0.09142262	1.28784905
B3	1.22298611	-0.21944564	2.13941466
C4	2.57574157	-0.58876318	1.25579977
C5	2.28920495	0.82765227	-0.12769946
C6	1.01083232	0.62367466	-0.71689747
H7	0.92742113	0.61159665	-1.79862254
H8	2.31150582	1.49549007	0.73127182
H9	3.49159998	-0.1961522	1.70434338
C10	2.77000792	-1.72363245	0.49608719
C11	-4.04295069	-0.05056043	-1.62463168
C12	-3.0758779	0.71780116	-2.27733111
C13	-1.79392254	0.82537965	-1.74567907
C14	-1.45865126	0.16050402	-0.55389112
C15	-2.44167892	-0.59815362	0.1028709
C16	-3.72238583	-0.70533527	-0.43350554
H17	-5.04486494	-0.13053209	-2.03876623
H18	-3.32544048	1.24389521	-3.19498873
H19	-1.05994143	1.45358836	-2.24171461
H20	-2.18685829	-1.0951603	1.03272752
H21	-4.47407513	-1.2978827	0.08112575
C22	0.0819232	2.83785096	3.51647733

C23	0.67809194	1.58089214	3.70769431
I24	0.50198388	3.97401262	1.75575807
O25	1.52148972	1.06221996	2.78352282
C26	-0.42531837	1.4754969	5.87016412
C27	0.44701899	0.90605676	4.93049284
C28	1.6526143	-0.52601251	6.56821368
C29	1.16688329	-0.34948105	5.26433108
C30	1.93701132	-2.58708491	4.75209647
C31	1.33704072	-1.39132545	4.31652581
I32	2.13066932	-4.23772468	3.4078925
C33	2.39660407	-2.754539	6.05510095
C34	2.26389395	-1.7094243	6.9672221
H35	2.85918536	-3.68983013	6.35192894
C36	-0.76687219	3.40140916	4.46609577
C37	-1.03345575	2.70598491	5.6438276
H38	-1.21855574	4.37090065	4.28426043
O39	0.86368106	-1.29278461	3.06078765
C40	3.48497797	0.97315152	-1.04223587
H41	3.48634476	0.23021066	-1.8463998
H42	3.45302996	1.96890826	-1.50620584
H43	4.42724458	0.89945394	-0.49192174
H44	3.78750363	-2.0761984	0.32017872
C45	1.67942055	-2.45360213	-0.19083868
H46	2.01957065	-3.37669532	-0.66629869
H47	0.85727642	-2.67412891	0.49973351
H48	1.24320834	-1.79174804	-0.96731651
H49	2.63710337	-1.82237024	7.98113514
H50	1.55367748	0.29337058	7.27426792
H51	-0.63068656	0.93272972	6.78803745
H52	-1.71097954	3.1289527	6.38026673

B3LYP/lacvp* Energy = -1238.22056

Number of Imaginary Frequencies = 1 (-288.44)

Product 1c+5c-Si-endo

B3LYP/lacvp* Geometry

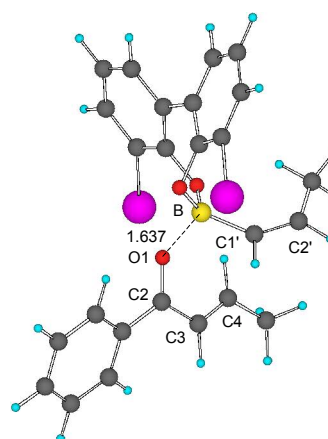
C1	0.42016709	-0.03978637	-0.05754751
O2	0.37743728	-0.70610382	1.15788306
B3	0.61561254	-0.23976382	2.40175443
C4	3.4525661	-0.70663395	0.7523229
C5	2.92194775	0.56602137	0.09776826
C6	1.55839687	0.46579513	-0.55918588
H7	1.48561132	0.87939235	-1.56172393
H8	2.83141751	1.30878887	0.90206258
H9	3.91768914	-0.54554551	1.72580257
C10	3.48350672	-1.95363356	0.26600098
C11	-3.3261679	-0.24966931	-2.15623444
C12	-2.39598975	0.73983871	-2.48241864
C13	-1.18766732	0.82303243	-1.79593833
C14	-0.87549068	-0.09108318	-0.7750866
C15	-1.8254409	-1.0725326	-0.44481424
C16	-3.0356116	-1.15135606	-1.13221159
H17	-4.27141876	-0.31038197	-2.68951952
H18	-2.61825687	1.4601993	-3.26571886
H19	-0.49075694	1.61953669	-2.03842798
H20	-1.60372538	-1.77996254	0.34716763

H21	-3.7534217	-1.92310992	-0.86541054
C22	0.32418286	3.07259086	3.68569584
C23	0.79508242	1.75495409	3.7853364
I24	-0.04526407	3.94759944	1.78295919
O25	1.00932161	1.06482876	2.61833312
C26	0.80191905	1.98798094	6.18734799
C27	1.071714	1.20237869	5.05380221
C28	2.59202988	-0.34771307	6.28731034
C29	1.66456261	-0.14787979	5.25008968
C30	1.78900635	-2.53390969	4.77925417
C31	1.28964214	-1.26079899	4.47115452
I32	1.17931505	-4.22262463	3.63901683
C33	2.6846733	-2.71350443	5.83045154
C34	3.09648093	-1.61031654	6.57707602
H35	3.06575139	-3.70401334	6.0550703
C36	0.0880464	3.84012499	4.82412224
C37	0.3189237	3.28638377	6.08153649
H38	-0.28307237	4.85441188	4.72688067
O39	0.41480124	-1.14605597	3.42588765
C40	3.95748119	1.12331777	-0.9048685
H41	4.09699125	0.43578549	-1.74702578
H42	3.63523033	2.09396928	-1.30228655
H43	4.93051141	1.26001629	-0.42144369
H44	3.94700784	-2.71555761	0.89449156
C45	2.95531223	-2.46090484	-1.04613935
H46	3.7503606	-2.96751709	-1.61073891
H47	2.16395285	-3.20480806	-0.8811391
H48	2.53987357	-1.6677639	-1.67112212
H49	3.81352882	-1.74063915	7.38254132
H50	2.92634652	0.50924494	6.86328326
H51	0.96240045	1.55486972	7.16944035
H52	0.1158207	3.86838771	6.9758289

B3LYP/lacvp* Energy = -1238.273362

Number of Imaginary Frequencies = 0

Complex 1c-5c-Si-exo



B3LYP/lacvp* Geometry

C1	0.17503587	-0.06723993	-0.14292351
O2	0.24538699	-0.1313398	1.11752078
B3	1.40851104	-0.06272088	2.26670844
C4	2.75594311	-0.66911275	1.65964737

C5	2.16744438	1.33645503	-0.56441824
C6	1.20351576	0.49377825	-0.99805731
H7	1.1771627	0.2048245	-2.04447712
H8	2.15331196	1.67530102	0.46563574
C9	4.04253007	-0.32925592	1.85397098
H10	2.60933163	-1.5818929	1.07407386
C11	-3.37622345	-1.76735624	-1.81740193
C12	-2.60559065	-0.89567545	-2.59056752
C13	-1.4450268	-0.33761203	-2.06262017
C14	-1.04727706	-0.64211573	-0.74819883
C15	-1.83891305	-1.50923155	0.02810669
C16	-2.99132666	-2.07235393	-0.50859313
H17	-4.2789169	-2.20664969	-2.23421138
H18	-2.9120242	-0.64806203	-3.60297467
H19	-0.86732457	0.35653772	-2.66444626
H20	-1.52722226	-1.73392841	1.0429767
H21	-3.59153278	-2.74978447	0.09212333
C22	0.1095085	3.11030578	3.45673751
C23	0.75155892	1.87821686	3.67301222
I24	0.20145947	4.04905441	1.53681599
O25	1.48757059	1.32641387	2.67963338
C26	-0.03192937	1.98602889	5.97037925
C27	0.69093673	1.31274021	4.97399571
C28	1.97845331	-0.11548723	6.58333954
C29	1.36928116	0.0387025	5.32869855
C30	1.8284738	-2.30211071	4.88328119
C31	1.32629856	-1.0662211	4.44543249
I32	1.67228743	-4.01783883	3.62334771
C33	2.41053386	-2.44644421	6.13999432
C34	2.49966106	-1.3411629	6.98625688
H35	2.79798677	-3.4106957	6.45217254
C36	-0.59100798	3.77287011	4.46117104
C37	-0.66535376	3.19982095	5.72874629
H38	-1.07772574	4.71939086	4.25250846
O39	0.752377	-0.93670899	3.23083335
H40	4.81280885	-0.97091845	1.41563899
C41	3.24528486	1.88717766	-1.43580028
H42	3.17886217	1.52796915	-2.46744825
H43	3.21378683	2.98492123	-1.43586171
H44	4.22475464	1.60645719	-1.02599568
C45	4.59241891	0.82917453	2.64224027
H46	5.25914949	1.44503466	2.0203661
H47	3.80488709	1.46726299	3.0443624
H48	5.20619378	0.46456004	3.47836614
H49	2.97307155	-1.44343027	7.95886692
H50	2.0464893	0.74334929	7.24478828
H51	-0.1077668	1.52778805	6.95200168
H52	-1.22229953	3.69633991	6.51830069

B3LYP/lacvp* Energy = -1238.239233

Number of Imaginary Frequencies = 0

TS 1c+5c-Si-exo

B3LYP/lacvp* Geometry

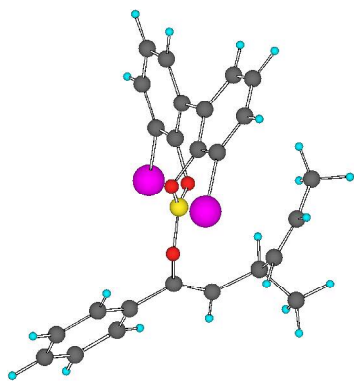
C1	-0.01933331	-0.0458439	-0.02489751
O2	-0.0141452	-0.06979991	1.28290221

B3	1.189176	-0.02482959	2.18860749
C4	2.54438461	-0.45951498	1.3338212
C5	2.24663262	0.89095498	-0.11689649
C6	1.10484776	0.32519082	-0.74989426
H7	1.17512048	0.02862413	-1.79165004
H8	2.0618126	1.67890987	0.60759427
C9	3.84599516	-0.2368767	1.72065538
H10	2.40480499	-1.41576823	0.82398015
C11	-3.6625595	-1.40845099	-1.81581538
C12	-2.74680734	-0.67820394	-2.57744378
C13	-1.56062414	-0.23145975	-2.00238997
C14	-1.27057162	-0.5146878	-0.65679953
C15	-2.20276893	-1.23918054	0.10467466
C16	-3.38764591	-1.68521924	-0.47471416
H17	-4.5904013	-1.75372925	-2.26494881
H18	-2.96338416	-0.44733436	-3.61715486
H19	-0.86948622	0.36387864	-2.59198588
H20	-1.98062283	-1.44591174	1.14613384
H21	-4.09995282	-2.24897771	0.12177488
C22	-0.23420871	2.94872917	3.47484444
C23	0.51745741	1.7844894	3.69779402
I24	-0.09819056	3.96412857	1.59987324
O25	1.35859263	1.31589646	2.74494878
C26	-0.39705281	1.71437295	5.94560102
C27	0.45192147	1.16970558	4.97152369
C28	1.89656558	-0.09395237	6.56943491
C29	1.29663543	-0.0050192	5.30560178
C30	2.18441906	-2.20598878	4.80272376
C31	1.46297992	-1.07291617	4.38784641
I32	2.37357537	-3.87825149	3.48570969
C33	2.76089738	-2.28646407	6.06753532
C34	2.6246291	-1.21664049	6.95170424
H35	3.31423768	-3.17359953	6.35761576
C36	-1.06195226	3.48729446	4.45689231
C37	-1.14950546	2.85777263	5.69754097
H38	-1.63642766	4.38465192	4.25247238
O39	0.87876299	-1.0485763	3.17741893
H40	4.59261423	-0.99757428	1.47959862
C41	3.46640652	1.11197042	-0.98586918
H42	3.7544339	0.20205027	-1.52260744
H43	3.21890905	1.87499659	-1.73715272
H44	4.32512256	1.47544248	-0.41749299
C45	4.3900499	0.96204714	2.42447413
H46	5.26202933	1.36516905	1.88867447
H47	3.64321018	1.74220315	2.56920088
H48	4.76221282	0.65795936	3.41447799
H49	3.08543397	-1.26476605	7.93454496
H50	1.79383895	0.74146447	7.25630791
H51	-0.47261528	1.21773159	6.90869941
H52	-1.80617613	3.26043498	6.46375582

B3LYP/lacvp* Energy = -1238.223847

Number of Imaginary Frequencies = 1 (-312.6)

Product 1c+5c-Si-exo



B3LYP/lacvp* Geometry

C1	0.47082887	-0.19034546	-0.11040768
O2	0.58515153	-0.80986593	1.12531623
B3	0.73135158	-0.23819097	2.34222964
C4	3.44015705	-0.24847475	0.76453741
C5	2.83988265	0.84628055	-0.09376142
C6	1.47955054	0.49885173	-0.66636576
H7	1.29424971	0.86869855	-1.67088884
H8	2.72430535	1.75509495	0.51243782
C9	4.13596485	-0.09966199	1.90004327
H10	3.32509824	-1.25575593	0.36493413
C11	-3.2700066	-1.11135893	-2.02284307
C12	-2.52956437	-0.0011222	-2.43498956
C13	-1.32363411	0.31088525	-1.81329462
C14	-0.82387557	-0.4874356	-0.77018479
C15	-1.5841308	-1.5942915	-0.35528973
C16	-2.79205592	-1.90320337	-0.97879997
H17	-4.21417832	-1.35037491	-2.50554593
H18	-2.90011462	0.63451392	-3.23527185
H19	-0.77941003	1.1975219	-2.1237348
H20	-1.21679293	-2.21676515	0.45355792
H21	-3.3607599	-2.76774604	-0.64533498
C22	-0.23858459	3.02570131	3.396637
C23	0.45775568	1.82480302	3.60065196
I24	-0.63294918	3.72033545	1.42561217
O25	0.85776289	1.12775521	2.48950766
C26	0.2700298	2.17965955	5.98101231
C27	0.75382314	1.40210094	4.91484845
C28	2.45583638	0.24591731	6.33091053
C29	1.57981817	0.20524359	5.23152715
C30	2.19881295	-2.13022249	4.92298206
C31	1.48484832	-0.99840425	4.50510847
I32	2.01602979	-3.95827913	3.85131018
C33	3.0364751	-2.07592518	6.03410928
C34	3.17348841	-0.87608157	6.73088043
H35	3.58609392	-2.95872429	6.34305443
C36	-0.68445262	3.7929642	4.47052138
C37	-0.43780707	3.35645099	5.77030456
H38	-1.22812537	4.71385432	4.29054932
O39	0.68110847	-1.11569225	3.40737414
H40	4.54027553	-1.00371259	2.35709217
C41	3.81120981	1.18193046	-1.25011396
H42	3.9847891	0.30287	-1.88240197
H43	3.40512169	1.97986743	-1.88436218

H44	4.77803421	1.51247369	-0.85784222
C45	4.45564357	1.17621114	2.63015346
H46	5.53932828	1.36032384	2.62935969
H47	3.968463	2.05163717	2.1919335
H48	4.14994685	1.11035569	3.68237216
H49	3.8445413	-0.82008906	7.58318975
H50	2.57694262	1.18004027	6.86994532
H51	0.44491208	1.83535945	6.9952936
H52	-0.80240958	3.9336358	6.61511861

B3LYP/lacvp* Energy = -1238.27825

Number of Imaginary Frequencies = 0

Conjugate Addition of 2d to 1c

Complex 1c-2d-endo

B3LYP/6-31G* Geometry

C1	-0.30132561	0.21752942	-0.29069591
O2	-0.16567238	0.18938588	0.93278553
B3	2.18663576	0.10091868	3.06965406
C4	2.7957291	-1.25199413	2.53668996
C5	1.8518018	1.35721347	-0.7050394
C6	0.67469702	0.90758982	-1.16775584
O7	1.11837446	0.26435498	3.90467524
O8	2.85892233	1.24540441	2.70429216
H9	0.41536547	1.0556472	-2.2127061
H10	2.09315186	1.19720999	0.34476035
C11	4.30932412	-1.3452462	2.55549477
H12	4.74734703	-0.46906629	2.06308352
C13	-3.75397085	-1.7437408	-1.95939881
C14	-2.69856572	-1.39648591	-2.80283534
C15	-1.57502595	-0.74996307	-2.28850012
C16	-1.49056687	-0.45102749	-0.92032142
C17	-2.55377962	-0.8177911	-0.08015366
C18	-3.67894435	-1.45262456	-0.5945272
H19	-4.63170185	-2.24233389	-2.36276106
H20	-2.74834419	-1.63110399	-3.86278
H21	-0.75683311	-0.50396917	-2.95764677
H22	-2.47217286	-0.59010343	0.97782175
H23	-4.49879099	-1.72322882	0.06582661
C24	2.3894934	2.51999551	3.13014376
H25	3.07234123	3.2728333	2.7244847
H26	1.37561989	2.70956183	2.76101569
H27	2.37857915	2.59458553	4.22331203
C28	0.27567247	-0.7651813	4.3878675
H29	-0.56917819	-0.90546806	3.70409013
H30	0.8092798	-1.71576739	4.49491387
H31	-0.10888324	-0.45433734	5.3652622
C32	2.87751069	2.06405541	-1.53286266
H33	2.55691171	2.19310489	-2.57188785
H34	3.09898987	3.05393907	-1.11119499
H35	3.82605713	1.51007876	-1.52678542
C36	1.99458335	-2.20851459	2.02696942
H37	0.92156866	-2.01813788	2.01910969
H38	4.69236401	-1.33997621	3.58535184
H39	4.69900123	-2.24213413	2.06555908

C40	2.37411273	-3.52589353	1.40618232
H41	1.8879459	-4.35690359	1.93646748
H42	2.02415609	-3.57870676	0.36568172
H43	3.45049688	-3.71462851	1.40840106

B3LYP/6-31G* Energy = -873.7787348
Number of Imaginary Frequencies = 0

TS 1c+2d-endo

B3LYP/6-31G* Geometry

C1	-0.0004659	0.00268252	-0.00056406
O2	0.00020593	0.00604814	1.30692585
B3	1.17807125	0.00441417	2.25663861
C4	2.57359055	-0.80802587	1.57929685
C5	2.42255138	0.34160102	-0.13536156
C6	1.16025373	0.10083106	-0.7456761
O7	0.66230628	-0.72873555	3.3736524
O8	1.6434618	1.34460772	2.51984862
H9	1.13403314	-0.22018816	-1.78266635
H10	2.46933163	1.1680154	0.57127487
C11	3.86492639	-0.41516301	2.2846031
H12	3.92767857	0.67115166	2.38422437
C13	-3.85872716	-0.70153875	-1.74123491
C14	-2.83456544	-0.16140556	-2.52203797
C15	-1.58091978	0.07537272	-1.96437326
C16	-1.32999391	-0.2303281	-0.61693731
C17	-2.37025397	-0.75916133	0.1639601
C18	-3.6225065	-0.996304	-0.39712573
H19	-4.83764142	-0.88470098	-2.17709921
H20	-3.01635216	0.08491019	-3.56495715
H21	-0.80001386	0.52323419	-2.57208408
H22	-2.17691597	-0.98110575	1.20804766
H23	-4.41761575	-1.41186419	0.21650991
C24	0.70036442	2.28355618	2.99530785
H25	1.24108938	3.18541523	3.30616505
H26	-0.02554885	2.56339398	2.21769589
H27	0.13682205	1.89812997	3.85637263
C28	1.3396982	-0.7564749	4.60086629
H29	0.61177737	-0.94825952	5.40002938
H30	2.0899379	-1.56575749	4.63828525
H31	1.85332987	0.19059915	4.81968532
C32	3.6634775	0.16078201	-0.97683104
H33	3.61972765	-0.745134	-1.59006828
H34	3.75199622	1.02042568	-1.65674734
H35	4.57207494	0.13525206	-0.37037183
C36	2.46039046	-2.05878906	1.04109679
H37	1.55953137	-2.27067645	0.46094826
H38	3.88395892	-0.82188259	3.30299476
H39	4.76482853	-0.77617835	1.7726732
C40	3.41367682	-3.20587626	1.1360888
H41	2.910133	-4.06767004	1.59793654
H42	3.72136125	-3.5410606	0.13373429
H43	4.30771526	-2.97933699	1.72078674

B3LYP/6-31G* Energy = -873.7278857
Number of Imaginary Frequencies = 1 (-360.83)

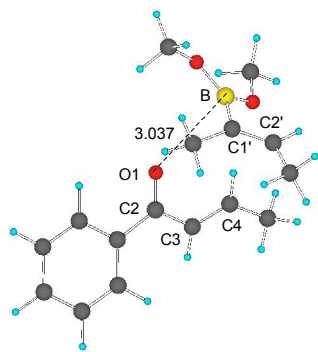
Product 1c+2d-endo

B3LYP/6-31G* Geometry

C1	0.1352164	-0.24407517	0.30747375
O2	0.10982925	-0.46055334	1.66870253
B3	0.49074495	0.38080436	2.6931675
C4	3.24603321	-1.41681912	0.68200522
C5	2.66777954	-0.04397601	0.29686854
C6	1.30060125	-0.09977843	-0.34697781
O7	0.8252049	-0.2577562	3.85270954
O8	0.53388006	1.74662291	2.65895658
H9	1.26031038	-0.03426703	-1.4307186
H10	2.5865464	0.53580437	1.22734145
C11	4.09006106	-1.39526881	1.93250616
H12	3.45972667	-1.17640045	2.80576289
C13	-3.75681784	-0.47884125	-1.5072775
C14	-2.69588894	0.10326967	-2.20461832
C15	-1.43516222	0.19090632	-1.62179316
C16	-1.20161182	-0.31162256	-0.32943162
C17	-2.27968093	-0.88452195	0.36580797
C18	-3.5418095	-0.96919165	-0.21967413
H19	-4.74196794	-0.54223372	-1.96202221
H20	-2.85392026	0.5027316	-3.20323411
H21	-0.6308585	0.67387683	-2.1684186
H22	-2.11489911	-1.27384179	1.36451681
H23	-4.35991769	-1.42242392	0.33448539
C24	0.02690981	2.57157466	1.61847645
H25	-0.15847425	3.56059275	2.04829905
H26	0.75411882	2.66675016	0.80524647
H27	-0.91000399	2.1805851	1.20795296
C28	1.10375683	0.4857948	5.03189084
H29	1.26093878	-0.23360775	5.84026796
H30	2.00587696	1.09711652	4.91368809
H31	0.27114643	1.14820511	5.29497147
C32	3.65483479	0.71887949	-0.61378303
H33	3.76218153	0.205161	-1.57625565
H34	3.30640846	1.74086323	-0.80721675
H35	4.64843574	0.78145154	-0.15725912
C36	3.00906393	-2.50322613	-0.06630591
H37	2.34927408	-2.3833315	-0.92622754
H38	4.60581294	-2.33997312	2.11989779
H39	4.85149637	-0.60476447	1.88409284
C40	3.51616343	-3.90443307	0.13079576
H41	2.6808022	-4.60147123	0.28603209
H42	4.05104886	-4.25495297	-0.76294732
H43	4.19275292	-4.00438035	0.98371127

B3LYP/6-31G* Energy = -873.8097288
Number of Imaginary Frequencies = 0

Complex 1c-2d-exo



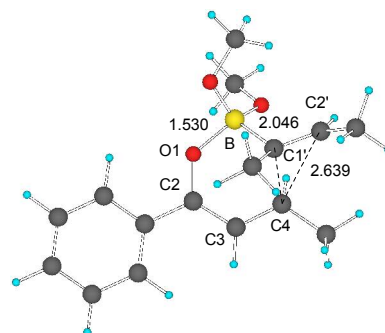
B3LYP/6-31G* Geometry

C1	-0.3981999	0.18405931	-0.28505679
O2	-0.23964682	-0.01344749	0.91991576
B3	2.09900116	0.21249404	3.24645768
C4	2.71557302	-1.02885948	2.49769219
C5	1.37388837	1.8955462	-0.43535615
C6	0.34999862	1.24131677	-1.00625315
O7	1.24465947	0.19131111	4.317748
O8	2.49806598	1.46256756	2.82858818
H9	0.044874	1.4940306	-2.01787327
H10	1.66421333	1.62265669	0.57867803
C11	3.97886413	-0.89375397	2.04478333
H12	4.46761772	0.06610454	2.21417596
C13	-3.25258965	-2.29692978	-2.34677496
C14	-2.35839384	-1.52984251	-3.0938261
C15	-1.4317543	-0.70957957	-2.45057706
C16	-1.38439745	-0.65382337	-1.04924589
C17	-2.28247593	-1.43920693	-0.30935972
C18	-3.21243488	-2.24983784	-0.95065977
H19	-3.97702234	-2.93238231	-2.84989796
H20	-2.37997365	-1.57190129	-4.17956695
H21	-0.73267017	-0.13514119	-3.04936005
H22	-2.22888468	-1.39394162	0.77364014
H23	-3.90645323	-2.84739963	-0.36523722
C24	2.05324983	2.62675441	3.51479208
H25	2.53524691	3.48896148	3.0434735
H26	0.96542905	2.73651849	3.44398382
H27	2.32736993	2.59565302	4.57536691
C28	0.80931398	-0.96689921	5.0051401
H29	0.37289551	-0.64250408	5.95524049
H30	0.04327354	-1.50308204	4.43388815
H31	1.63874708	-1.65151898	5.21866651
C32	4.83564072	-1.89659205	1.32282028
H33	5.75658954	-2.09517987	1.88913996
H34	4.33743278	-2.85451035	1.15308041
H35	5.15417696	-1.50290153	0.34711596
C36	2.16244055	2.98054314	-1.09717586
H37	1.80933959	3.19267803	-2.11183915
H38	2.10947145	3.90798834	-0.51048552
H39	3.22591756	2.71041099	-1.14646598
C40	1.89691905	-2.29053602	2.29264183
H41	1.82273227	-2.89075824	3.20909078
H42	0.87579785	-2.03723606	1.98712593
H43	2.31774503	-2.94065581	1.51943163

B3LYP/6-31G* Energy = -873.7773699

Number of Imaginary Frequencies = 0

TS 1c+2d-*exo*



B3LYP/6-31G* Geometry

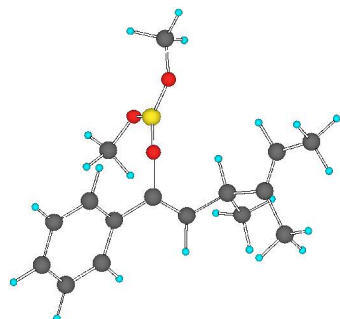
C1	-0.03054314	0.04420216	0.05350098
O2	-0.01978519	0.03463707	1.35869015
B3	1.19960784	0.0428748	2.28207212
C4	2.55989612	-0.53659864	1.42085118
C5	2.27040493	0.85829165	-0.04699137
C6	1.0994479	0.36366125	-0.68398182
O7	0.83956575	-0.9211764	3.2838722
O8	1.50263373	1.37573093	2.73994294
H9	1.14769435	0.06134051	-1.72548866
H10	2.12631588	1.62961968	0.70388253
C11	3.77596101	-0.111862	1.89168653
H12	3.81210318	0.89946967	2.29821742
C13	-3.68008804	-1.33842617	-1.71944919
C14	-2.7824916	-0.58614895	-2.48032916
C15	-1.59882401	-0.12534783	-1.91036196
C16	-1.29345287	-0.41491728	-0.57073733
C17	-2.20912493	-1.15798219	0.19136667
C18	-3.39055596	-1.61985544	-0.38272195
H19	-4.60377568	-1.69834179	-2.16554521
H20	-3.00971404	-0.35142339	-3.51695362
H21	-0.91859842	0.48184768	-2.50070556
H22	-1.97258423	-1.36941113	1.22887511
H23	-4.08784913	-2.2021657	0.21393037
C24	0.46784171	2.09667059	3.37838067
H25	0.90802686	2.97843234	3.85928406
H26	-0.2956276	2.43572102	2.66285597
H27	-0.03749875	1.49434743	4.14627109
C28	1.62163793	-0.99774557	4.44535934
H29	1.2242982	-1.80131732	5.07680318
H30	2.67752121	-1.2321042	4.21789423
H31	1.61483318	-0.06205567	5.02393972
C32	5.07408855	-0.85560234	1.91043674
H33	5.47797531	-0.89601093	2.93150808
H34	4.99200055	-1.87699624	1.53228441
H35	5.8280458	-0.32128938	1.31162086
C36	3.50615286	1.01862556	-0.90579452
H37	3.79324855	0.07778374	-1.38817277
H38	3.29059117	1.74168649	-1.70468139
H39	4.35989118	1.39405926	-0.33652739
C40	2.42526028	-1.94233397	0.86303978

H41	3.2005337	-2.18931838	0.12693653
H42	2.48736794	-2.67165599	1.67883343
H43	1.45453947	-2.08948445	0.38221694

B3LYP/6-31G* Energy = -873.73764

Number of Imaginary Frequencies = 1 (-298.71)

Product 1c+2d-*exo*



B3LYP/6-31G* Geometry

C1	0.18644734	-0.23819977	0.38155702
O2	0.27399373	-0.4786353	1.73599358
B3	0.52934339	0.40567043	2.76337712
C4	3.50252411	-0.83657398	0.22481406
C5	2.64231993	0.43405123	0.2144566
C6	1.25796623	0.15185956	-0.33114359
O7	1.04140021	-0.17190516	3.88950781
O8	0.29967778	1.75272081	2.76236286
H9	1.13610952	0.22259664	-1.40838797
H10	2.55241105	0.76162523	1.25620928
C11	3.86531477	-1.36799013	1.40250966
H12	3.51595331	-0.86620602	2.30569808
C13	-3.66613323	-1.24438371	-1.24646032
C14	-2.7928363	-0.43204921	-1.9731359
C15	-1.54841069	-0.09286832	-1.4503463
C16	-1.14224014	-0.56625701	-0.19032584
C17	-2.03489065	-1.37228121	0.53602441
C18	-3.28101164	-1.7096649	0.01041062
H19	-4.63931579	-1.50494198	-1.65427528
H20	-3.08723129	-0.0500154	-2.94734795
H21	-0.89611539	0.56354569	-2.01833731
H22	-1.73639311	-1.74218146	1.51083162
H23	-3.95237514	-2.34081702	0.58723629
C24	-0.41204853	2.47850464	1.76951865
H25	-0.78132648	3.39582055	2.23823086
H26	0.24423745	2.74423843	0.93403912
H27	-1.2634897	1.91060585	1.3799615
C28	1.22833851	0.59325535	5.07269493
H29	1.56598669	-0.09325453	5.8540666
H30	1.98477325	1.37314594	4.92764844
H31	0.29624951	1.07327876	5.39217782
C32	4.68390959	-2.60112505	1.66386172
H33	4.10914235	-3.32714441	2.25514488
H34	5.01767828	-3.10346744	0.75213073
H35	5.57783929	-2.35724872	2.25468352
C36	3.30345601	1.59062332	-0.56358747

H37	3.38385614	1.36632797	-1.63357305
H38	2.7141488	2.509737	-0.46345736
H39	4.31170579	1.78805117	-0.18266037
C40	3.86301492	-1.41529729	-1.12320307
H41	4.51063889	-0.73655866	-1.69373121
H42	4.38434019	-2.37155744	-1.04146012
H43	2.96447523	-1.58203591	-1.73150799

B3LYP/6-31G* Energy = -873.8109541

Number of Imaginary Frequencies = 0

Conjugate Addition of 5d to 1c

Complex 1c-5d-*Re-endo*

B3LYP/lacvp* Geometry

C1	2.63195428	0.36714273	-1.50757416
O2	1.74566058	0.67190461	-0.65968889
B3	1.212149	0.25174463	0.83467492
C4	2.31468283	0.52808365	1.96901755
C5	3.77405886	-1.52980573	-0.34561118
C6	3.7022172	-0.60013377	-1.32259198
C7	-0.33367256	-3.06913544	1.35808184
C8	-0.31168515	-1.76704315	0.81684229
I9	1.49716594	-4.03790548	1.89927685
C10	-2.73187727	-1.92596139	0.63836675
C11	-1.54941083	-1.20038792	0.40875772
C12	-2.64825309	0.29035116	-1.26843577
C13	-1.6732671	0.11593375	-0.27252085
C14	-1.22128847	2.49547411	-0.40638517
C15	-0.90398773	1.23336023	0.12424709
I16	-0.181049	4.22180819	0.29979393
C17	-2.21661262	2.65822409	-1.36584588
C18	-2.91713956	1.53989058	-1.81657692
H19	-2.43693116	3.64408061	-1.76204577
C20	-1.51181866	-3.78140088	1.55077097
C21	-2.72622284	-3.19592792	1.20006601
H22	-1.48166469	-4.77683522	1.98079483
O23	0.07998891	1.11914323	1.03962049
O24	0.88190673	-1.1662748	0.65493422
H25	4.51450402	-0.53445388	-2.04016125
H26	2.95469629	-1.63894071	0.35595987
C27	1.91678714	-0.00106654	3.33307858
H28	1.79563157	-1.09139187	3.31548153
C29	2.40446295	2.54969528	-5.18748235
C30	3.07624522	1.32543539	-5.15479159
C31	3.17138455	0.61482179	-3.96211815
C32	2.58018118	1.11547236	-2.78712915
C33	1.89021864	2.34019472	-2.83593007
C34	1.81379826	3.05497125	-4.02638481
H35	2.3386369	3.10728969	-6.11823072
H36	3.52270169	0.92253476	-6.05953254
H37	3.67445866	-0.3463333	-3.95795734
H38	1.43090037	2.72578402	-1.93283982
H39	1.29062184	4.00672811	-4.04869464
C40	4.92007962	-2.4701116	-0.18618785
H41	5.69920841	-2.32250141	-0.94054281

H42	5.36348065	-2.34595317	0.81142015
H43	4.56464292	-3.50817623	-0.2333352
C44	3.43203722	1.24476493	1.75584831
H45	2.63181474	0.24225593	4.12480396
H46	0.94353017	0.41540634	3.62493984
H47	3.61368737	1.61900019	0.7471368
C48	4.49914032	1.6566327	2.73671689
H49	4.55113315	2.75210302	2.81597057
H50	4.33901728	1.26008602	3.7425338
H51	5.49226829	1.32434068	2.40070801
H52	-3.65768052	-3.72819995	1.37021169
H53	-3.67866302	-1.46274035	0.37926674
H54	-3.20223887	-0.57643754	-1.61645184
H55	-3.67582819	1.6493445	-2.58665428

B3LYP/lacvp* Energy = -1277.523304
 Number of Imaginary Frequencies = 0

TS 1c+5d-Re-endo

B3LYP/lacvp* Geometry

C1	2.54042062	0.38081091	-1.50198746
O2	1.45317221	0.60742559	-0.79339978
B3	1.18215286	0.14125326	0.59216857
C4	2.54465698	0.1742156	1.60118934
C5	3.61211106	-0.94530409	0.2857915
C6	3.62507397	-0.30332411	-0.99301852
C7	-0.61188895	-3.0969531	1.11493577
C8	-0.51668821	-1.73007245	0.77248183
I9	1.14557744	-4.32044533	1.11368826
C10	-2.93190195	-1.62729913	1.03269601
C11	-1.72991228	-0.98887134	0.67865577
C12	-2.93551096	0.80127588	-0.58846182
C13	-1.82608807	0.41146348	0.18055616
C14	-1.07579125	2.72030387	0.11798396
C15	-0.86111914	1.38909569	0.50710715
I16	0.35488543	4.21262192	0.65692627
C17	-2.19818149	3.09747291	-0.61384848
C18	-3.12508102	2.122287	-0.9810274
H19	-2.34032281	4.13296575	-0.90501755
C20	-1.8157511	-3.71313007	1.43101429
C21	-2.98893124	-2.96211663	1.40925714
H22	-1.83577485	-4.76423489	1.69825493
O23	0.24319312	1.05613703	1.2117782
O24	0.7036103	-1.24416457	0.50062785
H25	4.58157932	-0.17949083	-1.49125448
H26	2.82652481	-1.68102113	0.44856881
C27	2.3400575	-0.61989561	2.88077135
H28	2.07009215	-1.65558771	2.65864437
C29	2.54647485	2.28034695	-5.34790955
C30	3.46941924	1.26879153	-5.07086172
C31	3.47011983	0.64508853	-3.82644631
C32	2.55104908	1.02800377	-2.83450153
C33	1.61623552	2.03455148	-3.1283349
C34	1.61954238	2.65718266	-4.37444487
H35	2.54538175	2.76564388	-6.32070695
H36	4.18270556	0.95825385	-5.82986474

H37	4.17075096	-0.16219618	-3.63436153
H38	0.89419948	2.32138556	-2.37211592
H39	0.89463542	3.43880817	-4.58611994
C40	4.93995432	-1.3444024	0.88785978
H41	5.69260787	-0.5542382	0.79857229
H42	4.84261663	-1.62723288	1.93936021
H43	5.31383668	-2.22604423	0.34820482
C44	3.34762236	1.28668087	1.6158245
H45	3.21798816	-0.63029347	3.53564835
H46	1.50353115	-0.1878008	3.44358782
H47	3.49877092	1.79878874	0.66427832
C48	4.07175792	1.90567566	2.76263393
H49	3.75625615	2.95472095	2.85844857
H50	3.89786784	1.40526539	3.7166297
H51	5.15444619	1.9357576	2.56482052
H52	-3.93592069	-3.41896123	1.68164636
H53	-3.84575266	-1.04160183	1.01999542
H54	-3.65403352	0.04685544	-0.8938936
H55	-3.99099344	2.39672295	-1.57722823

B3LYP/lacvp* Energy = -1277.501402
 Number of Imaginary Frequencies = 1 (-298.35)

Product 1c+5d-Re-endo

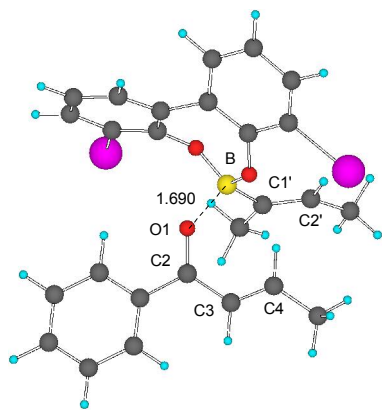
B3LYP/lacvp* Geometry

C1	2.9253832	0.52970293	-0.25356588
O2	1.79325859	0.89237272	0.47577552
B3	0.58123515	0.28941423	0.39183351
C4	5.18652881	0.76074156	2.57076981
C5	4.16333791	-0.14271615	1.86907616
C6	4.02591923	0.11946035	0.39257996
C7	-0.30722226	-3.08910823	-0.37090924
C8	-0.62402976	-1.72745627	-0.25536447
I9	1.69693276	-3.69699334	-0.74235328
C10	-2.93364716	-2.34463023	0.09054044
C11	-1.96485767	-1.33580518	-0.05227142
C12	-3.6436417	0.42714545	-0.6050078
C13	-2.40791038	0.08351207	-0.02975772
C14	-2.16935552	2.40498481	0.66541056
C15	-1.65656634	1.10262609	0.58879048
I16	-1.04892327	3.93552783	1.62749553
C17	-3.40957097	2.71675791	0.11347598
C18	-4.14199541	1.72292274	-0.53436426
H19	-3.79226704	3.72975734	0.17757996
C20	-1.28843311	-4.07042968	-0.24999848
C21	-2.60728569	-3.6918279	-0.00569537
H22	-1.02157798	-5.118062	-0.3358662
O23	-0.43055731	0.85311115	1.14769508
O24	0.39895555	-0.82559998	-0.39329842
H25	4.90853336	-0.06301626	-0.21597214
H26	3.1900556	0.04344408	2.3441983
C27	5.36536506	0.48030557	4.04746479
H28	4.39502065	0.29573529	4.52781831
C29	2.68647704	1.26677156	-4.48456351
C30	3.49626486	0.23948456	-3.99468501
C31	3.56533606	-0.01175346	-2.62604755

C32	2.83238254	0.76606716	-1.71463692
C33	2.01521067	1.7921782	-2.21878432
C34	1.94577988	2.03980571	-3.5892415
H35	2.62799015	1.45686989	-5.55308388
H36	4.06412735	-0.38157668	-4.68299327
H37	4.16802119	-0.83738724	-2.25995387
H38	1.44969191	2.41327745	-1.53004612
H39	1.31265156	2.84344511	-3.95704631
C40	4.50070855	-1.6419812	2.07786125
H41	5.47548468	-1.88407571	1.63620677
H42	4.53785745	-1.90337248	3.14033175
H43	3.74451736	-2.27344553	1.60062234
C44	5.84361286	1.73029764	1.91530421
H45	5.97952586	-0.41269177	4.22557156
H46	5.8392783	1.31203585	4.57434033
H47	5.61612577	1.86990725	0.85944724
C48	6.87680474	2.68349178	2.44987902
H49	6.5640091	3.72569798	2.29643578
H50	7.08491871	2.54885264	3.51455063
H51	7.8277013	2.56356768	1.91132907
H52	-3.37590891	-4.45015603	0.11251055
H53	-3.95887828	-2.05486648	0.29691107
H54	-4.2089082	-0.33765692	-1.12784227
H55	-5.09855687	1.96594249	-0.98807017

B3LYP/lacvp* Energy = -1277.566021
Number of Imaginary Frequencies = 0

Complex 1c-5d-Re-exo



B3LYP/lacvp* Geometry

C1	2.56999018	-12.8801078	-1.77218826
O2	1.65391696	-12.5990819	-0.94815929
B3	1.27716557	-12.9730949	0.6561669
C4	2.64226861	-13.0550769	1.49228632
C5	3.24959183	-15.0953446	-0.88577155
C6	3.49318608	-13.9942964	-1.62971164
C7	-1.05243614	-15.8043917	1.21912072
C8	-0.73142629	-14.4969328	0.79752049
I9	0.45962477	-17.3155545	1.31068911
C10	-3.09229402	-13.9686371	1.02983886
C11	-1.79881805	-13.5727624	0.64230659
C12	-2.69476151	-11.7000705	-0.73572916
C13	-1.65363126	-12.2117459	0.05814145

C14	-0.61119367	-10.0247782	-0.03921737
C15	-0.55293659	-11.374063	0.35315671
I16	0.93310927	-8.67363323	0.55594615
C17	-1.67225234	-9.52188645	-0.78755256
C18	-2.70712113	-10.3769407	-1.16255074
H19	-1.68531825	-8.47716123	-1.08019642
C20	-2.34431412	-16.1847548	1.56333542
C21	-3.37245219	-15.2482856	1.48907061
H22	-2.54216667	-17.1981756	1.89559689
O23	0.50992027	-11.8228284	1.05242748
O24	0.5550455	-14.2246029	0.50800877
H25	4.42766308	-13.9195904	-2.17811011
H26	2.29101508	-15.2033506	-0.38814436
C27	2.86070321	-14.0960238	2.31991166
H28	2.11159397	-14.8861923	2.33604176
C29	2.89943215	-10.2547543	-5.14164086
C30	3.53199532	-11.4998167	-5.17694733
C31	3.43641913	-12.3609875	-4.08797326
C32	2.69998187	-11.9872442	-2.94825157
C33	2.05065909	-10.7397544	-2.93255016
C34	2.15758234	-9.87843807	-4.01896041
H35	2.9819755	-9.58027308	-5.99007072
H36	4.09716912	-11.8005122	-6.05470464
H37	3.91388563	-13.3339386	-4.13934919
H38	1.47534767	-10.4565706	-2.05919477
H39	1.66340078	-8.91147775	-3.98930759
C40	4.00387396	-14.3274116	3.27189004
H41	4.49089669	-15.2923598	3.06711679
H42	4.7727746	-13.5514903	3.23082729
H43	3.63994993	-14.384522	4.30764854
C44	4.20869961	-16.2303994	-0.74746979
H45	5.14209391	-16.0634515	-1.29430419
H46	4.44344662	-16.3872851	0.31367897
H47	3.74938619	-17.1634421	-1.10073323
C48	3.58616553	-11.8779502	1.38398668
H49	4.41136643	-11.9127033	2.10144589
H50	4.0349147	-11.8152933	0.38057167
H51	3.04419313	-10.9379874	1.53615926
H52	-3.50801466	-12.3605103	-1.01974782
H53	-3.52359215	-10.0048758	-1.77515869
H54	-3.89159092	-13.2365634	0.97720249
H55	-4.38140418	-15.5197506	1.7858973

B3LYP/lacvp* Energy = -1277.526961
Number of Imaginary Frequencies = 0

TS 1c-5d-Re-exo

B3LYP/lacvp* Geometry

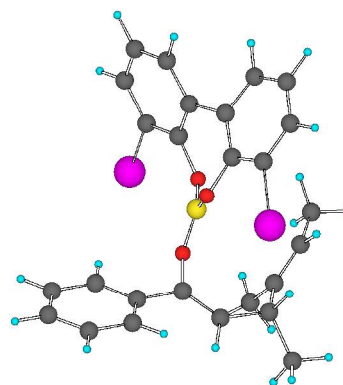
C1	2.45252058	-12.8099684	-1.84079001
O2	1.43366841	-12.5383312	-1.05324685
B3	1.2311599	-13.0384869	0.34317922
C4	2.73843751	-13.343198	1.05122412
C5	3.24565126	-14.6037226	-0.35178078
C6	3.40570384	-13.7448242	-1.4911695
C7	-1.1800673	-15.8113839	1.01474738
C8	-0.81480012	-14.491232	0.67075859

I9	0.26884025	-17.3852867	0.88528779
C10	-3.11068362	-13.8637602	1.15734749
C11	-1.83035082	-13.4948834	0.70678948
C12	-2.7030818	-11.4120552	-0.36258011
C13	-1.64484311	-12.081166	0.27554393
C14	-0.43577583	-9.97685031	0.31017386
C15	-0.46439552	-11.3576838	0.5655538
I16	1.27232318	-8.82130857	0.86495587
C17	-1.50888338	-9.32084356	-0.28799493
C18	-2.63984859	-10.0522026	-0.64739436
H19	-1.45620577	-8.25437266	-0.48105371
C20	-2.4613319	-16.1589832	1.42505372
C21	-3.43507198	-15.1662471	1.51254756
H22	-2.69183855	-17.1867154	1.68380961
O23	0.60390915	-11.9804535	1.11632119
O24	0.4517031	-14.2788139	0.2809328
H25	4.37001425	-13.7124626	-1.98718146
H26	2.31680073	-15.1643607	-0.31091885
C27	2.71297729	-14.2001737	2.13081109
H28	1.99300981	-15.0177776	2.09176302
C29	2.7640225	-10.3285192	-5.32258478
C30	3.47494713	-11.5294497	-5.25784968
C31	3.36986362	-12.3426189	-4.13313674
C32	2.55697095	-11.9644331	-3.05088075
C33	1.83087583	-10.7653039	-3.13330732
C34	1.94032476	-9.95288349	-4.25961395
H35	2.84651139	-9.69344397	-6.20107508
H36	4.10438806	-11.8369492	-6.08893824
H37	3.90231517	-13.2886375	-4.10552059
H38	1.18989381	-10.4782812	-2.30726599
H39	1.38086329	-9.02237408	-4.30699049
C40	3.55620854	-14.1596362	3.35823329
H41	3.99638691	-15.1473142	3.55680486
H42	4.34965068	-13.4106203	3.31894468
H43	2.91838084	-13.9370142	4.22749043
C44	4.46336388	-15.4216488	0.03705063
H45	5.3212599	-14.787343	0.28629803
H46	4.26125277	-16.0874547	0.88023754
H47	4.75557933	-16.0443492	-0.8191007
C48	3.69864391	-12.1640307	1.08581375
H49	4.73135075	-12.4643548	1.30291786
H50	3.70461523	-11.6242825	0.1365213
H51	3.37964165	-11.4532843	1.85509113
H52	-3.58647303	-11.9760639	-0.64503788
H53	-3.46894412	-9.55664312	-1.14485547
H54	-3.8660238	-13.0889735	1.24289905
H55	-4.43511102	-15.4099111	1.85933815

B3LYP/lacvp* Energy= -1277.506882

Number of Imaginary Frequencies= 1 (-252.62)

Product 1c+5d-Re-exo



B3LYP/lacvp* Geometry

C1	2.9098571	-13.1229748	-1.26442802
O2	2.21944715	-12.3773583	-0.31486994
B3	0.99434768	-12.6669894	0.18250488
C4	3.57273487	-13.9533678	1.66333675
C5	3.88717631	-14.8145516	0.44338246
C6	3.69912041	-14.1474827	-0.90798541
C7	-0.99445984	-15.657763	0.05665755
C8	-0.84602847	-14.2721983	0.22515201
I9	0.38265093	-16.7604245	-1.13344314
C10	-2.86712895	-14.2723093	1.54751157
C11	-1.82361986	-13.549124	0.94436027
C12	-3.08056086	-11.3944346	1.01650043
C13	-1.8452139	-12.0640944	1.04599873
C14	-0.77406152	-9.90697464	1.40514736
C15	-0.67878288	-11.292585	1.21439049
I16	0.98580311	-8.7484088	1.69856568
C17	-2.01165575	-9.26872038	1.40311417
C18	-3.16805496	-10.0187216	1.19473454
H19	-2.0693422	-8.19530134	1.54876288
C20	-2.05436728	-16.3478232	0.64069754
C21	-2.98502513	-15.6493823	1.40642878
H22	-2.14448654	-17.4198252	0.50376502
O23	0.56351443	-11.8645678	1.22411974
O24	0.23130409	-13.6722524	-0.37005307
H25	4.2674291	-14.5999419	-1.71744942
H26	3.19974129	-15.674367	0.46604777
C27	2.62192022	-14.3486363	2.52660124
H28	2.08123545	-15.2681555	2.29304524
C29	2.51724438	-11.546465	-5.24485603
C30	2.85795689	-12.8873705	-5.05433815
C31	2.97738691	-13.4068099	-3.76795843
C32	2.76999082	-12.5928122	-2.64156541
C33	2.41623256	-11.2481877	-2.84556835
C34	2.29464836	-10.7315373	-4.13458528
H35	2.41722948	-11.1442552	-6.24977349
H36	3.01478726	-13.5370166	-5.91183947
H37	3.20336214	-14.460486	-3.63565809
H38	2.24870085	-10.6060745	-1.98673653
H39	2.02577898	-9.68686446	-4.27015811
C40	2.20220689	-13.6833141	3.80831065
H41	2.35837003	-14.35398	4.6651814
H42	2.74984712	-12.7587161	4.00702013
H43	1.1318994	-13.4386043	3.78838768

C44	5.32045269	-15.390893	0.53316176
H45	6.075978	-14.5988936	0.48160135
H46	5.4567333	-15.9337138	1.47467976
H47	5.51116909	-16.0866925	-0.29295699
C48	4.4329357	-12.7236558	1.85551896
H49	5.38502623	-12.97861	2.34105756
H50	4.67498537	-12.2634151	0.89208423
H51	3.94074993	-11.9647699	2.46832393
H52	-3.98337844	-11.9689077	0.83524754
H53	-4.13501065	-9.52467171	1.16611309
H54	-3.59156821	-13.7326809	2.14909467
H55	-3.8008327	-16.1809255	1.88783294

B3LYP/lacvp* Energy = -1277.565402
Number of Imaginary Frequencies = 0

Complex 1c-5d-Si-endo

B3LYP/lacvp* Geometry

C1	16.227011	-13.0498892	-2.15087848
O2	15.1327117	-13.0667757	-1.52156811
B3	14.4551784	-13.6486171	-0.16237969
C4	15.016807	-15.1194442	0.19419178
C5	17.7559276	-13.5409961	-0.26856225
C6	17.5148313	-13.4155752	-1.59114382
H7	18.3157383	-13.6050419	-2.29888884
H8	16.9674615	-13.3047214	0.43871036
C9	15.2139651	-15.4360789	1.66456455
H10	15.8667165	-14.6992147	2.14966065
C11	15.8636366	-11.9080357	-6.26034864
C12	17.1206496	-11.8761511	-5.65200141
C13	17.2590909	-12.2483744	-4.31796294
C14	16.1347814	-12.6500229	-3.57405776
C15	14.8694849	-12.6619335	-4.1918437
C16	14.7395732	-12.3007045	-5.52801658
H17	15.7595059	-11.6233032	-7.30420692
H18	17.9921496	-11.5573005	-6.21675786
H19	18.2379768	-12.1960011	-3.85274016
H20	14.0054821	-12.9639964	-3.60880379
H21	13.761643	-12.3238654	-6.00049764
C22	14.597188	-10.4006493	1.50825572
C23	13.9996246	-11.651986	1.26881169
I24	16.6937461	-10.1281714	1.17965526
O25	14.7695902	-12.6951011	0.89100271
C26	11.8994407	-10.6690706	1.99708961
C27	12.6130566	-11.7896939	1.54417927
C28	10.8706733	-13.4254194	2.29319326
C29	11.8751766	-13.0701813	1.37955114
C30	11.22155	-14.9672436	0.01491952
C31	12.0931927	-13.8892301	0.24434255
I32	11.384877	-16.112228	-1.78014914
C33	10.2111978	-15.2912588	0.91713183
C34	10.052031	-14.5288438	2.07400151
H35	9.55801535	-16.1350832	0.72074557
C36	13.8776832	-9.30423354	1.97475707
C37	12.5124193	-9.44063111	2.21457664
H38	14.3766308	-8.35553801	2.14012086

O39	13.0736718	-13.5857995	-0.63004097
C40	19.0696385	-13.9505871	0.30585154
H41	19.8249982	-14.1410816	-0.46276745
H42	19.4426092	-13.1783945	0.9918534
H43	18.9424778	-14.860442	0.90843885
C44	15.203906	-16.0306517	-0.77841413
H45	14.2578736	-15.3814498	2.20313421
H46	15.6336069	-16.4311753	1.84329754
H47	15.0073524	-15.7163743	-1.80584099
C48	15.6218559	-17.4732024	-0.67531822
H49	14.820366	-18.1289831	-1.04459242
H50	16.5007153	-17.6740644	-1.30532902
H51	15.8618101	-17.7869909	0.34421859
H52	9.28233056	-14.7934865	2.79371172
H53	10.7363651	-12.8233494	3.18707785
H54	10.8311388	-10.770592	2.16277444
H55	11.932667	-8.58976879	2.56092497

B3LYP/lacvp* Energy = -1277.523393
Number of Imaginary Frequencies = 0

TS 1c+5d-Si-endo

B3LYP/lacvp* Geometry

C1	15.9795937	-12.7600883	-2.25204008
O2	14.7950169	-12.8547065	-1.67775421
B3	14.4699143	-13.5234855	-0.39780515
C4	15.4516874	-14.8761018	-0.04874626
C5	17.1412093	-13.8627893	-0.37493935
C6	17.1190035	-13.2860772	-1.68955864
H7	17.9846094	-13.4343325	-2.32720317
H8	16.7940305	-13.2153886	0.428798
C9	15.3893207	-15.2711017	1.42013188
H10	15.5781105	-14.4062815	2.06065296
C11	15.8751455	-10.9816059	-6.15393923
C12	17.0843116	-11.0621435	-5.4591957
C13	17.1246873	-11.6347899	-4.19083027
C14	15.9562952	-12.142818	-3.59886229
C15	14.742805	-12.043601	-4.29865251
C16	14.7061179	-11.4713534	-5.56824176
H17	15.843804	-10.5308821	-7.14275316
H18	17.9950131	-10.6663571	-5.90138745
H19	18.0628814	-11.6601495	-3.64468042
H20	13.8375777	-12.4206621	-3.83501086
H21	13.7612935	-11.4048735	-6.10140524
C22	14.4895382	-10.226488	0.89140215
C23	13.8948705	-11.498573	0.84824534
I24	16.6150605	-10.0260362	0.81363869
O25	14.6538174	-12.615024	0.73663327
C26	11.7418138	-10.4118114	1.11729932
C27	12.4918658	-11.5931869	1.01174994
C28	10.759837	-13.027288	2.0751927
C29	11.805857	-12.9051633	1.1468578
C30	11.3414452	-15.1810054	0.45005944
C31	12.1336023	-14.0219123	0.33372369
I32	11.7134466	-16.8464702	-0.83907441
C33	10.2922436	-15.2760515	1.35822564

C34	10.0098022	-14.1927656	2.18874653
H35	9.70710163	-16.1874767	1.42070589
C36	13.7342058	-9.0635452	1.02215
C37	12.3472811	-9.15960264	1.11644553
H38	14.2239203	-8.09587049	1.04290931
O39	13.1006497	-13.9828019	-0.59403558
C40	18.3594655	-14.6773118	0.00376399
H41	18.6589571	-15.372196	-0.7878708
H42	19.1965556	-13.9860147	0.1750196
H43	18.2083513	-15.2377545	0.93006638
C44	15.6805676	-15.8486223	-0.99342448
H45	14.3806727	-15.6279702	1.66226869
H46	16.0943292	-16.0654313	1.68854714
H47	15.7727433	-15.5156913	-2.02852136
C48	15.8591729	-17.3158664	-0.80712874
H49	15.0739773	-17.8424209	-1.36863829
H50	16.815881	-17.6449021	-1.24059164
H51	15.8050306	-17.6385532	0.23376763
H52	9.20707862	-14.2618917	2.91735886
H53	10.5424669	-12.1849225	2.72451166
H54	10.6609697	-10.4854404	1.19243724
H55	11.7455369	-8.25830866	1.1933882

B3LYP/lacvp* Energy = -1277.502536

Number of Imaginary Frequencies = 1 (-296.21)

Product 1c+5d-Si-endo

B3LYP/lacvp* Geometry

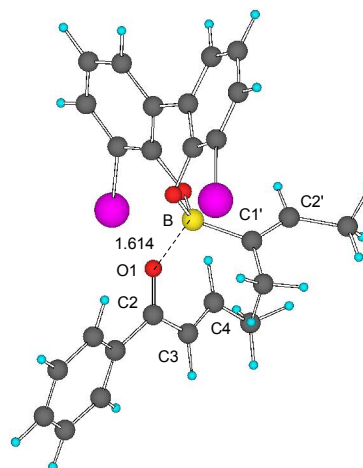
C1	15.8583285	-13.8672987	-1.87803098
O2	14.5096042	-13.9506188	-1.53175868
B3	13.8638703	-13.1289406	-0.6712066
C4	17.0397239	-16.8399949	-0.06929241
C5	16.5579755	-15.3878668	0.048388
C6	16.7710765	-14.5793412	-1.20265625
H7	17.7930397	-14.535754	-1.56863545
H8	15.4804734	-15.4250553	0.26497078
C9	16.9822478	-17.635662	1.21623549
H10	16.0384628	-17.4500709	1.74681798
C11	16.6132903	-11.5046205	-5.38788155
C12	17.6546527	-11.8006704	-4.50424265
C13	17.4146693	-12.5569596	-3.36084082
C14	16.1256348	-13.0456821	-3.0800019
C15	15.0860925	-12.7376521	-3.9730139
C16	15.329414	-11.9751962	-5.11509376
H17	16.8016133	-10.9060841	-6.27552486
H18	18.6565913	-11.4262024	-4.69916152
H19	18.2275818	-12.7441474	-2.66597859
H20	14.0863446	-13.1108826	-3.776026
H21	14.5102707	-11.7503427	-5.79358934
C22	14.5738326	-9.84721628	0.56403814
C23	13.9577454	-11.1025607	0.67607784
I24	16.3386639	-9.60460952	-0.59329271
O25	14.5471561	-12.1634403	0.03365715
C26	12.2794703	-10.099207	2.09449508
C27	12.8032514	-11.2465461	1.47501211
C28	11.5895312	-12.8217259	2.98791985

C29	12.1317594	-12.5500597	1.72093916
C30	11.2153316	-14.6716297	0.95251954
C31	11.9616981	-13.5114609	0.70589803
I32	10.9170274	-16.0965218	-0.59711864
C33	10.6615593	-14.9066668	2.20898148
C34	10.8640986	-13.982168	3.23275341
H35	10.0893068	-15.8104695	2.38871833
C36	14.0454573	-8.72882832	1.20489743
C37	12.8865354	-8.85651003	1.96684974
H38	14.5322463	-7.76530576	1.09969345
O39	12.5000527	-13.3305271	-0.54176697
C40	17.237071	-14.643691	1.22893446
H41	18.3223603	-14.5868535	1.07984841
H42	16.8499261	-13.6223075	1.2998173
H43	17.0529568	-15.1451742	2.18467394
C44	17.4404973	-17.3544022	-1.24274921
H45	17.0540252	-18.7118792	1.04211677
H46	17.7907889	-17.3597626	1.90639068
H47	17.4061873	-16.7049837	-2.11646159
C48	17.9329471	-18.7448976	-1.53654106
H49	17.2956073	-19.2339136	-2.28661503
H50	18.9449504	-18.7133339	-1.96458321
H51	17.9699657	-19.3908879	-0.6555399
H52	10.4565218	-14.1729068	4.22140521
H53	11.7552461	-12.111591	3.79210862
H54	11.3653198	-10.1926966	2.67200639
H55	12.4578522	-7.98495874	2.45309062

B3LYP/lacvp* Energy = -1277.56535

Number of Imaginary Frequencies = 0

Complex 1c-5d-Si-exo



B3LYP/lacvp* Geometry

C1	16.1428046	-0.39216797	-2.32982455
O2	15.058034	-0.31715836	-1.68008301
B3	14.5289247	-0.77095455	-0.22458902
C4	15.1963779	-2.18227299	0.17206836
C5	17.7410263	-0.51560158	-0.43591318
C6	17.4419686	-0.66365616	-1.74788314
H7	18.2127003	-1.00558244	-2.4322482
H8	16.9975063	-0.10843517	0.2390893

C9	15.593942	-2.3920517	1.44389484
H10	15.5123341	-1.55143838	2.13424068
C11	15.6972841	0.10262788	-6.55659603
C12	16.9631637	0.23927648	-5.98204689
C13	17.1262578	0.07768675	-4.60931052
C14	16.0184705	-0.21680609	-3.79409524
C15	14.7443597	-0.3356469	-4.38053645
C16	14.5895112	-0.18399108	-5.75378019
H17	15.5735216	0.22311091	-7.62973403
H18	17.8220347	0.4760517	-6.60365932
H19	18.1106562	0.20981133	-4.17209884
H20	13.8933958	-0.55484447	-3.74393677
H21	13.6048378	-0.28864463	-6.20046886
C22	14.6147176	2.63337454	1.11707764
C23	14.093802	1.32645078	1.06974252
I24	16.6146287	3.03524103	0.4706367
O25	14.8883077	0.30060518	0.69383998
C26	12.0289746	2.2301715	1.97826409
C27	12.7669022	1.12397318	1.52810995
C28	11.2372395	-0.53840565	2.59485857
C29	12.1055451	-0.2071689	1.54394327
C30	11.3496038	-2.18963373	0.37715505
C31	12.2253501	-1.09153572	0.44316227
I32	11.2646896	-3.39910992	-1.382393
C33	10.4704279	-2.48975292	1.41461817
C34	10.4389223	-1.67589861	2.54582122
H35	9.8188594	-3.35407759	1.34031021
C36	13.87465	3.71654383	1.58321297
C37	12.5668714	3.51109272	2.01506353
H38	14.3124634	4.70869013	1.59830346
O39	13.1031531	-0.83754544	-0.54906051
C40	16.1237644	-3.65288939	2.07345268
H41	17.1168711	-3.48168022	2.51490395
H42	15.4749285	-3.97705876	2.89946524
H43	16.2118915	-4.48584912	1.37102739
C44	19.0788365	-0.82650706	0.14678183
H45	19.7869805	-1.20492981	-0.59699544
H46	19.5029305	0.06814466	0.62228518
H47	18.9693104	-1.57483274	0.94303711
C48	15.2580623	-3.25599781	-0.89373913
H49	15.3917033	-4.26447039	-0.49038124
H50	14.3436145	-3.259898	-1.49510657
H51	16.092218	-3.07741962	-1.59023384
H52	9.7780841	-1.92135025	3.37250366
H53	11.1905481	0.11569544	3.46080222
H54	10.9997107	2.07322601	2.28603517
H55	11.9707757	4.3490753	2.36509559

B3LYP/lacvp* Energy = -1277.525999
Number of Imaginary Frequencies = 0

TS 1c+5d-Si-exo

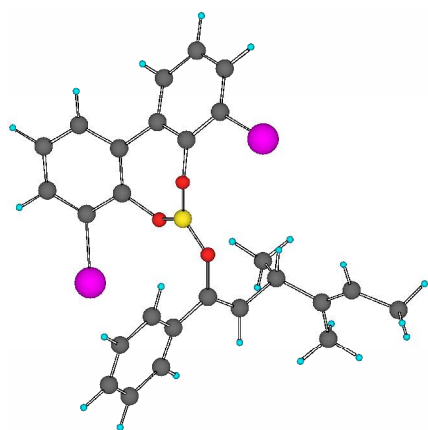
B3LYP/lacvp* Geometry

C1	15.927357	-0.11522801	-2.44285972
O2	14.7922441	-0.04398469	-1.78075352
B3	14.5172306	-0.61090211	-0.42775611

C4	15.5635916	-1.9118547	-0.12980576
C5	17.1724474	-0.80609722	-0.43930468
C6	17.0880014	-0.57084543	-1.84959539
H7	17.8974517	-0.91200589	-2.48707155
H8	16.8358381	0.0065255	0.19519163
C9	15.7628279	-2.21953717	1.19818778
H10	15.7599274	-1.38412542	1.89920654
C11	15.6332047	0.81783846	-6.61488192
C12	16.8803786	0.83181114	-5.98557277
C13	16.9811448	0.5368526	-4.6289289
C14	15.8351968	0.21633887	-3.88157449
C15	14.583844	0.22102722	-4.51878395
C16	14.4871188	0.51470924	-5.87686225
H17	15.5551881	1.05007696	-7.6740133
H18	17.7739155	1.0837641	-6.55081815
H19	17.9503041	0.58176301	-4.14060742
H20	13.698328	-0.01257136	-3.93779221
H21	13.5141195	0.50781363	-6.36099179
C22	14.4275471	2.76850109	0.61973128
C23	13.9260507	1.4621242	0.73940256
I24	16.499752	3.10068131	0.22644022
O25	14.7386271	0.38409575	0.62278066
C26	11.7482624	2.42202489	1.21343172
C27	12.5646923	1.28971867	1.07667163
C28	11.089213	-0.21320948	2.39421857
C29	11.9949309	-0.05719857	1.33402889
C30	11.5236098	-2.34213624	0.68757662
C31	12.2730936	-1.16494952	0.48841165
I32	11.6795535	-3.96887861	-0.6897438
C33	10.6131143	-2.47350737	1.73248408
C34	10.4127103	-1.40861593	2.60840284
H35	10.0648111	-3.40105427	1.85912661
C36	13.6099558	3.88582618	0.77674605
C37	12.2577799	3.70760072	1.0628134
H38	14.0243562	4.88251115	0.66948357
O39	13.1392186	-1.08628107	-0.5364133
C40	15.9904525	-3.563396	1.8041396
H41	16.9007391	-3.55885774	2.42186032
H42	15.1640836	-3.80473764	2.48927908
H43	16.0646075	-4.36390325	1.0652618
C44	18.433068	-1.49111235	0.05037117
H45	18.5732981	-2.47400148	-0.41308504
H46	19.2976137	-0.87367151	-0.22851655
H47	18.445115	-1.61092911	1.13674072
C48	15.5435668	-3.04428443	-1.14602662
H49	16.4773551	-3.62022477	-1.14476038
H50	14.7210846	-3.7321345	-0.93077359
H51	15.3890303	-2.66921408	-2.16032546
H52	9.72118616	-1.5107654	3.43991184
H53	10.9212658	0.62820296	3.05951654
H54	10.6932118	2.28199254	1.42939158
H55	11.6076388	4.57184066	1.16620087

B3LYP/lacvp* Energy = -1277.508523
Number of Imaginary Frequencies = 1 (-267.17)

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B3LYP/lacvp* Geometry

C1	15.6628211	-1.14225464	-1.98588769
O2	14.4097743	-1.2457147	-1.38214313
B3	13.8172531	-0.32457732	-0.58558742
C4	17.513691	-3.77788437	-0.22657066
C5	16.7449164	-2.45907416	-0.09423103
C6	16.7268476	-1.72678926	-1.41649952
H7	17.6606136	-1.68919813	-1.96966151
H8	15.7095608	-2.70585085	0.16470496
C9	16.8309511	-4.93315866	-0.25057283
H10	15.744705	-4.86937183	-0.16494113
C11	15.5854337	0.75347009	-5.84475731
C12	16.79517	0.59956487	-5.1622684
C13	16.8240281	-0.00236974	-3.90842818
C14	15.6435832	-0.47677664	-3.30823749
C15	14.433473	-0.31300276	-4.00274897
C16	14.4068355	0.2956305	-5.25750842
H17	15.5638629	1.23146098	-6.82073098
H18	17.7195696	0.96490567	-5.60275281
H19	17.7686012	-0.0797516	-3.3784444
H20	13.5119308	-0.68161091	-3.56407123
H21	13.4587393	0.40868566	-5.77739168
C22	14.6095218	3.1254779	-0.07243673
C23	13.9550291	1.9424952	0.30199113
I24	16.4275006	3.06165834	-1.16898745
O25	14.5201511	0.75195604	-0.08672422
C26	12.2670653	3.2803716	1.39389795
C27	12.7838592	2.00982583	1.08708607
C28	11.5395785	0.8965981	2.94034089
C29	12.1015121	0.81586181	1.65417085
C30	11.2171342	-1.44729114	1.49243708
C31	11.952443	-0.38919909	0.94102697
I32	10.9729119	-3.25650531	0.40134609
C33	10.6438398	-1.33435874	2.75656876
C34	10.8174504	-0.15858887	3.48532263
H35	10.0793001	-2.16206484	3.17217548
C36	14.0914051	4.3725877	0.2695403
C37	12.9039633	4.44767881	0.99290872
H38	14.6083655	5.27529399	-0.0374163
O39	12.4854963	-0.55903926	-0.30802162
C40	17.3559784	-6.33539004	-0.38772425
H41	17.0825416	-6.94163122	0.48732793

H42	16.9100082	-6.8322131	-1.26063361
H43	18.4428593	-6.38493277	-0.49624677
C44	17.3014848	-1.55310367	1.03016648
H45	18.3158319	-1.20442303	0.80650874
H46	16.6688954	-0.6676763	1.14900669
H47	17.328876	-2.09499583	1.98339362
C48	19.0182956	-3.67899771	-0.32931901
H49	19.4611287	-3.34806767	0.61943127
H50	19.483541	-4.63126808	-0.593966
H51	19.32431	-2.94440657	-1.08623951
H52	10.3929563	-0.07242426	4.48143874
H53	11.6893028	1.80071112	3.52148304
H54	11.3366483	3.34211156	1.94902373
H55	12.4796709	5.41619287	1.24135921

B3LYP/lacvp* Energy = -1277.566385
Number of Imaginary Frequencies = 0