

Supporting Information

Computational evidence for a reaction pathway bifurcation in Sasaki-type (4+3)-cycloadditions.

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Table S1: Free energies for conformers of α -methoxyacrolein-BF₃ adduct.

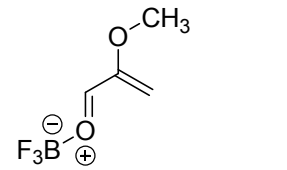
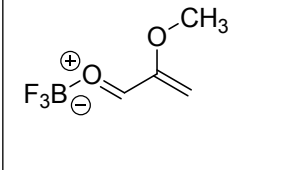
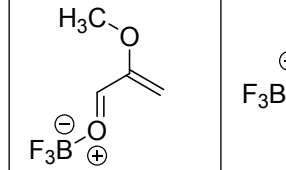
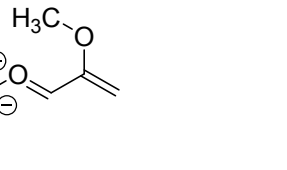
			
A $\Delta G_{\text{rel}} = 0$ kcal/mol	A-CHOtrans 0.43 kcal/mol	A-OMetrans 4.38 kcal/mol	A-CHOtrans-OMetrans 1.90 kcal/mol

Table S2: Energy (E, in Hartrees) of geometries from the potential energy surface (PES) surrounding **TS-1**.

C3-C4 bond (Å)	C1-C7 bond (Å)											
	2.7643	2.6643	2.5643	2.4643	2.3643	2.2643	2.1643	2.0643	1.9643	1.8643	1.7643	1.6643
2.0725	-786.9828625	-786.9827598	-786.9824248	-786.9818285	-786.980958	-786.9798708	-786.9787202	-786.9777216	-786.9772928	-786.9777307	-786.9788684	-786.9798311
1.9725	-786.9834919	-786.9837951	-786.9838044	-786.9836485	-786.9832018	-786.9825284	-786.9818514	-786.9813118	-786.9812823	-786.9819838	-786.9833384	-786.9844566
1.8725	-786.9857866	-786.9864437	-786.9869574	-786.9873839	-787.0109414	-787.0069282	-787.0046334	-786.9863474	-786.9864542	-786.9872662	-786.9884641	-786.9898351
1.7725	-787.0156647	-787.0204762	-787.0221765	-787.0254008	-787.0228362	-787.0191804	-787.0160105	-786.9922355	-786.992203	-786.9929475	-786.9942596	-786.9954083
1.6725	-787.0284712	-787.0298834	-787.0366909	-787.034941	-787.0352329	-787.0308115	-787.0273015	-787.0195194	-787.0112835	-786.9977466	-786.9894825	-786.9999683

Table S3: Energy (E) of geometries from the potential energy surface (PES) surrounding **TS-1-DCM**.

C3-C4 bond (Å)	C1-C7 bond (Å)											
	2.6965	2.5965	2.4965	2.3965	2.2965	2.1965	2.0965	1.9965	1.8965	1.7965	1.6965	1.5965
2.1783	-787.0097546	-787.0096526	-787.0094319	-787.0090626	-787.008696	-787.008628	-787.008775	-787.0104117	-787.0124134	-787.0162815	-787.0192967	-787.0207391
2.0783	-787.0102871	-787.0104637	-787.0105819	-787.0106252	-787.0107227	-787.0110712	-787.0119401	-787.0138062	-787.0167243	-787.0203907	-787.0238839	-787.0252747
1.9783	-787.0123553	-787.0128163	-787.0133806	-787.0138219	-787.014327	-787.015084	-787.0163669	-787.0186012	-787.0218163	-787.0257087	-787.029389	-787.0309543
1.8783	-787.0158059	-787.016721	-787.0175477	-787.0183794	-787.0192048	-787.0202988	-787.021829	-787.0243274	-787.0277254	-787.0317635	-787.0355839	-787.0373191
1.7783	-787.0199526	-787.0212919	-787.0225262	-787.0237102	-787.0246776	-787.026076	-787.0276972	-787.0302829	-787.0337424	-787.0377899	-787.0417998	-787.0437131
1.6783	-787.0237586	-787.0471135	-787.0523847	-787.0523342	-787.0520323	-787.0478251	-787.0446506	-787.035296	-787.0304484	-787.0428829	-787.0469517	-787.049049
1.5783	-787.0512911	-787.0571356	-787.0600842	-787.059691	-787.0600689	-787.0551306	-787.0524705	-787.037183	-787.0372177	-787.0448252	-787.0495812	-787.0512808

Table S4: Energy (E) of geometries from the potential energy surface (PES) surrounding **Dom-TS-1**.

C3-C4 bond (Å)	C1-C7 bond (Å)							
	2.862465	2.662465	2.462465	2.262465	2.062465	1.862465	1.662465	
2.023437	-2529.151323	-2529.150808	-2529.148994	-2529.14606	-2529.143138	-2529.142359	-2529.142698	
1.923437	-2529.151918	-2529.151635	-2529.15016	-2529.147699	-2529.145439	-2529.145317	-2529.146357	
1.823437	-2529.15357	-2529.153515	-2529.152401	-2529.150449	-2529.148745	-2529.149215	-2529.150897	
1.723437	-2529.155525	-2529.155664	-2529.154888	-2529.153354	-2529.152153	-2529.153156	-2529.15554	
1.623437	-2529.156178	-2529.156445	-2529.155954	-2529.154777	-2529.15398	-2529.155459	-2529.158665	

Computational data is listed as follows:

Optimised xyz coordinates

B3LYP electronic energy (E)

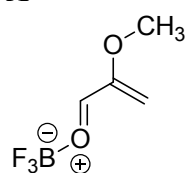
B3LYP enthalpy (H)

B3LYP free energy (G)

M06-2X single-point energies, enthalpies and free energies are listed below as appropriate.

All values are given in Hartrees.

A



C	-1.70160	0.25306	-0.00018
C	-1.98763	1.56791	-0.00008
O	-2.56162	-0.79736	-0.00011
H	-2.99782	1.95730	0.00007
H	-1.16691	2.27476	-0.00015
C	-0.31412	-0.23123	-0.00034
O	0.65591	0.53124	-0.00060
H	-0.16071	-1.31692	-0.00027
C	-3.95238	-0.49516	0.00023
H	-4.46926	-1.45509	0.00039
H	-4.22827	0.07558	0.89603
H	-4.22872	0.07552	-0.89546
B	2.30323	-0.10431	0.00011
F	2.08752	-1.45029	-0.00057
F	2.77459	0.41846	-1.15054
F	2.77294	0.41760	1.15186

0 imaginary frequencies

E = -631.0064567

H = -630.884761

G = -630.934563

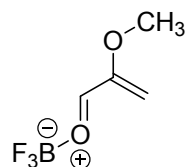
M06-2X

E = -630.9765869

H = -630.855264

G = -630.903185

A-DCM



C	1.67490	0.23429	-0.00075
C	1.93731	1.55784	-0.00071
O	2.55654	-0.79489	-0.00028
H	2.94400	1.95819	-0.00068
H	1.11137	2.25969	-0.00160
C	0.30985	-0.27144	-0.00363
O	-0.68337	0.48368	0.00213
H	0.16728	-1.35572	-0.01046
C	3.94479	-0.45457	0.00208
H	4.48494	-1.40213	0.00381
H	4.20641	0.12069	-0.89434
H	4.20309	0.12205	0.89858
B	-2.20428	-0.07981	0.00047
F	-2.10912	-1.45094	-0.04067
F	-2.72849	0.40207	1.16943
F	-2.74929	0.46989	-1.12814

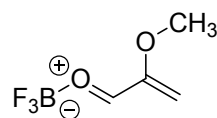
1 imaginary frequencies – **A-DCM** possesses a low frequency (-30 cm^{-1}) vibration corresponding to rotation around the B–O bond. Repeated attempts to locate alternative energy minimised structures (manually adjusting the dihedral, fine integration grid, quadratic convergence) returned the same geometry. The result is likely due to the low barrier to bond rotation in the solvent phase.

E = -155.9972548

H = -155.906249

G = -155.937602

A-CHOtrans



C	1.72691	0.45269	-0.00012
C	2.47312	1.57763	0.00015
O	2.14336	-0.82658	-0.00014
H	3.55592	1.57605	0.00032
H	1.98134	2.54328	0.00019
C	0.26981	0.60055	-0.00052
O	-0.49559	-0.36633	-0.00124
H	-0.13791	1.61750	-0.00024
C	3.54978	-1.05407	0.00012
H	3.67584	-2.13673	0.00009

H	4.01630	-0.62616	-0.89611
H	4.01595	-0.62625	0.89658
B	-2.22481	-0.11234	0.00016
F	-2.31920	1.25197	-0.00169
F	-2.57966	-0.72233	-1.15051
F	-2.57706	-0.71891	1.15349

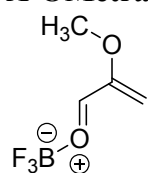
0 imaginary frequencies

E = -631.0066176

H = -630.884661

G = -630.933879

A-OMetrans



C	-1.80055	0.62153	-0.04079
C	-1.91377	1.95687	0.09622
O	-2.91680	-0.14267	-0.20882
H	-2.88835	2.43141	0.11651
H	-1.02306	2.56868	0.16447
C	-0.47505	-0.00361	-0.09907
O	0.56703	0.63805	0.09358
H	-0.39106	-1.07144	-0.32331
C	-2.87983	-1.52632	0.14891
H	-3.92282	-1.84143	0.20674
H	-2.37072	-2.13085	-0.61136
H	-2.40311	-1.67969	1.12502
B	2.11917	-0.15531	0.00091
F	1.76884	-1.44936	-0.26927
F	2.69924	0.51660	-1.01609
F	2.60043	0.07121	1.24176

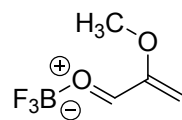
0 imaginary frequencies

E = -630.9981267

H = -630.876616

G = -630.92759

A-CHOtrans-OMetrans



C	-1.92908	0.55087	0.04165
C	-2.64393	1.69000	-0.08421

O	-2.54602	-0.61241	0.34555
H	-3.72420	1.68204	0.00928
H	-2.15015	2.64116	-0.24535
C	-0.47663	0.67894	-0.05627
O	0.31127	-0.25275	0.15323
H	-0.07914	1.66394	-0.32560
C	-2.05264	-1.85163	-0.19970
H	-2.86681	-2.56377	-0.05752
H	-1.83880	-1.75271	-1.26942
H	-1.15918	-2.18998	0.32630
B	2.03689	-0.00557	0.00267
F	2.11243	1.31493	-0.33780
F	2.45569	-0.31577	1.24735
F	2.33472	-0.88145	-0.98180

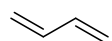
0 imaginary frequencies

E = -631.0025284

H = -630.880794

G = -630.931543

BD



C	-0.32610	-0.65172	0.00001
C	0.32610	0.65172	0.00001
C	0.32610	-1.82292	-0.00001
H	-1.41654	-0.64533	0.00003
H	-0.20119	-2.77210	-0.00001
H	1.41305	-1.86915	-0.00003
C	-0.32610	1.82292	-0.00001
H	1.41654	0.64533	0.00003
H	0.20119	2.77210	-0.00001
H	-1.41305	1.86915	-0.00003

0 imaginary frequencies

E = -155.9921449

H = -155.901063

G = -155.932441

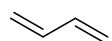
M06-2X

E = -155.9507634

H = -155.860099

G = -155.8913

BD-DCM



C	-0.32712	0.65185	-0.00000
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C	0.32712	-0.65185	-0.00000
C	0.32712	1.82317	0.00000
H	-1.41807	0.64570	-0.00001
H	-0.20202	2.77243	0.00001
H	1.41501	1.86933	0.00001
C	-0.32712	-1.82317	0.00000
H	1.41807	-0.64570	-0.00001
H	0.20202	-2.77243	0.00001
H	-1.41501	-1.86933	0.00001

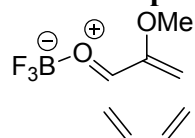
0 imaginary frequencies

E = -155.9972548

H = -155.906249

G = -155.937602

A•BD complex

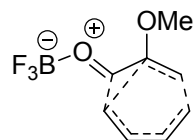


C	-0.69251	2.30175	-1.22959
C	0.57329	2.08647	-0.83816
C	1.17208	2.54726	0.42333
C	0.85864	3.68525	1.05599
C	-2.08707	-0.97556	1.68253
C	-1.84312	-0.84022	0.36624
O	-2.73030	-0.61124	-0.63548
C	-4.09887	-0.47981	-0.26976
C	-0.48441	-0.94527	-0.17810
O	0.49803	-1.17878	0.53833
B	2.06606	-1.30835	-0.12370
F	1.88182	-0.98766	-1.44412
F	2.74510	-0.37948	0.59988
F	2.37378	-2.60148	0.12111
H	1.22445	1.48914	-1.47564
H	-1.05810	1.95232	-2.19121
H	1.94344	1.89826	0.83403
H	1.33389	3.96067	1.99322
H	0.13475	4.38838	0.65023
H	-1.25225	-1.15985	2.34735
H	-3.07781	-0.90673	2.11343
H	-1.39966	2.84304	-0.60513
H	-0.36301	-0.83290	-1.25875
H	-4.64294	-0.30142	-1.19761
H	-4.46753	-1.39776	0.20561
H	-4.24174	0.36709	0.41333

0 imaginary frequencies

E = -786.9998742
H = -786.784897
G = -786.851326

TS-1



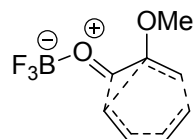
C	0.64618	1.19169	1.78098
C	0.06535	2.01986	0.86434
C	0.64317	2.35765	-0.38853
C	1.89066	1.91735	-0.82235
C	1.67365	-0.06863	-1.37364
C	1.32300	-0.80766	-0.24030
O	2.20247	-1.38837	0.62906
C	3.51336	-1.67994	0.15678
C	-0.04673	-0.91994	0.13708
O	-0.95866	-0.43873	-0.60336
B	-2.49580	-0.43285	-0.11460
F	-2.53574	-1.22768	1.01335
F	-2.74735	0.89600	0.15332
F	-3.19201	-0.93052	-1.17571
H	-0.96894	2.31082	1.01860
H	0.10039	0.88972	2.66979
H	0.00199	2.86839	-1.10317
H	2.26739	2.28963	-1.77161
H	2.66354	1.70250	-0.08937
H	0.88046	0.07965	-2.09535
H	2.67074	-0.16056	-1.79166
H	1.68374	0.88186	1.73156
H	-0.31426	-1.48157	1.03300
H	3.98624	-2.27502	0.93955
H	3.47865	-2.25853	-0.77505
H	4.10280	-0.76834	-0.00358

1 imaginary frequency

E = -786.9828625
H = -786.768171
G = -786.827128

M06-2X

E = -786.918718
H = -786.70506
G = -786.762796

TS-1-exo-cis

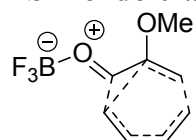
C	0.41628	1.62038	-1.25493
C	1.75164	1.79422	-1.01823
C	2.35575	1.78851	0.26732
C	1.67263	1.45556	1.43618
C	1.41269	-0.56705	1.46887
C	1.01359	-0.98390	0.19351
C	-0.33920	-0.87137	-0.22526
O	-1.24274	-0.48116	0.58034
B	-2.69937	-0.09362	0.02446
F	-3.55828	-0.47299	1.01015
O	1.88229	-1.36449	-0.78268
C	3.12124	-1.95291	-0.39329
F	-2.60622	1.27559	-0.15386
F	-2.85003	-0.77806	-1.16344
H	2.42127	1.87027	-1.87312
H	0.04783	1.55582	-2.27463
H	3.43718	1.90384	0.31369
H	2.18944	1.56741	2.38624
H	0.60169	1.63434	1.48401
H	2.38986	-0.85627	1.83881
H	0.62830	-0.53609	2.21719
H	-0.34948	1.68437	-0.49096
H	-0.61207	-1.17757	-1.23675
H	3.56642	-2.33898	-1.31170
H	3.80110	-1.21723	0.05089
H	2.96193	-2.77816	0.31216

1 imaginary frequency

E = -786.9805288

H = -786.765655

G = -786.765655

TS-1-endo-trans

C	0.50798	-1.43958	-1.16891
C	1.18507	-2.35001	-0.39998
C	2.46657	-2.12570	0.15829
C	3.15766	-0.92057	0.04780
C	2.05991	0.41178	1.19531

C	0.99194	0.88134	0.42080
C	-0.31909	0.32572	0.56817
O	-1.32602	0.79105	-0.03783
B	-2.71560	-0.01487	0.05939
F	-3.67903	0.94220	-0.00516
O	1.10999	1.82068	-0.54959
F	-2.67391	-0.86240	-1.03345
F	-2.67055	-0.70038	1.25961
H	0.65756	-3.24943	-0.08787
H	-0.53290	-1.58992	-1.43820
H	2.83641	-2.86148	0.87007
H	4.13764	-0.84730	0.51284
H	3.04707	-0.31931	-0.85039
H	1.80431	-0.21512	2.04124
H	2.91284	1.05960	1.36898
H	1.00236	-0.59775	-1.64146
H	-0.46191	-0.45632	1.31479
C	2.22117	2.71289	-0.50956
H	2.04516	3.43612	-1.30664
H	2.27092	3.23450	0.45421
H	3.17082	2.19687	-0.69564

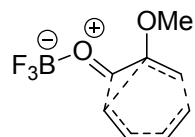
1 imaginary frequency

E = -786.9807844

H = -786.765697

G = -786.823327

TS-1-exo-trans



C	-0.44863	-1.88664	-0.38311
C	-1.58924	-1.62978	-1.09955
C	-2.82787	-1.29218	-0.50655
C	-2.98146	-1.11323	0.87284
C	-1.89683	0.52637	1.44569
C	-0.91755	0.82226	0.48469
O	-1.20356	1.42633	-0.68568
C	0.43141	0.38211	0.63565
H	-1.51243	-1.55387	-2.18182
H	0.51977	-1.99336	-0.86110
H	-3.63794	-0.98628	-1.16540
H	-3.97144	-0.87065	1.25115
H	-2.40869	-1.75050	1.54073
H	-2.75417	1.18550	1.52554
H	-1.52764	0.17646	2.40530
H	-0.48533	-2.13774	0.67226

O	1.35617	0.71459	-0.15950
H	0.68782	-0.17209	1.54168
C	-2.34683	2.27835	-0.76836
H	-2.31225	2.71445	-1.76733
H	-3.28210	1.72192	-0.64892
H	-2.29115	3.07679	-0.01866
B	2.78373	-0.00954	-0.01392
F	3.68978	0.91889	-0.42113
F	2.89261	-0.36731	1.31791
F	2.67294	-1.10867	-0.84681

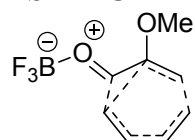
1 imaginary frequency

E = -786.9760011

H = -786.761113

G = -786.818869

TS-1-DCM



C	0.64436	1.19393	1.74189
C	0.24457	2.10589	0.80749
C	0.93765	2.39437	-0.40329
C	2.14447	1.83137	-0.77701
C	1.64451	-0.19724	-1.39311
C	1.25332	-0.86457	-0.23839
O	2.09444	-1.47779	0.64174
C	3.41309	-1.80333	0.19251
C	-0.10516	-0.87080	0.17780
O	-1.03320	-0.40758	-0.57951
B	-2.50578	-0.36414	-0.12567
F	-2.64154	-1.13445	1.02319
F	-2.80411	0.97002	0.11494
F	-3.23846	-0.87416	-1.18204
H	-0.74176	2.54963	0.91752
H	0.01104	0.97778	2.59796
H	0.41054	3.00370	-1.13461
H	2.59869	2.13491	-1.71601
H	2.83584	1.45516	-0.02918
H	0.86633	0.07226	-2.09517
H	2.63265	-0.34693	-1.81276
H	1.63662	0.75673	1.76001
H	-0.37308	-1.39198	1.09632
H	3.86413	-2.38301	0.99972
H	3.37909	-2.40966	-0.72062
H	4.01508	-0.90525	0.01503

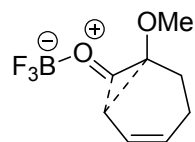
1 imaginary frequency

E = -787.0097596

H = -786.795465

G = -786.854522

TS-2



C	-0.32897	0.45704	-1.42190
C	-0.18667	1.82233	-0.90280
C	-1.04453	2.37660	-0.02852
C	-2.20457	1.63363	0.55962
C	-1.75720	0.27934	1.24211
C	-1.24511	-0.73285	0.28157
O	-2.02000	-1.62836	-0.31356
C	-3.45506	-1.58819	-0.20249
C	0.13707	-0.79928	-0.07611
O	1.04101	-0.27986	0.71750
B	2.49447	-0.28444	0.17151
F	2.70938	-1.54014	-0.38968
F	2.54903	0.70629	-0.81905
F	3.29610	-0.01248	1.24535
H	0.72842	2.34354	-1.16293
H	0.49835	0.15430	-2.06059
H	-0.83603	3.36913	0.36306
H	-2.69830	2.23320	1.32958
H	-2.96519	1.40799	-0.19866
H	-0.94806	0.49345	1.94365
H	-2.60697	-0.13046	1.79654
H	-1.28801	0.20164	-1.87567
H	0.42469	-1.65248	-0.69617
H	-3.80782	-2.39731	-0.84118
H	-3.76485	-1.77365	0.82982
H	-3.85699	-0.63606	-0.55496

1 imaginary frequency

E = -786.9994004

H = -786.782439

G = -786.837991

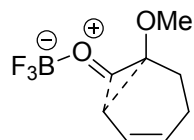
M06-2X

E = -786.947793

H = -786.731779

G = -786.785865

TS-2-DCM



C	0.59258	0.35761	1.39018
C	0.41473	1.75802	0.99328
C	1.21270	2.35022	0.08752
C	2.27696	1.59220	-0.64912
C	1.70323	0.28251	-1.28152
C	1.18124	-0.73123	-0.30667
O	1.92494	-1.74906	0.14058
C	3.35345	-1.60668	0.28575
C	-0.19702	-0.85603	-0.00749
O	-1.10994	-0.20480	-0.67344
B	-2.52934	-0.20256	-0.13255
F	-2.86495	-1.50158	0.25379
F	-2.57386	0.65713	0.96942
F	-3.32784	0.25087	-1.16793
H	-0.43905	2.28813	1.40535
H	-0.16274	-0.02752	2.07340
H	1.02834	3.38361	-0.19724
H	2.69345	2.19809	-1.45820
H	3.11111	1.32894	0.01368
H	0.87876	0.54850	-1.94694
H	2.47902	-0.19547	-1.88697
H	1.58354	0.07849	1.74876
H	-0.49622	-1.70438	0.60831
H	3.71064	-2.60179	0.55167
H	3.82413	-1.28490	-0.64664
H	3.58841	-0.90540	1.09140

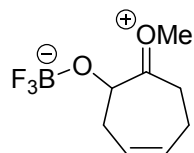
1 imaginary frequency

E = -787.0354412

H = -786.818543

G = -786.873498

Prod-1



C	-0.06451	0.51890	-1.43415
C	-0.03800	1.88700	-0.83404
C	-0.93995	2.37854	0.02787
C	-2.12689	1.62634	0.55874
C	-1.75472	0.24009	1.24637

C	-1.31378	-0.70444	0.20777
O	-2.12139	-1.49444	-0.43297
C	-3.54348	-1.56478	-0.14669
C	0.06510	-0.66958	-0.29925
O	0.96473	-0.37675	0.66952
B	2.42170	-0.36190	0.21946
F	2.59776	-1.44206	-0.65755
F	2.65437	0.84220	-0.46960
F	3.18037	-0.46218	1.35975
H	0.84287	2.47977	-1.05629
H	0.82907	0.35286	-2.03662
H	-0.77639	3.36904	0.44563
H	-2.63413	2.21281	1.32996
H	-2.86973	1.43251	-0.22711
H	-0.91154	0.39577	1.92242
H	-2.62405	-0.12940	1.79649
H	-0.94978	0.33127	-2.05558
H	0.28542	-1.57710	-0.87937
H	-3.93835	-2.25992	-0.88547
H	-3.69441	-1.95763	0.86107
H	-4.00937	-0.58507	-0.25797

0 imaginary frequencies

E = -787.0015267

H = -786.783196

G = -786.839684

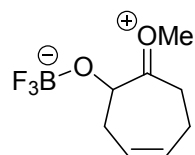
M06-2X

E = -786.9537159

H = -786.735864

G = -786.790183

Prod-1-DCM



C	-0.08624	0.70085	-1.45442
C	-0.22728	2.04372	-0.79080
C	-1.14905	2.39640	0.11648
C	-2.24572	1.52361	0.66771
C	-1.76494	0.13252	1.25063
C	-1.28432	-0.70573	0.14356
O	-2.01307	-1.54268	-0.49562
C	-3.42217	-1.79277	-0.16664
C	0.07703	-0.50815	-0.43833
O	0.99050	-0.26673	0.57211
B	2.41939	-0.35155	0.22440

F	2.67848	-1.54716	-0.47912
F	2.80576	0.74030	-0.58575
F	3.13312	-0.32743	1.42535
H	0.52484	2.78219	-1.05974
H	0.82269	0.68343	-2.05797
H	-1.10412	3.40390	0.52578
H	-2.73618	2.02751	1.50457
H	-3.02194	1.33364	-0.08455
H	-0.92843	0.30611	1.92981
H	-2.59533	-0.33323	1.78445
H	-0.92835	0.48196	-2.12503
H	0.32670	-1.39281	-1.03912
H	-3.74734	-2.51412	-0.91332
H	-3.48341	-2.21559	0.83680
H	-3.98572	-0.86396	-0.24895

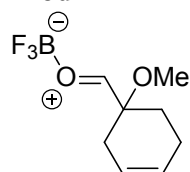
0 imaginary frequencies

E = -787.0513178

H = -786.83212

G = -786.887925

Prod-2



C	-0.94966	0.19504	-0.15914
C	-1.35713	-0.08901	1.29961
C	-2.78202	-0.56946	1.41189
C	-3.49408	-1.01782	0.37495
C	-2.94838	-1.09930	-1.02617
C	-1.41707	-0.97948	-1.06283
O	-1.53474	1.35797	-0.73785
C	-1.41556	2.57221	-0.00762
C	0.54708	0.29811	-0.33422
O	1.35042	-0.32729	0.35555
B	3.09800	-0.22821	0.04529
F	3.37060	-1.51527	-0.24820
F	3.14553	0.64692	-0.99730
F	3.53104	0.24146	1.23232
H	-3.22602	-0.53840	2.40503
H	-0.66151	-0.83469	1.70599
H	-4.52496	-1.33349	0.52513
H	-3.23574	-2.05290	-1.48837
H	-3.39757	-0.31109	-1.64463
H	-0.95097	-1.89945	-0.69318
H	-1.07191	-0.81551	-2.08965

H	-1.20579	0.80736	1.91299
H	0.91105	0.93062	-1.15661
H	-1.71453	3.36738	-0.69430
H	-2.07792	2.59228	0.86682
H	-0.38310	2.76371	0.32258

0 imaginary frequencies

E = -787.0488787

H = -786.830411

G = -786.888827

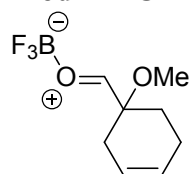
M06-2X

E = -786.995321

H = -786.777583

G = -786.833632

Prod-2-DCM



C	-0.93287	0.21500	-0.15664
C	-1.33506	-0.07501	1.30375
C	-2.75299	-0.57692	1.40846
C	-3.44776	-1.05211	0.37034
C	-2.88719	-1.14625	-1.02358
C	-1.35978	-0.98480	-1.05727
O	-1.55157	1.35565	-0.73820
C	-1.44917	2.58257	-0.01581
C	0.55005	0.35368	-0.34259
O	1.37051	-0.29931	0.32113
B	2.98389	-0.22806	0.05586
F	3.29565	-1.49809	-0.34153
F	3.16513	0.72332	-0.91746
F	3.48436	0.12315	1.27789
H	-3.20676	-0.53438	2.39705
H	-0.63518	-0.81479	1.71342
H	-4.47631	-1.38026	0.51288
H	-3.13934	-2.11903	-1.46576
H	-3.36008	-0.39024	-1.66451
H	-0.87052	-1.88635	-0.67455
H	-1.01343	-0.82046	-2.08311
H	-1.20027	0.82560	1.91339
H	0.90489	1.01785	-1.13912
H	-1.75326	3.36816	-0.71229
H	-2.11735	2.60374	0.85378
H	-0.42105	2.78753	0.31594

0 imaginary frequencies

E = -787.0694148

H = -786.851353

G = -786.908556