

Supporting Information (SI)

The Atmospheric Importance of Methylamine Additions to Criegee Intermediates

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1 Geometries and Harmonic Frequencies

1.1 Reactants

1.1.1 Simple Criegee Intermediate

CCSD(T)/ANO1 Coordinates (Angstroms)

C	1.135311597749	-0.244904665423	0.000000000000
H	1.055269236982	-1.324770697625	0.000000000000
H	2.049262657122	0.330767757421	0.000000000000
O	0.062849717504	0.449505680840	0.000000000000
O	-1.110217867173	-0.203137561719	0.000000000000

CCSD(T)/ANO1 Frequencies (cm^{-1})

534.2830 631.7639 841.9159 960.7317 1236.6206 1298.1543 1480.4939 3145.3618
3305.5852

1.1.2 Anti-Methylated Criegee Intermediate

CCSD(T)/ANO1 Coordinates (Angstroms)

C	-0.476590126260	0.447548996881	-0.000820985583
O	0.460313499348	-0.413324062707	-0.000054795581
O	1.740623141549	0.040664145239	-0.072127481339
H	-0.175063609056	1.489355759184	-0.059693934909
C	-1.878567833985	-0.037566060952	0.077556733906
H	-2.371740486419	0.373867606200	0.962212010764
H	-2.442829600846	0.294961429303	-0.797741053253
H	-1.898365618332	-1.125398053326	0.127128684272

CCSD(T)/ANO1 Frequencies (cm^{-1})

144.5429 247.0678 322.5822 556.5842 833.8044 906.9339 957.3256 1042.4121
1151.8449 1302.8293 1409.4247 1455.2864 1470.7105 1512.8059 3038.5353 3102.8803
3152.6613 3178.2967

1.1.3 Syn-Methylated Criegee Intermediate

CCSD(T)/ANO1 Coordinates (Angstroms)

C	-0.597770108223	-0.681470579020	0.000000000000
O	0.677522098625	-0.600770646932	0.000000000000
O	1.203265484433	0.653393318682	0.000000000000
H	-0.957336084276	-1.702966297843	0.000000000000
C	-1.425361972824	0.537479129035	0.000000000000
H	-1.158982553731	1.145304664107	-0.870830967641
H	-2.485075510902	0.291678508371	0.000000000000
H	-1.158982553731	1.145304664107	0.870830967641

CCSD(T)/ANO1 Frequencies (cm^{-1})

208.1820 304.6305 440.8503 671.9088 710.9220 925.7600 969.5007 1025.5769
1110.8520 1301.5664 1390.6076 1443.8630 1461.6846 1506.0096 3030.6664 3085.4452
3161.8836 3213.4876

1.1.4 Methylamine

CCSD(T)/ANO1 Coordinates (Angstroms)

N	-0.531760777045	-0.328886861588	-0.373340089624
H	-0.531677783170	-1.309986525589	-0.116046187140
H	-1.417474314867	0.036528147378	-0.040563701703
C	0.565164156925	0.353517423542	0.325953882100
H	1.516502046139	-0.054532785669	-0.019858990624
H	0.551411660505	1.412515512005	0.062383961837
H	0.540396091657	0.275873506449	1.420325858795

CCSD(T)/ANO1 Frequencies (cm^{-1})

311.8438	878.5676	977.0867	1063.0296	1190.0389	1359.1463	1458.4317	1506.1329
1524.8181	1668.0207	2998.0889	3081.3589	3118.2493	3498.1095	3579.6483	

1.2 Simple Criegee Intermediate Addition

1.2.1 Equatorial Pre-reactive Complex

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.229983892580	-1.127805284387	0.179772642242
O	-1.629796978803	0.105753663209	-0.259711715224
C	-1.118035541791	1.107830256279	0.316120827853
H	-1.421622854536	2.068288224353	-0.078044132891
H	-0.443200351674	0.955132685125	1.146234877083
H	0.751657340038	-0.647779716508	-0.470477312889
N	1.396321165995	0.137532621588	-0.546677778290
C	2.535648427784	-0.085919129096	0.351774537395
H	1.719765845606	0.149033360741	-1.507429593508
H	3.224610986331	0.758755515992	0.287464722533
H	3.101693938124	-1.004029614290	0.153180765283
H	2.173643675123	-0.137346682006	1.380978615468

CCSD(T)/ANO1 Frequencies (cm^{-1})

44.8323	63.8774	95.3523	142.3164	170.4133	224.8439	424.7773	521.2369
651.4353	868.9233	926.5170	933.5888	1011.0960	1068.7107	1195.8571	1231.0532
1353.1304	1375.0403	1457.6382	1503.6957	1508.0087	1526.6904	1677.2761	3004.7332
3076.4829	3110.3414	3154.1717	3307.9619	3453.9770	3563.5802		

1.2.2 Equatorial Transition State

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.398122163252	-1.019741455483	0.244552529686
O	-1.491028787864	0.323778044095	-0.222875999368
C	-0.625366435437	1.061653838540	0.320272664043
H	-0.561884039063	2.075613692559	-0.058726151476
H	-0.185323605775	0.754911222251	1.260139968056
H	0.499712714260	-0.800505957800	-0.448332724667
N	1.146037898034	-0.008716369921	-0.539179738456
C	2.370094243913	-0.234236142885	0.231273477129
H	1.341674853564	0.132989599106	-1.522740408202
H	3.028308578700	0.631921295747	0.145179909883
H	2.925600398892	-1.125287120147	-0.079441005029
H	2.107206206524	-0.355010800254	1.284284874366

CCSD(T)/ANO1 Frequencies (cm ⁻¹)							
218.9441i	135.8154	165.1162	240.0131	282.4324	411.2832	498.9613	615.2701
718.4296	826.3317	984.5735	1046.1001	1090.0150	1106.7387	1206.9914	1211.4101
1372.4071	1381.3666	1466.1116	1506.5023	1526.0870	1542.4226	1685.6793	2968.7504
3034.1992	3061.4717	3075.9461	3204.1492	3242.2629	3499.8507		

1.2.3 Equatorial Product

CCSD(T)/ANO1 Coordinates (Angstroms)			
O	-1.628895582780	-0.834954556015	0.136897743084
O	-1.319103907687	0.559341632610	-0.150793014835
C	0.003587123664	0.756196582814	0.293017307958
H	0.164250640955	1.833417798030	0.160925209293
H	0.097333256460	0.492554987276	1.351304493898
H	-0.895123440493	-1.255646867086	-0.346688161903
N	0.907204207129	-0.088574262462	-0.466989726022
C	2.194333362643	-0.305640992875	0.195143866424
H	1.053696556568	0.319616550331	-1.383290017718
H	2.741826713472	0.619481889274	0.420161094277
H	2.823278049626	-0.931063731029	-0.439130631140
H	2.026353737122	-0.838189919543	1.133313410895

CCSD(T)/ANO1 Frequencies (cm ⁻¹)							
84.9220	179.4516	244.1584	305.2110	388.8965	514.0305	588.9403	830.6076
853.4804	978.7791	1049.3313	1072.2440	1140.0508	1180.1368	1231.5870	1309.7884
1400.5914	1432.8033	1457.8120	1479.1494	1501.6648	1507.8504	1523.7595	2993.9304
3016.6441	3075.9697	3085.1259	3129.0083	3535.2876	3660.3290		

1.2.4 Axial Pre-reactive Complex

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.391372234353	-0.949786160089	0.018748077173
O	-1.201860260978	0.271833102884	-0.573367839264
C	-0.957475813917	1.242438199926	0.198308608771
H	-0.768223433098	2.186201285102	-0.295385740182
H	-0.969354839950	1.085794144771	1.267379935295
H	0.634808787423	-0.818190212127	0.806657264848
N	1.375803619851	-0.119593442716	0.782858452785
H	1.970696844517	-0.299342233974	1.583597353189
C	2.145761367150	-0.298114679527	-0.454958454162
H	2.937184693129	0.452522839750	-0.505034236560
H	1.483180642718	-0.141728251557	-1.308780728854
H	2.603578963549	-1.287875772412	-0.567639558347

CCSD(T)/ANO1 Frequencies (cm ⁻¹)							
63.9009	76.8051	113.4592	151.4147	173.5663	229.4044	429.8337	521.1106
653.5203	864.3299	919.8458	938.8919	1004.9300	1065.6385	1196.8735	1230.1182
1354.5199	1372.5617	1457.2056	1504.0544	1508.7119	1526.6325	1670.2439	3008.4915
3079.5316	3113.8119	3154.3914	3307.9440	3458.3550	3566.7451		

1.2.5 Axial Transition State

CCSD(T)/ANO1 Coordinates (Angstroms)			
O	-1.063993222931	0.618497605377	-1.222844971537
O	-1.035880833610	0.703011267823	0.198218613237
C	-1.011044173732	-0.438511844684	0.732684021612
H	-0.888057740510	-0.454343573258	1.809948363154
H	-1.337832070142	-1.295753075861	0.160382557554
H	0.628017085161	-0.540330281336	-0.913011111439
N	1.039562495480	-0.916518596186	-0.053182486889
H	1.444900130885	-1.822976308553	-0.251316022427
C	2.034903731837	0.022441042839	0.471128427421
H	2.469952273279	-0.375002090556	1.389690772111
H	1.531519759501	0.962792227257	0.705124806641
H	2.843059886961	0.240822450177	-0.233908003739

CCSD(T)/ANO1 Frequencies (cm ⁻¹)							
210.0426i	91.2661	145.4202	165.4591	224.7055	402.1931	501.8374	567.4496
766.2073	802.2501	946.4996	1035.3540	1051.9050	1082.0396	1193.8095	1212.9236
1365.4581	1388.6247	1455.8789	1502.5267	1525.3072	1544.9504	1662.9373	3024.4273
3093.0318	3122.9003	3138.2219	3277.0519	3367.6052	3575.5151		

1.2.6 Axial Product

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.582169822588	-0.877820732454	0.273771339947
O	-1.079262214005	0.214674996619	-0.547755912556
C	-0.122188768285	0.884032228288	0.247519572954
H	0.160261649750	1.745169162846	-0.372934112783
H	-0.575859942842	1.219627708543	1.184027784093
H	-0.735472960756	-1.310629114269	0.486529829149
N	0.975718708930	-0.010127997127	0.546073500825
H	1.420126216483	0.258730008075	1.413972741158
C	1.953742700861	-0.110539025107	-0.538750350335
H	2.430894709075	0.848669367960	-0.780465911766
H	1.446884091463	-0.475481914760	-1.432988837679
H	2.727047605099	-0.830610276614	-0.269509018031

CCSD(T)/ANO1 Frequencies (cm ⁻¹)							
109.2064	175.0204	214.9450	319.5195	450.4364	501.2865	615.8827	770.9030
853.9853	932.5456	1046.0258	1066.5241	1150.0205	1165.3791	1224.9048	1309.4713
1402.3972	1433.9756	1452.0401	1478.5577	1490.7173	1506.5059	1523.0451	2996.1074
3007.5100	3084.7263	3095.0777	3135.4507	3569.5112	3657.3573		

1.3 *Anti*-Methylated Criegee Intermediate Addition

1.3.1 Equatorial Pre-reactive Complex

CCSD(T)/ANO1 Coordinates (Angstroms)			
O	-0.512286228955	-1.782266406700	0.156123840316
O	-1.236581362156	-0.676446727900	-0.290794143309
C	-1.044343796308	0.395602950039	0.340785029773
C	-1.694819970410	1.638041943006	-0.139880804259
H	-0.411076550106	0.343445141878	1.218987340414
H	1.178651677304	-0.696376456607	-0.379554058383
N	1.575004511629	0.241719770946	-0.463976839623
C	2.714790925744	0.366464065960	0.452965141076
H	1.901410535447	0.325900072404	-1.420471767957
H	3.141956554444	1.368677719933	0.376681713524
H	3.518161801139	-0.360644747553	0.283949529512
H	2.363282356900	0.236182898504	1.479016267979
H	-2.308365966107	1.436568928961	-1.016416228009
H	-0.912800274648	2.357825337887	-0.395577106582
H	-2.308883458683	2.073757432452	0.651845942146

CCSD(T)/ANO0 Frequencies (cm ⁻¹)							
48.7393	60.6608	96.9438	139.0417	157.1677	172.9248	241.6579	273.6059
317.4122	465.5513	536.0227	783.7588	857.3019	929.8112	957.0337	1026.4776
1061.6624	1063.9815	1162.0321	1215.1375	1323.3472	1388.7375	1409.8747	1459.9876
1464.6901	1477.8015	1507.4960	1530.8142	1546.9619	1689.8420	3013.9873	3053.7695
3088.0607	3121.1816	3133.1233	3175.3632	3221.0992	3403.8276	* 3532.3493	

1.3.2 Equatorial Transition State

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-0.957832898945	-1.680844531255	-0.069736853132
O	-1.383325379096	-0.302388752554	-0.045168174879
C	-0.558939278313	0.408908009343	0.597924874675
C	-0.783232737514	1.881150697859	0.644324736483
H	0.070625025599	-0.097776399883	1.321843594118
H	0.636479431375	-0.889109877370	-0.816866035726
N	1.124931018829	0.016668355081	-0.751836376894
C	2.491604558380	-0.142565556173	-0.256310066985
H	1.100013714240	0.465955150212	-1.659526615998
H	2.971694820837	0.833183379035	-0.158733152641
H	3.117966478461	-0.774607611709	-0.894602871311
H	2.455707389102	-0.601872579283	0.734086368134
H	-1.348766385276	2.210167437487	-0.226165478820
H	0.177252880190	2.395112760723	0.679818051995
H	-1.341374517104	2.132870138295	1.550637039041

CCSD(T)/ANO0 Frequencies (cm^{-1})

210.1081i	98.0316	115.3360	150.6209	166.2680	246.6471	278.0783	317.8135
436.5258	521.3640	590.0067	752.3161	937.0336	956.6298	987.3318	1061.3421
1096.1804	1117.3169	1161.2598	1204.0701	1318.0757	1368.0493	1409.0067	1458.7994
1468.0588	1486.0440	1503.4493	1525.3747	1574.0837	1688.5636	3028.5322	3057.9343
3102.7249	3130.6302	3144.8058	3175.5524	3190.9125	3201.2098	3544.1726	

1.3.3 Equatorial Product

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.767552284368	-1.019996600209	0.093122136088
O	-1.329529942915	0.342439174837	-0.172340858832
C	0.009755571246	0.422928458412	0.279579354668
C	0.408509108826	1.877525903090	0.093012535231
H	0.055125306090	0.126895969157	1.333846742601
H	-1.049923212437	-1.495746896213	-0.365565996223
N	0.807325024348	-0.539144945250	-0.469854409092
C	2.041991753048	-0.936806944630	0.207356931984
H	1.021770007465	-0.146427158854	-1.381199283440
H	2.711948271526	-0.099884566024	0.446057466744
H	2.586024195334	-1.640903142806	-0.423189649393
H	1.788345638499	-1.446156362032	1.139135790823
H	0.304153056747	2.158285560933	-0.957816622759
H	1.448025430264	2.019242283686	0.395239865134
H	-0.223634786176	2.532374880669	0.693720771339

CCSD(T)/ANO0 Frequencies (cm^{-1})

100.3063	176.9857	206.2534	224.8019	271.6379	296.8321	396.1352	504.2347
552.9014	568.1791	794.7961	846.9508	904.4534	939.0401	1034.9604	1102.6317
1115.7894	1175.7792	1185.4963	1238.9385	1348.2068	1387.4759	1411.6597	1428.5874
1461.6005	1490.0615	1492.5001	1506.2678	1511.3941	1528.3363	3008.9141	3052.2228
3053.6233	3099.1945	3141.3385	3142.7278	3152.3852	3495.8247	3634.0030	

1.3.4 Axial Pre-reactive Complex

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-0.521640233234	-1.836170766645	0.012615719386
O	-0.941985970985	-0.591702627214	-0.462815378878
C	-1.081705116830	0.306401505137	0.408952656862
C	-1.415170788820	1.682688777448	-0.030123076941
H	-0.959509357338	0.012152805687	1.444708676240
H	1.218786419740	-0.814714512073	0.638051450450
N	1.576354626989	0.140818960686	0.689347193064
H	2.287816705134	0.147901562084	1.411367360230
C	2.183336654026	0.479109350938	-0.604296174022
H	2.573514872834	1.498869617384	-0.572600693260
H	1.412591536316	0.439143767437	-1.377627660531
H	2.994904663274	-0.189238254803	-0.914484912643
H	-1.520634864044	1.725831508531	-1.113057885206
H	-0.608761259088	2.348451817790	0.288623634814
H	-2.339063908541	2.018696154041	0.446576081034

CCSD(T)/ANO0 Frequencies (cm^{-1})

61.6502	75.6302	111.3023	142.3567	166.2675	176.2366	245.3381	274.5983
322.7424	487.6638	536.0789	780.7535	855.5274	930.1098	954.5317	1017.1797
1057.2754	1062.0797	1161.6395	1212.9023	1323.0125	1386.0429	1409.1874	1458.4974
1464.2836	1477.4035	1507.3741	1531.2930	1547.0670	1686.2686	3017.1619	3053.3813
3089.4693	3122.5922	3133.0161	3174.2475	3224.2419	3407.7255	3538.3386	

1.3.5 Axial Transition State

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-0.706405285455	0.311390216789	-1.789124731129
O	-0.856384575832	0.723159974170	-0.414764365834
C	-0.894821524978	-0.279863208897	0.355087318463
C	-0.950164154647	-0.036568312851	1.823651917885
H	-1.180610410482	-1.228657935613	-0.083801796348
H	0.837839903748	-0.654039517447	-1.066580937874
N	1.166427489341	-0.869892261530	-0.114811055088
H	1.568256012657	-1.799111069595	-0.096929711003
C	2.116876714689	0.149678970833	0.331380892363
H	2.439909706677	-0.060955372329	1.352954903709
H	1.610849388715	1.117689444567	0.318933675711
H	3.002595013751	0.228320590486	-0.306671942984
H	-0.504523781905	0.926189181471	2.070371187057
H	-0.422321612139	-0.834885779298	2.345118939096
H	-1.993497108847	-0.041529993556	2.151579639269

CCSD(T)/ANO0 Frequencies (cm^{-1})

232.0665i	101.6209	133.9449	149.3621	178.0902	250.8143	275.1757	318.1419
457.9987	524.2083	630.5803	748.7554	933.2748	961.1352	970.1179	1050.2416
1082.3409	1112.8580	1160.4555	1208.5230	1315.8475	1370.4321	1407.7553	1452.8463
1466.5614	1484.6118	1505.5409	1526.3273	1569.8398	1678.4001	3032.4018	3058.2287
3106.5731	3135.4282	3145.2207	3176.5762	3203.2173	3216.9430	3550.6172	

1.3.6 Axial Product

CCSD(T)/ANO1 Coordinates (Angstroms)			
O	-0.839012845034	0.317709455487	-1.826490091347
O	-0.820870815521	0.771974688724	-0.443404764535
C	-0.483930002148	-0.358565160389	0.344388586590
C	-0.627707397280	0.111902387951	1.784748098167
H	-1.189368939267	-1.168163457394	0.128903655976
H	0.031651623286	-0.123459730530	-1.847358607170
N	0.829938722988	-0.829190614994	-0.075955680930
H	0.925854994881	-1.814956149114	0.130817369945
C	1.970479988129	-0.069092738251	0.439602996290
H	2.104518161365	-0.143061817367	1.525301046376
H	1.836562457875	0.981851719568	0.178821333071
H	2.880187112556	-0.423052694581	-0.046867224781
H	-0.013978958451	0.993836266425	1.971596592883
H	-0.320841511636	-0.683051421790	2.467856243749
H	-1.668577588501	0.366690767523	1.985619694368

CCSD(T)/ANO0 Frequencies (cm ⁻¹)							
114.9279	182.1662	212.9311	243.2414	288.7908	292.0080	396.5739	541.9719
547.4310	612.8788	763.8032	811.5511	858.5813	937.2814	1009.8479	1091.3729
1111.5752	1164.5028	1182.8161	1221.2690	1343.5922	1397.4474	1423.3213	1435.4439
1456.9648	1476.3969	1489.1087	1509.5093	1512.5506	1531.5448	3023.8007	3051.8341
3060.0954	3109.9274	3146.6477	3149.1366	3159.8504	3540.6046	3621.4633	

1.4 *Syn*-Methylated Criegee Intermediate Addition

1.4.1 Equatorial Pre-reactive Complex

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.047659702914	0.926886170665	-0.782381305863
O	-1.272207373336	0.842061768682	0.571814735970
C	-1.256128808163	-0.323178823627	1.077493624164
C	-1.047451026329	-1.527386026892	0.256644112221
H	-0.011654638594	-1.514556209478	-0.097036714325
H	-1.690233900241	-1.466982215896	-0.625601028954
H	-1.239488462452	-2.426953982424	0.838147334724
H	-1.416753159343	-0.313085924301	2.149664645134
H	1.018115031118	0.729342718269	-0.409259536079
N	1.789902261599	0.242760626893	0.044194486216
C	2.665146829630	-0.324759935361	-0.990097352902
H	2.304315456165	0.949177818289	0.559341925167
H	2.098665047899	-1.050726438530	-1.578075511489
H	3.491467154770	-0.860599349831	-0.518012815948
H	3.088896218729	0.408114469001	-1.687807607216

CCSD(T)/ANO0 Frequencies (cm^{-1})

28.0727	47.2640	74.3500	120.1727	143.6911	177.4339	241.1662	305.4786
426.4085	450.1202	652.3783	733.7155	814.4519	944.8119	960.8195	1013.3751
1052.2900	1058.7756	1121.0367	1213.1039	1308.4990	1387.5628	1397.0721	1450.3701
1459.8622	1487.4736	1507.9669	1511.7771	1530.9751	1683.7792	3011.7063	3023.6724
3087.6474	3111.7347	3122.1602	3175.1531	3210.7600	3433.3156	3536.5757	

1.4.2 Equatorial Transition State

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-0.548381051857	1.242243746207	-1.224363159853
O	-0.538231332626	1.407606067390	0.213217330557
C	-0.633326405324	0.285952874591	0.810296239739
C	-1.399984385328	-0.872173610760	0.268813604235
H	-1.192355423599	-1.006844037789	-0.788280688019
H	-2.463474693393	-0.634297366693	0.378234786539
H	-1.178508027594	-1.770155023842	0.845559894985
H	-0.496113371152	0.374346719266	1.886304821705
H	1.002454843683	0.116144218564	-0.693537549913
N	1.266757478658	-0.379670338093	0.171229762451
C	1.736834127593	-1.741837922605	-0.084921703271
H	1.966002493578	0.178374337942	0.647523003499
H	0.945103572511	-2.302129996309	-0.583801418181
H	1.963509961023	-2.240845938850	0.858822789404
H	2.628032444060	-1.774564121852	-0.719961725447

CCSD(T)/ANO0 Frequencies (cm^{-1})

288.1897i	53.6264	98.7295	112.1548	142.0717	259.9580	303.0127	336.0683
440.7508	578.7387	623.6785	775.9166	899.5554	949.5555	976.6485	1063.1730
1103.3129	1111.0841	1158.0545	1192.9616	1343.9051	1356.3189	1383.5420	1455.1410
1465.3894	1491.6371	1502.8900	1522.3191	1568.2588	1691.7313	3044.7240	3066.0368
3125.0252	3157.6041	3166.9839	3171.4866	3176.0565	3227.5020	3586.3822	

1.4.3 Equatorial Product

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.728670487464	-0.580268493582	0.649222995346
O	-1.295539442196	-0.169930220041	-0.682715219014
C	0.014538546894	0.363004544000	-0.551667370095
C	0.067347350684	1.578681351103	0.358804225523
H	-0.074728553807	1.289833310693	1.399985306152
H	-0.733176443299	2.260431649901	0.071159796944
H	1.020952215138	2.099646912796	0.256277340588
H	0.236492814244	0.662168605857	-1.586766998231
H	-0.975007497671	-1.150852336409	0.886264116817
N	0.868160206606	-0.724442507153	-0.081575268969
C	2.247888324707	-0.344872481906	0.231743195729
H	0.879363511544	-1.428946498702	-0.812355951650
H	2.271911663400	0.262665347396	1.136229856237
H	2.744655448698	0.214923409812	-0.573151025298
H	2.823198503503	-1.250998218177	0.424400704496

CCSD(T)/ANO0 Frequencies (cm^{-1})

101.3362	171.5933	212.9396	250.9838	290.9888	323.4840	411.0817	473.8164
534.4198	638.2680	789.3399	843.1487	885.0548	953.1747	1046.7578	1087.8233
1106.1721	1151.3012	1196.3972	1224.9560	1353.6594	1372.5588	1410.0296	1425.3490
1461.5327	1495.2103	1497.5363	1501.6778	1509.3458	1529.3465	3001.1557	3003.8097
3065.7519	3108.8934	3149.3027	3155.5829	3169.2373	3496.9686	3646.8521	

1.4.4 Axial Pre-reactive Complex

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.221353733151	-0.476384335985	0.971550118733
O	-1.242878266062	0.139380847714	-0.258049934738
C	-0.670646918702	1.270848932453	-0.333360390539
C	-0.060387397695	1.914794004977	0.841671245009
H	0.810641425255	1.322178837314	1.136036650185
H	-0.770791316757	1.874944821648	1.671928018737
H	0.234924206808	2.936273207480	0.610250878810
H	-0.700549846505	1.686916440628	-1.334085857953
H	0.786101091248	-1.080778299629	0.530406781714
N	1.605280946951	-0.885014224381	-0.042432720277
H	2.406905921773	-1.184091627333	0.502523352203
C	1.530517143708	-1.694068963653	-1.266509331233
H	2.390937139598	-1.475721809786	-1.902886928426
H	0.631444233138	-1.416809117113	-1.820756965180
H	1.495896405093	-2.777640686031	-1.099867174757

CCSD(T)/ANO0 Frequencies (cm^{-1})

22.6015	49.9817	76.3223	110.9161	145.9579	171.6454	214.4682	305.5827
420.8937	451.3564	651.7345	729.9989	813.5973	947.8738	960.5176	1005.8001
1045.8794	1055.8599	1120.0406	1209.5348	1308.8195	1379.8161	1387.6146	1450.1194
1460.0544	1483.6163	1507.6140	1512.9755	1530.4708	1696.2166	3011.9800	3042.4662
3087.2092	3121.4791	3124.8365	3176.5350	3211.4116	3439.3691	3537.6530	

1.4.5 Axial Transition State

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.311833231457	-0.556418928537	1.021567047693
O	-1.180115631261	-0.051267296934	-0.323257063581
C	-0.303970391266	0.868948897212	-0.396292167436
C	-0.002098999222	1.807765292655	0.721826637117
H	0.101264983559	1.269741627677	1.658904423800
H	-0.857259226647	2.485561447189	0.816908141154
H	0.888660408718	2.389980712720	0.487126925024
H	-0.101909674120	1.171356242617	-1.422055861688
H	0.688041173108	-0.824538357219	0.704523533858
N	1.317839584175	-0.458694149319	-0.021786415148
H	2.205358433477	-0.204614094936	0.394758565978
C	1.468259223545	-1.435815861740	-1.102066417625
H	2.125767842340	-1.035121648056	-1.875466096938
H	0.482706171247	-1.614151533813	-1.536497749953
H	1.867886681561	-2.395699641498	-0.762147125179

CCSD(T)/ANO0 Frequencies (cm^{-1})

285.2352i	108.7207	152.3474	157.4698	178.2147	241.7961	272.1577	351.7806
471.3395	593.6929	656.3753	726.9083	888.9901	942.3229	984.5599	1058.0628
1082.1500	1085.6673	1147.0931	1208.6560	1342.1055	1369.2732	1388.5626	1452.1780
1464.3585	1490.4738	1505.2431	1525.6453	1566.6643	1675.8464	3037.6071	3054.6439
3114.5323	3143.1943	3143.9457	3151.9215	3212.5489	3239.4714	3550.3030	

1.4.6 Axial Product

CCSD(T)/ANO1 Coordinates (Angstroms)

O	-1.410686505382	-0.660090983798	0.955214782499
O	-1.180651964159	-0.077800051082	-0.361562087344
C	0.062572841061	0.615012537082	-0.300777503991
C	0.048981395498	1.769072876905	0.686928797548
H	-0.019150216871	1.395046386174	1.708357678870
H	-0.812592992342	2.406862259249	0.490157115872
H	0.958452674921	2.366101095174	0.581582962258
H	0.148354652970	0.988469359173	-1.331747279732
H	-0.559698132129	-1.124134685929	1.064578615131
N	1.099152266817	-0.345159285421	0.030485664359
H	1.891416703734	0.127583509923	0.446019977900
C	1.517620140503	-1.164472168162	-1.108704292027
H	1.939028456871	-0.574556841453	-1.933709538540
H	0.649914512099	-1.707436627134	-1.485402166173
H	2.260389542804	-1.893030226122	-0.781800171744

CCSD(T)/ANO0 Frequencies (cm ⁻¹)							
106.9612	160.8119	197.2998	212.7235	275.2338	310.2046	388.3847	522.0939
529.1973	657.0805	777.9560	802.7621	852.2343	939.9378	1065.1921	1076.1349
1110.3181	1155.1862	1162.6823	1234.0540	1356.8695	1369.8131	1411.6358	1427.1395
1456.4041	1478.8991	1493.6749	1504.5231	1509.7571	1527.4669	3004.8325	3009.1152
3058.2474	3108.4242	3146.3574	3150.4381	3169.7541	3542.2010	3632.9861	

2 Kinetics

2.1 Rate Constants

Rate constants for each SCI addition with and without the full $\Delta_{(Q)}$ contribution

Species		CCSD(T)	CCSD(T) + $\Delta_{(Q)}$
Simple	Equatorial	2.73×10^{-12}	3.55×10^{-13}
	Axial	1.29×10^{-11}	1.77×10^{-12}
<i>Anti</i>	Equatorial	7.45×10^{-12}	1.54×10^{-12}
	Axial	2.52×10^{-11}	5.29×10^{-12}
<i>Syn</i>	Equatorial	4.25×10^{-15}	9.37×10^{-16}
	Axial	3.98×10^{-15}	8.95×10^{-16}