

## Supplementary Information

### **Mechanistic Study of the Complex Photooxidation of Allyl Methyl Sulfide (AMS). Reaction Paths and Products of Addition at Different Atmospheric Conditions.**

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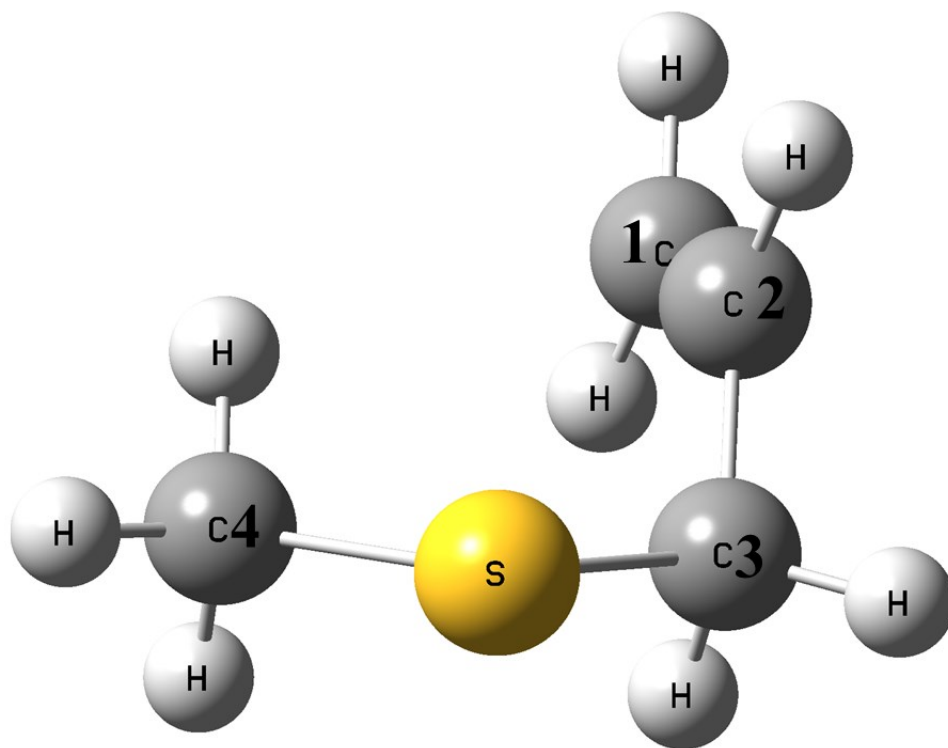
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# Contents

<b>I.</b>	Optimized geometries and vibrational frequencies of species considered in the Allyl Methyl Sulfide oxidation initiated by OH radicals.....	3
	Table S1. IUPAC nomenclature and given names for reactants, products and intermediaries optimized in this work.....	4
A.	AMS and simple molecules.....	6
B.	Products (P).....	12
C.	Intermediaries ( $_Im$ ).....	32
1.	Addition of OH at C1 and C2.....	32
2.	Reactions of the peroxy radicals (A1O2, A2O2) with NO <sub>2</sub> .....	42
3.	Intramolecular rearrangement mechanism in RO <sub>2</sub> intermediates (A1O2-A2O2).....	45
4.	MSP decomposition.....	59
D.	Transitions States (TS) and Postreaction Wells (PW).....	75
1.	Addition of OH at C1 and C2.....	75
2.	Reactions of the peroxy radicals (A1O2, A2O2) with NO <sub>2</sub> .....	102
3.	Intramolecular rearrangement mechanism in RO <sub>2</sub> intermediates (A1O2-A2O2).....	106
4.	MSP decomposition.....	147
<b>II.</b>	Thermochemistry tables.....	164
A.	Table S2. Calculated relative energies (kcal mol <sup>-1</sup> ) of the gas phase oxidation of AMS initiated by OH radicals in the absence of NO <sub>x</sub> radicals.....	165
B.	Table S3. Calculated relative energies (kcal mol <sup>-1</sup> ) for the gas phase decomposition of the A1O2 intermediate: C1 addition.....	167
C.	Table S4. Calculated relative energies (kcal mol <sup>-1</sup> ) for the gas phase decomposition of the A2O2 intermediate: C2 addition.....	168
D.	Table S5. Calculated relative energies (kcal mol <sup>-1</sup> ) for the gas phase decomposition of the MSP intermediate.....	169

I. Optimized geometries and vibrational frequencies of species considered in the Allyl Methyl Sulfide oxidation initiated by OH radicals.

This section includes the optimized geometries in XYZ format and vibrational frequencies at the M06-2X-GD3/aug-cc-pVTZ level of theory. Calculated energies for all methods used in this work are also included. For each transitions state (TS), a postreaction well (PW) and the intrinsic reaction coordinate (IRC) were determined.



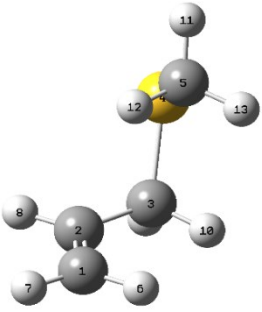
*Figure S 1. Numbering of carbon atoms in the AMS molecule: C1 and C2 are attached by a double bond, C3 is between double bond and sulfur and C4 is the methyl carbon bonded to sulfur.*

Table S1. IUPAC nomenclature and given names for reactants, products and intermediaries optimized in this work.

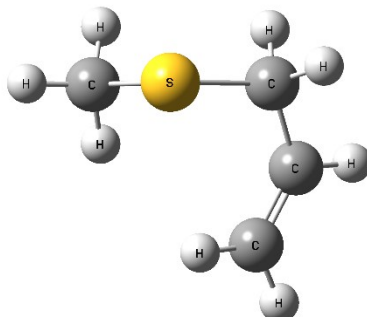
IUPAC Nomenclature	Given Name
allyl methyl sulfide	AMS
1-hydroxy-3-(methylthio)-2-propyl radical	A1
2-hydroxy-3-(methylthio)-1-propyl radical	A2
2-peroxy-3-(methylthio)-propan-1-ol radical	A1O2
1-peroxy-3-(methylthio)-propan-2-ol radical	A2O2
2-hydroxy-1-[(methylthio)-methyl]-ethoxyl radical	A1O
2-hydroxy-3-(methylthio)-propoxyl radical	A2O
methyl thiomethyl radical	Ad_Im1
1-hydroxy-2-(methylthio)-ethyl radical	Ad_Im2
1-hydroxy-2-(methylthio)-ethyldioxyl radical	Ad_Im2-O2
1-hydroxy-2-(methylthio)-ethoxyl radical	Ad_Im2-O
hydroxymethyl radical	P3_Im1
hydroxy methylene	P3_Im2
methyl hydroperoxide	P3_Im3
methylthio radical	MeS
methylthiodioxyl radical	MeS-O2
methylthiooxyl radical	MeS-O
2-hydroxyacetaldehyde	P1
1,2-ethenediol	P1'
2-methyl thio acetaldehyde	P2
formaldehyde	P3
formic acid	P4
acetaldehyde	P5
vinyl alcohol	P5'
sulfur dioxide	P6
nitric acid	P7
2-hydroxy-3-(methylthio)-propanal	P8
2-propen-1-ol	P9
1-hydroxy-3-(methylthio)-propan-2-one	P10
(E)-3-(methylthio)-prop-2-en-1-ol	P11
thioformaldehyde S-methylide	P12
(Z)-2-(methylthio)-ethen-1-ol	P13
methanethial	P14
sulfur monoxide	P15
carbon oxide sulfide	P16
formic thioanhydride	P17
dimethyl disulfide	DMDS
3-hydroxy-2-(methylthiodioxy)-propyl radical	A1_Im1_1

IUPAC Nomenclature	Given Name
2-hydroperoxy-3-(methylthio)-propoxyl radical	A1_Im1_2
2-hydroperoxy-1-hydroxy-3-(methylthio)-2-propyl radical	A1_Im2_1
2-hydroperoxy-3-hydroxy-1-(methylthio)-propyl radical	A1_Im3_1
(2-hydroperoxy-3-hydroxypropylthio)-methyl radical	A1_Im3_2
1-hydroperoxy-2-hydroxy-3-(methylthio)-2-propyl radical	A2_Im1_1
2-hydroperoxy-1-[(methylthio)-methyl]-ethoxyl radical	A2_Im1_2
3-hydroperoxy-2-hydroxy-1-(methylthio)-propyl radical	A2_Im2_1
1-hydroxy-2-(methylthio)-ethyl radical	P2_Im1
methyl thiomethylperoxyl radical	MSP
(hydroxymethoxymethylthio)-methyl radical	MSP-1
(hydroxymethoxymethylthio)-methyl dioxyl radical	MSP-2
(hydroperoxymethylthio)-hydroxymethoxymethyl radical	MSP-3
(thio)-carbonylmethyl hydroperoxide	MSP-3a
(thio) carbonylmethoxyl radical	MSP-3b
(thio)-methyl hydroperoxide	P-Im1a
1,2λ <sup>4</sup> -oxathiiran-2-one	P-Im1b
methylenedioxyl radical	P-Im2
1,2-oxathiirane	P-Im3
carbothioic O-acid	P-Im4
Thiomethyldioxyl radical	P-Im5a
1,2,3-dioxathietane	P-Im5b

A. AMS and simple molecules.

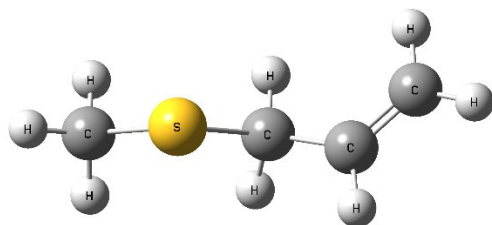
AMS_1						
						
Method	Ee		E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-555.383676		-555.273468	-555.265757	-555.304243	
M06-2X/DG3/aug-cc-pVTZ	-555.386004		-555.275839	-555.268135	-555.306588	
MN15/cc-pVTZ	-555.150612		-555.040974	-555.033210	-555.071805	
MN15/aug-cc-pVTZ	-555.156155		-555.046699	-555.038927	-555.077554	
SVECV-f12	-555.279005		-555.168841	-555.161137	-555.199590	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.001633	0.018122	-0.006185	92.4976	999.9976	3074.8757
C	0.002130	-0.001624	1.318673	104.002	1042.2559	3128.1329
C	1.240370	0.005966	2.149407	178.2029	1107.1492	3149.6425
S	1.466460	-1.560450	3.053456	258.7735	1238.7919	3157.601
C	1.740345	-2.660918	1.648497	313.3585	1253.557	3168.9723
H	0.923567	0.068897	-0.568502	418.7191	1324.2892	3175.3446
H	-0.923362	-0.009423	-0.570817	616.293	1353.3887	3248.3028
H	-0.933508	-0.064418	1.864176	734.6886	1443.5981	
H	1.190478	0.767964	2.926660	783.2981	1468.6434	
H	2.123669	0.194381	1.538717	865.6934	1474.3424	
H	1.875738	-3.661819	2.050502	949.8983	1489.0076	
H	0.882871	-2.653571	0.979381	969.0969	1727.761	
H	2.637683	-2.370014	1.10493	978.7292	3067.8917	

**AMS\_2**



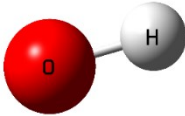
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-555.381520	-555.271375	-555.263743	-555.301806		
M06-2X/DG3/aug-cc-pVTZ	-555.383787	-555.273667	-555.266050	-555.304052		
MN15/cc-pVTZ	-555.149065	-555.039346	-555.031727	-555.069683		
MN15/aug-cc-pVTZ	-555.154629	-555.045029	-555.037415	-555.075349		
SVECV-f12	-555.276736	-555.166616	-555.158999	-555.197001		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.006210	-0.018046	0.008560	113.6376	1011.005	3071.4004
C	0.005133	0.005492	1.330995	152.8212	1040.2346	3100.3191
C	1.209022	-0.007058	2.230692	162.0531	1071.4215	3151.769
S	2.810864	-0.313497	1.448024	236.8529	1215.4846	3152.908
C	2.608870	-2.067841	1.060880	290.6119	1301.0063	3168.334
H	0.931856	-0.055644	-0.552008	526.7767	1327.5978	3169.691
H	-0.920533	0.010175	-0.547314	566.621	1354.4351	3255.3603
H	-0.943924	0.046797	1.857968	717.3662	1438.4343	
H	1.069277	-0.743013	3.025322	755.3842	1451.1601	
H	1.306239	0.961088	2.72557	879.8988	1471.8425	
H	3.526722	-2.39661	0.579995	935.9621	1490.8761	
H	2.459661	-2.642204	1.973276	976.419	1735.1324	
H	1.771906	-2.222932	0.384196	984.9716	3059.5098	

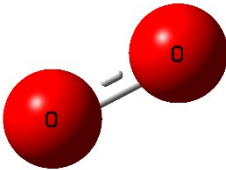
**AMS\_3**

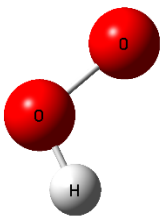


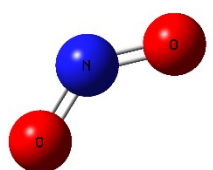
Method	E <sub>e</sub>	E+ZPE	ΔH	ΔG		
M06-2X/GD3/cc-pVTZ	-555.380609	-555.270573	-555.262707	-555.301783		
M06-2X/DG3/aug-cc-pVTZ	-555.383080	-555.273123	-555.265252	-555.304362		
MN15/cc-pVTZ	-555.147117	-555.037669	-555.029745	-555.068977		
MN15/aug-cc-pVTZ	-555.152929	-555.043607	-555.035691	-555.074903		
SVECV-f12	-555.276404	-555.166446	-555.158575	-555.197685		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.012972	-0.004374	0.013075	64.1303	997.7248	3067.2611
C	0.005489	0.002085	1.336795	87.1343	1037.1571	3114.8844
C	1.237902	0.004313	2.178981	175.3865	1094.7821	3145.3977
S	1.342756	-1.560992	3.106936	201.9017	1226.116	3162.6724
C	2.688987	-1.118052	4.227722	313.5573	1255.8714	3165.8008
H	0.942465	-0.003024	-0.543395	421.5961	1325.4516	3176.3456
H	-0.905847	-0.011254	-0.556671	607.7776	1351.9965	3252.3813
H	-0.936890	-0.013557	1.873954	741.5249	1448.7566	
H	1.201644	0.814422	2.909334	800.2421	1473.2901	
H	2.129073	0.122555	1.56318	893.0483	1484.8283	
H	2.881008	-1.981983	4.859046	949.0202	1488.0099	
H	3.592457	-0.879425	3.669866	972.8778	1734.7719	
H	2.406754	-0.274562	4.854994	973.9316	3060.1302	



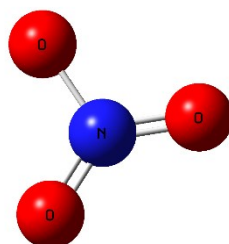
OH				
				
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-75.730486	-75.721884	-75.718580	-75.738804
M06-2X/DG3/aug-cc-pVTZ	-75.733810	-75.725222	-75.721918	-75.742143
MN15/cc-pVTZ	-75.683738	-75.675135	-75.671830	-75.692061
MN15/aug-cc-pVTZ	-75.687249	-75.678673	-75.675368	-75.695600
SVECV-f12	-75.726817	-75.718229	-75.714925	-75.735150
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )	
O	0.000000	0.000000	0.106696	3769.6136
H	0.000000	0.000000	-0.865234	

O <sub>2</sub>				
				
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-150.321735	-150.317729	-150.314423	-150.337669
M06-2X/DG3/aug-cc-pVTZ	-150.324795	-150.320798	-150.317492	-150.340738
MN15/cc-pVTZ	-150.225415	-150.221486	-150.218179	-150.241435
MN15/aug-cc-pVTZ	-150.228786	-150.224861	-150.221554	-150.244810
SVECV-f12	-150.303405	-150.299408	-150.296102	-150.319348
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )	
O	0.000000	0.000000	0.000000	1754.4579
O	0.000000	0.000000	1.189850	

<b>_OOH</b>						
						
Method			Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ			-150.904167	-150.889552	-150.885756	-150.911696
M06-2X/DG3/aug-cc-pVTZ			-150.908095	-150.893517	-150.889721	-150.915660
MN15/cc-pVTZ			-150.814457	-150.799939	-150.796141	-150.822090
MN15/aug-cc-pVTZ			-150.818537	-150.804066	-150.800268	-150.826216
SVECV-f12			-150.890724	-150.876146	-150.872350	-150.898289
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
O	0.017219	0.000000	-0.019469	1252.762		
O	-0.030895	0.000000	1.287852	1459.4343		
H	0.894501	0.000000	1.587493	3686.8681		

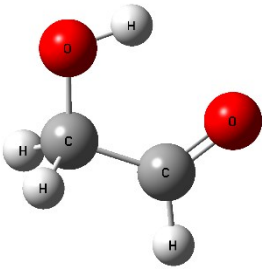
<b>NO<sub>2</sub></b>						
						
Method			Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ			-205.070765	-205.061555	-205.057688	-205.084869
M06-2X/DG3/aug-cc-pVTZ			-205.074636	-205.065465	-205.061598	-205.089431
MN15/cc-pVTZ			-204.938870	-204.929761	-204.925887	-204.953748
MN15/aug-cc-pVTZ			-204.943091	-204.934013	-204.930139	-204.957997
SVECV-f12			-205.051490	-205.042319	-205.038452	-205.066286
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
N	0.096272	0.000000	0.055593	783.4383		
O	-0.057361	0.000000	1.225779	1465.8194		
O	1.032883	0.000000	-0.662572	1776.1539		

**NO<sub>3</sub>**

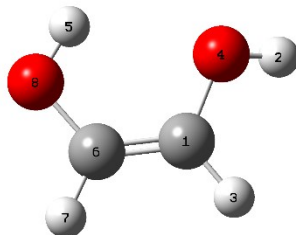


Method	Ee	E+ZPE	ΔH	ΔG	
M06-2X/GD3/cc-pVTZ	-280.208273	-280.195218	-280.190763	-280.221538	
M06-2X/DG3/aug-cc-pVTZ	-280.213675	-280.200605	-280.196178	-280.226895	
MN15/cc-pVTZ	-280.035793	-280.023933	-280.019361	-280.050263	
MN15/aug-cc-pVTZ	-280.041539	-280.029865	-280.025232	-280.056256	
SVECV-f12	-280.182839	-280.169769	-280.165342	-280.196059	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )	
N	0.046566	0	0.027307	332.011	1377.8004
O	-0.07377	0	1.214024	677.8461	1669.4979
O	1.020022	0	-0.662005	816.1297	
O	-1.098819	0	-0.640526	863.8924	

B. Products (P)

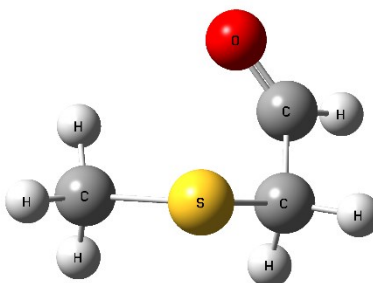
P1						
						
Method			Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ			-229.040609	-228.97865	-228.973261	-229.005219
M06-2X/DG3/aug-cc-pVTZ			-229.04574	-228.983824	-228.978448	-229.010378
MN15/cc-pVTZ			-228.883092	-228.821423	-228.816091	-228.847915
MN15/aug-cc-pVTZ			-228.889409	-228.827891	-228.822549	-228.85439
SVECV-f12			-229.0184336	-228.9565176	-228.9511416	-228.9830716
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.031047	-0.008823	-0.043160	217.4757	1265.5261	3043.7897
H	-0.018764	0.028708	1.053348	301.6945	1306.6404	3781.1445
H	1.013937	0.054777	-0.371594	393.1325	1400.9188	
O	-0.632539	-1.178372	-0.500453	729.6279	1445.486	
H	-1.388216	-0.914981	-1.042794	771.6247	1485.3511	
C	-0.740007	1.221396	-0.53441	885.4352	1853.0833	
H	-0.324647	2.192263	-0.215268	1117.5118	2988.8341	
O	-1.710678	1.155417	-1.239282	1167.0425	3023.7816	

**P1'**



Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-229.030318	-228.96784	-228.96228	-228.994522		
M06-2X/DG3/aug-cc-pVTZ	-229.036294	-228.973972	-228.968326	-229.000786		
MN15/cc-pVTZ	-228.874395	-228.812268	-228.806667	-228.83899		
MN15/aug-cc-pVTZ	-228.881557	-228.819683	-228.813942	-228.846694		
SVECV-f12	-229.0070739	-228.9447519	-228.9391059	-228.9715659		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.014246	0.025940	0.011264	168.0979	1133.2435	3829.1832
H	0.083879	-0.096521	1.938551	253.2623	1196.2215	3908.5978
H	1.056872	0.034074	-0.119490	457.8197	1276.3663	
O	-0.526592	-0.33678	1.239755	557.7217	1366.6035	
H	-2.413673	0.042615	0.06985	740.5899	1432.0207	
C	-0.855625	0.287128	-0.977628	768.9088	1789.5954	
H	-0.515209	0.526585	-1.97203	918.363	3236.164	
O	-2.206543	0.264248	-0.845654	1056.2917	3267.1968	

**P2**



Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-591.313675	-591.227722	-591.220331	-591.258060		
M06-2X/DG3/aug-cc-pVTZ	-591.317055	-591.231159	-591.223756	-591.261521		
MN15/cc-pVTZ	-591.068061	-590.982535	-590.975115	-591.012894		
MN15/aug-cc-pVTZ	-591.074322	-590.988926	-590.981499	-591.019299		
SVECV-f12	-591.203094	-591.117198	-591.109795	-591.147561		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.037108	-0.033394	-0.023807	107.3317	980.8841	3047.4089
C	0.101466	0.064799	1.481388	142.4702	1045.9156	3075.3981
S	1.730530	-0.095148	2.224941	183.074	1222.9174	3101.7462
C	2.511300	1.391055	1.552962	212.0087	1291.3647	3159.734
H	-0.526950	-0.727346	1.894413	279.4299	1350.8651	3181.3593
H	-0.372951	1.007938	1.771054	630.4509	1413.5913	
H	3.496692	1.455458	2.007419	677.5848	1421.4725	
H	2.611009	1.314387	0.474498	732.2782	1470.4977	
H	1.939598	2.276616	1.825115	776.3466	1494.6988	
H	-0.99046	0.036426	-0.43247	941.1035	1868.0534	
O	0.975655	-0.159569	-0.755512	961.6016	2934.2304	

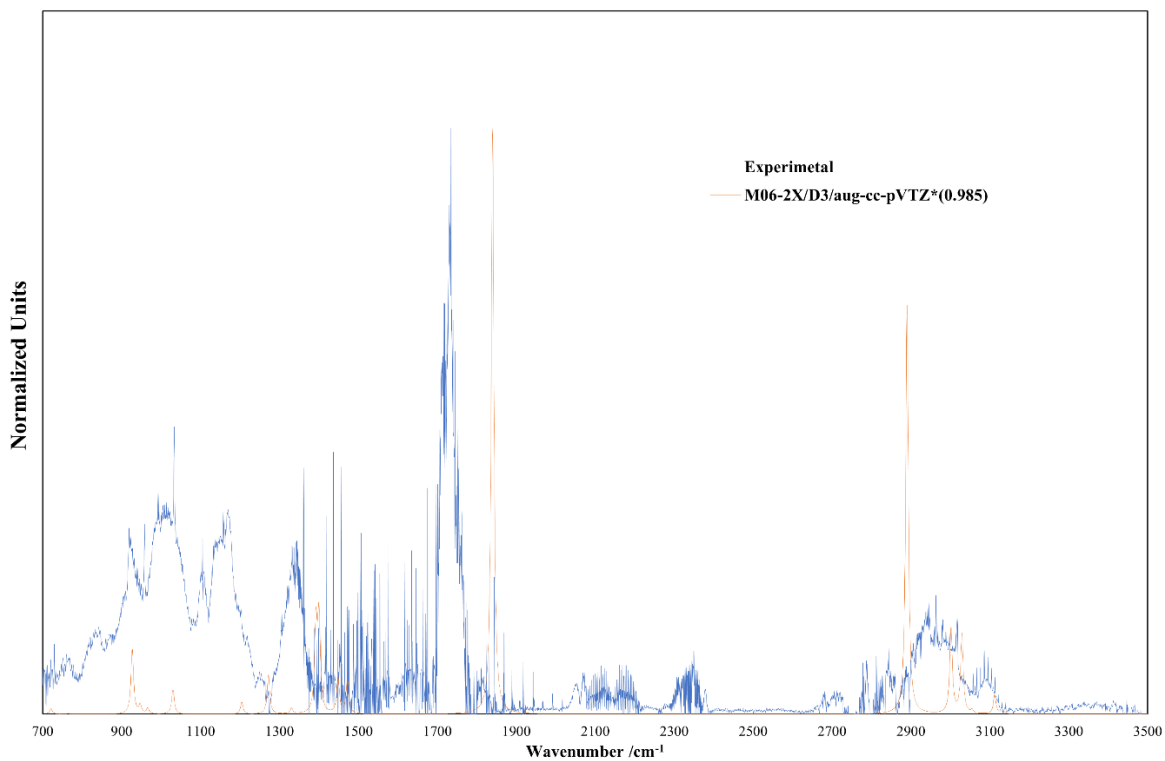


Figure S 2. Comparison between experimental and theoretical IR spectra of 2-methyl thioacetaldehyde (**P2**) calculated at the M06-2X/GD3/aug-cc-pVTZ level of theory (scaled by 0.985).

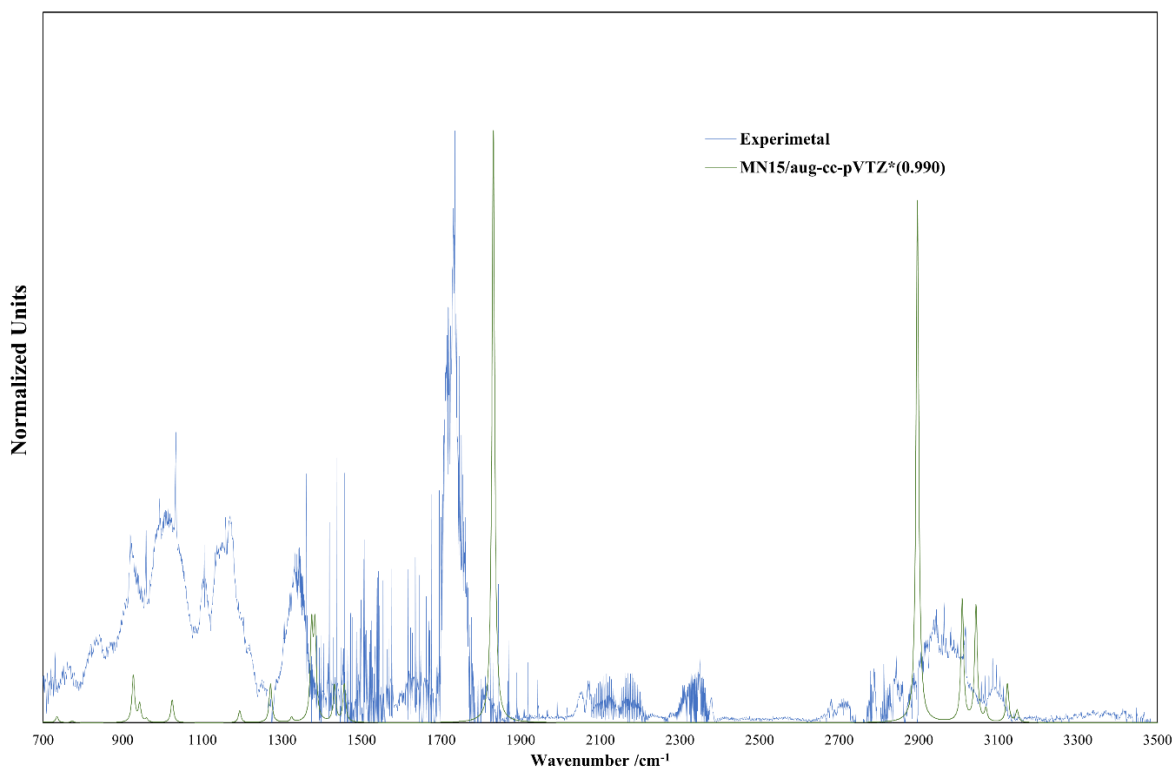
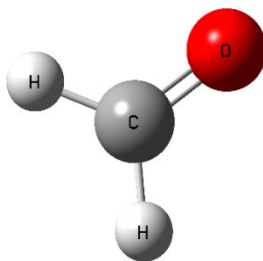


Figure S 3. Comparison between experimental and theoretical IR spectra of 2-methyl thioacetaldehyde (**P2**) calculated at the MN15/aug-cc-pVTZ level of theory (scaled by 0.990).

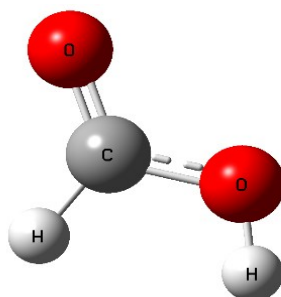
**P3**



Method	Ee			E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-114.496616			-114.469571	-114.465762	-114.491216
M06-2X/DG3/aug-cc-pVTZ	-114.498971			-114.471958	-114.468148	-114.492949
MN15/cc-pVTZ	-114.417742			-114.390864	-114.387052	-114.412514
MN15/aug-cc-pVTZ	-114.420636			-114.393807	-114.389994	-114.414804
SVECV-f12	-114.4872821			-114.4602691	-114.4564591	-114.4812601
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>		
C	-0.725883	-0.088050	0.000000	1213.5626	2945.4693	
H	-0.203116	-1.059481	0.000000	1273.4858	3015.7189	
H	-1.828540	-0.121380	0.000000	1539.8781		
O	-0.128035	0.947827	0.000000	1869.1147		

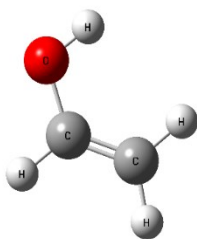


**P4**



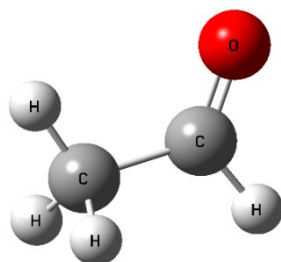
Method/Base	Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-189.758341	-189.724279	-189.720099	-189.748345	
M06-2X/DG3/aug-cc-pVTZ	-189.762579	-189.7286	-189.72442	-189.752668	
MN15/cc-pVTZ	-189.634074	-189.600274	-189.59608	-189.624351	
MN15/aug-cc-pVTZ	-189.638946	-189.60524	-189.601047	-189.629316	
SVECV-f12	-189.7389772	-189.7049972	-189.7008172	-189.7290662	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )		
C	-0.017950	0.000000	-0.009380	519.0422	1431.3763
O	-0.001516	0	1.335139	673.8219	1911.408
O	0.975801	0	-0.657857	1058.0938	3026.8633
H	-1.030572	0	-0.440829	1140.6833	3865.7675
H	-0.898734	0.000000	1.683251	1288.1358	

**P5**



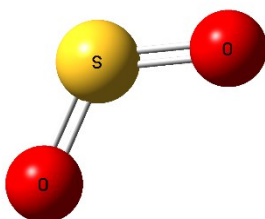
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-153.805133	-153.747969	-153.743424	-153.772396	
M06-2X/DG3/aug-cc-pVTZ		-153.808177	-153.751075	-153.746526	-153.775506	
MN15/cc-pVTZ		-153.693929	-153.637085	-153.632508	-153.661528	
MN15/aug-cc-pVTZ		-153.69796	-153.641201	-153.636623	-153.665648	
SVECV-f12		-153.8052193	-153.7492653	-153.7444353	-153.7741903	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.010778	0.038119	0.022072	458.1265	1329.2061	3856.4518
C	0.011703	-0.088032	1.340026	496.7739	1354.5662	
H	0.892951	0.149563	1.922308	723.5819	1449.0658	
H	-0.865732	-0.435982	1.860716	864.0791	1732.1096	
H	1.775246	0.66295	-0.22205	967.9914	3177.1252	
H	-0.884684	-0.195745	-0.570823	1018.643	3218.7795	
O	1.008178	0.461002	-0.766739	1137.1648	3280.6649	

**P5'**



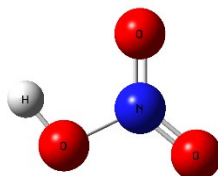
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-153.818126	-153.762145	-153.757316	-153.78707		
M06-2X/DG3/aug-cc-pVTZ	-153.820805	-153.76485	-153.76002	-153.789775		
MN15/cc-pVTZ	-153.705867	-153.650214	-153.645372	-153.675133		
MN15/aug-cc-pVTZ	-153.709414	-153.653852	-153.649004	-153.678777		
SVECV-f12	-153.8052193	-153.7492653	-153.7444353	-153.7741903		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
O	0.009342	0.016897	0.002236	157.7096	1430.1129	3179.8869
C	-0.003091	-0.000861	1.201899	513.5302	1464.924	
C	1.224611	-0.000044	2.061508	775.7494	1474.8385	
H	-0.967056	-0.019408	1.74591	900.8864	1866.0199	
H	1.220155	-0.886443	2.69827	1138.3645	2944.7846	
H	2.120622	0.018785	1.447635	1145.7648	3062.972	
H	1.200954	0.866962	2.724026	1380.5524	3125.2017	

**P6**



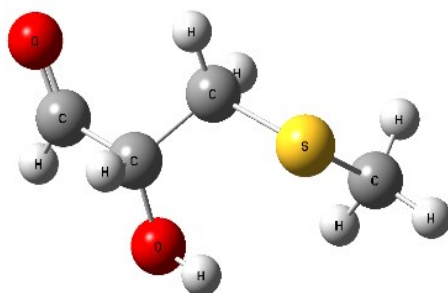
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-548.614765	-548.607451	-548.603456	-548.63161
M06-2X/DG3/aug-cc-pVTZ	-548.619472	-548.612207	-548.608209	-548.636369
MN15/cc-pVTZ	-548.426317	-548.418985	-548.41499	-548.443794
MN15/aug-cc-pVTZ	-548.432575	-548.425292	-548.421295	-548.44945
SVECV-f12	-549.0987169	-549.0914519	-549.0874539	-549.1156129
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )	
O	-0.262602	0.000000	-0.178041	535.2882
S	0.084560	0.000000	1.215440	1234.4605
O	1.478041	0.000000	1.562602	1419.2867

**P7**



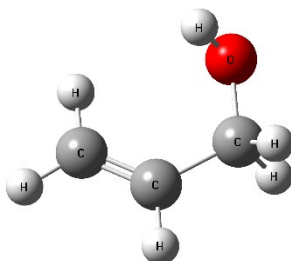
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-280.891715	-280.864226	-280.85985	-280.889893	
M06-2X/DG3/aug-cc-pVTZ	-280.897333	-280.869981	-280.865598	-280.895652	
MN15/cc-pVTZ	-280.715325	-280.68819	-280.683777	-280.713879	
MN15/aug-cc-pVTZ	-280.721435	-280.69443	-280.690013	-280.720122	
SVECV-f12	-280.8641479	-280.8367959	-280.8324129	-280.8624659	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )	
H	0.018848	0.016258	0.021556	506.1591	1358.7488
O	-0.005191	-0.004839	2.155606	621.5287	1415.7078
N	1.046545	-0.00338	1.575598	706.1928	1808.6919
O	2.151719	-0.012163	2.004871	825.2425	3781.4187
O	0.972309	0.010602	0.19838	982.6155	

P8



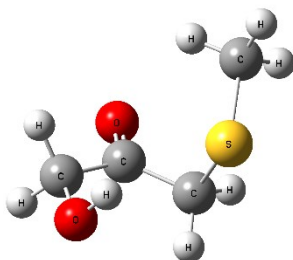
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-705.847948	-705.728288	-705.718474	-705.762901		
M06-2X/DG3/aug-cc-pVTZ	-705.853707	-705.734216	-705.724333	-705.769158		
MN15/cc-pVTZ	-705.523128	-705.404134	-705.394314	-705.438631		
MN15/aug-cc-pVTZ	-705.532503	-705.413749	-705.403863	-705.448580		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.031390	0.083501	0.010452	40.324	981.350	1866.364
C	-0.001786	-0.023482	1.522010	79.572	985.351	2977.759
C	1.442083	-0.043186	2.020213	80.094	1043.211	3022.852
S	1.540312	-0.326705	3.812488	159.493	1065.937	3075.020
C	1.912320	-2.100710	3.827348	186.320	1163.213	3090.791
H	-0.497770	0.872296	1.915837	246.079	1218.946	3155.735
H	1.914029	0.909292	1.790819	290.392	1239.443	3159.992
H	2.006355	-0.830632	1.520964	411.132	1261.773	3171.069
H	1.918443	-2.413662	4.868475	430.487	1354.200	3827.551
H	1.157971	-2.663985	3.283675	458.736	1360.333	
H	2.893644	-2.281693	3.395033	588.044	1384.910	
O	-0.719989	-1.183313	1.866558	726.119	1425.937	
H	-0.749071	-1.229085	2.828717	761.031	1459.701	
H	-0.680569	-0.654356	-0.494983	843.825	1474.232	
O	0.600428	0.900972	-0.596880	887.759	1495.210	

P9



Method	E <sub>e</sub>	E+ZPE	ΔH	ΔG		
M06-2X/GD3/cc-pVTZ	-193.104659	-193.018552	-193.012844	-193.045359		
M06-2X/DG3/aug-cc-pVTZ	-193.108118	-193.022198	-193.016446	-193.049052		
MN15/cc-pVTZ	-192.959172	-192.873646	-192.867871	-192.900504		
MN15/aug-cc-pVTZ	-192.964295	-192.878955	-192.873152	-192.905845		
SVECV-f12	-193.374516	-193.288596	-193.282844	-193.315450		
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.018952	-0.005166	0.001486	196.9399	1159.5468	3165.8129
C	0.014190	0.033897	1.499892	293.9888	1220.4702	3177.4295
C	1.113321	-0.030676	2.233907	323.0222	1318.4794	3257.8497
H	-0.374998	0.953441	-0.381205	579.8972	1374.3833	3865.4876
H	-0.746708	-0.759295	-0.320829	618.8155	1419.2892	
H	1.068829	-0.006218	3.313466	903.5955	1449.4864	
H	2.092281	-0.091564	1.776205	968.6929	1500.8568	
O	1.235603	-0.225512	-0.60006	1000.1051	1736.2174	
H	1.583412	-1.06296	-0.281847	1026.8377	3021.5943	
H	-0.955479	0.115620	1.980735	1048.7245	3086.9964	

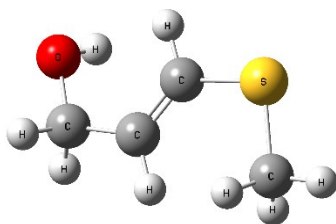
**P10**



<b>P10</b>						
<b>Method</b>			<b>Ee</b>	<b>E+ZPE</b>	<b><math>\Delta H</math></b>	<b><math>\Delta G</math></b>
M06-2X/GD3/cc-pVTZ			-705.857618	-705.737052	-705.727449	-705.771067
M06-2X/DG3/aug-cc-pVTZ			-705.863611	-705.743268	-705.733576	-705.777576
MN15/cc-pVTZ			-705.532523	-705.412704	-705.403002	-705.446903
MN15/aug-cc-pVTZ			-705.542190	-705.422617	-705.412864	-705.457165
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>		
C	-0.109557	-0.275938	0.344779	48.171	954.887	1832.415
C	0.238689	0.654984	1.499442	96.570	984.921	3056.577
C	1.593605	0.515229	2.141096	102.519	1022.824	3078.329
S	1.562118	-0.998393	3.153275	149.986	1131.495	3105.585
C	0.325830	-0.512904	4.381417	173.259	1141.660	3115.206
H	-0.308462	0.358476	-0.519843	272.197	1205.670	3165.397
H	-1.049494	-0.773817	0.599621	304.993	1241.786	3174.264
H	2.374903	0.359341	1.400980	432.063	1284.918	3175.815
H	0.206355	-1.361403	5.050193	488.722	1361.111	3835.080
H	0.678808	0.346907	4.945864	513.143	1367.777	
H	-0.627097	-0.279645	3.913008	574.328	1404.152	
H	1.013626	-1.815822	0.691912	709.910	1447.940	
O	0.901522	-1.179062	-0.021705	754.596	1469.753	
H	1.804764	1.381542	2.762802	799.394	1472.845	
O	-0.581951	1.436148	1.912479	889.873	1484.489	

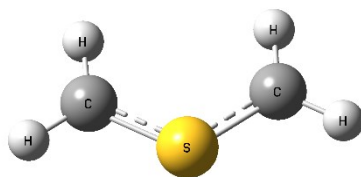


**P11**



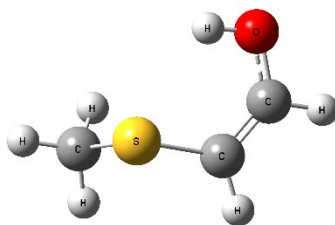
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-630.609130	-630.493248	-630.484656	-630.525303		
M06-2X/DG3/aug-cc-pVTZ	-630.613579	-630.497805	-630.489204	-630.529845		
MN15/cc-pVTZ	-630.330770	-630.215407	-630.206803	-630.247431		
MN15/aug-cc-pVTZ	-630.339088	-630.223907	-630.215297	-630.255930		
SVECV-f12	-631.271887	-631.156113	-631.147512	-631.188153		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.003759	-0.003039	0.062775	74.944	989.221	3023.221
C	0.052128	0.202073	1.551449	173.721	994.010	3068.971
C	1.137044	-0.021270	2.283926	196.594	1001.424	3084.255
S	1.342766	0.165841	4.009300	223.127	1148.957	3148.978
C	-0.288473	0.741888	4.505299	238.102	1209.578	3173.577
H	-0.066848	0.962006	-0.443037	270.625	1257.846	3191.484
H	-0.904988	-0.558979	-0.194390	332.742	1320.756	3194.241
H	2.050805	-0.353078	1.805140	411.805	1351.706	3866.322
H	-0.252791	0.885905	5.581710	597.537	1378.307	
H	-0.524772	1.687831	4.021758	741.946	1414.176	
H	-1.047245	-0.0006	4.265091	774.193	1472.889	
H	1.210729	-1.516172	-0.093648	860.133	1489.629	
O	1.145954	-0.634673	-0.470983	958.024	1506.934	
H	-0.868183	0.554158	2.002143	970.799	1708.024	

**P12**



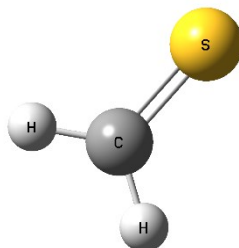
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-476.706236	-476.654931	-476.649857	-476.679935		
M06-2X/DG3/aug-cc-pVTZ	-476.708399	-476.657126	-476.652055	-476.682781		
MN15/cc-pVTZ	-476.543034	-476.491855	-476.486774	-476.51751		
MN15/aug-cc-pVTZ	-476.547606	-476.496344	-476.491294	-476.52198		
SVECV-f12	-477.1772726	-477.1259996	-477.1209286	-477.1516546		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
S	0.120133	-0.069140	0.098002	345.2366	1040.8635	3327.1833
C	0.019391	-0.082305	1.715402	400.0121	1122.2984	
H	0.774574	-0.518905	2.348287	583.4919	1405.3464	
C	1.448014	-0.765211	-0.517211	616.1545	1434.9717	
H	2.216983	-1.208128	0.09434	663.5194	3202.2083	
H	-0.861657	0.379151	2.125227	880.8866	3202.8382	
H	1.516306	-0.757165	-1.590714	955.8397	3325.4666	

**P13**

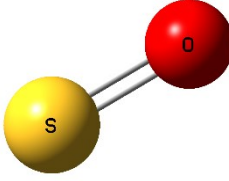


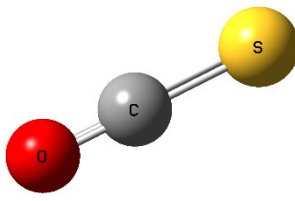
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-591.311195	-591.223802	-591.216549	-591.254367	
M06-2X/DG3/aug-cc-pVTZ		-591.315059	-591.227761	-591.220486	-591.258417	
MN15/cc-pVTZ		-591.067521	-590.980476	-590.973207	-591.011063	
MN15/aug-cc-pVTZ		-591.074265	-590.987307	-590.980042	-591.017853	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.004686	0.001190	0.004916	45.7897	985.6827	3167.1156
C	0.009705	-0.001317	1.337942	162.8718	999.2222	3171.9015
S	1.529413	-0.003868	2.233812	214.4008	1105.2678	3206.544
C	1.552703	1.707936	2.842798	243.29	1224.8563	3229.6289
H	-0.916954	-0.036776	-0.561114	461.6154	1344.089	3722.9315
H	-0.922764	-0.046966	1.880301	629.4396	1365.0802	
H	2.462535	1.824777	3.426944	645.1895	1388.47	
H	1.556539	2.407126	2.011343	725.1229	1471.2874	
H	0.690382	1.887806	3.479543	757.1914	1486.0065	
O	1.086555	0.044821	-0.788788	817.6441	1699.5159	
H	1.871011	0.070335	-0.218856	971.6809	3077.5344	

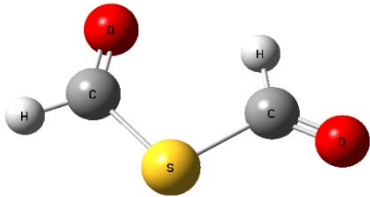
**P14**

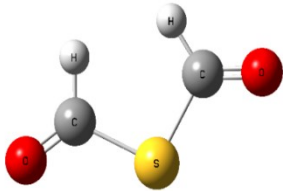


<b>Method</b>					<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>
M06-2X/GD3/cc-pVTZ					-437.454125	-437.429159	-437.425288	-437.451462
M06-2X/DG3/aug-cc-pVTZ					-437.455269	-437.430309	-437.426437	-437.452612
MN15/cc-pVTZ					-437.321875	-437.296904	-437.293031	-437.319201
MN15/aug-cc-pVTZ					-437.324756	-437.299773	-437.2959	-437.322071
SVECV-f12					-437.850338	-437.825379	-437.821507	-437.847682
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>				
S	0.000000	0.000000	-0.338555	1002.9277	3098.983			
C	0.000000	0.000000	1.262464	1040.107	3183.7447			
H	0.921809	0.000000	1.838046	1128.3775				
H	-0.921809	0.000000	1.838046	1501.8407				

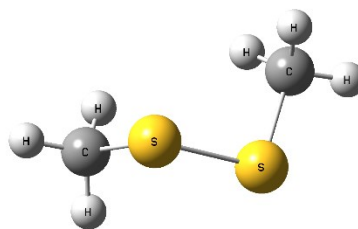
P15				
				
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-473.359898	-473.357118	-473.353798	-473.37898
M06-2X/DG3/aug-cc-pVTZ	-473.362833	-473.360061	-473.356741	-473.381922
MN15/cc-pVTZ	-473.211212	-473.208419	-473.205099	-473.230272
MN15/aug-cc-pVTZ	-473.215875	-473.213082	-473.209762	-473.234934
SVECV-f12	-473.7210453	-473.7182723	-473.7149523	-473.7401343
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )	
O	0.000000	0.000000	-0.092802	1216.9374
S	0.000000	0.000000	1.392802	

P16				
				
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-511.540741	-511.531338	-511.527582	-511.553822
M06-2X/DG3/aug-cc-pVTZ	-511.542731	-511.533341	-511.529586	-511.555823
MN15/cc-pVTZ	-511.362279	-511.352865	-511.349108	-511.375347
MN15/aug-cc-pVTZ	-511.365852	-511.356448	-511.352692	-511.378929
SVECV-f12	-511.9970653	-511.9876753	-511.9839203	-512.0101583
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )	
C	0.000000	0.000000	-0.035976	539.433
S	0.000000	0.000000	1.528519	886.0667
O	0.000000	0.000000	-1.184543	2156.6686

P17						
						
Method			Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ			-626.032216	-625.992787	-625.98633	-626.022242
M06-2X/DG3/aug-cc-pVTZ			-626.036581	-625.997206	-625.990729	-626.026703
MN15/cc-pVTZ			-625.775632	-625.736254	-625.729815	-625.765654
MN15/aug-cc-pVTZ			-625.782443	-625.743141	-625.736683	-625.772595
SVECV-f12			-625.9100418	-625.8706678	-625.8641908	-625.9001648
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.077915	-0.134725	0.093659	127.2049	945.432	3065.877
S	0.096421	0.750239	1.648582	152.3736	969.6345	
C	1.699531	0.202372	2.267592	194.7619	1346.7254	
H	-0.849212	0.068396	-0.462587	413.6635	1386.4683	
H	2.209136	-0.483264	1.579061	513.0691	1814.8367	
O	0.938933	-0.853886	-0.311078	725.8905	1844.1277	
O	2.121017	0.569600	3.315787	769.9636	3013.4012	

P17						
						
Method			Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ			-626.02975	-625.990427	-625.984002	-626.019059
M06-2X/DG3/aug-cc-pVTZ			-626.034711	-625.995405	-625.988984	-626.024675
MN15/cc-pVTZ			-625.773485	-625.734281	-625.727881	-625.763501
MN15/aug-cc-pVTZ			-625.780874	-625.741705	-625.735307	-625.770923
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
S	-0.119178	-0.069814	-0.097627	107.3919	938.218	2984.4168
C	-0.035476	0.143731	1.674861	199.8709	941.6918	
H	0.889270	0.637885	2.018062	211.2353	1352.4503	
O	-0.897516	-0.214528	2.410436	419.7768	1417.1868	
C	1.450464	0.673187	-0.519416	484.0183	1820.112	
H	2.016349	1.039061	0.354085	691.7716	1864.3959	
O	1.843585	0.762388	-1.637487	846.3651	2974.4501	

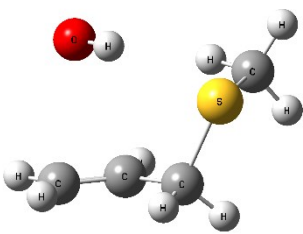
**DMDS**



<b>Method</b>				<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>
M06-2X/GD3/cc-pVTZ				-876.198483	-876.120592	-876.113226	-876.150325
M06-2X/DG3/aug-cc-pVTZ				-876.20073	-876.122874	-876.115504	-876.15262
MN15/cc-pVTZ				-875.930476	-875.852828	-875.845478	-875.883128
MN15/aug-cc-pVTZ				-875.936061	-875.858528	-875.851178	-875.88818
SVECV-f12				-876.990167	-876.912311	-876.904941	-876.942056
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>			
S	0.438244	0.180460	1.229979	93.617	976.8339	3160.2848	
S	0.283756	2.221540	1.229979	150.7051	977.7661	3160.716	
C	1.661401	-0.107008	-0.079014	165.742	1338.6807	3175.1533	
C	-0.939401	2.509008	-0.079014	236.2853	1347.2095	3175.2272	
H	1.819804	-1.183606	-0.121396	266.3204	1463.1058		
H	1.286068	0.238112	-1.038801	527.4481	1468.7437		
H	2.594531	0.39209	0.165232	719.8289	1479.3901		
H	-1.097804	3.585606	-0.121396	722.2997	1483.4613		
H	-0.564068	2.163888	-1.038801	967.2223	3073.7864		
H	-1.872531	2.00991	0.165232	970.2753	3074.9082		

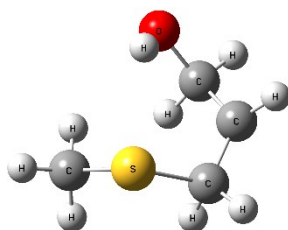
C. Intermediaries (\_Im).

1. Addition of OH at C1 and C2.

CR_add						
						
Method	Ee			E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-631.12471			-631.002952	-630.992701	-631.037876
M06-2X/DG3/aug-cc-pVTZ	-631.129235			-631.007704	-630.997363	-631.042985
MN15/cc-pVTZ	-630.844751			-630.723463	-630.713161	-630.758592
MN15/aug-cc-pVTZ	-630.852843			-630.731785	-630.721441	-630.767122
SVECV-f12	-631.0175668			-630.8960358	-630.8856948	-630.9313168
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.000768	0.051670	0.009725	57.5151	947.9705	3068.9031
C	-0.002071	-0.035024	1.338546	84.6513	969.306	3076.4319
C	1.239963	-0.033715	2.168333	112.3329	970.0492	3134.2161
S	1.70192	-1.684417	2.763181	130.3167	981.6448	3154.8962
C	0.229179	-2.085493	3.710922	144.5338	1020.2054	3170.7512
H	0.926819	0.148813	-0.54238	198.9826	1101.5711	3173.8012
H	-0.917017	0.021726	-0.56088	248.4827	1221.6912	3195.8592
H	-0.943758	-0.138936	1.864721	326.979	1250.6536	3272.1255
H	1.137119	0.618071	3.037321	400.6452	1310.6971	3659.6078
H	2.092218	0.309867	1.582906	449.8827	1349.298	
H	0.432259	-3.008587	4.248254	550.4144	1430.9328	
H	0.018159	-1.299064	4.434747	615.4864	1452.3627	
H	-0.625039	-2.2372	3.053538	736.8591	1456.3873	
O	-0.499597	-2.523169	0.405436	785.9785	1478.0667	
H	0.386474	-2.550145	0.823558	851.3457	1697.4493	

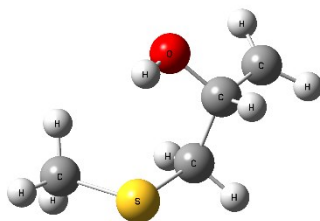


**A1**



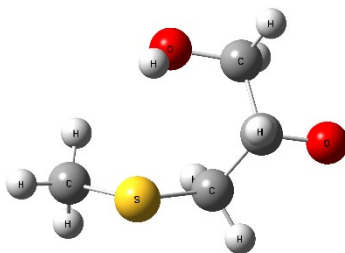
<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			$\Delta H$			$\Delta G$		
M06-2X/GD3/cc-pVTZ							-631.169438			-631.043704			-631.034626			-631.076763		
M06-2X/DG3/aug-cc-pVTZ							-631.174097			-631.048493			-631.039378			-631.081689		
MN15/cc-pVTZ							-630.890697			-630.76558			-630.756485			-630.798609		
MN15/aug-cc-pVTZ							-630.89901			-630.774153			-630.765011			-630.807331		
SVECV-f12							-631.05701			-630.931406			-630.922291			-630.964603		
<b>Coordinates (xyz)</b>										<b>Vibrations (cm<sup>-1</sup>)</b>								
C	0.047799	-0.104937	0.001055	87.7476	987.3062	3026.1644												
C	-0.035159	0.217096	1.449726	113.4153	1037.3301	3068.625												
C	1.097252	-0.062172	2.349927	123.5006	1077.5924	3072.4922												
S	1.420496	-1.881935	2.543012	216.0425	1159.6271	3098.5875												
C	2.533735	-2.168226	1.142773	256.3752	1190.7126	3148.921												
H	1.085544	-0.021993	-0.341754	264.1104	1220.1946	3156.3684												
H	-0.553107	0.587395	-0.58899	367.0467	1262.1469	3164.3279												
H	-1.019787	0.346172	1.879661	406.1246	1325.4238	3194.3501												
H	0.920652	0.301978	3.358616	423.0419	1358.7635	3816.8718												
H	2.034152	0.363154	1.98592	593.6488	1394.2161													
H	2.880343	-3.195255	1.231188	668.5772	1438.8624													
H	2.026515	-2.049174	0.187828	740.2726	1466.6789													
H	3.390761	-1.500394	1.201874	844.9944	1476.2104													
O	-0.460462	-1.408977	-0.292044	895.8755	1489.6693													
H	-0.270628	-1.977748	0.462536	976.0409	1525.4085													

**A2**



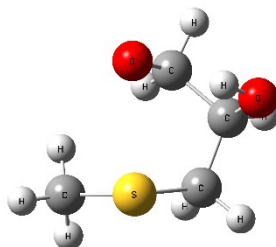
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-631.167788	-631.044282	-631.034703	-631.078064		
M06-2X/DG3/aug-cc-pVTZ	-631.172284	-631.048958	-631.039298	-631.083072		
MN15/cc-pVTZ	-630.888943	-630.765771	-630.756268	-630.799363		
MN15/aug-cc-pVTZ	-630.897068	-630.774134	-630.764575	-630.80794		
SVECV-f12	-631.055302	-630.931977	-630.922317	-630.96609		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.006500	0.032736	-0.007362	62.4062	960.9728	2984.7663
C	-0.000589	0.009011	1.473127	90.4849	982.9228	3074.2086
C	1.437707	-0.028198	2.019545	102.2478	1027.9736	3081.8057
S	1.498793	-0.215831	3.828956	160.232	1073.8663	3141.3405
C	1.800323	-1.999342	3.945071	220.0767	1140.0759	3158.7162
H	0.377707	0.896979	-0.534904	282.5542	1214.8683	3170.8496
H	-0.264625	-0.857216	-0.552394	328.6943	1252.594	3183.9059
H	-0.471304	0.924478	1.85819	419.4877	1269.7479	3297.2628
H	1.951387	0.89696	1.762786	445.6531	1353.1975	3823.6089
H	1.983078	-0.859244	1.572313	472.7354	1355.999	
H	1.767667	-2.259593	5.000172	484.627	1404.5233	
H	1.037766	-2.558193	3.40843	724.5414	1449.681	
H	2.783971	-2.240475	3.548613	768.5163	1464.8645	
O	-0.736495	-1.120456	1.897635	839.8354	1474.0181	
H	-0.764574	-1.093097	2.860673	894.3559	1495.5268	

**A10**



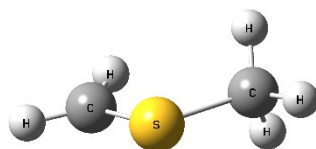
<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			<b><math>\Delta H</math></b>			<b><math>\Delta G</math></b>																																																																																															
M06-2X/GD3/cc-pVTZ							-706.380428			-706.250143			-706.240228			-706.284735																																																																																															
M06-2X/DG3/aug-cc-pVTZ							-706.386279			-706.256052			-706.246134			-706.290676																																																																																															
MN15/cc-pVTZ							-706.056221			-705.926485			-705.916624			-705.96085																																																																																															
MN15/aug-cc-pVTZ							-706.066087			-705.936481			-705.926595			-705.970974																																																																																															
SVECV-f12							-706.166063			-706.035835			-706.025917			-706.070459																																																																																															
<b>Coordinates (xyz)</b>							<b>Vibrations (cm<sup>-1</sup>)</b>																																																																																																								
C	0.032194	-0.010880	-0.002860	70.9721	984.2576	1518.6574	C	0.007305	0.002282	1.561647	97.7455	1000.4063	2958.2696	C	1.410624	0.0041	2.1762	132.1558	1046.6799	3072.6271	S	2.090047	-1.679847	2.342373	184.7572	1098.1912	3075.2312	C	3.603144	-1.526824	1.360788	204.0308	1151.8445	3091.3893	H	0.308454	0.984889	-0.346684	269.5969	1168.1453	3132.2666	H	-0.976254	-0.237127	-0.351721	287.969	1181.0625	3149.8109	H	-0.541049	-0.904802	1.864442	335.9687	1255.6297	3163.1498	H	1.351439	0.456741	3.163241	380.943	1271.382	3171.1969	H	2.0944	0.592995	1.565844	410.3753	1343.6118	3816.6976	H	4.0643	-2.511215	1.337378	479.9557	1351.8985		H	3.361551	-1.209729	0.349191	727.4647	1381.2155		H	4.289633	-0.824858	1.827428	745.7611	1421.2609		O	0.989206	-0.89767	-0.513864	780.7059	1464.6027		H	0.918943	-1.743181	-0.05637	873.9148	1478.4909		O	-0.728902	1.096185	1.881967	936.3819	1496.5404	

**A20**



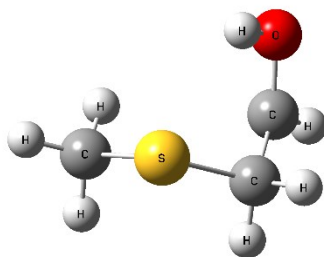
<b>Method</b>				<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>
M06-2X/GD3/cc-pVTZ				-706.388008	-706.257243	-706.247712	-706.291202
M06-2X/DG3/aug-cc-pVTZ				-706.393995	-706.263378	-706.253799	-706.297484
MN15/cc-pVTZ				-706.066313	-705.935708	-705.926378	-705.969162
MN15/aug-cc-pVTZ				-706.076341	-705.945989	-705.936637	-705.979472
SVECV-f12				-706.266941	-706.136324	-706.126745	-706.17043
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>			
C	-0.029807	0.039869	-0.014940	76.4409	975.3534	1483.294	
C	0.010010	-0.016269	1.519772	107.1938	985.196	2964.023	
C	1.45883	-0.011456	2.013192	137.0928	1014.6713	3018.2589	
S	2.450246	-1.334574	1.270365	170.7684	1100.6239	3073.733	
C	3.334148	-0.425	-0.019091	213.3131	1122.4778	3078.1691	
H	0.551204	0.8919	-0.393449	244.3521	1152.2103	3089.1237	
H	-1.083354	0.180045	-0.305274	317.7894	1200.8568	3145.544	
H	1.456402	-0.178838	3.088671	382.1484	1253.6601	3164.9964	
H	1.942038	0.94418	1.810725	440.2895	1280.6687	3175.2306	
H	3.998285	-1.139282	-0.4992	496.1983	1341.0353	3791.2562	
H	2.645472	-0.032595	-0.762138	667.7518	1349.5982		
H	3.92789	0.372258	0.42245	746.087	1364.4248		
O	0.350125	-1.161053	-0.547415	773.2125	1425.9777		
H	-0.433291	-1.876722	1.384642	844.0344	1445.2675		
H	-0.502488	0.857034	1.929459	852.4687	1453.8244		
O	-0.678719	-1.149742	1.972514	941.4612	1474.1794		

### Ad\_Im1



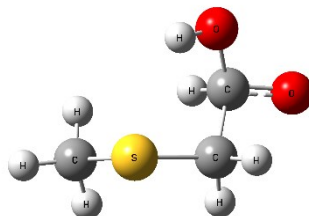
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-477.33585	-477.274164	-477.268013	-477.302011	
M06-2X/DG3/aug-cc-pVTZ		-477.337743	-477.276094	-477.269919	-477.304007	
MN15/cc-pVTZ		-477.170709	-477.10907	-477.102899	-477.137029	
MN15/aug-cc-pVTZ		-477.175096	-477.113361	-477.107269	-477.141164	
SVECV-f12		-477.240136	-477.178488	-477.172313	-477.206401	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.067803	-0.079664	0.099211	120.0078	1027.4791	3189.2872
S	-0.086689	-0.142757	1.79604	179.9037	1348.1442	3315.0295
C	1.640039	0.02227	2.293987	299.3286	1407.9069	
H	-0.830284	-0.175969	-0.48685	344.6281	1472.2998	
H	0.99969	0.211092	-0.35786	732.3431	1485.8485	
H	1.6677	0.010814	3.380023	858.3843	3076.441	
H	2.220379	-0.810591	1.90475	897.3256	3161.0065	
H	2.042969	0.964806	1.930698	968.3239	3176.8964	

**Ad\_Im2**



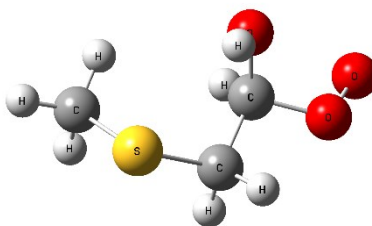
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-591.871873	-591.775221	-591.767303	-591.806809		
M06-2X/DG3/aug-cc-pVTZ	-591.876384	-591.779816	-591.771891	-591.811368		
MN15/cc-pVTZ	-591.628125	-591.532102	-591.524073	-591.563639		
MN15/aug-cc-pVTZ	-591.635563	-591.539699	-591.53167	-591.571238		
SVECV-f12	-591.761333	-591.664766	-591.656841	-591.696317		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.141064	0.148604	-0.026128	76.3648	980.2232	3072.9577
C	0.129472	0.041535	1.450134	136.2481	1006.9793	3117.6064
S	1.818031	-0.06345	2.148099	178.1463	1174.4309	3155.4642
C	2.463353	1.530306	1.58785	225.0987	1191.6568	3171.4298
H	-0.349103	-0.880284	1.802636	313.4133	1267.6518	3236.9572
H	-0.399727	0.885002	1.890761	381.051	1350.5114	3745.9706
H	3.492623	1.596063	1.930818	541.3566	1352.5918	
H	2.435614	1.595973	0.502626	563.7716	1442.2513	
H	1.886836	2.344141	2.022842	706.1539	1455.8754	
H	1.58022	-1.073017	-0.17059	752.0143	1470.9821	
H	-0.677796	0.586296	-0.574961	865.8673	1485.9019	
O	0.870595	-0.741759	-0.740265	964.0101	3005.5657	

**Ad\_Im2\_O**



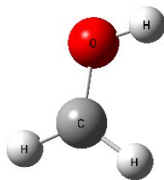
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-667.087459	-666.986348	-666.977826	-667.019306		
M06-2X/DG3/aug-cc-pVTZ	-667.093507	-666.992579	-666.984022	-667.025551		
MN15/cc-pVTZ	-666.797401	-666.696711	-666.688209	-666.729463		
MN15/aug-cc-pVTZ	-666.806643	-666.706231	-666.697693	-666.7391		
SVECV-f12	-666.826467	-666.725539	-666.716982	-666.758511		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.063424	-0.019677	-0.055695	51.237	970.2075	2899.6224
C	0.029055	0.001549	1.501312	116.6261	975.1533	3071.4355
S	1.723596	-0.030422	2.108542	192.5299	1031.2684	3099.1123
C	2.29345	1.577623	1.510391	227.5595	1130.8236	3153.2946
H	-0.451606	-0.89937	1.878385	275.5703	1168.0111	3163.3206
H	-0.501462	0.875544	1.871508	335.7525	1227.233	3171.3083
H	3.293769	1.725743	1.908838	362.4401	1256.0348	3792.4424
H	2.340904	1.601784	0.423508	475.099	1302.63	
H	1.642319	2.368823	1.876037	573.8562	1334.2773	
H	1.498535	-1.161444	-0.084081	714.7797	1357.75	
O	0.707402	-1.035368	-0.623073	757.2307	1446.1741	
H	0.271112	0.970308	-0.424176	821.3302	1475.1804	
O	-1.356336	-0.122573	-0.357988	885.9963	1486.8744	

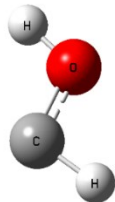
**Ad\_Im2\_O2**



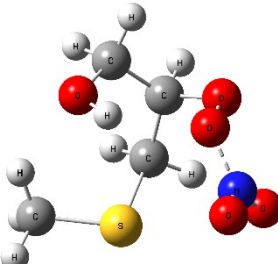
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-742.248689	-742.141931	-742.132208	-742.176885		
M06-2X/DG3/aug-cc-pVTZ	-742.255256	-742.148681	-742.138911	-742.183777		
MN15/cc-pVTZ	-741.913181	-741.806878	-741.797215	-741.841722		
MN15/aug-cc-pVTZ	-741.923219	-741.817147	-741.807452	-741.85207		
SVECV-f12	-742.119829	-742.013254	-742.003484	-742.04835		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.011141	0.169072	-0.022051	54.0229	952.5095	1490.0263
C	0.022528	0.060249	1.497873	86.6355	969.2466	3072.3473
S	1.685668	-0.024891	2.194128	97.1238	985.8634	3084.897
C	2.367033	1.511108	1.525085	169.8043	1052.4275	3119.4532
H	-0.471176	-0.867401	1.790159	205.3307	1179.6188	3140.6628
H	-0.536254	0.888684	1.930127	246.4762	1193.3241	3156.771
H	3.365915	1.619366	1.939217	274.8147	1265.1933	3173.3936
H	2.433317	1.462713	0.440381	346.3669	1289.5139	3805.3361
H	1.760983	2.360758	1.833172	380.9526	1335.3786	
H	1.317182	-1.227017	-0.072282	540.1957	1355.2988	
O	0.908491	-0.604348	-0.685569	598.9455	1392.1528	
H	0.06243	1.193041	-0.385599	726.6068	1450.161	
O	-1.357783	-0.263425	-0.371322	794.4541	1466.3748	
O	-1.717539	0.200939	-1.529878	852.9885	1476.2238	



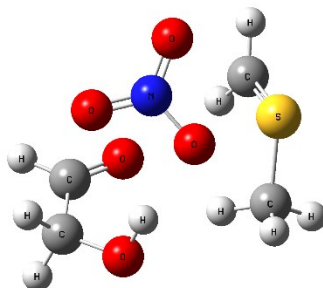
P3_Im1					
					
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-115.052657	-115.014983	-115.010697	-115.037962	
M06-2X/DG3/aug-cc-pVTZ	-115.056127	-115.018536	-115.014232	-115.041523	
MN15/cc-pVTZ	-114.975028	-114.937888	-114.933374	-114.961027	
MN15/aug-cc-pVTZ	-114.979314	-114.94234	-114.937753	-114.96556	
SVECV-f12	-115.043941	-115.00635	-115.002046	-115.029337	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )		
C	0.00545	0.002071	0.000246	408.8737	1494.903
H	-0.001567	-0.007276	1.077017	583.2139	3160.8342
H	0.934522	0.006823	-0.550792	1063.2462	3298.4584
O	-1.085765	-0.583982	-0.560655	1236.2151	3895.9641
H	-0.98958	-0.616906	-1.514844	1358.9451	

P3_Im2					
					
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-114.415051	-114.387937	-114.384107	-114.409632	
M06-2X/DG3/aug-cc-pVTZ	-114.418013	-114.390928	-114.387097	-114.41262	
MN15/cc-pVTZ	-114.338116	-114.311186	-114.307352	-114.332887	
MN15/aug-cc-pVTZ	-114.34156	-114.314662	-114.310827	-114.33636	
SVECV-f12	-114.4040481	-114.3769631	-114.3731321	-114.3986551	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )		
H	0.017978	-0.000140	-0.000872	1087.5314	2911.6041
C	-0.003793	0.000104	1.857863	1224.728	3779.7916
H	0.812721	-0.000115	2.610072	1376.9712	
O	0.649322	-0.000291	0.730513	1508.4146	

2. Reactions of the peroxy radicals (A1O2, A2O2) with NO<sub>2</sub>

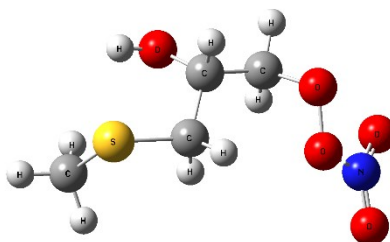
A1O2-NO <sub>2</sub>						
						
Method	Ee		E+ZPE	ΔH	ΔG	
M06-2X/GD3/cc-pVTZ	-986.658867		-986.508045	-986.494958	-986.546692	
M06-2X/DG3/aug-cc-pVTZ	-986.668341		-986.517712	-986.504603	-986.556428	
MN15/cc-pVTZ	-986.158012		-986.008433	-985.995116	-986.047489	
MN15/aug-cc-pVTZ	-986.172309		-986.023072	-986.009702	-986.062295	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.118636	0.093140	-0.030252	64.6622	813.2374	1451.6264
C	-0.038572	-0.014456	1.480555	77.7527	833.1851	1471.3948
C	1.205048	-0.266457	2.326571	84.6991	855.0344	1495.3471
S	2.164976	-1.795009	2.101015	109.0869	870.9558	1502.0509
C	3.419527	-1.243904	0.922915	129.6953	958.9188	1835.768
H	0.730143	0.973721	-0.235249	170.3494	982.9907	3039.5227
H	-0.876917	0.274359	-0.44863	187.8036	984.7475	3058.2891
H	0.894912	-0.264665	3.370095	201.1324	1022.9367	3073.9366
H	1.886908	0.573571	2.184721	234.0226	1057.7917	3079.2847
H	4.08428	-2.09045	0.767173	264.2365	1108.855	3100.4049
H	2.962151	-0.962761	-0.020718	314.4912	1159.6791	3136.2519
H	3.99212	-0.420752	1.345876	339.2751	1245.2327	3159.0129
H	0.343392	-1.807485	-0.39979	345.1361	1261.1517	3182.0442
O	0.752001	-0.982742	-0.677698	425.0134	1291.2008	3870.2456
H	-0.439763	0.951125	1.805685	490.9592	1342.9107	
O	-1.150844	-0.857133	1.84233	561.7704	1357.3869	
O	-0.998213	-2.12784	1.29561	662.7342	1369.9688	
N	-0.638411	-3.079675	2.327534	710.0884	1395.0433	
O	-0.51161	-2.665902	3.425816	745.3385	1418.1614	
O	-0.543561	-4.163688	1.863298	779.1409	1436.5175	

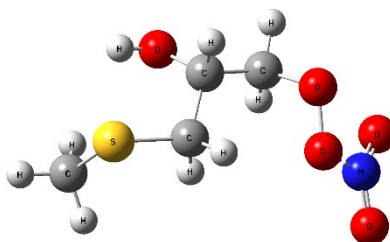
**A1O2-NO<sub>2</sub>-PW**



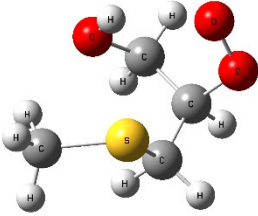
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-986.691867	-986.545696	-986.530853	-986.586895	
M06-2X/DG3/aug-cc-pVTZ		-986.702874	-986.556981	-986.54206	-986.598462	
MN15/cc-pVTZ		-986.190583	-986.045448	-986.030412	-986.087109	
MN15/aug-cc-pVTZ		-986.206428	-986.061634	-986.046537	-986.103513	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.093472	0.010928	0.083329	44.9942	735.5701	1460.5452
C	-0.181714	0.285933	1.534651	71.3202	742.1799	1466.1513
C	2.858320	-0.173672	4.244091	79.1798	776.99	1475.6736
S	3.870489	-0.679014	3.121014	92.232	871.4538	1591.4673
C	3.857332	0.605622	1.864279	119.9503	882.5214	1844.6528
H	-0.389536	0.810118	-0.489766	125.1507	928.461	2973.9151
H	-0.427797	-0.920918	-0.164932	138.2382	930.9546	3035.617
H	2.765896	-0.794321	5.123913	149.32	995.7424	3067.8884
H	2.18794	0.658652	4.08338	174.0439	1045.3487	3084.4758
H	4.242944	0.145357	0.959545	187.8305	1092.2877	3174.2508
H	2.828408	0.923294	1.712067	203.0951	1102.7933	3192.447
H	4.506317	1.409501	2.200788	217.7011	1123.553	3197.0384
H	1.848724	-0.773753	0.221107	227.5914	1182.9439	3292.7283
O	1.445196	-0.017379	-0.240184	252.8896	1263.991	3633.899
H	-1.247468	0.245816	1.824687	301.5457	1348.1141	
O	0.663676	0.545223	2.353359	344.2071	1376.797	
O	2.733272	-1.867794	1.476543	621.7213	1400.4132	
N	1.75938	-2.462249	2.084201	640.6975	1414.2832	
O	1.960709	-2.918922	3.198881	715.9417	1449.8274	
O	0.679736	-2.514352	1.513474	722.5586	1454.3759	

**A2O2-NO<sub>2</sub>**

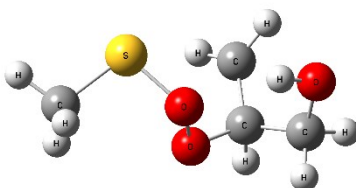


<b>A2O2-NO<sub>2</sub></b>						
						
<b>Method</b>		<b>E<sub>c</sub></b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>	
M06-2X/GD3/cc-pVTZ		-986.663129	-986.512375	-986.499097	-986.552975	
M06-2X/DG3/aug-cc-pVTZ		-986.67314	-986.522608	-986.509294	-986.563282	
MN15/cc-pVTZ		-986.1633	-986.013568	-986.000227	-986.054104	
MN15/aug-cc-pVTZ		-986.177869	-986.028501	-986.015116	-986.06913	
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>		
C	0.142050	-0.132091	0.076305	34.7767	790.6216	1462.5489
C	0.043362	-0.051907	1.591059	44.5665	846.0566	1475.1876
C	1.402184	-0.080468	2.284291	75.586	863.1229	1482.2158
S	1.239529	-0.249279	4.089253	90.4621	893.6401	1495.5705
C	1.542957	-2.027817	4.264783	95.8157	983.9573	1826.7588
H	0.624596	-1.05866	-0.238085	122.3319	986.418	3032.513
H	-0.462571	0.883824	1.854213	171.6365	1010.2995	3076.0094
H	1.945301	0.84128	2.087223	189.7382	1055.8785	3083.9371
H	2.004199	-0.913834	1.920284	229.2387	1082.4509	3088.6221
H	1.396688	-2.271463	5.314163	292.5774	1104.1541	3149.0876
H	0.850356	-2.605516	3.657814	317.1481	1161.5405	3152.0088
H	2.567126	-2.262177	3.983948	413.7136	1225.9494	3161.142
O	-0.75526	-1.15991	1.946742	427.9919	1254.0193	3172.3438
H	-0.88041	-1.125102	2.902346	443.0097	1271.5971	3813.5348
H	-0.855183	-0.093483	-0.358926	471.1681	1306.9063	
O	0.816653	0.991748	-0.491303	568.4068	1357.4327	
O	2.187184	0.796819	-0.418815	593.4397	1365.4456	
N	2.652841	0.174399	-1.641399	716.9096	1401.5706	
O	3.833626	0.075274	-1.629401	730.4767	1411.2844	
O	1.835788	-0.142077	-2.434962	767.3759	1435.5785	

3. Intramolecular rearrangement mechanism in RO<sub>2</sub> intermediates (A1O2-A2O2)

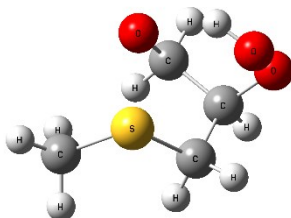
A1_Im1						
						
Method		Ee	E+ZPE	ΔH	ΔG	
M06-2X/GD3/cc-pVTZ		-781.547593	-781.411338	-781.400765	-781.446998	
M06-2X/DG3/aug-cc-pVTZ		-781.55404	-781.417921	-781.407321	-781.453627	
MN15/cc-pVTZ		-781.178299	-781.042763	-781.032171	-781.07828	
MN15/aug-cc-pVTZ		-781.188915	-781.053596	-781.042966	-781.08921	
SVECV-f12		-781.4141	-781.277981	-781.267381	-781.313687	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.054596	-0.012950	-0.010353	64.7925	938.2931	1496.0619
C	0.021564	-0.000231	1.508299	93.9673	981.8735	1500.5351
C	1.366853	-0.003036	2.234704	123.4313	983.7647	3045.0999
S	2.287721	-1.571301	2.241042	166.5044	1024.2309	3072.8755
C	3.629275	-1.179658	1.092217	181.7545	1089.3528	3077.4282
H	0.354934	0.983366	-0.337221	211.1167	1152.7383	3090.8093
H	-0.965368	-0.188471	-0.367429	241.4585	1219.9765	3109.3225
H	1.187925	0.257883	3.275766	288.4625	1242.0232	3142.291
H	2.002153	0.769593	1.802148	310.1428	1267.46	3159.3685
H	4.247218	-2.072331	1.028555	428.0757	1277.6353	3174.3564
H	3.227466	-0.940725	0.111659	484.0718	1343.2854	3825.791
H	4.232959	-0.360753	1.477196	508.541	1358.9733	
H	0.763772	-1.785742	-0.226006	668.7668	1398.7832	
O	0.963944	-0.913792	-0.585904	741.3595	1404.0621	
H	-0.528678	0.890116	1.82188	799.5151	1442.4292	
O	-0.795208	-1.075431	2.042133	826.549	1457.3022	
O	-0.715089	-2.167845	1.341427	860.3876	1474.1059	

**A1\_Im1\_1**



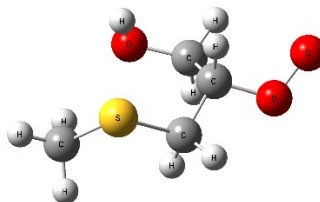
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.50707	-781.375035	-781.363661	-781.411849	
M06-2X/DG3/aug-cc-pVTZ		-781.514271	-781.38249	-781.371034	-781.419452	
MN15/cc-pVTZ		-781.13793	-781.006481	-780.995055	-781.043346	
MN15/aug-cc-pVTZ		-781.14075	-781.010186	-780.998558	-781.046694	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.092108	0.296657	0.045912	49.9651	813.6386	1484.8209
C	-0.014873	-0.274084	1.457104	76.3515	861.4778	1497.4549
C	1.272801	0.005827	2.136295	94.2575	941.7931	3033.1134
S	1.685598	-3.208341	1.619757	144.9072	973.1295	3047.583
C	0.706951	-4.667213	1.998357	166.0203	977.4171	3072.607
H	-0.18431	1.380819	0.118282	167.6569	993.513	3110.3081
H	-0.995591	-0.093732	-0.432275	203.7104	1020.9739	3160.0635
H	1.393382	-0.241331	3.17889	280.1655	1130.5002	3175.9232
H	2.094087	0.441042	1.590406	336.5712	1166.8592	3186.495
H	1.345462	-5.306688	2.607301	350.2052	1244.7575	3299.1662
H	-0.173421	-4.386417	2.570194	430.3489	1320.9344	3859.4175
H	0.430719	-5.188121	1.085793	464.9032	1339.233	
O	1.053509	0.049219	-0.73662	486.1659	1342.6015	
H	1.189996	-0.902495	-0.765423	545.7257	1391.7049	
H	-0.854497	0.133617	2.032895	721.4389	1435.8884	
O	-0.36181	-1.673895	1.481063	738.7823	1454.3964	
O	0.600565	-2.390588	0.678019	790.4009	1462.0139	

**A1\_Im1\_2**



Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.518973	-781.383549	-781.373402	-781.418123	
M06-2X/DG3/aug-cc-pVTZ		-781.525919	-781.390476	-781.380366	-781.424953	
MN15/cc-pVTZ		-781.153486	-781.018804	-781.008648	-781.053316	
MN15/aug-cc-pVTZ		-781.113247	-780.98078	-780.969748	-781.017539	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.001265	-0.006335	-0.001857	108.9253	955.2663	1484.4635
C	-0.002876	0.004697	1.526557	130.6075	961.1401	1501.9991
C	1.439197	0.008337	2.038425	141.8173	971.4408	2951.6858
S	2.52659	-1.017453	1.017126	181.3761	1008.4754	3014.3211
C	3.328005	0.218334	-0.018309	208.6913	1030.6771	3078.6531
H	0.416484	0.947917	-0.366802	237.8956	1111.1325	3080.8413
H	-1.043496	-0.061049	-0.33681	253.0029	1146.6874	3103.1527
H	1.470971	-0.397883	3.046521	327.0027	1175.3246	3165.3819
H	1.839196	1.02044	2.042568	355.0743	1236.8727	3168.1515
H	4.041021	-0.313303	-0.642727	433.0839	1261.9528	3178.2471
H	2.593502	0.708033	-0.652243	503.4133	1315.1017	3622.4281
H	3.855851	0.94232	0.598594	607.6314	1342.2957	
O	0.673766	-1.110999	-0.479598	697.726	1353.7226	
H	0.074725	-2.346831	0.929331	748.2079	1377.7457	
H	-0.533726	0.88326	1.901148	819.4509	1443.7093	
O	-0.750419	-1.073646	2.052891	837.9543	1465.7142	
O	-0.019431	-2.286277	1.898904	885.4496	1468.5893	

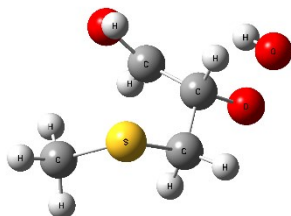
**A1\_Im2**



<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			<b><math>\Delta H</math></b>			<b><math>\Delta G</math></b>																																																																																																						
M06-2X/GD3/cc-pVTZ							-781.545523			-781.409882			-781.398781			-781.446837																																																																																																						
M06-2X/DG3/aug-cc-pVTZ							-781.552317			-781.416749			-781.405662			-781.453816																																																																																																						
MN15/cc-pVTZ							-781.175816			-781.040875			-781.02978			-781.077525																																																																																																						
MN15/aug-cc-pVTZ							-781.186311			-781.05162			-781.040577			-781.088107																																																																																																						
<b>Coordinates (xyz)</b>							<b>Vibrations (cm<sup>-1</sup>)</b>																																																																																																															
C	-0.270464	0.139268	-0.008262	35.6848	984.4445	1498.1118	C	-0.095405	0.049170	1.502913	78.912	986.7928	1524.2004	C	1.341921	0.024134	1.995998	103.7003	1019.9357	3059.8104	S	2.078871	-1.639997	1.955411	148.0597	1052.3738	3076.5899	C	3.251215	-1.462275	0.588396	168.722	1132.2585	3083.8898	H	0.188663	1.06568	-0.356572	190.9317	1160.5479	3090.0996	H	-1.339978	0.184612	-0.228006	249.8516	1180.1844	3114.0829	H	-0.656024	-0.792876	1.912982	266.7882	1261.9322	3143.4002	H	1.355959	0.362331	3.030646	311.0638	1275.8675	3163.5787	H	1.968089	0.698104	1.4123	316.7874	1290.6523	3177.0465	H	3.728918	-2.431528	0.46583	405.1354	1324.383	3851.4755	H	2.728146	-1.192601	-0.324548	442.3615	1351.8021		H	4.010034	-0.723824	0.835762	581.3268	1378.6111		O	0.362579	-0.912313	-0.699358	726.7641	1394.0047		H	0.141826	-1.750403	-0.281532	786.8436	1431.9429		O	-0.690785	1.250226	2.061285	826.9865	1470.6166		O	-1.98797	1.209139	2.017496	913.3443	1475.5571	

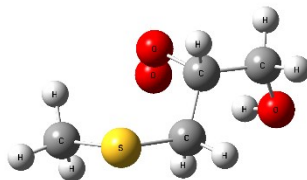


**A1\_Im2\_1**



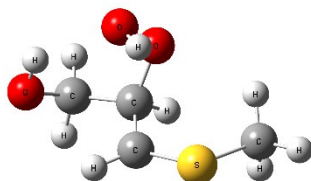
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.532934	-781.399072	-781.387675	-781.435377	
M06-2X/DG3/aug-cc-pVTZ		-781.540568	-781.407069	-781.395546	-781.44367	
MN15/cc-pVTZ		-781.165429	-781.032751	-781.021152	-781.069225	
MN15/aug-cc-pVTZ		-781.17708	-781.044911	-781.033159	-781.081668	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.022737	-0.019188	-0.006463	67.6382	845.8587	1480.0247
C	-0.010545	0.005223	1.482769	83.3762	966.8326	1488.6314
C	1.378162	-0.005053	2.125053	138.4358	985.6329	3032.5743
S	2.316769	-1.500875	1.706402	148.1472	1017.0091	3078.0792
C	3.204103	-0.94281	0.229981	176.4583	1042.1141	3086.7869
H	0.256068	0.852388	-0.583275	184.2235	1085.3873	3145.602
H	-2.091721	1.340509	0.792985	248.5905	1127.4349	3164.0111
H	-0.57529	-0.854112	1.863099	262.4954	1166.7022	3175.3963
H	1.270297	0.015369	3.208208	274.0852	1226.6122	3203.6959
H	1.948677	0.871413	1.819082	315.7515	1261.5931	3780.1551
H	3.850542	-1.764444	-0.069266	341.9889	1298.0081	3805.6933
H	2.519573	-0.712367	-0.581699	386.5332	1327.4462	
H	3.818589	-0.078379	0.470772	455.6607	1357.4137	
O	0.04223	-1.192241	-0.680965	552.5143	1382.3482	
H	0.172617	-1.92034	-0.060648	577.9527	1416.7295	
O	-0.616795	1.201374	1.9548	724.3753	1454.4494	
O	-2.01357	1.113138	1.730189	784.0244	1474.6511	

**A1\_Im3**



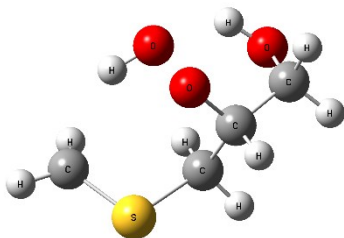
<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			<b><math>\Delta</math>H</b>			<b><math>\Delta</math>G</b>																																																																																																						
M06-2X/GD3/cc-pVTZ							-781.55176			-781.415681			-781.404915			-781.452349																																																																																																						
M06-2X/DG3/aug-cc-pVTZ							-781.558488			-781.422483			-781.41176			-781.458824																																																																																																						
MN15/cc-pVTZ							-781.18228			-781.046871			-781.036139			-781.083138																																																																																																						
MN15/aug-cc-pVTZ							-781.193033			-781.057908			-781.047131			-781.094289																																																																																																						
<b>Coordinates (xyz)</b>							<b>Vibrations (cm<sup>-1</sup>)</b>																																																																																																															
C	0.003165	-0.004597	-0.010149	43.7237	964.8384	1493.5805	C	0.005419	0.010907	1.513880	81.353	970.6104	1499.9069	C	1.396950	0.020312	2.117254	115.3522	981.6556	3042.9824	S	1.465045	0.317381	3.900493	150.1336	1033.6312	3076.8474	C	1.007962	-1.31269	4.543725	189.8119	1103.5916	3093.2804	H	0.264338	0.996896	-0.352768	214.3905	1149.8432	3111.6418	H	-1.013022	-0.223942	-0.35357	248.8021	1216.5698	3118.2765	H	1.960854	0.829791	1.65434	278.0848	1235.9879	3145.7851	H	1.910654	-0.909284	1.87754	323.0467	1251.5266	3162.3896	H	1.267614	-1.308699	5.599414	407.4411	1278.6843	3179.1173	H	-0.05361	-1.509341	4.431154	466.4143	1336.1455	3841.6051	H	1.58365	-2.086361	4.038943	498.1957	1361.4223		H	0.765786	-1.764855	-0.237621	678.0295	1392.6049		O	0.94427	-0.881473	-0.576706	725.3761	1408.4704		H	-0.577389	0.857998	1.874898	787.2957	1434.27		O	-0.753632	-1.125108	2.022488	820.7603	1441.4524		O	-0.271887	-2.259696	1.616562	873.5514	1470.8013	

**A1\_Im3\_1**



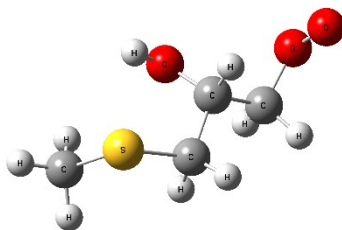
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.539964	-781.404941	-781.393933	-781.440984	
M06-2X/DG3/aug-cc-pVTZ		-781.547205	-781.412453	-781.401378	-781.448613	
MN15/cc-pVTZ		-781.172579	-781.038209	-781.027235	-781.07396	
MN15/aug-cc-pVTZ		-781.184099	-781.050043	-781.039013	-781.08591	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.002059	0.000977	0.008326	58.1453	886.8851	1493.0538
C	0.010693	-0.013433	1.532433	95.7649	964.1947	1499.7321
C	1.388957	0.001433	2.088694	112.1081	969.4666	3041.087
S	1.729733	-0.120747	3.764459	170.5933	993.8552	3051.1376
C	0.249709	0.581466	4.533166	183.5625	999.3453	3081.2083
H	0.349838	0.976501	-0.333041	203.8943	1055.2961	3111.8214
H	-1.03278	-0.131815	-0.32143	235.5549	1141.3278	3169.6963
H	2.22509	-0.218432	1.442	300.4464	1154.7564	3182.9219
H	0.468055	-2.449488	2.456766	335.3735	1232.603	3225.2051
H	0.412002	0.530722	5.606253	349.8856	1249.495	3765.0959
H	0.13601	1.621081	4.235137	412.6941	1337.408	3845.6584
H	-0.631927	0.005802	4.26643	457.509	1346.4563	
H	0.62685	-1.813946	-0.195729	507.2277	1363.9048	
O	0.854038	-0.957858	-0.573325	566.0556	1404.9599	
H	-0.579485	0.840795	1.883098	708.2951	1407.6987	
O	-0.781858	-1.101829	2.054351	743.9148	1441.4355	
O	-0.157143	-2.335701	1.725863	819.9695	1472.8005	

**A1\_Im3\_2**



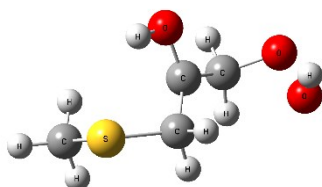
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.536429	-781.40125	-781.390711	-781.436391	
M06-2X/DG3/aug-cc-pVTZ		-781.543537	-781.408533	-781.397959	-781.443742	
MN15/cc-pVTZ		-781.168799	-781.034355	-781.023778	-781.069523	
MN15/aug-cc-pVTZ		-781.180035	-781.045897	-781.035274	-781.08114	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.241314	-0.078327	0.159309	74.6637	860.7009	1460.4867
C	0.699163	-0.101949	1.615194	109.4678	880.8471	1501.335
C	2.220903	-0.068732	1.724927	144.752	943.9658	3048.7651
S	2.818495	-0.259762	3.426336	175.0682	973.4428	3079.7817
C	3.16558	-1.929969	3.479679	198.8527	993.3743	3102.1548
H	0.479874	0.8955	-0.270666	263.5212	1072.0618	3107.644
H	-0.846102	-0.198496	0.148718	271.0276	1123.0365	3150.9717
H	2.579704	0.892124	1.359465	336.7432	1158.1035	3159.0596
H	2.671176	-0.845904	1.111858	362.2415	1209.8514	3278.0452
H	3.446323	-2.322602	4.44455	395.1084	1246.596	3667.779
H	1.256597	-2.643545	2.483616	466.2821	1266.7144	3844.9091
H	3.52483	-2.424762	2.58682	503.3845	1335.7305	
O	0.87457	-1.040641	-0.652679	525.1549	1377.2524	
H	0.736895	-1.901563	-0.244239	621.2206	1403.5731	
H	0.274115	0.767457	2.123447	679.5862	1409.7306	
O	0.109083	-1.170185	2.340374	777.5869	1428.3714	
O	0.587237	-2.40594	1.819072	829.3448	1441.4509	

**A2\_Im1**



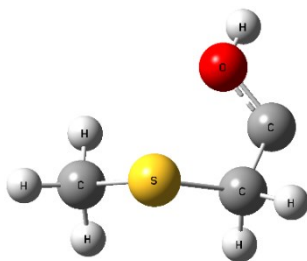
<b>Method</b>				<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>
M06-2X/GD3/cc-pVTZ				-781.55	-781.414064	-781.403241	-781.450671
M06-2X/DG3/aug-cc-pVTZ				-781.557104	-781.421353	-781.410475	-781.458127
MN15/cc-pVTZ				-781.180561	-781.045436	-781.034567	-781.082035
MN15/aug-cc-pVTZ				-781.191576	-781.05674	-781.045829	-781.093461
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>			
C	-0.090191	-0.074416	0.073637	58.8005	973.4326	1474.204	
C	-0.054383	-0.073681	1.585327	61.7594	981.8142	1495.8862	
C	1.392866	-0.022800	2.069869	103.5057	987.7003	3050.0554	
S	1.531087	-0.244187	3.867824	127.2089	1056.6569	3073.5482	
C	1.900622	-2.016902	3.937474	153.468	1076.8611	3076.7839	
H	0.541122	0.710601	-0.340135	187.7221	1163.6017	3095.6265	
H	0.197849	-1.051468	-0.311492	264.3764	1213.0913	3134.0533	
H	-0.58208	0.818682	1.937165	286.0617	1240.3404	3160.6016	
H	1.832552	0.943169	1.824559	333.0802	1264.3052	3160.8918	
H	1.987866	-0.801344	1.589607	420.4043	1282.7607	3173.5318	
H	1.932139	-2.291085	4.989043	455.6003	1323.6395	3832.1869	
H	1.131095	-2.594999	3.432774	495.3429	1355.9651		
H	2.871275	-2.215619	3.488693	590.3132	1363.6384		
O	-0.717145	-1.241611	2.015099	728.6701	1405.7076		
H	-0.803177	-1.189965	2.973303	778.749	1436.4388		
O	-1.427695	0.138805	-0.415996	844.6329	1459.617		
O	-1.80396	1.366292	-0.228266	912.442	1472.8956		

**A2\_Im1\_1**



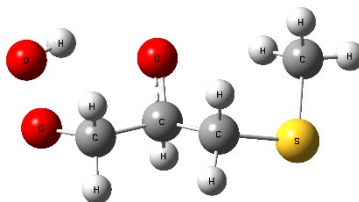
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-781.541651	-781.407412	-781.395872	-781.445523		
M06-2X/DG3/aug-cc-pVTZ	-781.549741	-781.41565	-781.404083	-781.453696		
MN15/cc-pVTZ	-781.174464	-781.041017	-781.02948	-781.078784		
MN15/aug-cc-pVTZ	-781.186533	-781.053342	-781.04177	-781.091153		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.113928	-0.363582	0.302877	36.5591	868.3312	1481.2002
C	-0.155877	-0.070007	1.747820	51.7393	909.4763	1486.0198
C	0.989629	0.481733	2.511549	82.3563	978.3066	3015.618
S	0.969969	-0.031307	4.265981	108.0526	995.0185	3067.2242
C	1.08452	-1.822158	4.042863	156.0413	1012.0847	3072.5751
H	0.885107	-0.695698	0.013929	195.3665	1047.8625	3119.9702
H	-0.849008	-1.126939	0.041698	211.609	1141.4434	3123.7159
H	-0.063109	2.460732	0.023097	219.4313	1189.3217	3154.3475
H	0.966331	1.576667	2.559061	301.882	1251.0418	3171.9097
H	1.930586	0.193543	2.045641	347.1116	1271.1824	3735.5319
H	1.089482	-2.26847	5.033821	387.7254	1353.4627	3831.7374
H	0.231444	-2.196205	3.480912	463.4714	1358.6648	
H	2.00879	-2.078412	3.528987	559.5822	1392.3719	
O	-1.396545	0.055404	2.277828	640.1766	1414.2178	
H	-1.307245	0.191757	3.232966	710.9744	1431.4297	
O	-0.496027	0.731	-0.539776	754.2736	1457.6863	
O	0.475748	1.75568	-0.354598	829.3762	1471.6816	

**P2\_Im1**



Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-591.235195	-591.149517	-591.141984	-591.18006
M06-2X/DG3/aug-cc-pVTZ				-591.239233	-591.153606	-591.146067	-591.184166
MN15/cc-pVTZ				-590.991987	-590.906738	-590.89918	-590.937269
MN15/aug-cc-pVTZ				-590.998764	-590.913635	-590.90606	-590.944224
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	-0.029247	-0.028885	0.064096	90.1314	973.3393	3074.0188	
C	-0.007268	-0.068110	1.558301	134.2221	995.4962	3095.2009	
S	1.543040	0.004580	2.502620	179.2651	1165.7046	3156.0152	
C	1.99603	1.729782	2.201249	221.7954	1234.0988	3171.2702	
H	-0.509453	-0.999677	1.83287	272.4349	1325.8928	3811.0729	
H	-0.692529	0.719373	1.889026	591.579	1355.8046		
H	2.86823	1.939534	2.815339	635.2784	1365.4995		
H	2.245226	1.892037	1.156456	728.3058	1412.4799		
H	1.186539	2.392425	2.502324	767.9368	1474.2189		
O	1.181106	0.098956	-0.402428	876.5909	1492.4247		
H	1.137483	0.113036	-1.36609	934.3116	3051.5754		

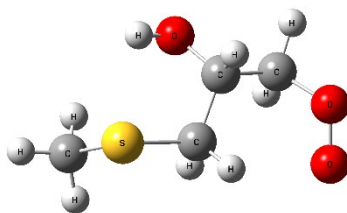
**A2\_Im1\_2**



Method	Ee			E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-781.518913			-781.384892	-781.374165	-781.420962
M06-2X/DG3/aug-cc-pVTZ	-781.525946			-781.392052	-781.381313	-781.428137
MN15/cc-pVTZ	-781.150934			-781.017837	-781.007064	-781.054007
MN15/aug-cc-pVTZ	-781.161967			-781.029101	-781.018322	-781.065273
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.008452	0.015048	0.003923	62.7667	910.0094	1469.292
C	0.006337	-0.036014	1.589599	80.8409	961.1252	1475.1545
C	1.472418	-0.025052	2.040043	101.2277	972.5901	2999.8338
S	1.652975	0.386727	3.786186	172.4149	1000.0846	3060.0542
C	0.772783	-1.010465	4.511993	213.333	1024.2202	3072.4685
H	0.446394	0.963022	-0.282556	226.1471	1109.0807	3079.5708
H	0.552528	-0.834656	-0.385406	233.0509	1157.8008	3133.1484
H	-0.522774	0.869761	1.91765	299.913	1176.1652	3141.7512
H	2.032572	0.738459	1.500036	354.1925	1242.93	3152.7717
H	1.910878	-1.001697	1.832032	391.8292	1276.2412	3169.5472
H	0.833352	-0.894477	5.591242	449.342	1297.0725	3669.3288
H	-0.273189	-1.010013	4.205286	475.2698	1340.5271	
H	1.235491	-1.949984	4.218641	571.7028	1362.0322	
O	-0.649538	-1.16189	1.916085	724.6958	1373.0267	
H	-1.985201	-1.43886	0.449471	768.9792	1441.7184	
O	-1.303814	0.035153	-0.493522	800.5087	1460.3883	
O	-1.802805	-1.287718	-0.495361	857.0227	1461.5181	

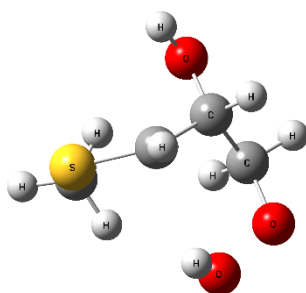


**A2\_Im2**



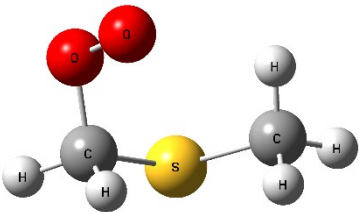
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.550274	-781.414209	-781.403419	-781.450743	
M06-2X/DG3/aug-cc-pVTZ		-781.557253	-781.421333	-781.410509	-781.457996	
MN15/cc-pVTZ		-781.180939	-781.045647	-781.034833	-781.082122	
MN15/aug-cc-pVTZ		-781.191812	-781.056835	-781.045969	-781.093473	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.058222	-0.014170	0.010338	55.7041	982.4516	1487.6063
C	0.084249	0.034279	1.530280	82.339	985.7615	1495.2754
C	1.496834	-0.072576	2.095633	96.0899	1003.5785	3032.8339
S	1.485595	-0.272612	3.904958	118.0314	1061.0853	3076.2067
C	1.724934	-2.065689	4.021768	163.8928	1083.8377	3088.9917
H	0.527713	-0.92199	-0.364263	192.8784	1159.8759	3103.9415
H	-0.354073	0.984354	1.856176	240.0951	1214.887	3151.8708
H	2.065708	0.825263	1.863897	292.3751	1246.9587	3161.053
H	2.020777	-0.924284	1.661675	387.5337	1267.3189	3170.7203
H	1.659918	-2.325753	5.07539	427.6798	1280.4352	3171.969
H	0.95771	-2.600705	3.467662	453.9982	1319.1143	3810.5267
H	2.709387	-2.336854	3.647666	483.5391	1355.9135	
O	-0.731986	-1.045146	1.929872	584.0206	1363.1984	
H	-0.764545	-1.03238	2.893836	727.8904	1405.9288	
H	-0.966941	0.062203	-0.345198	765.053	1430.7722	
O	0.749035	1.1171	-0.545255	845.2893	1461.9675	
O	2.019765	0.886076	-0.692372	897.7028	1473.9056	

**A2\_Im2\_1**

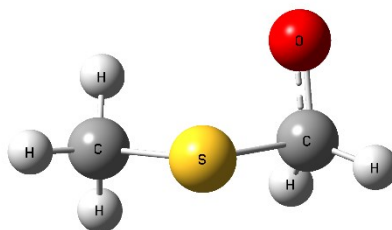


<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			<b><math>\Delta H</math></b>			<b><math>\Delta G</math></b>																																																																																																						
M06-2X/GD3/cc-pVTZ							-781.535392			-781.400441			-781.38944			-781.436105																																																																																																						
M06-2X/DG3/aug-cc-pVTZ							-781.542809			-781.40802			-781.396984			-781.443745																																																																																																						
MN15/cc-pVTZ							-781.167522			-781.03337			-781.022298			-781.069102																																																																																																						
MN15/aug-cc-pVTZ							-781.179164			-781.045268			-781.034177			-781.081022																																																																																																						
<b>Coordinates (xyz)</b>							<b>Vibrations (cm<sup>-1</sup>)</b>																																																																																																															
C	0.002069	-0.007692	0.004280	75.1568	924.3261	1482.7258	C	-0.004094	-0.000381	1.538488	105.6191	971.6148	1505.6841	C	1.334289	0.000590	2.208272	123.8129	977.1332	3034.848	S	2.386391	-1.335607	2.420938	177.5259	993.0504	3083.1398	C	1.9778	-2.476791	1.078332	207.5999	1044.2409	3092.8345	H	0.307346	-0.976808	-0.386188	229.2422	1074.212	3151.7232	H	-0.496787	0.928596	1.844078	253.6865	1119.6085	3177.2274	H	1.583268	0.824558	2.862739	284.3944	1147.9823	3183.5962	H	2.491156	0.774926	0.267434	302.577	1253.8478	3205.6503	H	2.572703	-3.367894	1.260405	365.681	1285.989	3759.2138	H	0.920449	-2.723434	1.104044	402.5053	1323.4266	3869.4786	H	2.252555	-2.037759	0.122932	410.3995	1351.7703		O	-0.813204	-1.120827	1.889454	487.677	1362.1479		H	-0.829848	-1.197413	2.847436	584.9147	1392.1401		H	-1.008979	0.20616	-0.343742	621.9711	1407.7772		O	0.808309	1.012672	-0.540374	703.4089	1417.5892		O	2.146316	0.540549	-0.606853	767.2993	1468.9594	

## 4. MSP decomposition

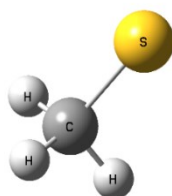
MSP						
						
Method	Ee		E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-627.707413		-627.63398	-627.626686	-627.665201	
M06-2X/DG3/aug-cc-pVTZ	-627.712042		-627.638631	-627.631354	-627.669815	
MN15/cc-pVTZ	-627.450945		-627.377787	-627.370478	-627.40904	
MN15/aug-cc-pVTZ	-627.45831		-627.385225	-627.377927	-627.416446	
SVECV-f12	-627.590561		-627.517153	-627.509872	-627.548362	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.006460	0.003403	0.047089	82.7949	981.1007	3103.6011
S	-0.013252	0.294449	1.812126	114.0785	1038.5244	3167.1805
C	1.731494	-0.022063	2.167991	188.4199	1226.5954	3174.7835
H	-0.986736	0.273025	-0.336809	256.6521	1306.3094	3180.2447
H	0.787882	0.552441	-0.453322	367.233	1334.7441	
H	1.872843	0.189001	3.224949	538.2842	1362.8132	
H	1.981436	-1.060391	1.967425	717.6909	1445.8275	
H	2.365550	0.635107	1.577498	766.0617	1469.9585	
O	1.426988	-1.684666	-0.439986	892.6159	1484.3777	
O	0.172285	-1.391153	-0.273178	945.4856	3078.2171	

**MSO**



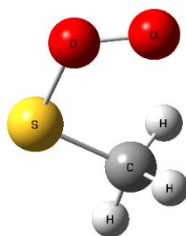
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-552.544637	-552.476321	-552.469815	-552.505714	
M06-2X/DG3/aug-cc-pVTZ		-552.548542	-552.480285	-552.473757	-552.509745	
MN15/cc-pVTZ		-552.33308	-552.264768	-552.258337	-552.294049	
MN15/aug-cc-pVTZ		-552.339634	-552.27144	-552.264985	-552.300804	
SVECV-f12		-552.437202	-552.368945	-552.362417	-552.398405	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.004601	-0.041188	-0.077552	102.6913	1111.8586	3081.9634
S	0.002272	-0.059553	1.769052	157.0228	1203.2504	3169.8311
C	1.784486	0.025295	2.051502	239.65	1263.6919	3183.7282
H	-1.015300	0.215018	-0.379699	303.3571	1346.9111	
H	0.729707	0.709129	-0.408660	582.3724	1469.7157	
H	1.936212	-0.058486	3.124715	733.0835	1485.7234	
H	2.272654	-0.805773	1.552040	918.1339	1518.0351	
H	2.180607	0.974546	1.699225	968.8336	3017.7661	
O	0.364574	-1.316496	-0.275672	1023.6712	3080.1418	

**MeS**



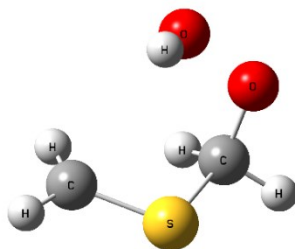
<b>Method</b>					<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>
M06-2X/GD3/cc-pVTZ					-438.046809	-438.012842	-438.008887	-438.037052
M06-2X/DG3/aug-cc-pVTZ					-438.048284	-438.012934	-438.008657	-438.037291
MN15/cc-pVTZ					-437.912357	-437.876652	-437.872519	-437.900902
MN15/aug-cc-pVTZ					-437.91537	-437.879712	-437.87558	-437.903959
SVECV-f12					-437.949675	-437.914325	-437.910048	-437.938683
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>				
S	-0.689551	0.019268	0.045929	391.1284	1477.5619			
C	1.101820	-0.011108	-0.018060	737.3702	3054.1732			
H	1.529315	0.907615	0.375059	868.4326	3129.3659			
H	1.504331	-0.879678	0.496533	1335.1263	3145.7596			
H	1.370421	-0.086199	-1.074490	1377.8804				

**MeS-O2**



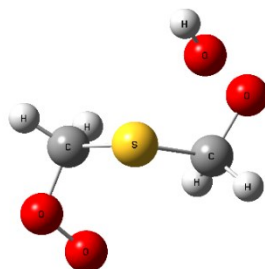
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-588.383406	-588.339586	-588.333331	-588.369333		
M06-2X/DG3/aug-cc-pVTZ	-588.388035	-588.344196	-588.33797	-588.373819		
MN15/cc-pVTZ	-588.159994	-588.116288	-588.110062	-588.145795		
MN15/aug-cc-pVTZ	-588.166847	-588.123178	-588.116972	-588.152636		
SVECV-f12	-588.270455	-588.226615	-588.220389	-588.256238		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
S	0.055018	-0.071107	-0.018460	46.6159	976.301	3185.7322
C	-0.064094	0.058235	1.756647	210.5086	1249.6989	
H	0.947991	-0.153893	2.102273	278.2735	1342.4521	
H	-0.355808	1.060715	2.054870	463.8794	1442.7693	
H	-0.754733	-0.678836	2.155071	623.7602	1476.1118	
O	-2.393982	0.523071	0.506701	735.9773	3076.5429	
O	-1.582718	0.279435	-0.458731	970.571	3164.1115	

**MSP\_1**



Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-627.690988	-627.619578	-627.611829	-627.650786		
M06-2X/DG3/aug-cc-pVTZ	-627.696043	-627.624655	-627.616915	-627.655872		
MN15/cc-pVTZ	-627.436723	-627.365551	-627.357769	-627.396802		
MN15/aug-cc-pVTZ	-627.444711	-627.373589	-627.365822	-627.404809		
SVECV-f12	-627.576769	-627.505381	-627.497641	-627.536599		
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.111924	-0.014533	0.113593	74.5438	888.293	3165.0742
S	-0.019967	-0.237008	1.912817	164.2856	954.7031	3180.1065
C	1.577982	0.123867	2.420415	206.9358	1026.7125	3307.6361
H	-0.897393	0.153902	-0.255603	291.8835	1111.7113	3767.4223
H	0.750000	0.845856	-0.088103	336.0382	1292.7241	
H	1.774696	0.072548	3.478400	380.7256	1325.3597	
H	2.259542	0.627029	1.753271	419.3092	1405.76	
O	0.568637	-1.144230	-0.572519	516.0658	1422.3362	
O	1.955798	-1.281341	-0.321186	721.4112	1447.5049	
H	1.969125	-1.775208	0.512248	843	3086.1774	

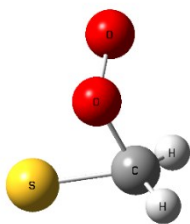
**MSP\_2**



Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-778.06207	-777.979207	-777.970026	-778.013782	
M06-2X/DG3/aug-cc-pVTZ		-778.069772	-777.987153	-777.977882	-778.021906	
MN15/cc-pVTZ		-777.716998	-777.634546	-777.62536	-777.668925	
MN15/aug-cc-pVTZ		-777.72786	-777.645621	-777.636389	-777.680114	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.032905	-0.167892	-0.116868	51.3786	887.6462	1465.782
S	-0.037723	-0.057382	1.700420	81.2733	930.1649	3103.784
C	1.691428	0.228599	2.090102	120.4403	967.7801	3112.4698
H	-0.873469	0.286382	-0.510870	149.5702	1027.6835	3172.6324
H	0.913399	0.370018	-0.462848	241.3453	1107.0463	3187.7678
H	1.883350	-0.134865	3.095681	294.4414	1233.644	3798.2538
O	0.007825	-1.481920	-0.598638	318.6051	1280.1671	
O	1.228815	-2.101538	-0.229647	363.3503	1287.8852	
H	0.958615	-2.614293	0.544224	512.7354	1325.9448	
H	2.333837	-0.257320	1.359960	550.2797	1352.2983	
O	2.043454	1.626235	2.140546	728.9115	1412.8812	
O	2.057208	2.157608	0.957772	747.7096	1451.5098	

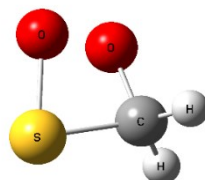


**P-Im1a**



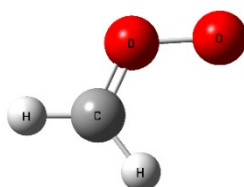
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ		-587.714161	-587.67986	-587.674756	-587.706925
M06-2X/DG3/aug-cc-pVTZ		-587.719672	-587.685589	-587.680433	-587.712712
MN15/cc-pVTZ		-587.496779	-587.462381	-587.457255	-587.489488
MN15/aug-cc-pVTZ		-587.503677	-587.46936	-587.464216	-587.496486
SVECV-f12		-588.254721	-588.220638	-588.215482	-588.247761
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )	
S	0.013924	0.015161	-0.012749	189.3155	1010.8314
C	-0.001527	-0.000468	1.759197	405.7408	1173.4439
H	0.959471	0.002716	2.259262	499.3085	1225.4342
H	-0.830783	0.474289	2.266574	719.9511	1471.917
O	-0.364340	-1.327213	1.355301	934.8262	3139.2266
O	-1.624207	-1.643748	1.611225	942.0582	3248.721

**P-Im1b**



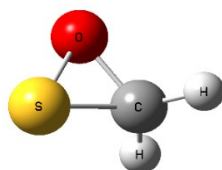
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ		-587.714161	-587.67986	-587.674756	-587.706925
M06-2X/DG3/aug-cc-pVTZ		-587.719672	-587.685589	-587.680433	-587.712712
MN15/cc-pVTZ		-587.496779	-587.462381	-587.457255	-587.489488
MN15/aug-cc-pVTZ		-587.503677	-587.46936	-587.464216	-587.496486
SVECV-f12		-588.307089	-588.271493	-588.266703	-588.298186
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )	
S	0.013924	0.015161	-0.012749	189.3155	1010.8314
C	-0.001527	-0.000468	1.759197	405.7408	1173.4439
H	0.959471	0.002716	2.259262	499.3085	1225.4342
H	-0.830783	0.474289	2.266574	719.9511	1471.917
O	-0.364340	-1.327213	1.355301	934.8262	3139.2266
O	-1.624207	-1.643748	1.611225	942.0582	3248.721

**P-Im2**



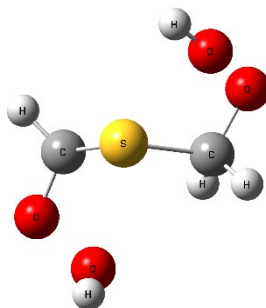
<b>Method</b>					<b>Ee</b>	<b>E+ZPE</b>	<b><math>\Delta H</math></b>	<b><math>\Delta G</math></b>
M06-2X/GD3/cc-pVTZ					-189.570184	-189.538406	-189.534217	-189.562444
M06-2X/DG3/aug-cc-pVTZ					-189.57547	-189.543684	-189.539493	-189.567728
MN15/cc-pVTZ					-189.450699	-189.419141	-189.414924	-189.443194
MN15/aug-cc-pVTZ					-189.456507	-189.424976	-189.420758	-189.449035
SVECV-f12					-189.777862	-189.746076	-189.741885	-189.77012
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>				
C	0.002171	0.003752	0.001295	538.8687	1434.5589			
H	-0.003865	0.002602	1.082487	699.6491	1630.2589			
H	0.888508	-0.003339	-0.622944	929.327	3141.3197			
O	-1.109927	0.014179	-0.544771	1024.2081	3292.0899			
O	-1.168475	0.016208	-1.886825	1262.2725				

**P-Im3**



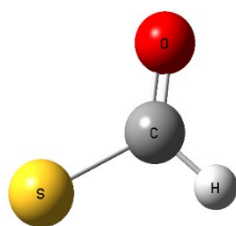
<b>Method</b>					<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>
M06-2X/GD3/cc-pVTZ					-512.653516	-512.622247	-512.618146	-512.6473
M06-2X/DG3/aug-cc-pVTZ					-512.656913	-512.625665	-512.621562	-512.650717
MN15/cc-pVTZ					-512.47346	-512.442285	-512.438178	-512.467328
MN15/aug-cc-pVTZ					-512.478941	-512.447775	-512.443669	-512.472817
SVECV-f12					-513.11389	-513.082643	-513.07854	-513.107695
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>				
C	0.003538	0.000873	0.009718	679.2236	1196.3841			
S	-0.004658	-0.000703	1.779845	762.8491	1510.8389			
H	0.974562	-0.004291	-0.470636	912.3574	3128.3703			
H	-0.797324	-0.541345	-0.478400	1144.8072	3231.5297			
O	-0.362693	1.201979	0.602059	1149.8063				

**MSP\_3**



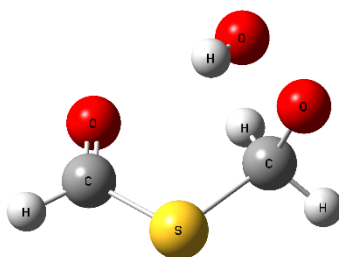
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-778.04673	-777.965967	-777.95602	-778.001295		
M06-2X/DG3/aug-cc-pVTZ	-778.054706	-777.974054	-777.964057	-778.009469		
MN15/cc-pVTZ	-777.703775	-777.623674	-777.613584	-777.659064		
MN15/aug-cc-pVTZ	-777.714792	-777.634942	-777.62478	-777.670554		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.178160	-0.257344	-0.264354	44.1817	703.0836	1452.9249
S	0.134920	0.196631	1.417601	76.8175	803.1386	3103.4971
C	1.890204	-0.037610	1.917583	133.5252	927.701	3178.9855
H	-0.214797	0.416704	-1.012260	146.2654	973.0123	3218.1587
H	2.013245	2.166147	0.523191	184.5527	1004.7228	3779.5881
H	1.887908	-0.425580	2.934198	254.333	1116.9842	3798.7309
O	-0.007315	-1.537946	-0.667501	294.4993	1159.1261	
O	0.776390	-2.431111	0.114491	319.7678	1291.7143	
H	0.123392	-2.755609	0.750018	365.3574	1313.8524	
H	2.346719	-0.735953	1.220219	461.7816	1342.8787	
O	2.598606	1.161682	1.991252	518.1929	1418.8235	
O	2.805645	1.630363	0.671532	594.0617	1421.9128	

**P-Im4**



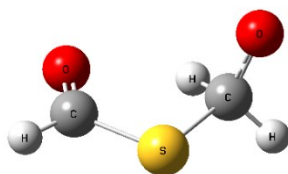
<b>Method</b>					<b>Ee</b>	<b>E+ZPE</b>	<b><math>\Delta H</math></b>	<b><math>\Delta G</math></b>
M06-2X/GD3/cc-pVTZ					-512.063348	-512.044925	-512.040593	-512.07079
M06-2X/DG3/aug-cc-pVTZ					-512.066588	-512.048151	-512.043831	-512.074004
MN15/cc-pVTZ					-511.883843	-511.865574	-511.861205	-511.891473
MN15/aug-cc-pVTZ					-511.888711	-511.870459	-511.866092	-511.896357
SVECV-f12					-512.528179	-512.509742	-512.505422	-512.535595
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>				
C	-0.054337	0.000000	-0.112590	342.7914	1791.1023			
S	0.016073	0.000000	1.647978	687.7133	2971.4708			
H	0.952412	0.000000	-0.565132	944.5961				
O	-1.066466	0.000000	-0.746409	1355.1824				

**MSP\_3a**



Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-702.372949	-702.305648	-702.297636	-702.337515	
M06-2X/DG3/aug-cc-pVTZ		-702.379135	-702.311909	-702.303898	-702.343752	
MN15/cc-pVTZ		-702.072243	-702.005212	-701.997216	-702.036907	
MN15/aug-cc-pVTZ		-702.081273	-702.014391	-702.006372	-702.046131	
SVECV-f12		-702.245511	-702.178285	-702.170274	-702.210128	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.010563	-0.032539	-0.011391	60.9612	921.2026	3007.548
S	-0.001495	0.041207	1.765975	129.2401	957.3743	3102.6277
C	1.794453	0.012698	2.085619	205.914	1011.0878	3177.7967
H	-1.041068	0.019908	-0.394865	216.0932	1120.3068	3796.0466
H	1.453594	2.617997	1.571957	250.1938	1295.4577	
H	1.979822	-0.684720	2.898243	359.0488	1325.9905	
O	0.945114	-0.139849	-0.717280	510.3977	1379.1956	
H	2.281822	-0.299655	1.163257	525.5226	1417.1545	
O	2.280046	1.241106	2.538019	717.5254	1452.1644	
O	2.284066	2.139710	1.443326	752.3057	1817.8341	

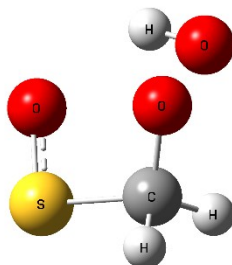
**MSP\_3b**



Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-626.564044	-626.514965	-626.508297	-626.546149
M06-2X/DG3/aug-cc-pVTZ				-626.568958	-626.520073	-626.513374	-626.551213
MN15/cc-pVTZ				-626.307663	-626.258677	-626.252098	-626.289171
MN15/aug-cc-pVTZ				-626.315196	-626.266322	-626.259725	-626.296869
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	-0.093482	-0.089313	0.059234	29.5348	954.4281	3018.6005	
S	0.053326	0.619378	1.676231	211.8002	1097.6731	3055.7683	
C	1.752956	0.052510	2.073830	246.9573	1113.7968		
H	-1.063292	0.156842	-0.397293	388.7837	1251.9976		
H	1.761589	-0.320254	3.102919	518.391	1357.2935		
O	0.733220	-0.760342	-0.485754	618.8929	1377.533		
H	1.950292	-0.800284	1.401970	698.3722	1801.8644		
O	2.726839	0.953031	1.859080	760.9455	2955.3337		

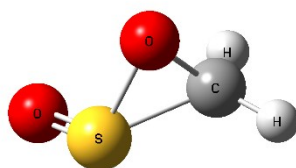


**P-Im5a**



Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-663.625253	-663.574697	-663.568059	-663.605174		
M06-2X/DG3/aug-cc-pVTZ	-663.632265	-663.581859	-663.575189	-663.612372		
MN15/cc-pVTZ	-663.355977	-663.305702	-663.299064	-663.336047		
MN15/aug-cc-pVTZ	-663.365558	-663.315403	-663.308753	-663.345724		
SVECV-f12	-664.236001	-664.185596	-664.178926	-664.216109		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.001482	0.003149	0.006387	61.2032	974.8488	3143.9258
S	0.011085	0.003705	1.852309	196.2984	1090.0406	3716.9222
H	1.039862	-0.012893	-0.316389	264.6977	1140.1742	
H	-0.535527	-0.879825	-0.345495	398.4231	1268.378	
O	-0.581711	1.167767	-0.478579	496.2636	1305.1817	
O	-1.991679	0.990768	-0.480240	534.9375	1442.0163	
H	-2.206872	1.156855	0.452551	650.1647	1466.5549	
O	-1.320160	0.612172	2.217338	902.1617	3073.2963	

**P-Im5b**

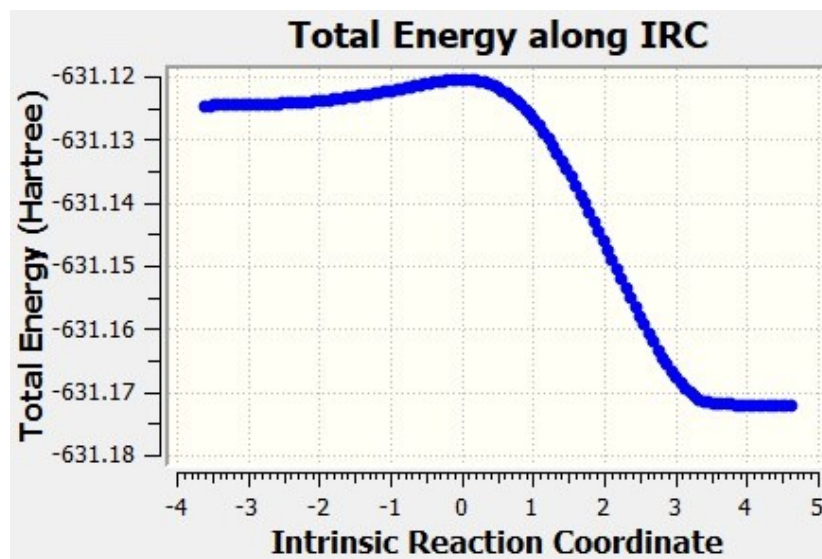


Method		Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ		-587.873353	-587.838017	-587.833194	-587.864547
M06-2X/DG3/aug-cc-pVTZ		-587.879231	-587.843957	-587.839127	-587.870493
MN15/cc-pVTZ		-587.650283	-587.614974	-587.610147	-587.641496
MN15/aug-cc-pVTZ		-587.658351	-587.623081	-587.618252	-587.649605
SVECV-f12		-588.415849	-588.380575	-588.375745	-588.407111
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )	
C	0.090414	-0.107221	-0.048333	358.3521	1139.518
S	-0.143285	0.644808	1.540317	398.7369	1153.6842
H	1.085374	-0.235818	-0.456410	651.7173	1239.4589
H	-0.658329	-0.854019	-0.285301	690.3225	1485.2531
O	-0.388234	1.227904	-0.007829	899.1318	3125.9071
O	-1.386652	0.200347	2.163174	1104.2341	3237.2798

D. Transitions States (TS) and Postreaction Wells (PW).

1. Addition of OH at C1 and C2.

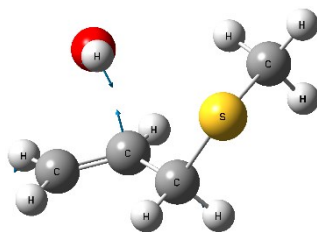
TS1-0_PRC-->A1						
Method	Ee			E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-631.120548			-630.998125	-630.988927	-631.031607
M06-2X/DG3/aug-cc-pVTZ	-631.125475			-631.003261	-630.993976	-631.037044
MN15/cc-pVTZ	-630.844336			-630.722517	-630.713267	-630.755963
MN15/aug-cc-pVTZ	-630.852689			-630.731241	-630.721897	-630.764938
SVECV-f12	-631.013807			-630.8915928	-630.882308	-630.925376
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.008006	0.063288	-0.009739	<b>437.3872i</b>	951.0969	3068.1432
C	-0.006343	-0.05208	1.330755	60.9597	979.8318	3081.4933
C	1.230379	-0.051659	2.162033	100.1155	983.401	3137.3804
S	1.902332	-1.7287	2.469849	144.166	991.3619	3152.5363
C	0.44224	-2.513766	3.192334	170.4438	1003.4141	3169.811
H	0.904306	0.277605	-0.550686	205.8889	1108.2694	3178.7634
H	-0.930472	0.107577	-0.566709	261.2082	1235.4482	3189.4186
H	-0.945309	-0.224548	1.842907	364.7342	1253.7794	3277.2074
H	1.054724	0.419747	3.128402	411.5482	1315.6363	3720.5355
H	2.039341	0.476581	1.659838	435.1902	1355.8423	
H	0.74848	-3.505316	3.515701	645.9031	1442.6332	
H	0.095388	-1.950509	4.056912	736.1198	1472.1147	
H	-0.350286	-2.606145	2.452583	770.0242	1478.5002	
O	0.022599	-2.041416	-0.342273	806.8137	1493.8323	
H	0.811344	-2.224081	0.197036	860.6312	1631.8542	



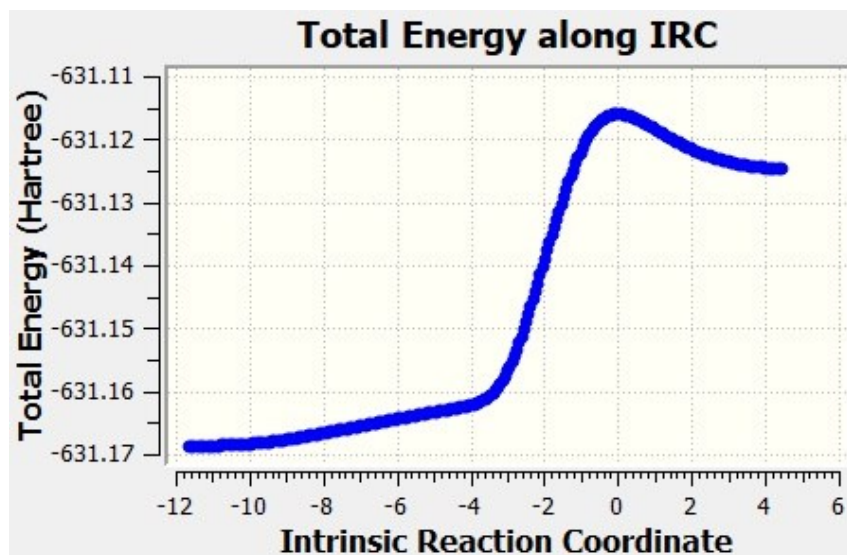
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-3.59552	-631.124659	-0.83469	-631.1219625	1.92623	-631.144597
-3.53132	-631.12465	-0.77049	-631.1218158	1.99044	-631.146099
-3.46713	-631.12464	-0.70628	-631.1216688	2.05465	-631.14761
-3.40293	-631.124629	-0.64207	-631.1215227	2.11886	-631.149125
-3.33873	-631.124618	-0.57786	-631.1213792	2.18307	-631.150641
-3.27453	-631.124606	-0.51365	-631.1212397	2.24727	-631.15215
-3.21033	-631.124593	-0.44944	-631.1211059	2.31148	-631.15365
-3.14614	-631.124579	-0.38524	-631.1209796	2.37569	-631.155133
-3.08194	-631.124564	-0.32103	-631.1208635	2.4399	-631.156595
-3.01774	-631.124547	-0.25682	-631.1207603	2.50411	-631.15803
-2.95355	-631.124529	-0.19262	-631.1206734	2.56832	-631.159432
-2.88935	-631.12451	-0.12842	-631.1206065	2.63253	-631.160795
-2.82515	-631.124488	-0.06422	-631.1205635	2.69674	-631.162113
-2.76095	-631.124463	<b>0</b>	<b>-631.12055</b>	2.76095	-631.163379
-2.69674	-631.124436	0.06422	-631.1205647	2.82516	-631.164587
-2.63254	-631.124406	0.12842	-631.1206164	2.88937	-631.165729
-2.56833	-631.124373	0.19262	-631.1207072	2.95358	-631.166798
-2.50413	-631.124338	0.25682	-631.1208409	3.01779	-631.167786
-2.43992	-631.124299	0.32103	-631.1210218	3.082	-631.168685
-2.37571	-631.124256	0.38523	-631.1212538	3.14621	-631.169487
-2.31151	-631.124211	0.44944	-631.121541	3.21042	-631.170182
-2.2473	-631.124162	0.51365	-631.1218867	3.27463	-631.170762
-2.18309	-631.124109	0.57785	-631.1222939	3.33882	-631.171218
-2.11888	-631.124053	0.64206	-631.1227648	3.40297	-631.171544
-2.05467	-631.123994	0.70627	-631.1233014	3.46674	-631.17174
-1.99046	-631.12393	0.77048	-631.1239047	3.52876	-631.171839

-1.92625	-631.123862	0.83468	-631.1245753	3.59249	-631.171901
-1.86204	-631.123789	0.89889	-631.1253131	3.65647	-631.17195
-1.79784	-631.123711	0.9631	-631.1261176	3.72043	-631.17199
-1.73363	-631.123628	1.02731	-631.1269876	3.78447	-631.172025
-1.66942	-631.12354	1.09152	-631.1279215	3.84859	-631.172055
-1.60521	-631.123446	1.15572	-631.1289175	3.91276	-631.172083
-1.541	-631.123348	1.21993	-631.1299731	3.97696	-631.172109
-1.47679	-631.123244	1.28414	-631.1310857	4.04115	-631.172134
-1.41258	-631.123135	1.34835	-631.1322524	4.10536	-631.172157
-1.34837	-631.123022	1.41256	-631.1334701	4.16956	-631.172178
-1.28416	-631.122905	1.47677	-631.1347353	4.23376	-631.172197
-1.21995	-631.122783	1.54098	-631.1360444	4.29796	-631.172215
-1.15574	-631.122656	1.60519	-631.1373936	4.36217	-631.172231
-1.09153	-631.122525	1.66939	-631.138779	4.42637	-631.172246
-1.02732	-631.122389	1.7336	-631.1401964	4.49058	-631.172259
-0.96311	-631.12225	1.79781	-631.1416415	4.55478	-631.172271
-0.8989	-631.122108	1.86202	-631.1431101	4.61899	-631.172281

TS1-0\_PRC-->A2



Method	Ee	E+ZPE	ΔH	ΔG		
M06-2X/GD3/cc-pVTZ	-631.116072	-630.993859	-630.984684	-631.027076		
M06-2X/DG3/aug-cc-pVTZ	-631.120886	-630.998882	-630.989634	-631.032217		
MN15/cc-pVTZ	-630.840204	-630.718587	-630.709401	-630.751725		
MN15/aug-cc-pVTZ	-630.848569	-630.727226	-630.71799	-630.760421		
SVECV-f12	-631.009218	-630.8872138	-630.877966	-630.920549		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.004062	0.00652	1.537424	<b>432.601i</b>	928.9024	3063.759
C	1.959801	-0.005094	1.961348	67.0133	945.2913	3069.792
S	2.827538	-1.373287	1.394174	126.5364	978.2729	3126.8251
C	3.234426	-0.907083	-0.303387	184.0057	989.4728	3155.1488
H	0.787902	0.588009	-0.416629	205.0168	1024.1629	3169.1222
H	-0.967982	0.442847	-0.293176	224.1817	1114.9658	3171.1037
H	1.846808	-0.014678	3.037712	243.5329	1241.4038	3213.1799
H	2.240907	0.950829	1.529886	303.693	1272.9909	3273.0256
H	4.044277	-1.559358	-0.619332	390.7919	1299.983	3775.7798
H	2.367221	-1.062149	-0.939079	417.1123	1347.586	
H	3.573015	0.126104	-0.333261	591.7634	1443.2935	
O	0.08187	-1.328951	-0.457089	723.479	1467.9076	
H	-0.222138	-1.887293	0.274934	773.1853	1472.6673	
H	-0.09472	1.009061	1.987551	795.2476	1496.9423	
O	-0.454182	-0.987449	2.131938	852.3666	1614.2811	



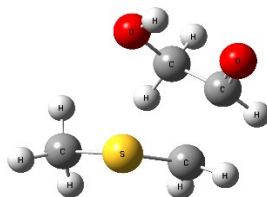
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-11.6581	-631.168809	-6.24272	-631.1647281	-0.82824	-631.119933
-11.59439	-631.168799	-6.17901	-631.1646552	-0.76453	-631.119306
-11.53067	-631.168789	-6.1153	-631.1645824	-0.70081	-631.118737
-11.46696	-631.168779	-6.05158	-631.16451	-0.6371	-631.118227
-11.40325	-631.168768	-5.98787	-631.1644378	-0.57339	-631.117777
-11.33953	-631.168757	-5.92416	-631.164366	-0.50968	-631.117385
-11.27582	-631.168746	-5.86044	-631.1642945	-0.44597	-631.117049
-11.21211	-631.168734	-5.79673	-631.1642235	-0.38226	-631.116769
-11.14839	-631.168721	-5.73302	-631.1641527	-0.31855	-631.116541
-11.08468	-631.168709	-5.66931	-631.1640823	-0.25484	-631.116362
-11.02097	-631.168695	-5.6056	-631.1640121	-0.19113	-631.11623
-10.95726	-631.168681	-5.54188	-631.1639424	-0.12742	-631.11614
-10.89354	-631.168667	-5.47817	-631.1638731	-0.06372	-631.116088
-10.82983	-631.168652	-5.41446	-631.1638046	<b>0</b>	<b>-631.11607</b>
-10.76612	-631.168637	-5.35075	-631.1637369	0.06372	-631.116087
-10.70241	-631.16862	-5.28704	-631.16367	0.12742	-631.116131
-10.6387	-631.168603	-5.22332	-631.1636041	0.19113	-631.1162
-10.57499	-631.168586	-5.15961	-631.1635391	0.25484	-631.116292
-10.51128	-631.168568	-5.0959	-631.1634748	0.31855	-631.116405
-10.44757	-631.168549	-5.03219	-631.1634113	0.38226	-631.116536
-10.38386	-631.168529	-4.96848	-631.1633482	0.44597	-631.116684
-10.32015	-631.168508	-4.90477	-631.1632856	0.50968	-631.116847
-10.25645	-631.168486	-4.84106	-631.1632232	0.57339	-631.117022
-10.19274	-631.168464	-4.77735	-631.163161	0.6371	-631.117207
-10.12903	-631.16844	-4.71365	-631.1630988	0.70081	-631.117402
-10.06532	-631.168415	-4.64994	-631.1630365	0.76452	-631.117604

-10.00162	-631.168388	-4.58624	-631.162974	0.82824	-631.117811
-9.93791	-631.168361	-4.52254	-631.162911	0.89195	-631.118023
-9.87421	-631.168332	-4.45884	-631.162847	0.95566	-631.118239
-9.81051	-631.168301	-4.39514	-631.1627819	1.01937	-631.118457
-9.74681	-631.168268	-4.33146	-631.1627151	1.08308	-631.118677
-9.6831	-631.168233	-4.26778	-631.1626458	1.1468	-631.118896
-9.6194	-631.168197	-4.20411	-631.1625733	1.21051	-631.119116
-9.55569	-631.168158	-4.14045	-631.1624963	1.27422	-631.119333
-9.49198	-631.168117	-4.07679	-631.1624132	1.33793	-631.11955
-9.42827	-631.168073	-4.01315	-631.1623219	1.40165	-631.119763
-9.36457	-631.168028	-3.94951	-631.1622198	1.46536	-631.119974
-9.30086	-631.16798	-3.88587	-631.162104	1.52907	-631.120181
-9.23715	-631.16793	-3.82222	-631.1619712	1.59278	-631.120384
-9.17344	-631.167877	-3.75856	-631.1618184	1.6565	-631.120584
-9.10973	-631.167823	-3.69489	-631.1616421	1.72021	-631.12078
-9.04602	-631.167766	-3.63122	-631.1614393	1.78392	-631.120971
-8.98231	-631.167708	-3.56755	-631.1612063	1.84764	-631.121158
-8.9186	-631.167649	-3.50389	-631.1609392	1.91135	-631.121339
-8.85489	-631.167588	-3.44023	-631.1606328	1.97506	-631.121516
-8.79118	-631.167525	-3.37657	-631.1602813	2.03878	-631.121688
-8.72747	-631.167461	-3.31291	-631.1598782	2.10249	-631.121854
-8.66375	-631.167396	-3.24924	-631.1594172	2.1662	-631.122015
-8.60004	-631.167331	-3.18555	-631.1588935	2.22992	-631.122171
-8.53633	-631.167264	-3.12186	-631.1583037	2.29363	-631.122321
-8.47262	-631.167197	-3.05816	-631.1576463	2.35734	-631.122466
-8.40891	-631.167129	-2.99446	-631.1569216	2.42106	-631.122605
-8.3452	-631.167061	-2.93076	-631.1561309	2.48477	-631.122739
-8.28149	-631.166993	-2.86705	-631.155277	2.54848	-631.122868
-8.21778	-631.166924	-2.80334	-631.1543631	2.6122	-631.122992
-8.15407	-631.166855	-2.73963	-631.1533931	2.67591	-631.12311
-8.09036	-631.166786	-2.67591	-631.1523713	2.73962	-631.123224
-8.02665	-631.166717	-2.6122	-631.151302	2.80334	-631.123333
-7.96294	-631.166648	-2.54849	-631.1501898	2.86705	-631.123437
-7.89923	-631.166578	-2.48478	-631.1490393	2.93076	-631.123536
-7.83552	-631.166509	-2.42106	-631.1478551	2.99448	-631.123631
-7.77181	-631.16644	-2.35735	-631.1466419	3.05819	-631.123721
-7.7081	-631.16637	-2.29364	-631.1454042	3.1219	-631.123806
-7.64438	-631.166301	-2.22992	-631.1441468	3.18562	-631.123887
-7.58067	-631.166231	-2.16621	-631.1428742	3.24933	-631.123963
-7.51696	-631.166161	-2.1025	-631.141591	3.31305	-631.124035
-7.45325	-631.166091	-2.03878	-631.1403016	3.37676	-631.124103
-7.38954	-631.166021	-1.97507	-631.1390105	3.44048	-631.124167



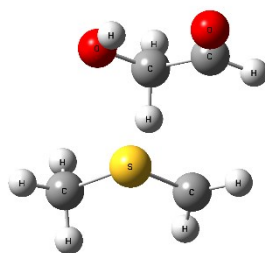
-7.32583	-631.16595	-1.91136	-631.137722	3.50419	-631.124226
-7.26211	-631.16588	-1.84765	-631.1364403	3.56791	-631.124282
-7.1984	-631.165809	-1.78393	-631.1351696	3.63162	-631.124334
-7.13469	-631.165738	-1.72022	-631.1339141	3.69533	-631.124381
-7.07098	-631.165666	-1.65651	-631.1326778	3.75905	-631.124425
-7.00727	-631.165595	-1.59279	-631.1314645	3.82276	-631.124466
-6.94355	-631.165523	-1.52908	-631.1302781	3.88648	-631.124503
-6.87984	-631.165451	-1.46537	-631.1291223	3.95019	-631.124536
-6.81613	-631.165379	-1.40165	-631.1280005	4.01391	-631.124566
-6.75242	-631.165307	-1.33794	-631.1269162	4.07762	-631.124593
-6.6887	-631.165235	-1.27423	-631.1258726	4.14133	-631.124617
-6.62499	-631.165163	-1.21051	-631.1248727	4.20505	-631.124637
-6.56128	-631.165091	-1.1468	-631.1239192	4.26876	-631.124655
-6.49757	-631.165019	-1.08309	-631.123015	4.33247	-631.12467
-6.43386	-631.164946	-1.01938	-631.1221622	4.39618	-631.124682
-6.37014	-631.164874	-0.95566	-631.1213632	4.45988	-631.124691
-6.30643	-631.164801	-0.89195	-631.1206198		

TS1-1\_A1O-->Pw1

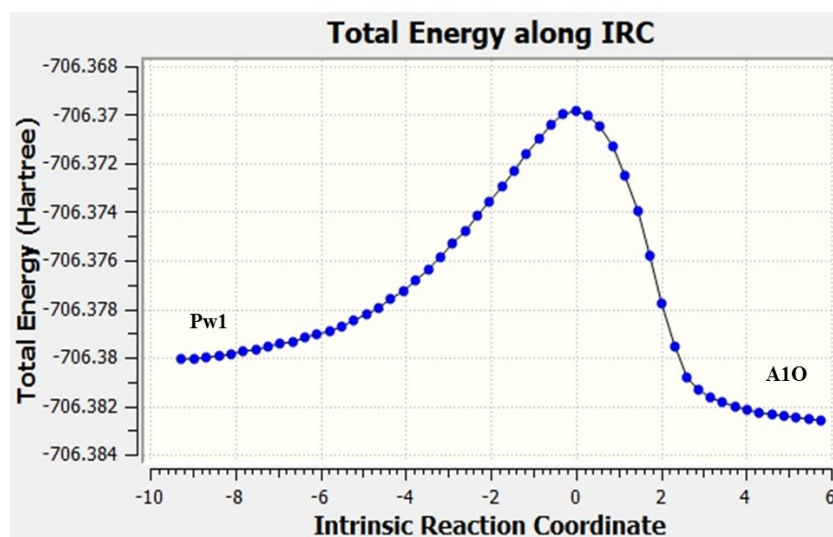


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-706.372631	-706.244149	-706.234636	-706.278099		
M06-2X/DG3/aug-cc-pVTZ	-706.378811	-706.250456	-706.240916	-706.28446		
MN15/cc-pVTZ	-706.047984	-705.9201	-705.910625	-705.953903		
MN15/aug-cc-pVTZ	-706.057957	-705.930311	-705.920801	-705.964181		
SVECV-f12	-706.249713	-706.121358	-706.111818	-706.155362		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.01634	-0.013824	0.010754	<b>322.8753i</b>	925.2187	1559.9129
C	0.004062	0.00652	1.537424	82.8225	959.4282	2951.0094
C	1.959801	-0.005094	1.961348	123.5189	980.9239	3004.9018
S	2.827538	-1.373287	1.394174	159.2951	987.005	3081.8199
C	3.234426	-0.907083	-0.303387	180.9035	1063.7081	3087.5014
H	0.787902	0.588009	-0.416629	219.399	1100.8333	3117.331
H	-0.967982	0.442847	-0.293176	231.8654	1147.9583	3172.0119
H	1.846808	-0.014678	3.037712	307.6595	1239.4514	3187.0818
H	2.240907	0.950829	1.529886	344.3953	1314.8658	3233.5655
H	4.044277	-1.559358	-0.619332	420.6083	1342.4689	3734.0615
H	2.367221	-1.062149	-0.939079	515.0442	1351.1529	
H	3.573015	0.126104	-0.333261	690.2412	1416.4478	
O	0.08187	-1.328951	-0.457089	733.9934	1442.4889	
H	-0.222138	-1.887293	0.274934	747.1656	1464.8531	
H	-0.09472	1.009061	1.987551	829.9593	1496.4564	
O	-0.454182	-0.987449	2.131938	874.8602	1517.1814	

Pw1

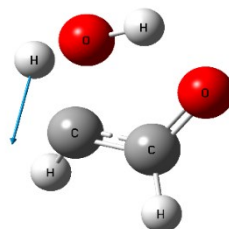


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-706.386081	-706.260459	-706.248621	-706.298413		
M06-2X/DG3/aug-cc-pVTZ	-706.39189	-706.26655	-706.254614	-706.304656		
MN15/cc-pVTZ	-706.063029	-705.938084	-705.926141	-705.976128		
MN15/aug-cc-pVTZ	-706.072604	-705.948029	-705.935983	-705.986417		
SVECV-f12	-706.264316	-706.138976	-706.12704	-706.177082		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.000363	-0.03769	0.00394	48.3174	863.1452	1852.2459
C	0.030074	0.009788	1.506851	62.3161	883.3843	2985.9158
C	3.179305	0.001772	1.257552	81.6434	905.012	3022.6141
S	3.170824	-1.635417	0.782822	88.7179	972.9873	3045.5843
C	3.272013	-1.476618	-1.012838	117.9991	1031.074	3078.0541
H	0.876549	0.514919	-0.356541	130.9481	1111.341	3167.5887
H	-0.888508	0.51137	-0.331571	168.2226	1162.2006	3169.3689
H	3.111382	0.197626	2.315798	234.7451	1265.0983	3176.3956
H	3.574066	0.755467	0.592675	284.7295	1311.4958	3292.0151
H	3.42507	-2.474785	-1.414018	288.0327	1348.4013	3762.941
H	2.338366	-1.075757	-1.399934	316.0943	1397.0623	
H	4.115366	-0.844718	-1.28119	370.1264	1407.8051	
O	-0.019869	-1.345427	-0.479998	503.479	1444.463	
H	0.092912	-1.92697	0.285569	727.1641	1470.4837	
H	0.09086	1.012998	1.961922	731.4057	1475.7971	
O	-0.017311	-0.985434	2.177535	772.4884	1489.1552	

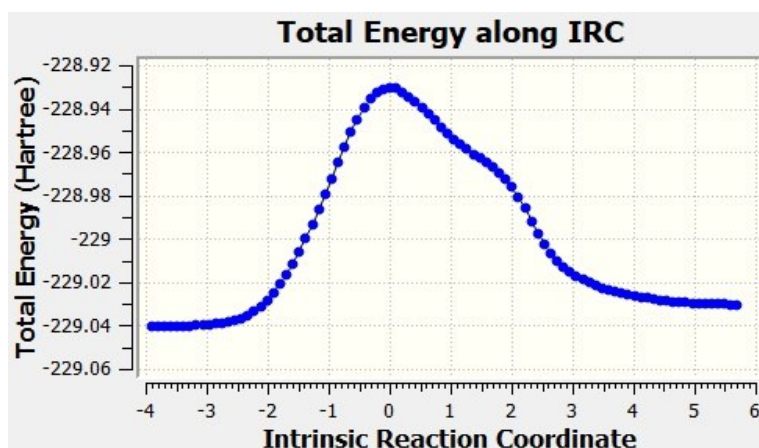


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-6.95196	-706.386009	-3.47893	-706.382837	<b>0</b>	<b>-706.3726</b>
-6.66306	-706.385963	-3.18901	-706.382112	0.28992	-706.372812
-6.37486	-706.3859	-2.89907	-706.381294	0.5797	-706.373379
-6.08585	-706.385814	-2.60915	-706.380391	0.86958	-706.374362
-5.79673	-706.385705	-2.31921	-706.379408	1.15937	-706.37575
-5.50749	-706.38556	-2.02929	-706.378362	1.44925	-706.377419
-5.21791	-706.385373	-1.73936	-706.37726	1.73892	-706.379054
-4.92829	-706.385136	-1.44947	-706.376131	2.02621	-706.380141
-4.63848	-706.384834	-1.15955	-706.375029	2.2954	-706.380535
-4.34864	-706.384462	-0.86967	-706.374052	2.58147	-706.380749
-4.05875	-706.384011	-0.57975	-706.373287	2.86548	-706.380855
-3.76885	-706.383471	-0.28991	-706.372801	3.15039	-706.380902

**TS\_P1**

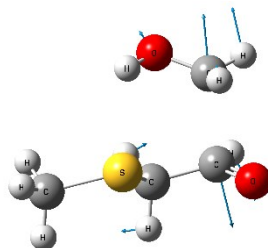


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-228.930282	-228.874149	-228.869097	-228.900335		
M06-2X/DG3/aug-cc-pVTZ	-228.935276	-228.879224	-228.874158	-228.905424		
MN15/cc-pVTZ	-228.776634	-228.720568	-228.715585	-228.746671		
MN15/aug-cc-pVTZ	-228.782753	-228.726774	-228.72179	-228.752877		
SVECV-f12	-228.906497	-228.850445	-228.845379	-228.876645		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.011872	-0.013671	-0.014986	<b>1663.5052i</b>	1089.6402	3175.8854
H	0.001838	-0.001555	1.319941	278.287	1165.9798	3274.2473
H	0.903104	0.004488	-0.581971	446.3785	1301.3211	
O	0.030972	-1.107912	1.08898	526.047	1369.8605	
H	-0.920605	-1.410486	1.009326	721.5501	1415.108	
C	-1.312789	-0.079231	-0.564813	757.0429	1691.1072	
H	-1.537055	0.552896	-1.43227	864.2118	2468.5877	
O	-2.17472	-0.800181	-0.053724	1000.2628	3058.376	



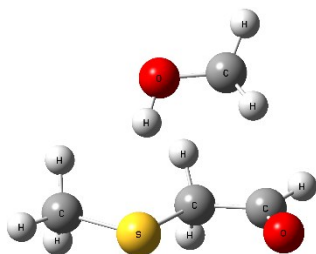
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-3.90658	-229.040612	-0.63422	-228.951046	2.64059	-229.006975
-3.8015	-229.0406	-0.52851	-228.944942	2.74576	-229.010278
-3.69609	-229.040566	-0.42281	-228.93974	2.85119	-229.012966
-3.5906	-229.040508	-0.3171	-228.935622	2.95672	-229.015215
-3.48505	-229.040424	-0.2114	-228.932655	3.06227	-229.017133
-3.37943	-229.040308	-0.10571	-228.93087	3.16783	-229.018785
-3.27378	-229.040158	<b>0</b>	<b>-228.9303</b>	3.27342	-229.020219
-3.16811	-229.039969	0.1057	-228.930825	3.37903	-229.021469
-3.06245	-229.039737	0.21134	-228.932281	3.48464	-229.022562
-2.95679	-229.039458	0.31703	-228.934371	3.59026	-229.023521
-2.85117	-229.039126	0.42271	-228.936856	3.69588	-229.024367
-2.74565	-229.03873	0.52841	-228.939598	3.80153	-229.025116
-2.64046	-229.038249	0.63411	-228.942491	3.90718	-229.025785
-2.53565	-229.037613	0.73981	-228.945456	4.01285	-229.026385
-2.43056	-229.0367	0.8455	-228.948409	4.11853	-229.026926
-2.32515	-229.035387	0.95119	-228.951274	4.22423	-229.027412
-2.21958	-229.0336	1.05686	-228.953989	4.32992	-229.027849
-2.11396	-229.031295	1.16251	-228.956519	4.43562	-229.028243
-2.0083	-229.028449	1.26812	-228.958845	4.54133	-229.028596
-1.90263	-229.025046	1.3737	-228.960993	4.64703	-229.02891
-1.79695	-229.021086	1.47922	-228.963008	4.75273	-229.029187
-1.69127	-229.016571	1.5847	-228.964997	4.85843	-229.029427
-1.58557	-229.011517	1.6902	-228.967097	4.96414	-229.029636
-1.47988	-229.005948	1.79572	-228.969511	5.06983	-229.029813
-1.37418	-228.999899	1.9013	-228.972472	5.17553	-229.029963
-1.26847	-228.993419	2.00692	-228.976213	5.28121	-229.030082
-1.16277	-228.98658	2.11259	-228.980813	5.38691	-229.030177
-1.05706	-228.979468	2.21829	-228.986138	5.49256	-229.030245
-0.95135	-228.972199	2.32398	-228.991866	5.59827	-229.030291
-0.84564	-228.964913	2.42966	-228.997567	5.70371	-229.03031
-0.73993	-228.957789	2.53526	-229.002733		

TS1-2\_A1O-->Pw2



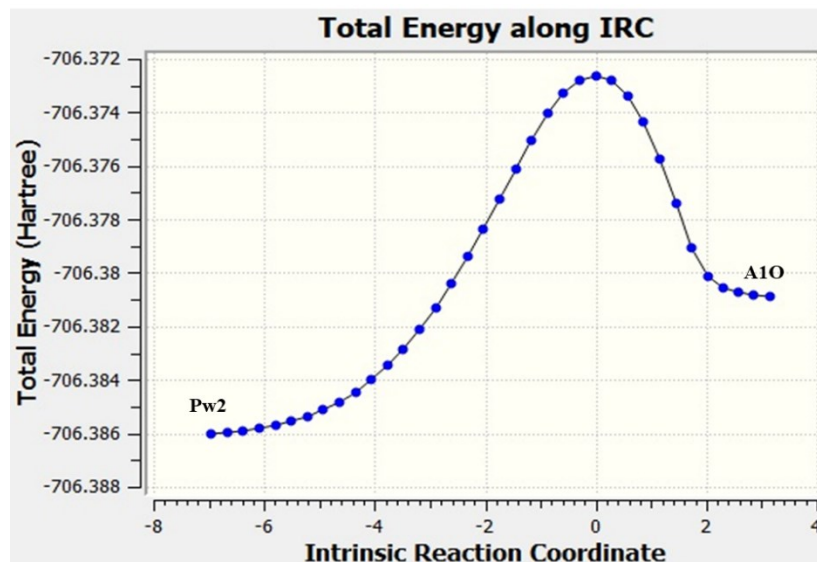
Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-706.36984	-706.241894	-706.231985	-706.276937
M06-2X/DG3/aug-cc-pVTZ				-706.376107	-706.248245	-706.238326	-706.28327
MN15/cc-pVTZ				-706.045564	-705.918058	-705.908214	-705.95285
MN15/aug-cc-pVTZ				-706.05559	-705.928254	-705.918395	-705.963061
SVECV-f12				-706.246767	-706.118905	-706.108986	-706.15393
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	-0.029012	-0.031711	-0.027313	<b>316.9004i</b>	943.4709	1595.9688	
C	0.012476	0.027186	2.087292	46.5785	962.8376	2951.976	
C	1.517942	-0.012251	2.300446	112.9263	981.1808	3062.7666	
S	2.243464	-1.552764	1.67127	137.6114	998.0255	3070.1181	
C	3.980998	-1.159199	1.984076	164.4956	1047.5459	3120.041	
H	-0.879776	0.610464	-0.207558	191.1766	1120.1856	3132.258	
H	-0.184267	-1.103023	-0.068496	224.685	1157.8971	3150.1425	
H	1.700553	0.054919	3.375174	254.7087	1248.2223	3169.0324	
H	1.987813	0.839596	1.809146	335.5911	1280.2895	3259.9009	
H	4.570888	-1.998242	1.624253	363.0424	1357.0096	3704.404	
H	4.281288	-0.256421	1.455785	544.5354	1374.3275		
H	4.152315	-1.036561	3.051338	623.5569	1411.7323		
O	1.114832	0.449149	-0.545098	722.2037	1457.9646		
H	1.805306	-0.219518	-0.410385	750.1214	1475.1354		
H	-0.396568	1.052697	2.091343	757.5662	1489.078		
O	-0.711121	-0.932441	2.365269	869.0533	1505.5689		

Pw2



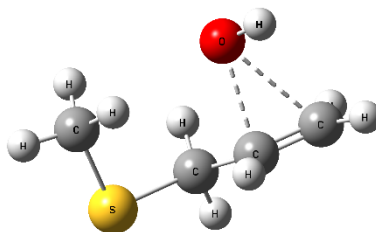
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-706.380149	-706.254175	-706.242415	-706.291834		
M06-2X/DG3/aug-cc-pVTZ	-706.386257	-706.260395	-706.248605	-706.298237		
MN15/cc-pVTZ	-706.056307	-705.931004	-705.91918	-705.968778		
MN15/aug-cc-pVTZ	-706.066109	-705.941024	-705.929168	-705.978905		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.047129	0.014027	0.029548	44.9487	800.846	1855.6458
C	0.011205	0.005261	3.198729	61.9505	958.3122	2970.263
C	1.494824	-0.004816	2.955979	100.1813	978.7246	3051.7241
S	2.091055	-1.674431	2.601277	112.3173	999.4632	3069.1929
C	3.793702	-1.21964	2.186338	137.1662	1009.8738	3097.3757
H	-0.399146	0.792242	-0.628401	170.5665	1100.4177	3150.2267
H	-0.734137	-0.697605	0.466302	174.5233	1199.5461	3150.8623
H	1.991461	0.401522	3.841592	183.8967	1241.7741	3170.3955
H	1.708989	0.660611	2.115699	221.2589	1296.805	3284.337
H	4.314331	-2.136723	1.923429	256.0087	1357.9581	3689.0035
H	3.812095	-0.538635	1.337082	260.0285	1407.6356	
H	4.287512	-0.763509	3.041518	615.0828	1413.3175	
O	1.225466	-0.383699	-0.214748	634.6959	1438.8514	
H	1.443646	-1.118922	0.379113	672.2301	1475.9703	
H	-0.426054	1.01302	3.318453	707.9371	1488.3984	
O	-0.668318	-0.979423	3.274819	741.7853	1495.5792	



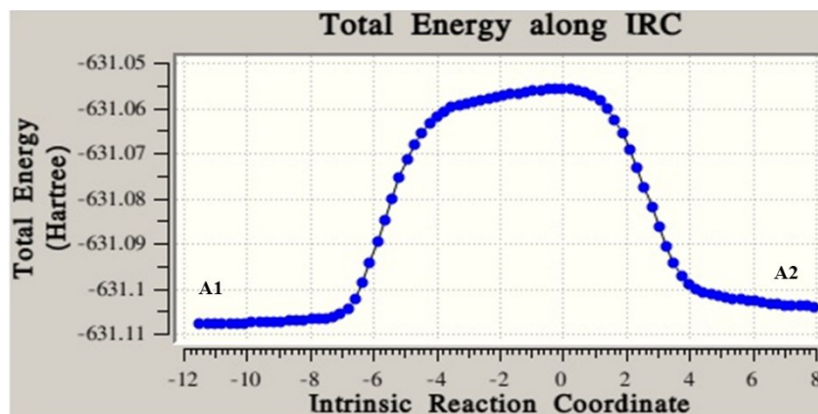


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-9.25657	-706.380081	-4.05046	-706.377242	1.15726	-706.37248
-8.96723	-706.380039	-3.76117	-706.376826	1.4466	-706.373975
-8.67785	-706.379984	-3.47185	-706.376365	1.7359	-706.375782
-8.3885	-706.379922	-3.18252	-706.375865	2.02524	-706.377758
-8.09914	-706.379848	-2.89317	-706.375331	2.31444	-706.379579
-7.80981	-706.379766	-2.60383	-706.374768	2.60232	-706.380822
-7.52047	-706.379672	-2.31448	-706.374178	2.87595	-706.381343
-7.23119	-706.379571	-2.02515	-706.373566	3.16124	-706.381638
-6.94194	-706.379459	-1.7358	-706.372934	3.44988	-706.381867
-6.65275	-706.379338	-1.44647	-706.372286	3.73872	-706.382051
-6.36361	-706.379204	-1.15713	-706.371632	4.02713	-706.382189
-6.07456	-706.379057	-0.86786	-706.370997	4.31439	-706.382292
-5.78553	-706.378889	-0.57857	-706.370423	4.60187	-706.382372
-5.4965	-706.378699	-0.28936	-706.369999	4.89039	-706.38244
-5.20737	-706.378479	<b>0</b>	<b>-706.3698</b>	5.1795	-706.382499
-4.91818	-706.378227	0.28938	-706.370007	5.4688	-706.382552
-4.62895	-706.377939	0.57865	-706.370505	5.75811	-706.382595
-4.33972	-706.377613	0.86799	-706.371331		

TS1-3\_A1<-->A2

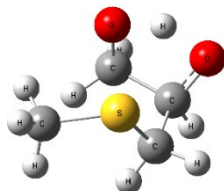


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-631.115841	-630.994818	-630.985009	-631.029875		
M06-2X/DG3/aug-cc-pVTZ	-631.120908	-630.999956	-630.99015	-631.034844		
MN15/cc-pVTZ	-630.839313	-630.718699	-630.708983	-630.752966		
MN15/aug-cc-pVTZ	-630.848067	-630.727598	-630.717881	-630.761767		
SVECV-f12	-631.011037	-630.890085	-630.880279	-630.924973		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.091764	0.094728	0.085393	<b>278.5832i</b>	935.4022	3074.7312
C	0.015293	-0.08556	1.414864	33.0072	946.1079	3080.5674
C	1.333489	-0.05609	2.136581	87.712	977.9305	3122.6585
S	1.246291	-0.348009	3.918729	124.2013	998.6393	3164.9051
C	0.828481	-2.107249	3.948516	182.6422	1023.9013	3165.8234
H	0.787184	0.156439	-0.542791	185.6846	1131.8883	3178.6986
H	-1.057674	0.158942	-0.396408	228.4949	1211.2437	3190.2104
H	-0.876654	-0.105151	2.029792	266.0534	1264.505	3259.9602
H	1.772856	0.937786	2.042391	314.0578	1310.2287	3801.804
H	2.019706	-0.767872	1.677803	411.6978	1360.1578	
H	0.836428	-2.405578	4.994189	555.2532	1433.1315	
H	-0.151916	-2.286039	3.518412	694.6032	1448.1934	
H	1.571447	-2.680831	3.399094	721.89	1466.1472	
O	0.053244	-2.207019	0.949369	776.5143	1479.6069	
H	-0.766944	-2.324941	0.447782	850.3733	1633.277	

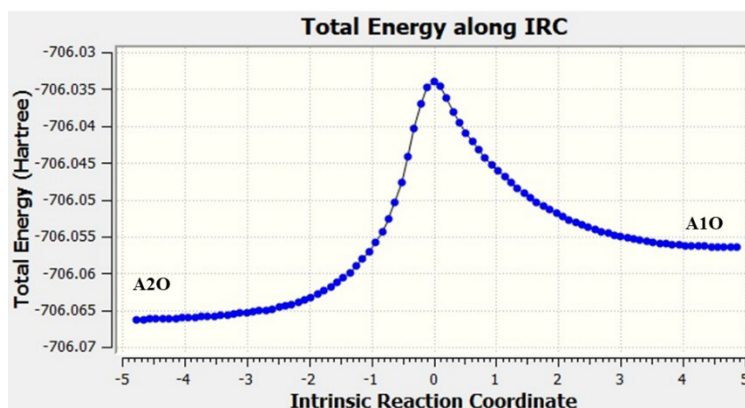


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-11.48097	-631.107987	-4.92841	-631.071629	1.64303	-631.062582
-11.24619	-631.107953	-4.69361	-631.068233	1.87784	-631.065584
-11.01141	-631.107914	-4.45881	-631.065501	2.11265	-631.069165
-10.77661	-631.107869	-4.22403	-631.063417	2.34746	-631.073225
-10.54182	-631.107819	-3.98929	-631.061877	2.58227	-631.077597
-10.30703	-631.107763	-3.7546	-631.060785	2.81708	-631.082099
-10.07224	-631.107702	-3.51996	-631.059989	3.05189	-631.08653
-9.83745	-631.107635	-3.28544	-631.059394	3.28668	-631.090668
-9.60268	-631.107564	-3.05091	-631.058939	3.52142	-631.094275
-9.3679	-631.107487	-2.81632	-631.058554	3.75595	-631.0971
-9.13314	-631.107405	-2.58163	-631.058213	3.9891	-631.098982
-8.89837	-631.107316	-2.34698	-631.057891	4.21916	-631.100078
-8.66364	-631.107224	-2.11234	-631.057596	4.45249	-631.10082
-8.42893	-631.107125	-1.87763	-631.057315	4.68665	-631.101365
-8.19439	-631.107021	-1.64289	-631.057049	4.9206	-631.101772
-7.96044	-631.106908	-1.40816	-631.056794	5.15397	-631.102065
-7.72869	-631.106774	-1.17345	-631.056553	5.38694	-631.102279
-7.49779	-631.106568	-0.93873	-631.056326	5.61998	-631.102479
-7.26429	-631.10624	-0.70404	-631.05612	5.85406	-631.102672
-7.03228	-631.10573	-0.46927	-631.055955	6.08824	-631.102881
-6.80638	-631.104647	-0.23468	-631.055838	6.32244	-631.103101
-6.57204	-631.102262	<b>0</b>	<b>-631.0558</b>	6.5567	-631.103329
-6.33727	-631.098754	0.23453	-631.055852	6.79065	-631.103546
-6.10247	-631.094484	0.46918	-631.056066	7.02489	-631.103732
-5.86766	-631.089777	0.70392	-631.056514	7.24874	-631.103863
-5.63284	-631.08491	0.93867	-631.057277	7.47961	-631.103944
-5.39803	-631.080125	1.17344	-631.058481	7.70422	-631.103987
-5.16322	-631.075636	1.40823	-631.060226	7.93825	-631.104017

TS1-4\_A1O<-->A2O

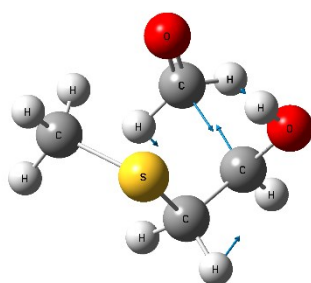


Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-706.35277	-706.226772	-706.218015	-706.259817
M06-2X/DG3/aug-cc-pVTZ				-706.358956	-706.232993	-706.224207	-706.26615
MN15/cc-pVTZ				-706.033975	-705.908156	-705.899465	-705.940995
MN15/aug-cc-pVTZ				-706.044011	-705.918387	-705.909678	-705.951275
SVECV-f12				-706.231886	-706.105923	-706.097137	-706.13908
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	-0.008725	-0.011435	-0.002784	<b>i1987.6492</b>	947.9591	1501.7801	
C	-0.008285	0.009031	1.566384	98.4452	964.5608	2037.9832	
C	1.5501	-0.003021	1.984837	117.699	997.3712	2978.0151	
S	2.443909	-1.337957	1.250352	138.5394	1089.3478	3037.5914	
C	3.191287	-0.601392	-0.21878	200.8762	1121.6237	3081.4324	
H	0.769884	0.58611	-0.481432	261.0047	1147.0946	3085.0079	
H	-0.992669	0.37942	-0.301392	319.7174	1184.3867	3096.3672	
H	1.553161	-0.165502	3.059932	387.3026	1221.6415	3169.1962	
H	2.005167	0.95439	1.739507	520.1951	1249.2154	3174.8186	
H	4.074142	-1.191918	-0.449229	668.3462	1267.3662	3176.7496	
H	2.493461	-0.654058	-1.050144	702.5509	1292.8642		
H	3.487126	0.425252	-0.018823	719.6969	1344.7749		
O	0.100478	-1.352451	-0.26534	770.5969	1353.7921		
H	-0.339164	-1.65162	0.773109	781.6003	1433.9666		
H	-0.433624	0.909563	2.022574	841.8241	1464.419		
O	-0.60571	-1.127859	1.912343	866.8984	1476.8087		



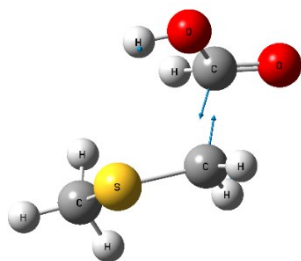
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-4.76199	-706.066286	-1.44801	-706.060637	1.8627	-706.051397
-4.65846	-706.06627	-1.34443	-706.059889	1.96629	-706.051871
-4.55489	-706.066248	-1.24087	-706.05905	2.06988	-706.052312
-4.45134	-706.066223	-1.13734	-706.058104	2.17348	-706.05272
-4.34775	-706.066192	-1.03385	-706.057031	2.27707	-706.053099
-4.24418	-706.066157	-0.93042	-706.055798	2.38066	-706.05345
-4.1406	-706.066117	-0.82704	-706.05435	2.48425	-706.053774
-4.03702	-706.066073	-0.72369	-706.052614	2.58784	-706.054072
-3.93342	-706.066023	-0.62054	-706.050451	2.69143	-706.054346
-3.82984	-706.065969	-0.51759	-706.047699	2.79503	-706.054598
-3.72625	-706.06591	-0.41424	-706.044184	2.89862	-706.054827
-3.62266	-706.065846	-0.31071	-706.04037	3.00221	-706.055037
-3.51908	-706.065778	-0.20714	-706.036984	3.10579	-706.055226
-3.41551	-706.065704	-0.10359	-706.034713	3.20938	-706.055397
-3.31194	-706.065625	0	-706.034	3.31296	-706.05555
-3.20839	-706.065541	0.1035	-706.03466	3.41654	-706.055687
-3.10484	-706.065449	0.20684	-706.036257	3.52012	-706.055808
-3.00131	-706.065349	0.31006	-706.038049	3.62368	-706.055914
-2.89779	-706.065239	0.41305	-706.0396	3.72724	-706.056007
-2.79427	-706.065117	0.51635	-706.040973	3.83078	-706.056087
-2.69076	-706.064981	0.61977	-706.042178	3.93431	-706.056156
-2.58724	-706.064826	0.72328	-706.043281	4.03782	-706.056216
-2.48371	-706.064649	0.82683	-706.0443	4.14133	-706.056267
-2.38018	-706.064446	0.9304	-706.045249	4.24485	-706.056311
-2.27663	-706.064212	1.03398	-706.046133	4.34839	-706.056349
-2.17307	-706.063943	1.13756	-706.046959	4.45195	-706.056381
-2.0695	-706.063634	1.24115	-706.047731	4.55553	-706.056409
-1.96593	-706.06328	1.34474	-706.048452	4.65912	-706.056431
-1.86235	-706.062875	1.44833	-706.049126	4.76271	-706.05645
-1.75876	-706.062414	1.55192	-706.049754	4.86631	-706.056463
-1.65518	-706.061891	1.65551	-706.050341		
-1.55159	-706.061301	1.75911	-706.050888		

TS1-5\_A2O-->P3+Ad\_Im2

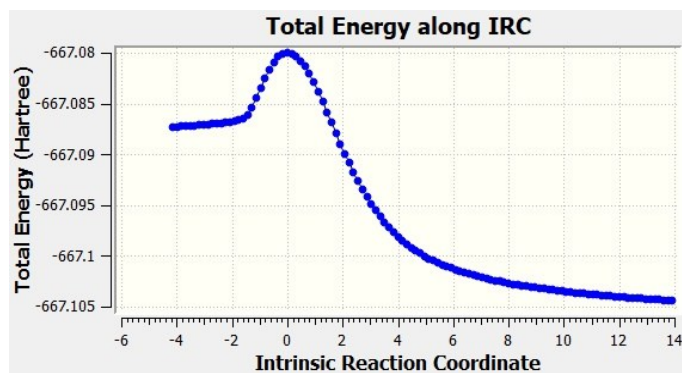


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-706.37034	-706.242963	-706.232971	-706.277886		
M06-2X/DG3/aug-cc-pVTZ	-706.376379	-706.24911	-706.239087	-706.284185		
MN15/cc-pVTZ	-706.046231	-705.919438	-705.90948	-705.954354		
MN15/aug-cc-pVTZ	-706.056031	-705.929449	-705.919449	-705.964651		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.009993	0.006917	0.000658	<b>282.2994i</b>	912.5461	1640.9549
C	0.001669	-0.00748	2.143453	51.6125	970.8248	2927.7847
C	1.437912	-0.012733	2.5891	77.8052	993.6654	3008.8372
S	2.285306	-1.607796	2.427255	172.8656	1013.202	3041.6078
C	3.051769	-1.442447	0.79501	177.8649	1107.1188	3073.0471
H	0.829281	0.724473	-0.037404	199.3255	1201.1518	3119.8583
H	-1.014504	0.455877	0.015928	209.7861	1206.8417	3158.1404
H	1.45749	0.215067	3.659395	232.4311	1249.714	3161.9127
H	2.00918	0.76355	2.081883	309.5805	1272.588	3180.6454
H	3.6436	-2.343371	0.650933	372.376	1353.4652	3695.4118
H	2.293586	-1.376515	0.02026	548.8457	1362.4752	
H	3.715669	-0.580516	0.788383	574.0036	1441.8312	
O	0.145757	-1.167825	-0.329433	650.469	1451.5304	
H	-0.210001	-1.872067	2.292779	699.0651	1469.4885	
H	-0.542125	0.92199	2.278908	748.0516	1480.0143	
O	-0.748778	-1.075456	2.435763	840.8366	1504.647	

TS1-6\_Ad\_Im-O-->P4+Ad\_Im1



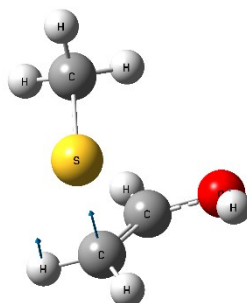
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-667.080007	-666.980836	-666.972264	-667.013821		
M06-2X/DG3/aug-cc-pVTZ	-667.086317	-666.987211	-666.978645	-667.020184		
MN15/cc-pVTZ	-666.788231	-666.689722	-666.681089	-666.72272		
MN15/aug-cc-pVTZ	-666.797806	-666.699372	-666.69076	-666.732325		
SVECV-f12	-666.961463	-666.862357	-666.853791	-666.89533		
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.010109	0.014367	0.03438	<b>i434.9979</b>	945.123	2930.3824
C	0.007612	-0.005261	1.931561	75.5042	970.2699	3077.8913
S	1.634503	0.007276	2.550633	109.3797	972.9906	3134.4113
C	2.001735	1.774999	2.473124	149.3814	1067.4961	3162.9069
H	-0.483428	-0.957729	2.088424	194.8127	1070.7467	3179.125
H	-0.596027	0.860187	2.179113	290.1392	1129.7539	3239.4575
H	3.005333	1.912464	2.866042	325.71	1253.9563	3833.5001
H	1.968218	2.129118	1.445145	402.8092	1347.5992	
H	1.292534	2.328856	3.083024	443.2326	1354.975	
H	1.655246	-0.983651	-0.014037	619.3966	1416.0904	
O	0.746583	-1.097701	-0.315068	724.6573	1474.0045	
H	0.590797	0.949912	-0.059079	764.946	1480.9617	
O	-1.204035	0.013398	-0.202187	802.7314	1558.0857	



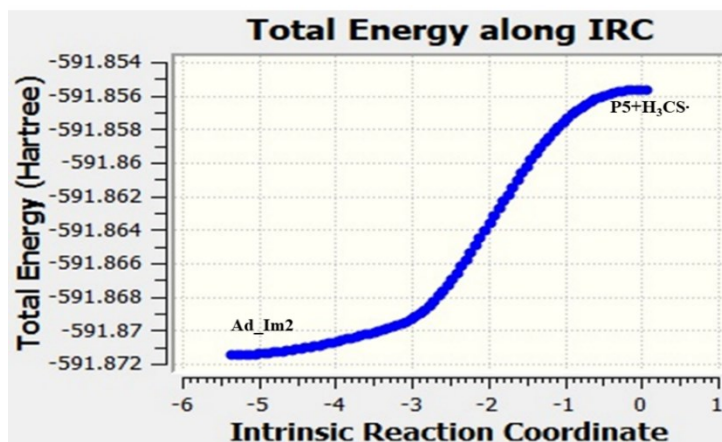
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-4.14888	-667.087318	1.92107	-667.088956	8.00442	-667.1027
-3.98878	-667.087295	2.08117	-667.089936	8.16451	-667.10278
-3.82868	-667.087269	2.24126	-667.090875	8.32461	-667.102856
-3.66858	-667.087242	2.40136	-667.091769	8.48471	-667.102929
-3.50848	-667.087213	2.56146	-667.092618	8.64481	-667.102999
-3.34838	-667.087182	2.72155	-667.093418	8.80491	-667.103067
-3.18828	-667.087148	2.88165	-667.094168	8.96501	-667.103131
-3.02818	-667.087111	3.04175	-667.094868	9.12511	-667.103194
-2.86809	-667.087072	3.20184	-667.095518	9.28521	-667.103254
-2.708	-667.08703	3.36193	-667.09612	9.44531	-667.103311
-2.54791	-667.086985	3.52202	-667.096675	9.6054	-667.103367
-2.38786	-667.086936	3.68211	-667.097188	9.7655	-667.103421
-2.22789	-667.086883	3.8422	-667.097659	9.92559	-667.103473
-2.06827	-667.086826	4.00228	-667.098091	10.08569	-667.103524
-1.90953	-667.086754	4.16236	-667.098486	10.24578	-667.103573
-1.75122	-667.086663	4.32244	-667.098848	10.40588	-667.103621
-1.59818	-667.086512	4.48252	-667.09918	10.56598	-667.103667
-1.44053	-667.086133	4.64259	-667.099483	10.72607	-667.103713
-1.28064	-667.085422	4.80267	-667.099762	10.88617	-667.103757
-1.12059	-667.084496	4.96274	-667.100018	11.04627	-667.1038
-0.9605	-667.083489	5.12281	-667.100254	11.20637	-667.103842
-0.80042	-667.08251	5.28289	-667.100473	11.36646	-667.103882
-0.64033	-667.081636	5.44297	-667.100676	11.52656	-667.103922
-0.48025	-667.080925	5.60305	-667.100866	11.68665	-667.10396
-0.32017	-667.080409	5.76314	-667.101044	11.84674	-667.103998
-0.16011	-667.080105	5.92323	-667.101211	12.00684	-667.104035
<b>0</b>	<b>-667.08</b>	6.08332	-667.101368	12.16693	-667.10407
0.16011	-667.080101	6.24341	-667.101515	12.32703	-667.104105
0.32017	-667.08037	6.4035	-667.101654	12.48713	-667.104139
0.48025	-667.080803	6.56359	-667.101785	12.64723	-667.104172
0.64034	-667.08138	6.72367	-667.101909	12.80732	-667.104203
0.80043	-667.082089	6.88377	-667.102026	12.96741	-667.104234
0.96052	-667.082909	7.04386	-667.102137	13.1275	-667.104264
1.12062	-667.083825	7.20395	-667.102242	13.28759	-667.104292
1.28071	-667.084814	7.36404	-667.102342	13.44768	-667.10432
1.4408	-667.085848	7.52413	-667.102438	13.60777	-667.104346
1.60089	-667.086899	7.68423	-667.102529	13.76786	-667.104371
1.76098	-667.08794	7.84432	-667.102616	13.92795	-667.104395



TS1-7\_Ad\_Im2-->P5+MeS

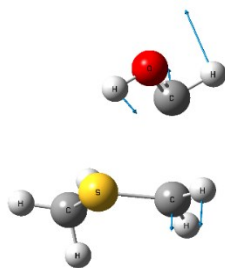


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-591.855645	-591.759874	-591.751903	-591.792309		
M06-2X/DG3/aug-cc-pVTZ	-591.859895	-591.764241	-591.756225	-591.796875		
MN15/cc-pVTZ	-591.610183	-591.514923	-591.506988	-591.547046		
MN15/aug-cc-pVTZ	-591.61718	-591.522118	-591.514139	-591.554363		
SVECV-f12	-591.742783	-591.647129	-591.639113	-591.679763		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.01555	-0.021458	-0.006817	<b>245.0066i</b>	952.0016	3143.2245
C	0.030725	-0.00269	1.347392	50.1281	968.6993	3148.4032
S	2.413106	-0.010992	1.814287	83.0705	989.2049	3182.6439
C	2.896709	1.060356	0.443866	135.2951	1146.6687	3223.7854
H	-0.009087	-0.925972	1.907893	189.7146	1308.845	3281.9277
H	-0.265657	0.899936	1.857388	273.0476	1336.1882	3816.2429
H	3.977671	1.18051	0.504933	486.2067	1363.7238	
H	2.653758	0.611997	-0.517613	514.7682	1451.5608	
H	2.434325	2.041577	0.526738	731.5208	1464.6739	
H	0.661573	-1.795828	-0.194675	765.2948	1484.5594	
H	-0.162786	0.860877	-0.60533	889.5933	1616.7178	
O	0.327622	-1.088024	-0.75966	925.5004	3063.5416	



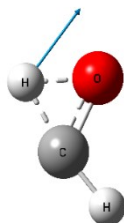
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-5.35116	-591.871513	-3.48708	-591.870122	-1.62361	-591.861055
-5.29107	-591.871504	-3.42695	-591.870047	-1.56348	-591.860646
-5.23096	-591.871492	-3.36684	-591.86997	-1.50334	-591.860249
-5.17084	-591.871477	-3.30674	-591.86989	-1.44321	-591.859863
-5.11071	-591.87146	-3.24669	-591.869807	-1.38307	-591.859491
-5.05058	-591.87144	-3.18669	-591.869717	-1.32294	-591.859135
-4.99045	-591.871418	-3.1267	-591.869616	-1.2628	-591.858794
-4.93031	-591.871392	-3.06668	-591.869498	-1.20267	-591.85847
-4.87018	-591.871365	-3.00662	-591.869359	-1.14253	-591.858163
-4.81005	-591.871335	-2.94653	-591.869195	-1.0824	-591.857875
-4.74991	-591.871302	-2.88642	-591.869004	-1.02227	-591.857605
-4.68978	-591.871267	-2.82629	-591.868786	-0.96213	-591.857354
-4.62964	-591.87123	-2.76617	-591.868542	-0.902	-591.857122
-4.56951	-591.87119	-2.70604	-591.868271	-0.84186	-591.856909
-4.50937	-591.871148	-2.6459	-591.867976	-0.78173	-591.856715
-4.44924	-591.871104	-2.58577	-591.867658	-0.72159	-591.856538
-4.3891	-591.871057	-2.52564	-591.867318	-0.66146	-591.85638
-4.32897	-591.871008	-2.4655	-591.86696	-0.60133	-591.856239
-4.26883	-591.870957	-2.40537	-591.866585	-0.54119	-591.856116
-4.2087	-591.870904	-2.34523	-591.866196	-0.48106	-591.856008
-4.14856	-591.870849	-2.2851	-591.865793	-0.42093	-591.855916
-4.08843	-591.870792	-2.22496	-591.865379	-0.36079	-591.85584
-4.02829	-591.870733	-2.16483	-591.864957	-0.30066	-591.855777
-3.96816	-591.870672	-2.10469	-591.864527	-0.24053	-591.855727
-3.90802	-591.870609	-2.04456	-591.864091	-0.1804	-591.85569
-3.84788	-591.870544	-1.98442	-591.863652	-0.12027	-591.855665
-3.78775	-591.870478	-1.92429	-591.863211	-0.06014	-591.855651
-3.72761	-591.87041	-1.86415	-591.862771	<b>0</b>	<b>-591.8556</b>
-3.66748	-591.87034	-1.80402	-591.862333	0.06014	-591.85565
-3.60734	-591.870269	-1.74388	-591.8619		
-3.54721	-591.870196	-1.68375	-591.861474		

TS1-8\_Ad\_Im2-->P3\_Im+Ad\_Im1

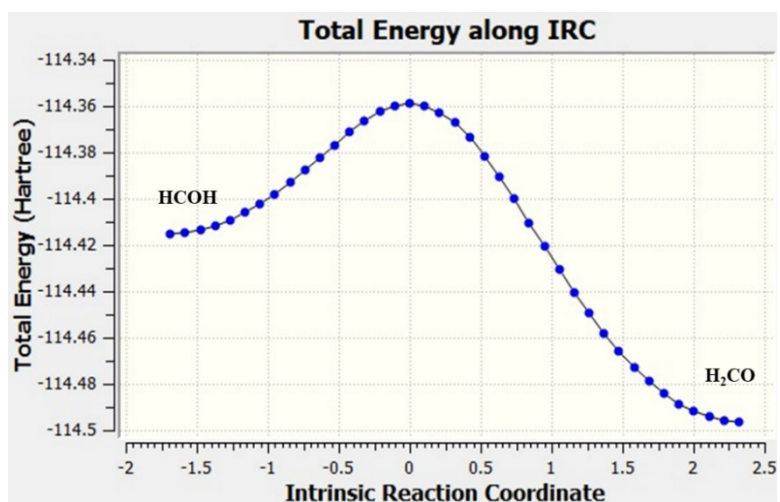


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-591.762086	-591.670989	-591.662217	-591.703451		
M06-2X/DG3/aug-cc-pVTZ	-591.766159	-591.675141	-591.666342	-591.707652		
MN15/cc-pVTZ	-591.521081	-591.43028	-591.421535	-591.462628		
MN15/aug-cc-pVTZ	-591.528077	-591.437378	-591.428614	-591.469788		
SVECV-f12	-591.652387	-591.561369	-591.55257	-591.59388		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.04113	-0.034755	0.006297	<b>220.2568i</b>	907.8265	3071.2249
C	0.01211	0.016973	2.773602	95.0518	980.8543	3161.7879
S	1.72945	0.008351	2.768298	133.387	1033.9813	3177.8548
C	2.037503	1.695624	2.198698	150.0742	1066.5682	3179.5934
H	-0.479842	-0.898327	3.061477	189.6349	1248.0512	3304.3429
H	-0.512508	0.956843	2.826934	211.9487	1340.705	3587.3616
H	3.108868	1.805332	2.055208	290.3568	1362.3621	
H	1.504167	1.840226	1.261227	308.0135	1408.8861	
H	1.695911	2.402614	2.95107	328.3298	1468.6781	
H	1.48262	-0.961701	0.521963	484.343	1489.1125	
H	-0.952283	-0.31992	-0.559101	725.9304	1496.053	
O	0.694267	-1.107792	-0.034972	837.608	2912.3602	

TS\_P3\_P3\_Im2->P3

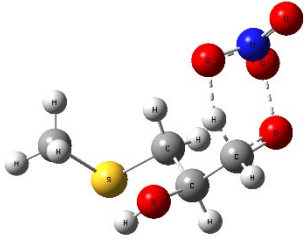


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ	-114.358842	-114.337882	-114.333985	-114.359609
M06-2X/DG3/aug-cc-pVTZ	-114.361808	-114.340928	-114.337024	-114.362656
MN15/cc-pVTZ	-114.282761	-114.261904	-114.25801	-114.283634
MN15/aug-cc-pVTZ	-114.28612	-114.265344	-114.261443	-114.287075
SVECV-f12	-114.34922	-114.328341	-114.324437	-114.350069
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )	
H	-0.176906	-0.002154	0.371716	<b>2162.1125i</b> 2663.468
C	0.116944	-0.0195	1.585923	699.9808 2956.2586
H	0.564728	-0.024115	2.598579	1345.9434
O	0.965769	0.045769	0.619757	1499.4818

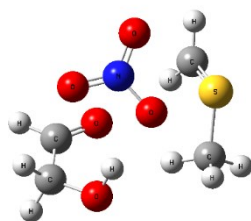


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-1.68687	-114.415023	-0.31634	-114.366509	1.05448	-114.430751
-1.58152	-114.414526	-0.2109	-114.362497	1.15993	-114.440445
-1.47611	-114.413382	-0.10547	-114.359801	1.26538	-114.449613
-1.37071	-114.411591	0	-114.3588	1.37082	-114.458138
-1.26529	-114.409138	0.10547	-114.359818	1.47627	-114.465926
-1.15987	-114.406034	0.21091	-114.362675	1.58171	-114.472907
-1.05443	-114.402293	0.31635	-114.367311	1.68715	-114.47903
-0.94899	-114.397959	0.42179	-114.37364	1.79259	-114.484259
-0.84354	-114.393107	0.52724	-114.381484	1.89803	-114.488565
-0.73809	-114.38785	0.63269	-114.390499	2.00346	-114.491939
-0.63265	-114.382339	0.73814	-114.400278	2.10888	-114.494378
-0.52721	-114.376773	0.84359	-114.410443	2.21422	-114.495906
-0.42178	-114.371392	0.94903	-114.420685	2.31906	-114.49657

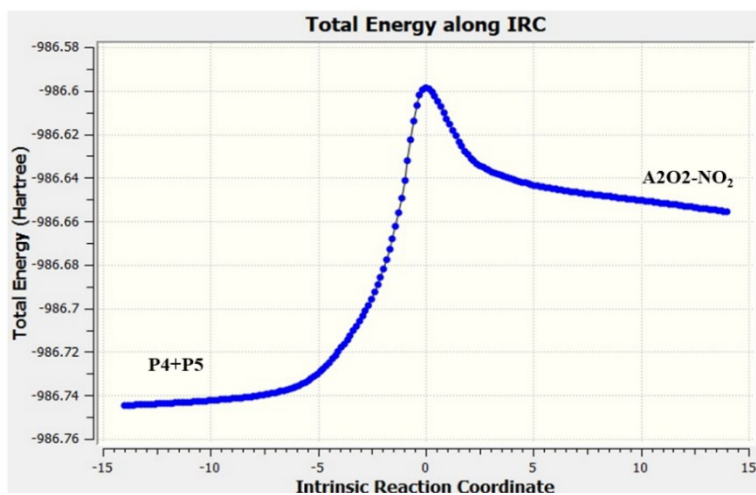
2. Reactions of the peroxy radicals (A1O2, A2O2) with NO<sub>2</sub>

TSnox_A2O2-NO <sub>2</sub> -->P4+P5						
						
Method	Ee			E+ZPE	ΔH	ΔG
M06-2X/GD3/cc-pVTZ	-986.598769			-986.454112	-986.441133	-986.494144
M06-2X/DG3/aug-cc-pVTZ	-986.609214			-986.464811	-986.451782	-986.504998
MN15/cc-pVTZ	-986.103342			-985.959756	-985.946634	-985.999839
MN15/aug-cc-pVTZ	-986.118334			-985.975065	-985.96189	-986.015318
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.366733	0.317411	0.026104	<b>1311.8239i</b>	767.2092	1437.5802
C	0.063071	-0.052805	1.470228	40.5896	820.5131	1461.4621
C	1.300853	0.091249	2.349368	50.4916	847.904	1473.5817
S	1.003581	-0.541121	4.027494	70.7438	856.5276	1495.4044
C	1.777328	-2.174339	3.883582	87.2813	910.942	1659.2399
H	1.171097	-0.505787	-0.3586	108.4441	975.7821	1792.2491
H	-0.719918	0.615928	1.846179	115.7491	981.9923	3018.7931
H	1.583216	1.139639	2.422977	159.9552	1027.7306	3028.512
H	2.140426	-0.455708	1.920208	193.8636	1058.2966	3076.4957
H	1.594252	-2.693969	4.820771	245.8369	1099.0461	3089.8863
H	1.34576	-2.7417	3.062883	289.6219	1142.0503	3150.0792
H	2.849579	-2.06859	3.737185	409.6294	1188.9587	3162.0882
O	-0.413379	-1.37715	1.411771	430.7763	1220.4644	3172.4257
H	-0.674203	-1.627832	2.305675	458.0517	1244.9303	3818.3127
H	-0.406464	0.095939	-0.723189	472.6112	1266.7971	283.238661
O	0.945877	1.471337	-0.195682	506.6416	1279.8258	1115.54725
O	2.687773	1.317111	-0.325209	585.0992	1356.7075	
N	2.843612	0.392869	-1.223101	685.6267	1379.9774	
O	3.17553	0.656162	-2.339542	696.705	1384.1272	
O	2.535962	-0.756661	-0.821688	727.0856	1404.7512	

**A1O2-NO<sub>2</sub>-PW**



<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			<b><math>\Delta</math>H</b>			<b><math>\Delta</math>G</b>																																																																																																																											
M06-2X/GD3/cc-pVTZ							-986.691867			-986.545696			-986.530853			-986.586895																																																																																																																											
M06-2X/DG3/aug-cc-pVTZ							-986.702874			-986.556981			-986.54206			-986.598462																																																																																																																											
MN15/cc-pVTZ							-986.190583			-986.045448			-986.030412			-986.087109																																																																																																																											
MN15/aug-cc-pVTZ							-986.206428			-986.061634			-986.046537			-986.103513																																																																																																																											
<b>Coordinates (xyz)</b>							<b>Vibrations (cm<sup>-1</sup>)</b>																																																																																																																																				
C	0.093472	0.010928	0.083329	44.9942	735.5701	1460.5452	C	-0.181714	0.285933	1.534651	71.3202	742.1799	1466.1513	C	2.858320	-0.173672	4.244091	79.1798	776.99	1475.6736	S	3.870489	-0.679014	3.121014	92.232	871.4538	1591.4673	C	3.857332	0.605622	1.864279	119.9503	882.5214	1844.6528	H	-0.389536	0.810118	-0.489766	125.1507	928.461	2973.9151	H	-0.427797	-0.920918	-0.164932	138.2382	930.9546	3035.617	H	2.765896	-0.794321	5.123913	149.32	995.7424	3067.8884	H	2.18794	0.658652	4.08338	174.0439	1045.3487	3084.4758	H	4.242944	0.145357	0.959545	187.8305	1092.2877	3174.2508	H	2.828408	0.923294	1.712067	203.0951	1102.7933	3192.447	H	4.506317	1.409501	2.200788	217.7011	1123.553	3197.0384	H	1.848724	-0.773753	0.221107	227.5914	1182.9439	3292.7283	O	1.445196	-0.017379	-0.240184	252.8896	1263.991	3633.899	H	-1.247468	0.245816	1.824687	301.5457	1348.1141		O	0.663676	0.545223	2.353359	344.2071	1376.797		O	2.733272	-1.867794	1.476543	621.7213	1400.4132		N	1.75938	-2.462249	2.084201	640.6975	1414.2832		O	1.960709	-2.918922	3.198881	715.9417	1449.8274		O	0.679736	-2.514352	1.513474	722.5586	1454.3759	

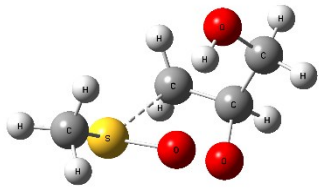


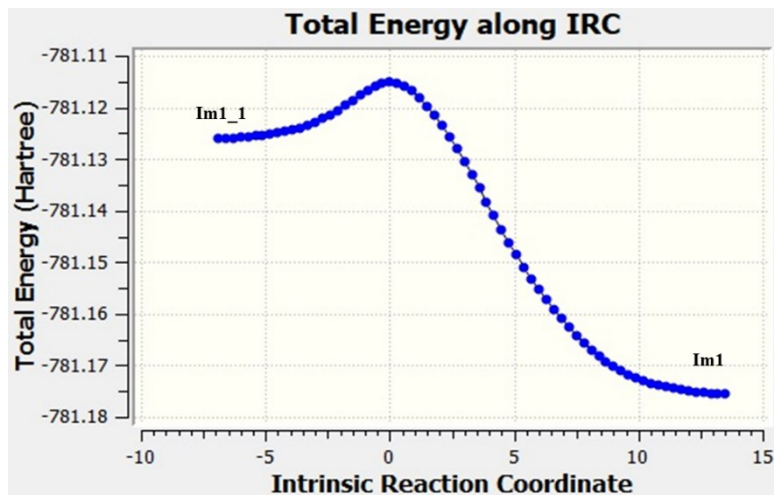
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-14.00359	-986.744706	-4.61953	-986.726361	4.75996	-986.642802
-13.86352	-986.744634	-4.47946	-986.724844	4.90003	-986.64313
-13.72344	-986.744562	-4.33945	-986.72325	5.04009	-986.643443
-13.58337	-986.744491	-4.19938	-986.721576	5.18015	-986.643742
-13.4433	-986.744419	-4.05937	-986.71985	5.32021	-986.644028
-13.30323	-986.744347	-3.91931	-986.71806	5.46027	-986.644302
-13.16316	-986.744274	-3.7793	-986.716222	5.60033	-986.644564
-13.02308	-986.744202	-3.63927	-986.714333	5.74039	-986.644816
-12.88301	-986.744128	-3.49926	-986.712393	5.88045	-986.645059
-12.74294	-986.744054	-3.35923	-986.710381	6.02051	-986.645293
-12.60286	-986.74398	-3.2192	-986.708282	6.16057	-986.645519
-12.46279	-986.743905	-3.07917	-986.706074	6.30063	-986.645739
-12.32272	-986.743829	-2.93913	-986.703738	6.4407	-986.645951
-12.18264	-986.743752	-2.79909	-986.701252	6.58076	-986.646158
-12.04257	-986.743675	-2.65905	-986.698594	6.72082	-986.646359
-11.9025	-986.743596	-2.51901	-986.695742	6.86089	-986.646555
-11.76242	-986.743516	-2.37896	-986.692672	7.00095	-986.646747
-11.62235	-986.743435	-2.23893	-986.689358	7.14102	-986.646935
-11.48228	-986.743352	-2.09889	-986.685771	7.28109	-986.647119
-11.34221	-986.743268	-1.95887	-986.681874	7.42116	-986.6473
-11.20213	-986.743183	-1.81887	-986.677631	7.56122	-986.647479
-11.06206	-986.743096	-1.67887	-986.672993	7.70129	-986.647656
-10.92199	-986.743008	-1.53888	-986.667912	7.84136	-986.64783
-10.78192	-986.742919	-1.39891	-986.66233	7.98144	-986.648003
-10.64185	-986.742827	-1.25903	-986.656192	8.12151	-986.648175



-10.50178	-986.742734	-1.11947	-986.649286	8.26158	-986.648346
-10.36171	-986.742639	-0.9799	-986.641295	8.40165	-986.648516
-10.22164	-986.742541	-0.84002	-986.632094	8.54172	-986.648686
-10.08157	-986.742441	-0.69999	-986.622566	8.6818	-986.648855
-9.9415	-986.742339	-0.55992	-986.613919	8.82187	-986.649023
-9.80144	-986.742234	-0.41985	-986.607006	8.96195	-986.649192
-9.66137	-986.742125	-0.2798	-986.602164	9.10202	-986.649361
-9.52131	-986.742013	-0.13984	-986.599515	9.2421	-986.64953
-9.38125	-986.741896	0	-986.5988	9.38217	-986.649699
-9.24118	-986.741776	0.13972	-986.599318	9.52225	-986.649869
-9.10112	-986.74165	0.27946	-986.600666	9.66233	-986.650039
-8.96105	-986.74152	0.4195	-986.602603	9.8024	-986.65021
-8.82099	-986.741384	0.55951	-986.604888	9.94248	-986.650382
-8.68092	-986.741243	0.69955	-986.607426	10.08255	-986.650554
-8.54085	-986.741096	0.8396	-986.610106	10.22263	-986.650728
-8.40078	-986.740943	0.97966	-986.612855	10.36271	-986.650902
-8.26071	-986.740783	1.11972	-986.615605	10.50279	-986.651077
-8.12064	-986.740616	1.25978	-986.6183	10.64286	-986.651253
-7.98058	-986.740441	1.39984	-986.620891	10.78294	-986.65143
-7.84052	-986.740256	1.5399	-986.623337	10.92302	-986.651608
-7.70046	-986.740059	1.67996	-986.625599	11.0631	-986.651786
-7.56041	-986.739848	1.82	-986.627648	11.20317	-986.651966
-7.42036	-986.739621	1.96002	-986.62946	11.34325	-986.652146
-7.2803	-986.739375	2.09999	-986.631024	11.48333	-986.652326
-7.14024	-986.739108	2.23988	-986.632345	11.62341	-986.652508
-7.00018	-986.738819	2.37966	-986.633454	11.76349	-986.652689
-6.86011	-986.738506	2.51944	-986.634399	11.90357	-986.652872
-6.72005	-986.738168	2.65929	-986.635229	12.04365	-986.653055
-6.57999	-986.737802	2.79923	-986.635977	12.18373	-986.653239
-6.43993	-986.737408	2.93923	-986.636666	12.32381	-986.653423
-6.29987	-986.736979	3.07925	-986.637308	12.46389	-986.653607
-6.15983	-986.73651	3.2193	-986.63791	12.60396	-986.653792
-6.01979	-986.735993	3.35934	-986.638477	12.74404	-986.653977
-5.87977	-986.735417	3.49939	-986.639013	12.88412	-986.654161
-5.73975	-986.734777	3.63945	-986.639521	13.0242	-986.654346
-5.59973	-986.734061	3.77951	-986.640004	13.16428	-986.65453
-5.45972	-986.733265	3.91957	-986.640463	13.30436	-986.654714
-5.31969	-986.732371	4.05963	-986.640901	13.44444	-986.654897
-5.17967	-986.731386	4.1997	-986.641319	13.58452	-986.65508
-5.03963	-986.730286	4.33977	-986.641717	13.7246	-986.655263
-4.89961	-986.729086	4.47983	-986.642096	13.86468	-986.655444
-4.75955	-986.727771	4.6199	-986.642457	14.00476	-986.655625

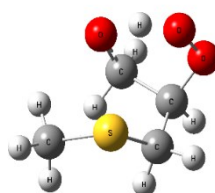
3. Intramolecular rearrangement mechanism in RO<sub>2</sub> intermediates (A1O2-A2O2)

TS2-1-A1_Im1-->A1_Im1_1						
						
Method	E <sub>c</sub>		E+ZPE	ΔH	ΔG	
M06-2X/GD3/cc-pVTZ	-781.484483		-781.350927	-781.340944	-781.385921	
M06-2X/DG3/aug-cc-pVTZ	-781.492081		-781.358634	-781.348644	-781.393598	
MN15/cc-pVTZ	-781.115151		-780.982249	-780.972219	-781.017264	
MN15/aug-cc-pVTZ	-781.127202		-780.994529	-780.984481	-781.029539	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.025151	0.061749	-0.008075	<b>283.2242i</b>	878.2876	1471.9089
C	-0.000958	-0.000554	1.511549	56.1622	922.967	1499.4977
C	1.366082	0.012518	2.098971	87.1392	944.3168	3043.9959
S	1.56415	-2.21532	2.604931	144.0541	954.5332	3064.8851
C	2.034058	-3.80359	1.845576	189.9149	993.1797	3070.7022
H	0.265111	1.065907	-0.319082	241.8463	1016.2373	3110.7987
H	-1.050528	-0.1191	-0.345143	277.5077	1044.6566	3158.0532
H	1.47534	0.40402	3.102118	286.3521	1122.0725	3166.9548
H	2.197277	0.17923	1.429427	383.306	1164.5886	3173.1242
H	2.962897	-4.095793	2.3301	447.0348	1239.378	3257.8666
H	1.259039	-4.543464	2.032925	455.2148	1310.2242	3852.3041
H	2.199284	-3.677291	0.778428	537.4686	1321.9877	
O	0.879534	-0.827217	-0.626835	626.4706	1352.8393	
H	0.666742	-1.713076	-0.317214	684.7803	1393.5132	
H	-0.633083	0.798786	1.908992	686.1972	1436.6506	
O	-0.696611	-1.17776	1.994665	770.937	1455.1229	
O	0.099888	-2.289036	1.680829	818.1631	1463.0627	

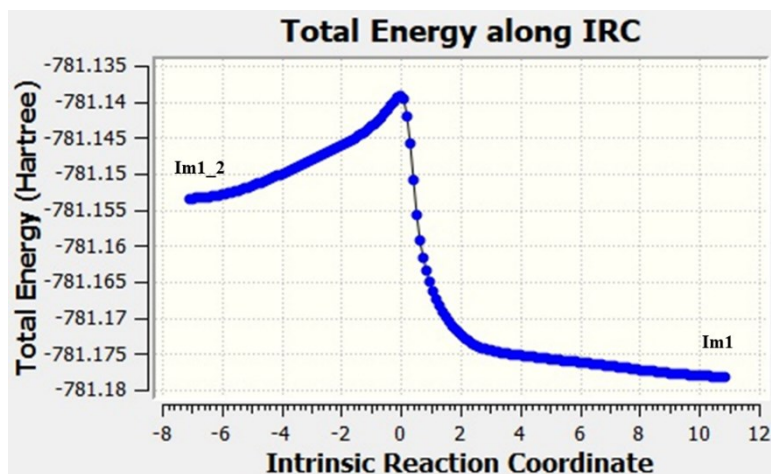


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-6.9004	-781.125985	<b>0</b>	<b>-781.1151</b>	6.89979	-781.160992
-6.60081	-781.125939	0.29294	-781.115282	7.2002	-781.162666
-6.30199	-781.125885	0.59305	-781.115874	7.5006	-781.164225
-6.00329	-781.125815	0.89339	-781.116877	7.801	-781.165664
-5.70379	-781.125722	1.19367	-781.118219	8.10139	-781.166986
-5.4038	-781.125597	1.49392	-781.119826	8.40177	-781.168185
-5.10361	-781.125437	1.7941	-781.121628	8.70214	-781.169264
-4.80334	-781.125235	2.09421	-781.123597	9.0025	-781.170223
-4.5031	-781.124989	2.39435	-781.125721	9.30282	-781.171068
-4.20286	-781.124692	2.69453	-781.128011	9.60312	-781.171804
-3.90265	-781.124338	2.9948	-781.130455	9.90339	-781.172441
-3.60242	-781.123918	3.29511	-781.133026	10.20359	-781.172989
-3.30217	-781.123423	3.59546	-781.135677	10.50379	-781.173461
-3.00188	-781.122843	3.89582	-781.138357	10.80388	-781.173864
-2.70157	-781.122174	4.19619	-781.141019	11.10404	-781.174215
-2.40122	-781.121413	4.49657	-781.14363	11.40407	-781.174513
-2.10087	-781.120564	4.79696	-781.146161	11.70408	-781.174775
-1.8005	-781.119639	5.09736	-781.1486	12.00406	-781.174988
-1.50013	-781.118664	5.39776	-781.150936	12.30365	-781.175165
-1.19975	-781.117677	5.69816	-781.153167	12.60335	-781.175301
-0.89939	-781.116742	5.99857	-781.155289	12.90269	-781.175404
-0.59902	-781.115936	6.29898	-781.157302	13.20222	-781.175479
-0.29891	-781.115363	6.59938	-781.159204	13.50187	-781.175533

TS2-2-A1\_Im1-->A1\_Im1\_2



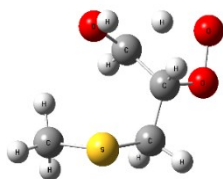
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.504877	-781.374753	-781.365243	-781.408706	
M06-2X/DG3/aug-cc-pVTZ		-781.511182	-781.381206	-781.371676	-781.41519	
MN15/cc-pVTZ		-781.139175	-781.009853	-781.000271	-781.043863	
MN15/aug-cc-pVTZ		-781.149665	-781.020623	-781.011001	-781.054704	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.014627	-0.000537	-0.014787	<b>1241.7664i</b>	903.6886	1499.6131
C	0.006557	-0.006901	1.589853	99.6435	948.5954	1521.8175
C	1.422727	0.013674	2.174171	141.0975	957.4216	1852.6558
S	2.696636	-1.119314	1.590281	168.3186	978.004	2971.3227
C	3.254738	-0.314313	0.073504	204.7395	1009.2737	3043.0387
H	0.720731	0.773209	-0.283908	245.5646	1068.7555	3065.797
H	-1.025591	0.313567	-0.297306	252.972	1129.4873	3070.329
H	1.327457	-0.192442	3.240773	271.1183	1179.3983	3099.2712
H	1.797388	1.03273	2.065789	373.0403	1223.1355	3126.5346
H	4.224754	-0.745563	-0.161911	462.265	1259.7954	3154.5357
H	2.563547	-0.513382	-0.741754	509.6488	1273.5291	3170.2914
H	3.37863	0.756292	0.232732	660.9953	1315.3816	
O	0.312323	-1.221825	-0.468433	703.3346	1325.8655	
H	0.090847	-2.026364	0.583421	727.4523	1349.9036	
H	-0.530737	0.880567	1.928889	751.7129	1390.1484	
O	-0.788977	-1.067319	1.982404	840.2925	1433.6038	
O	-0.194959	-2.250928	1.609018	855.9208	1463.4155	



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-7.05001	-781.153461	-0.97301	-781.143486	5.09576	-781.175782
-6.94157	-781.153441	-0.86451	-781.143087	5.2043	-781.175833
-6.83318	-781.153417	-0.75601	-781.142654	5.31283	-781.175884
-6.72474	-781.153385	-0.6475	-781.142187	5.42137	-781.175934
-6.61631	-781.153346	-0.53899	-781.141686	5.52991	-781.175985
-6.50784	-781.153299	-0.43049	-781.141154	5.63844	-781.176036
-6.39936	-781.153244	-0.32206	-781.140606	5.74698	-781.176087
-6.29085	-781.15318	-0.2137	-781.140046	5.85552	-781.176139
-6.18233	-781.153106	-0.10748	-781.139516	5.96406	-781.176191
-6.0738	-781.153023	<b>0</b>	<b>-781.1392</b>	6.07259	-781.176243
-5.96527	-781.152932	0.10828	-781.139734	6.18113	-781.176296
-5.85673	-781.152831	0.21674	-781.14195	6.28967	-781.176349
-5.74819	-781.152722	0.32525	-781.145879	6.39821	-781.176403
-5.63966	-781.152605	0.43376	-781.150825	6.50675	-781.176457
-5.53112	-781.15248	0.54218	-781.155672	6.61529	-781.176512
-5.42258	-781.152348	0.64985	-781.159269	6.72383	-781.176567
-5.31404	-781.152208	0.75667	-781.161677	6.83237	-781.176623
-5.20549	-781.152063	0.86491	-781.163509	6.94091	-781.176679
-5.09695	-781.151911	0.97323	-781.165024	7.04945	-781.176735
-4.98841	-781.151753	1.08153	-781.166288	7.15799	-781.176792
-4.87987	-781.15159	1.18989	-781.167366	7.26653	-781.176849
-4.77133	-781.151421	1.29831	-781.168308	7.37506	-781.176905
-4.66279	-781.151248	1.4068	-781.169144	7.4836	-781.176962
-4.55425	-781.151071	1.51531	-781.16989	7.59214	-781.177019
-4.44571	-781.150889	1.62384	-781.170558	7.70068	-781.177075
-4.33717	-781.150704	1.73236	-781.171153	7.80922	-781.177132

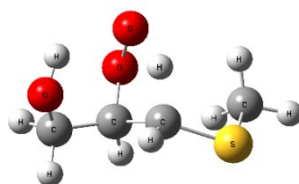
-4.22863	-781.150515	1.84089	-781.171684	7.91776	-781.177187
-4.12009	-781.150322	1.94942	-781.172154	8.0263	-781.177243
-4.01155	-781.150127	2.05795	-781.172569	8.13484	-781.177298
-3.90301	-781.149929	2.16647	-781.172935	8.24338	-781.177352
-3.79447	-781.149729	2.27499	-781.173254	8.35192	-781.177405
-3.68593	-781.149526	2.3835	-781.173532	8.46046	-781.177457
-3.57739	-781.149321	2.492	-781.173773	8.569	-781.177508
-3.46885	-781.149114	2.60049	-781.173981	8.67754	-781.177558
-3.36032	-781.148906	2.70896	-781.17416	8.78607	-781.177606
-3.25178	-781.148696	2.81741	-781.174314	8.89461	-781.177654
-3.14324	-781.148484	2.92585	-781.174446	9.00315	-781.177699
-3.0347	-781.148271	3.03426	-781.174562	9.11169	-781.177743
-2.92617	-781.148058	3.14268	-781.174664	9.22023	-781.177786
-2.81763	-781.147842	3.25111	-781.174756	9.32877	-781.177827
-2.7091	-781.147626	3.35956	-781.174839	9.43731	-781.177866
-2.60056	-781.147409	3.46803	-781.174917	9.54584	-781.177904
-2.49203	-781.14719	3.57652	-781.17499	9.65438	-781.17794
-2.3835	-781.14697	3.68501	-781.175059	9.76292	-781.177974
-2.27498	-781.146748	3.79351	-781.175124	9.87146	-781.178006
-2.16645	-781.146524	3.90201	-781.175187	9.97999	-781.178037
-2.05794	-781.146297	4.01052	-781.175248	10.08853	-781.178066
-1.94942	-781.146066	4.11904	-781.175306	10.19707	-781.178094
-1.84092	-781.14583	4.22755	-781.175363	10.30561	-781.178119
-1.73242	-781.145588	4.33607	-781.175418	10.41415	-781.178143
-1.62392	-781.145337	4.44459	-781.175472	10.52269	-781.178166
-1.51543	-781.145075	4.55312	-781.175525	10.63122	-781.178186
-1.40695	-781.144799	4.66164	-781.175577	10.73976	-781.178205
-1.29847	-781.144506	4.77017	-781.175629	10.8483	-781.178223
-1.18998	-781.144192	4.8787	-781.175681		
-1.0815	-781.143853	4.98723	-781.175732		

TS2-3-A1\_Im2-->A1\_Im2\_1



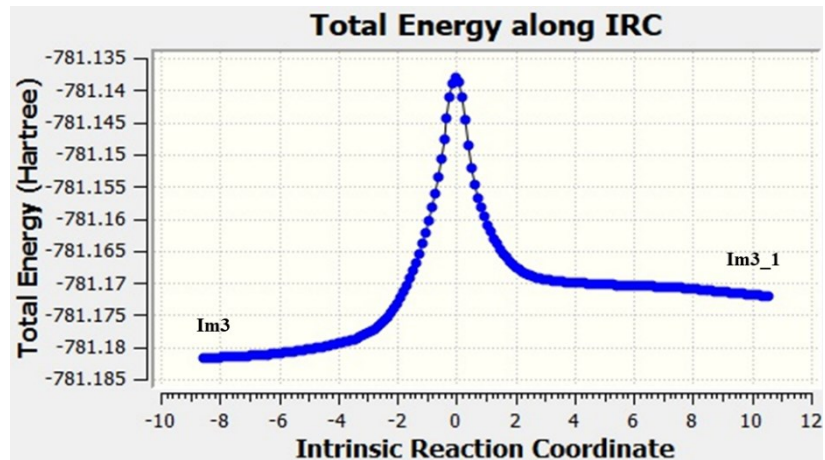
Method							Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ							-781.497426	-781.367048	-781.356822	-781.40228
M06-2X/DG3/aug-cc-pVTZ							-781.504749	-781.37457	-781.364301	-781.409896
MN15/cc-pVTZ							-781.131094	-781.001702	-780.991325	-781.037113
MN15/aug-cc-pVTZ							-781.142495	-781.013357	-781.002974	-781.048808
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )						
C	0.019832	-0.013367	0.011468	<b>2004.7816i</b>	929.1373	1474.6455				
C	0.014118	-0.026337	1.542756	75.5828	972.5871	1494.3447				
C	1.355966	0.002096	2.245695	87.6582	982.7411	1794.5998				
S	2.321703	-1.510875	1.992965	139.8312	1033.1994	3014.6134				
C	3.203326	-1.102126	0.465871	193.2613	1044.1303	3076.382				
H	0.680609	0.725484	-0.441955	210.6387	1083.4058	3085.0162				
H	-1.14792	0.56272	0.03977	224.8807	1139.3767	3120.3147				
H	-0.573213	-0.89297	1.874254	286.4509	1170.6294	3140.6503				
H	1.190527	0.089118	3.318707	327.0294	1230.8241	3162.6244				
H	1.939028	0.864725	1.923637	348.8286	1253.4492	3173.9631				
H	3.911743	-1.909994	0.298484	389.855	1263.1616	3833.6343				
H	2.529324	-1.041697	-0.38375	489.1692	1292.8348					
H	3.754202	-0.172283	0.590292	577.8319	1344.6424					
O	0.099099	-1.197482	-0.653968	676.7222	1358.2033					
H	-0.283861	-1.903976	-0.121737	724.9783	1392.2439					
O	-0.678779	1.169716	1.838858	784.6963	1444.8666					
O	-1.801733	1.119068	1.013146	831.3703	1467.1136					

TS2-4-A1\_Im3-->A1\_Im3\_1



Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.503494	-781.372444	-781.362546	-781.407131	
M06-2X/DG3/aug-cc-pVTZ		-781.510595	-781.379668	-781.369755	-781.414368	
MN15/cc-pVTZ		-781.138096	-781.007776	-780.997837	-781.042474	
MN15/aug-cc-pVTZ		-781.149579	-781.019481	-781.009523	-781.054197	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.005774	-0.000552	-0.006558	<b>1999.046i</b>	924.3155	1471.4312
C	0.006015	-0.004212	1.516755	83.9101	952.3773	1503.7994
C	1.445886	-0.003623	2.064247	110.8923	965.2995	1757.9099
S	1.775829	0.690683	3.618739	153.6236	994.5494	3039.6767
C	0.472559	-0.05247	4.622836	205.4904	1008.4239	3078.5297
H	0.298527	0.985763	-0.360386	221.5273	1045.2962	3085.2151
H	-1.036101	-0.177676	-0.331663	232.2512	1066.1415	3103.6961
H	2.207856	0.294602	1.351476	266.7593	1149.5876	3166.1379
H	1.389349	-1.287332	2.133588	327.5539	1233.017	3170.9394
H	0.641612	0.276492	5.644196	385.3186	1241.3962	3182.994
H	-0.509817	0.268544	4.286153	487.0842	1256.3886	3808.686
H	0.540874	-1.136267	4.555076	586.7573	1314.7746	
O	0.880731	-0.934397	-0.571806	623.403	1360.5088	
H	0.73926	-1.780693	-0.130342	718.7401	1363.3612	
H	-0.601679	0.822739	1.891563	759.3709	1396.6746	
O	-0.575254	-1.183962	2.059599	866.5591	1441.4124	
O	0.411253	-2.164359	1.946433	890.7642	1467.9687	

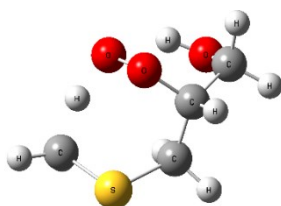




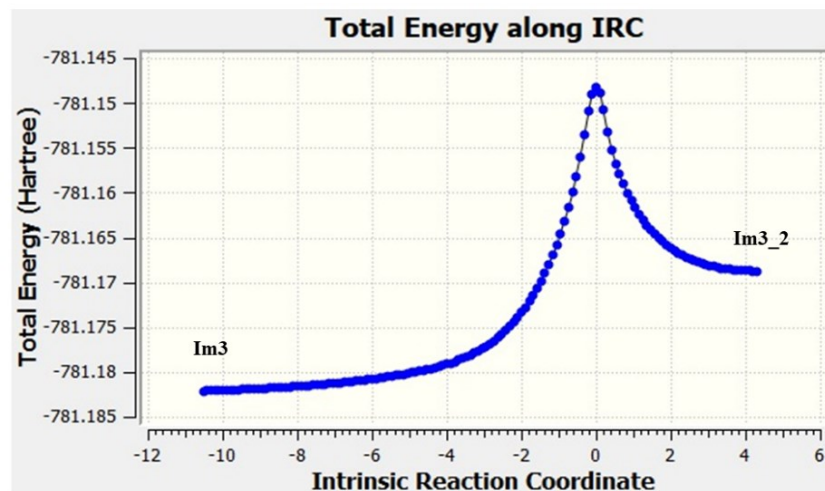
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-8.53907	-781.181713	-2.10757	-781.174057	4.31943	-781.170092
-8.43362	-781.181692	-2.00212	-781.173281	4.42487	-781.170122
-8.32816	-781.181671	-1.89666	-781.172426	4.53032	-781.170151
-8.22271	-781.181649	-1.79121	-781.171487	4.63576	-781.170179
-8.11726	-781.181627	-1.68576	-781.170463	4.74121	-781.170205
-8.01182	-781.181605	-1.58031	-781.169349	4.84666	-781.170229
-7.90637	-781.181583	-1.47487	-781.168141	4.95211	-781.170252
-7.80093	-781.18156	-1.36945	-781.166834	5.05756	-781.170274
-7.69549	-781.181537	-1.26404	-781.165419	5.16301	-781.170294
-7.59005	-781.181513	-1.15865	-781.16388	5.26846	-781.170314
-7.48461	-781.181489	-1.05328	-781.162198	5.37392	-781.170333
-7.37917	-781.181463	-0.94793	-781.160346	5.47937	-781.170351
-7.27374	-781.181436	-0.84258	-781.158293	5.58482	-781.170368
-7.1683	-781.181409	-0.73723	-781.156014	5.69026	-781.170385
-7.06286	-781.18138	-0.6319	-781.153481	5.79571	-781.170402
-6.95742	-781.181349	-0.52666	-781.15068	5.90115	-781.170419
-6.85198	-781.181317	-0.42148	-781.147567	6.00659	-781.170435
-6.74654	-781.181283	-0.3162	-781.144274	6.11204	-781.170452
-6.64109	-781.181247	-0.21082	-781.141183	6.21748	-781.170469
-6.53564	-781.18121	-0.10543	-781.138931	6.32292	-781.170487
-6.4302	-781.18117	0	-781.138069	6.42837	-781.170506
-6.32475	-781.181127	0.10537	-781.138861	6.53382	-781.170525
-6.2193	-781.181083	0.21079	-781.141207	6.63926	-781.170546
-6.11384	-781.181036	0.31623	-781.144693	6.74471	-781.170567
-6.00839	-781.180986	0.42163	-781.148636	6.85016	-781.17059
-5.90294	-781.180934	0.52683	-781.152201	6.95561	-781.170614
-5.79748	-781.180879	0.63116	-781.15478	7.06106	-781.17064

-5.69203	-781.180822	0.73591	-781.156733	7.16651	-781.170668
-5.58658	-781.180761	0.84111	-781.158328	7.27197	-781.170697
-5.48112	-781.180697	0.94643	-781.159722	7.37742	-781.170728
-5.37567	-781.180631	1.05183	-781.160962	7.48287	-781.170761
-5.27021	-781.180561	1.15725	-781.162074	7.58833	-781.170796
-5.16476	-781.180488	1.26269	-781.163072	7.69378	-781.170833
-5.05931	-781.180412	1.36813	-781.163965	7.79923	-781.170871
-4.95386	-781.180332	1.47357	-781.164761	7.90468	-781.170911
-4.8484	-781.180249	1.57901	-781.165469	8.01014	-781.170952
-4.74295	-781.180162	1.68446	-781.166094	8.11559	-781.170996
-4.6375	-781.180072	1.7899	-781.166644	8.22104	-781.17104
-4.53205	-781.179978	1.89533	-781.167125	8.3265	-781.171086
-4.4266	-781.179881	2.00077	-781.167544	8.43195	-781.171133
-4.32115	-781.179779	2.10619	-781.167906	8.5374	-781.171181
-4.21571	-781.179674	2.21161	-781.168217	8.64285	-781.17123
-4.11026	-781.179564	2.31702	-781.168482	8.7483	-781.171279
-4.00482	-781.17945	2.42241	-781.168707	8.85376	-781.171329
-3.89938	-781.179331	2.52778	-781.168897	8.95921	-781.171379
-3.79395	-781.179207	2.63313	-781.169057	9.06466	-781.17143
-3.68853	-781.179076	2.73846	-781.169192	9.17011	-781.17148
-3.58311	-781.17894	2.84379	-781.169307	9.27556	-781.171531
-3.47772	-781.178794	2.94912	-781.169406	9.38101	-781.171581
-3.37235	-781.178639	3.05446	-781.169493	9.48646	-781.171631
-3.267	-781.178469	3.15982	-781.16957	9.59191	-781.171681
-3.16166	-781.178282	3.2652	-781.169639	9.69736	-781.171731
-3.05632	-781.178071	3.37059	-781.169702	9.80281	-781.17178
-2.95097	-781.177829	3.47599	-781.169759	9.90826	-781.171829
-2.84559	-781.17755	3.5814	-781.169811	10.01371	-781.171877
-2.74019	-781.177228	3.68681	-781.16986	10.11916	-781.171924
-2.63478	-781.176854	3.79224	-781.169905	10.22461	-781.171971
-2.52935	-781.176426	3.89767	-781.169947	10.33006	-781.172017
-2.42391	-781.175936	4.00311	-781.169987	10.43551	-781.172061
-2.31847	-781.17538	4.10855	-781.170024	10.54096	-781.172105
-2.21302	-781.174755	4.21399	-781.170059		

TS2-5-A1\_Im3-->A1\_Im3\_2



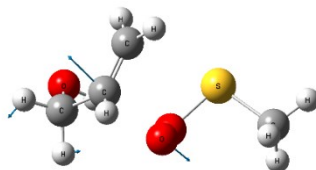
Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-781.516276	-781.384996	-781.375681	-781.418703
M06-2X/DG3/aug-cc-pVTZ				-781.523087	-781.391968	-781.382628	-781.425718
MN15/cc-pVTZ				-781.148226	-781.017697	-781.008333	-781.051384
MN15/aug-cc-pVTZ				-781.159251	-781.029004	-781.019611	-781.062742
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	0.008203	-0.007148	-0.002357	<b>1962.5448i</b>	900.4099	1471.1991	
C	0.000247	-0.001669	1.520688	80.2542	958.1124	1482.5334	
C	1.404218	0.022147	2.118518	145.806	983.8615	1499.9185	
S	1.37682	-0.528139	3.852493	208.465	1020.9474	3044.6487	
C	1.512341	-2.243319	3.559974	252.6789	1036.9844	3091.0726	
H	0.391888	0.95132	-0.356195	270.6608	1089.0321	3098.4938	
H	-1.026962	-0.105124	-0.343966	306.8339	1120.0456	3101.7422	
H	1.802409	1.034352	2.092258	329.5542	1156.433	3104.6843	
H	2.080596	-0.624975	1.563807	406.5752	1207.1804	3158.5605	
H	1.346712	-2.826248	4.459057	479.9257	1250.0323	3207.6168	
H	0.573761	-2.466451	2.679477	495.401	1263.9934	3821.5239	
H	2.39901	-2.535369	3.00116	538.2169	1279.5704		
O	0.831475	-1.004402	-0.560498	605.2852	1342.9331		
H	0.570473	-1.843998	-0.16502	690.5492	1376.4059		
H	-0.561586	0.868371	1.866337	768.8201	1402.1114		
O	-0.78158	-1.081073	2.048252	811.7664	1424.758		
O	-0.207923	-2.294858	1.727247	826.5948	1442.3449		



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-10.51783	-781.182129	-5.46809	-781.180472	-0.42011	-781.156063
-10.41262	-781.182113	-5.36289	-781.180402	-0.31538	-781.153592
-10.30742	-781.182096	-5.2577	-781.18033	-0.2103	-781.150987
-10.20221	-781.182079	-5.1525	-781.180255	-0.10515	-781.148982
-10.097	-781.182061	-5.0473	-781.180177	0	-781.148213
-9.9918	-781.182043	-4.94211	-781.180096	0.10507	-781.148904
-9.88659	-781.182025	-4.83692	-781.180012	0.21022	-781.150806
-9.78139	-781.182006	-4.73173	-781.179924	0.31531	-781.153254
-9.67619	-781.181987	-4.62654	-781.179831	0.41952	-781.155306
-9.57098	-781.181968	-4.52135	-781.179734	0.52309	-781.156784
-9.46578	-781.181948	-4.41616	-781.179631	0.62811	-781.157986
-9.36058	-781.181928	-4.31098	-781.179523	0.73325	-781.159063
-9.25537	-781.181907	-4.20579	-781.179407	0.8384	-781.160026
-9.15017	-781.181887	-4.1006	-781.179284	0.94355	-781.160891
-9.04497	-781.181865	-3.99541	-781.179152	1.04872	-781.161672
-8.93977	-781.181843	-3.89022	-781.179011	1.15388	-781.162379
-8.83456	-781.181821	-3.78503	-781.178859	1.25906	-781.163021
-8.72936	-781.181797	-3.67984	-781.178696	1.36424	-781.163605
-8.62416	-781.181773	-3.57465	-781.178521	1.46943	-781.164137
-8.51896	-781.181748	-3.46945	-781.178332	1.57461	-781.164622
-8.41376	-781.181723	-3.36426	-781.178129	1.6798	-781.165063
-8.30856	-781.181696	-3.25907	-781.17791	1.78499	-781.165465
-8.20335	-781.181668	-3.15387	-781.177673	1.89018	-781.16583
-8.09815	-781.18164	-3.04868	-781.177418	1.99537	-781.166163
-7.99295	-781.18161	-2.94349	-781.177142	2.10056	-781.166464
-7.88775	-781.181579	-2.83829	-781.176844	2.20575	-781.166738

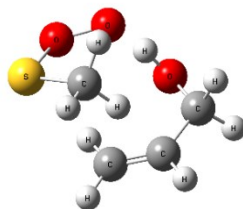
-7.78255	-781.181547	-2.7331	-781.176522	2.31094	-781.166987
-7.67735	-781.181514	-2.6279	-781.176174	2.41614	-781.167212
-7.57215	-781.18148	-2.52271	-781.175797	2.52133	-781.167415
-7.46694	-781.181444	-2.41751	-781.17539	2.62652	-781.167599
-7.36174	-781.181408	-2.31231	-781.17495	2.73172	-781.167764
-7.25654	-781.181369	-2.20712	-781.174473	2.83691	-781.167912
-7.15134	-781.18133	-2.10192	-781.173957	2.94211	-781.168045
-7.04614	-781.181289	-1.99672	-781.173399	3.04731	-781.168162
-6.94094	-781.181246	-1.89152	-781.172796	3.1525	-781.168266
-6.83573	-781.181202	-1.78632	-781.172145	3.25769	-781.168356
-6.73053	-781.181157	-1.68113	-781.171441	3.36287	-781.168434
-6.62533	-781.18111	-1.57594	-781.17068	3.46805	-781.168501
-6.52013	-781.181061	-1.47075	-781.169858	3.5732	-781.168557
-6.41492	-781.18101	-1.36557	-781.168969	3.67833	-781.168604
-6.30972	-781.180958	-1.2604	-781.168005	3.78342	-781.168643
-6.20451	-781.180904	-1.15524	-781.166958	3.88847	-781.168675
-6.09931	-781.180848	-1.05009	-781.165815	3.99349	-781.168701
-5.99411	-781.18079	-0.94495	-781.164564	4.09852	-781.168722
-5.8889	-781.180731	-0.83982	-781.163189	4.20358	-781.16874
-5.7837	-781.180669	-0.73469	-781.161676	4.30869	-781.168755
-5.6785	-781.180606	-0.62958	-781.160009		
-5.5733	-781.18054	-0.52462	-781.158176		

TS2-6\_A1\_Im1\_1-->Pw3

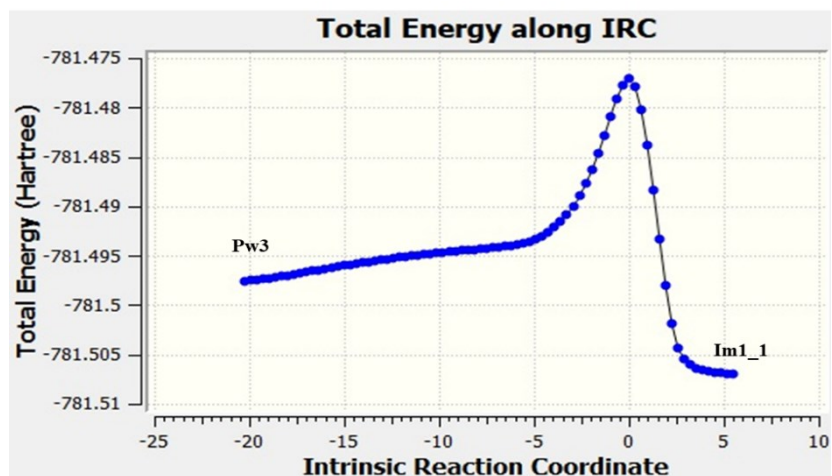


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-781.477072	-781.346077	-781.334816	-781.383596		
M06-2X/DG3/aug-cc-pVTZ	-781.48432	-781.353493	-781.342181	-781.391168		
MN15/cc-pVTZ	-781.11047	-780.980052	-780.968773	-781.017409		
MN15/aug-cc-pVTZ	-781.121754	-780.991668	-780.980311	-781.029425		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.022736	-0.026186	-0.029852	<b>583.6835i</b>	867.7162	1499.7326
C	0.00986	0.075918	1.472418	36.2445	896.414	1562.121
C	1.15759	0.088006	2.209735	44.308	916.212	3056.722
S	1.269505	-3.23546	2.46688	89.9236	971.1372	3075.2498
C	0.177778	-4.139515	3.568689	130.6137	974.691	3095.7816
H	0.031651	0.982723	-0.447527	151.9779	977.6513	3163.4586
H	-0.898192	-0.513203	-0.359412	173.752	1027.9137	3177.8984
H	1.137068	0.301017	3.267802	227.2767	1069.6829	3178.969
H	2.102966	-0.174066	1.756647	291.1815	1155.6293	3182.0535
H	0.814916	-4.53979	4.356453	313.7307	1222.9832	3279.649
H	-0.550533	-3.459427	4.001146	404.2746	1270.8245	3845.6679
H	-0.308865	-4.954304	3.039632	452.2028	1336.0798	
O	1.162037	-0.682562	-0.532642	462.9273	1395.5289	
H	1.099003	-1.606543	-0.269957	552.1839	1417.7906	
H	-0.895145	0.487297	1.90437	636.5536	1433.2366	
O	-0.697087	-1.727181	1.9036	719.2531	1452.5659	
O	0.14166	-2.673685	1.366051	751.1208	1485.322	

Pw3



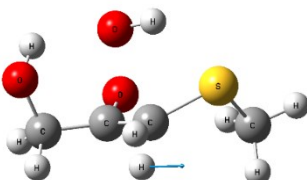
Pw3						
Method			Ee	E+ZPE	ΔH	ΔG
M06-2X/GD3/cc-pVTZ			-781.499224	-781.367701	-781.355272	-781.407321
M06-2X/DG3/aug-cc-pVTZ			-781.506303	-781.37501	-781.362524	-781.41479
MN15/cc-pVTZ			-781.130358	-780.999664	-780.987143	-781.039723
MN15/aug-cc-pVTZ			-781.141397	-781.010934	-780.998419	-781.05073
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.253223	-0.056374	0.232513	29.6964	901.3761	1489.7426
C	0.157309	0.109076	1.667137	56.8095	969.0786	1734.0753
C	1.398783	0.015031	2.116988	71.355	975.6899	3012.3953
S	2.061056	-3.364062	2.851688	83.1356	979.4153	3071.6426
C	0.305129	-3.364968	3.157638	95.1824	998.5423	3077.3397
H	-0.720005	0.869765	-0.11114	123.5003	1027.1664	3149.4758
H	-1.024772	-0.834233	0.171475	149.6277	1050.571	3161.3297
H	1.631043	0.151732	3.16428	214.258	1166.5402	3169.6585
H	2.220047	-0.187873	1.441518	226.4867	1233.18	3183.1115
H	0.227896	-3.526364	4.233283	287.1318	1243.1986	3252.9859
H	-0.118042	-2.400578	2.888249	290.673	1316.2399	3823.2093
H	-0.183574	-4.173811	2.623138	455.0763	1339.7523	
O	0.807535	-0.327088	-0.647638	475.7759	1398.993	
H	1.074739	-1.243858	-0.518296	582.4673	1417.2975	
H	-0.654642	0.328445	2.355521	620.4208	1441.4402	
O	0.930214	-2.974366	0.580828	633.264	1443.0799	
O	2.077768	-3.058455	1.161271	735.4316	1474.2028	



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-20.25539	-781.497563	-11.43252	-781.495015	-2.61405	-781.488947
-19.93013	-781.497514	-11.10566	-781.49494	-2.28722	-781.48773
-19.60406	-781.497453	-10.77885	-781.494867	-1.96039	-781.486304
-19.27741	-781.497381	-10.45205	-781.494798	-1.63361	-781.484664
-18.95064	-781.497299	-10.12526	-781.494732	-1.30681	-781.482843
-18.62381	-781.497208	-9.79845	-781.494668	-0.9801	-781.480944
-18.29696	-781.497107	-9.47166	-781.494607	-0.65332	-781.479132
-17.97009	-781.496999	-9.14485	-781.494547	-0.32677	-781.477687
-17.64319	-781.496887	-8.81807	-781.494488	<b>0</b>	<b>-781.4771</b>
-17.31631	-781.496778	-8.49136	-781.494429	0.3269	-781.477836
-16.98944	-781.496666	-8.16469	-781.49437	0.65371	-781.48017
-16.66256	-781.496553	-7.83805	-781.494313	0.98056	-781.483831
-16.33566	-781.496438	-7.51147	-781.494256	1.30739	-781.488363
-16.00879	-781.496326	-7.18513	-781.494198	1.63424	-781.493261
-15.68189	-781.496216	-6.85914	-781.494137	1.96105	-781.497956
-15.35501	-781.496109	-6.5334	-781.494067	2.28765	-781.501853
-15.02811	-781.496005	-6.20761	-781.493982	2.61259	-781.504369
-14.70123	-781.495905	-5.88154	-781.493875	2.92535	-781.505489
-14.37435	-781.495805	-5.55534	-781.493735	3.24648	-781.50605
-14.04748	-781.495705	-5.22874	-781.493548	3.56969	-781.506379
-13.72058	-781.495607	-4.90194	-781.493301	3.89116	-781.506567
-13.39371	-781.495512	-4.57507	-781.492989	4.21235	-781.506683
-13.06683	-781.495421	-4.24824	-781.492608	4.53847	-781.506773
-12.73997	-781.495334	-3.92142	-781.492132	4.86509	-781.50685
-12.41308	-781.49525	-3.59459	-781.491541	5.19171	-781.506912
-12.08622	-781.495171	-3.26773	-781.490822	5.51844	-781.506964
-11.75936	-781.495092	-2.94089	-781.489968		

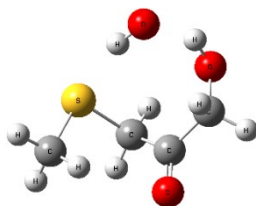


TS2-7\_A1\_Im3\_1-->Pw4

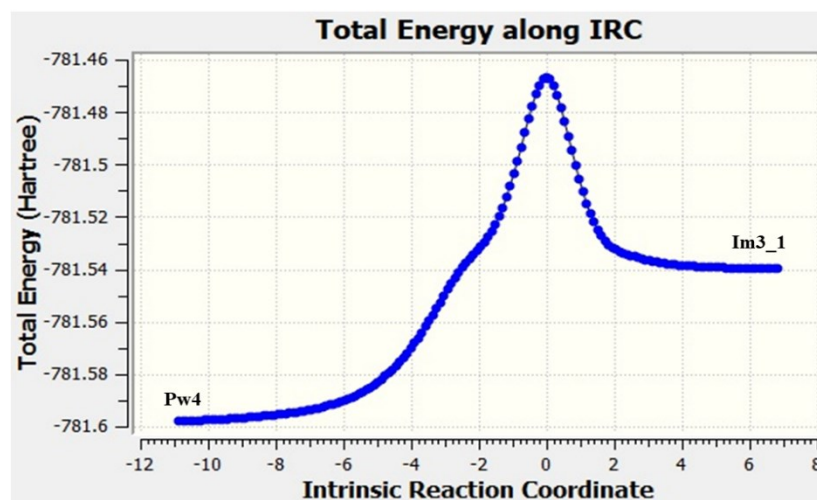


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-781.466816	-781.33799	-781.326788	-781.374381		
M06-2X/DG3/aug-cc-pVTZ	-781.474851	-781.346386	-781.335084	-781.382919		
MN15/cc-pVTZ	-781.129275	-781.000337	-780.989413	-781.035983		
MN15/aug-cc-pVTZ	-781.142652	-781.013861	-781.002879	-781.049624		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.004865	0.021517	0.018904	<b>1825.5109i</b>	737.7184	1494.047
C	0.014044	-0.044638	1.516271	64.4641	793.0784	1498.6507
C	1.305785	-0.005615	2.234786	76.7267	898.1233	2155.7315
S	1.534735	-0.705518	3.828844	108.6614	974.6206	3062.86
C	0.365457	0.258684	4.835076	144.0612	985.023	3078.0687
H	0.658298	0.818456	-0.335534	172.2921	994.8919	3119.7444
H	-1.014519	0.229619	-0.314608	189.2112	1070.2244	3168.5657
H	2.18945	0.207318	1.650266	219.3323	1131.8639	3182.1051
H	-0.196706	-2.247475	2.817399	283.9397	1194.3586	3217.6975
H	0.470774	-0.10764	5.853305	329.171	1235.3769	3704.0026
H	0.636204	1.311533	4.798434	371.1873	1312.3862	3830.8522
H	-0.65376	0.107283	4.492679	436.6236	1318.0274	
H	0.04643	-1.916159	-0.102451	472.9087	1336.1927	
O	0.494474	-1.184119	-0.541273	481.0478	1351.5259	
H	0.442542	0.996608	2.155007	568.9352	1379.6876	
O	-1.026563	-0.646296	2.125264	634.514	1432.9079	
O	-0.797175	-2.133512	2.061219	709.0842	1469.1625	

Pw4



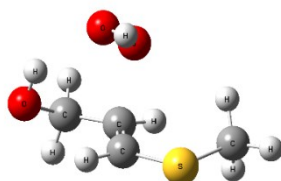
Pw4						
Method		Ee	E+ZPE	ΔH	ΔG	
M06-2X/GD3/cc-pVTZ		-781.601363	-781.469846	-781.457576	-781.508422	
M06-2X/DG3/aug-cc-pVTZ		-781.609065	-781.47792	-781.465521	-781.516841	
MN15/cc-pVTZ		-781.229018	-781.098298	-781.085907	-781.137063	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.078027	-0.222841	0.32311	29.2368	743.6938	1486.2205
C	0.257801	0.63403	1.536976	59.1243	800.521	1830.921
C	1.601698	0.452807	2.194261	78.983	897.5435	3044.7812
S	1.50416	-0.994425	3.295314	112.5396	965.7649	3079.7345
C	0.318425	-0.377066	4.514466	134.3286	987.8136	3096.4961
H	-0.45237	0.460901	-0.441623	167.6854	1015.2324	3110.9158
H	-0.914898	-0.87046	0.60417	182.8409	1132.0144	3168.8656
H	2.378198	0.224171	1.47014	194.4606	1148.3761	3176.7072
H	0.386593	-2.669331	2.05957	265.7798	1208.5403	3184.7875
H	0.154167	-1.184719	5.223158	281.0901	1247.562	3515.9782
H	0.737522	0.482204	5.032239	312.5118	1287.7522	3817.0467
H	-0.621197	-0.101343	4.043054	375.357	1360.4974	
H	0.879642	-1.879951	0.035403	487.2184	1363.8874	
O	1.011241	-0.949877	-0.180689	520.9922	1397.7504	
H	1.849355	1.332433	2.783115	557.0076	1444.6536	
O	-0.561111	1.39996	1.981447	649.4068	1469.2042	
O	-0.050726	-3.165592	1.330461	703.7178	1470.5735	



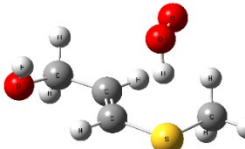
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-10.86302	-781.598052	-4.88741	-781.582013	1.08648	-781.510478
-10.75437	-781.597998	-4.77875	-781.580845	1.19512	-781.514866
-10.64572	-781.597941	-4.6701	-781.579593	1.30376	-781.518757
-10.53707	-781.597881	-4.56145	-781.578254	1.41238	-781.522132
-10.42841	-781.597819	-4.45279	-781.576823	1.52099	-781.524986
-10.31976	-781.597754	-4.34414	-781.575299	1.62957	-781.527338
-10.21111	-781.597686	-4.23549	-781.573678	1.73809	-781.529216
-10.10246	-781.597616	-4.12683	-781.571962	1.84653	-781.530667
-9.99381	-781.597543	-4.01818	-781.570149	1.95481	-781.53176
-9.88516	-781.597468	-3.90953	-781.568242	2.06291	-781.532583
-9.77651	-781.597389	-3.80087	-781.566241	2.17101	-781.533323
-9.66786	-781.597308	-3.69222	-781.56415	2.2793	-781.533779
-9.55921	-781.597223	-3.58357	-781.561973	2.38778	-781.534273
-9.45056	-781.597135	-3.47492	-781.559719	2.49636	-781.534733
-9.34192	-781.597043	-3.36627	-781.557398	2.60497	-781.535165
-9.23327	-781.596948	-3.25762	-781.555025	2.7136	-781.535571
-9.12463	-781.596848	-3.14898	-781.552616	2.82223	-781.535951
-9.01598	-781.596744	-3.04033	-781.550193	2.93087	-781.536307
-8.90734	-781.596635	-2.93169	-781.547786	3.0395	-781.536637
-8.79869	-781.596521	-2.82305	-781.545431	3.14814	-781.536945
-8.69005	-781.596403	-2.71441	-781.543173	3.25677	-781.537227
-8.5814	-781.59628	-2.60578	-781.541054	3.36539	-781.537486
-8.47276	-781.596151	-2.49718	-781.53911	3.47401	-781.537721
-8.36411	-781.596018	-2.38863	-781.537355	3.58263	-781.537933
-8.25546	-781.595879	-2.28016	-781.535772	3.69124	-781.538123
-8.14682	-781.595734	-2.17178	-781.534298	3.79984	-781.538293

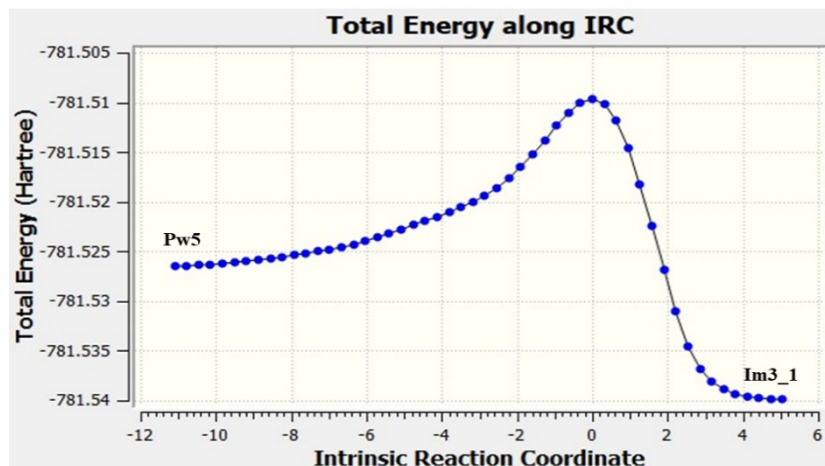
-8.03818	-781.595583	-2.06341	-781.532844	3.90842	-781.538443
-7.92953	-781.595425	-1.955	-781.531306	4.01699	-781.538576
-7.82089	-781.59526	-1.84652	-781.529598	4.12555	-781.538694
-7.71225	-781.595087	-1.738	-781.527649	4.2341	-781.538798
-7.6036	-781.594905	-1.62946	-781.525404	4.34265	-781.538892
-7.49496	-781.594712	-1.52089	-781.522813	4.45122	-781.538977
-7.38632	-781.594507	-1.4123	-781.519835	4.5598	-781.539054
-7.27768	-781.594288	-1.30369	-781.516439	4.6684	-781.539126
-7.16904	-781.594055	-1.19507	-781.512615	4.77701	-781.539192
-7.0604	-781.593804	-1.08644	-781.508362	4.88563	-781.539255
-6.95176	-781.593536	-0.9778	-781.503707	4.99426	-781.539313
-6.84311	-781.593248	-0.86916	-781.498702	5.10289	-781.539368
-6.73447	-781.592939	-0.76051	-781.493429	5.21153	-781.53942
-6.62582	-781.592607	-0.65187	-781.488018	5.32017	-781.53947
-6.51717	-781.592252	-0.54322	-781.482655	5.42882	-781.539516
-6.40853	-781.59187	-0.43458	-781.477593	5.53747	-781.53956
-6.29988	-781.591459	-0.32593	-781.473163	5.64612	-781.539602
-6.19123	-781.591016	-0.21729	-781.469721	5.75477	-781.539642
-6.08258	-781.590538	-0.10866	-781.467556	5.86342	-781.539679
-5.97393	-781.590023	<b>0</b>	<b>-781.4668</b>	5.97207	-781.539713
-5.86528	-781.589466	0.10867	-781.467574	6.08073	-781.539745
-5.75663	-781.588865	0.2173	-781.469843	6.18938	-781.539775
-5.64798	-781.588214	0.32594	-781.47349	6.29804	-781.539802
-5.53933	-781.587513	0.43458	-781.478186	6.40669	-781.539827
-5.43067	-781.586757	0.54323	-781.483531	6.51534	-781.53985
-5.32202	-781.585942	0.65188	-781.489178	6.624	-781.53987
-5.21337	-781.585063	0.76053	-781.494865	6.73265	-781.539888
-5.10471	-781.584117	0.86918	-781.500394	6.8413	-781.539904
-4.99606	-781.583102	0.97783	-781.505632		

TS2-8\_A1\_Im3\_1-->Pw5



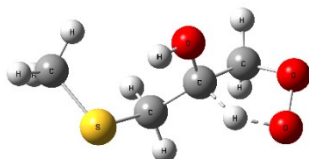
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-781.50962	-781.376534	-781.365453	-781.413079		
M06-2X/DG3/aug-cc-pVTZ	-781.517062	-781.384213	-781.373057	-781.420977		
MN15/cc-pVTZ	-781.143219	-781.010838	-780.999755	-781.047143		
MN15/aug-cc-pVTZ	-781.154927	-781.022889	-781.011731	-781.059349		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.005016	0.013342	0.028799	<b>485.0489i</b>	867.6214	1504.4489
C	0.012792	-0.050533	1.534197	41.5289	927.2461	1560.7002
C	1.195521	-0.032286	2.212832	85.7821	959.6841	3053.9731
S	1.420516	-0.083849	3.915921	121.0534	973.5407	3076.6827
C	-0.272655	-0.020461	4.531356	136.0715	996.0002	3091.293
H	0.067131	1.050737	-0.304348	172.0405	1004.1397	3164.1416
H	-0.960423	-0.385993	-0.320073	235.3649	1062.0843	3180.7653
H	2.123255	-0.12464	1.66173	249.182	1143.2914	3196.4495
H	0.942833	-3.00388	2.246432	256.0569	1229.0206	3207.4265
H	-0.211931	-0.122292	5.611162	286.5473	1256.5394	3776.4374
H	-0.73174	0.933941	4.283403	352.1158	1285.4126	3812.6107
H	-0.846712	-0.842331	4.109451	421.9236	1350.4542	
H	1.043289	-1.585809	-0.235504	435.8903	1390.9577	
O	1.080291	-0.673391	-0.547424	497.0689	1401.3953	
H	-0.910986	0.201547	2.037658	622.2289	1433.2245	
O	-0.537813	-1.990397	1.730435	733.0114	1473.1261	
O	0.50355	-2.828703	1.40321	796.3483	1493.0393	

Pw5						
						
Method			Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ			-781.527521	-781.395027	-781.382506	-781.434743
M06-2X/DG3/aug-cc-pVTZ			-781.534965	-781.402774	-781.390177	-781.442781
MN15/cc-pVTZ			-781.159256	-781.027396	-781.014821	-781.067012
MN15/aug-cc-pVTZ			-781.17071	-781.039141	-781.026532	-781.078903
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.002142	0.137303	-0.049444	27.2712	853.1507	1517.5112
C	0.010139	0.127418	1.453247	46.6093	957.2895	1715.5267
C	1.11342	-0.026679	2.170997	60.104	980.9165	3033.2117
S	1.2584	-0.081431	3.920615	102.9852	986.9346	3076.5158
C	-0.441028	0.208062	4.448975	114.7845	995.7356	3086.0793
H	-0.234551	1.140262	-0.41003	171.6724	1002.9893	3166.501
H	-0.797317	-0.521928	-0.404267	193.0902	1149.3868	3179.1762
H	2.073895	-0.133374	1.68137	199.1465	1212.2267	3195.495
H	1.119573	-2.344863	3.711359	231.5422	1250.9031	3197.0134
H	-0.432162	0.184665	5.535301	237.6716	1274.3525	3395.7424
H	-0.77091	1.187418	4.108902	267.6672	1321.9643	3865.4584
H	-1.091345	-0.575889	4.06921	349.42	1349.465	
H	1.419104	-1.130861	-0.443324	406.9949	1384.6135	
O	1.237792	-0.206353	-0.63331	486.5364	1410.8334	
H	-0.957275	0.243792	1.926832	596.2564	1471.8248	
O	-0.530262	-2.905578	3.161868	733.4309	1492.043	
O	0.720274	-3.194785	3.408395	773.6455	1503.3247	



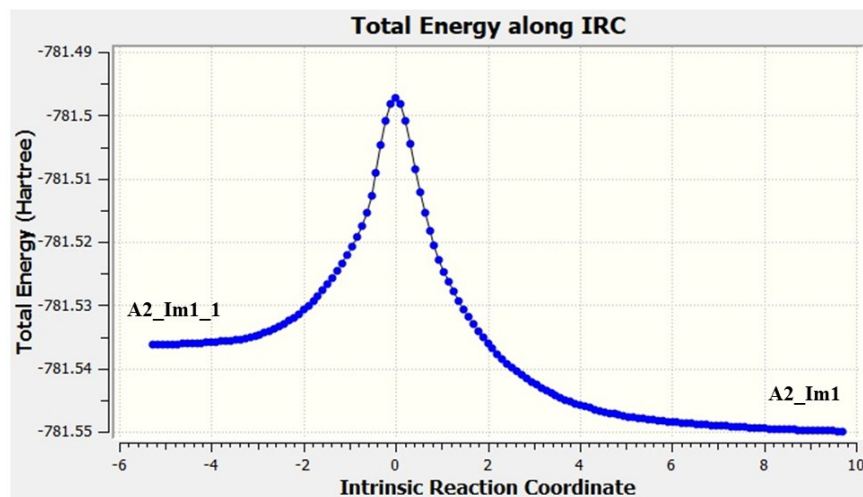
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-11.09248	-781.526468	-5.39292	-781.523181	0.31751	-781.510133
-10.77569	-781.526425	-5.07597	-781.52278	0.63492	-781.511787
-10.45872	-781.526371	-4.75909	-781.522362	0.95239	-781.514563
-10.14139	-781.526303	-4.44185	-781.521961	1.26983	-781.51822
-9.82401	-781.526221	-4.1249	-781.521544	1.5873	-781.522444
-9.50657	-781.526123	-3.8077	-781.521097	1.90475	-781.526859
-9.18921	-781.526011	-3.49061	-781.520603	2.22215	-781.531044
-8.87195	-781.525883	-3.17339	-781.520031	2.5393	-781.534519
-8.55476	-781.525741	-2.85616	-781.519369	2.85466	-781.536884
-8.23819	-781.525581	-2.5389	-781.518584	3.16501	-781.538168
-7.92143	-781.525403	-2.2216	-781.51764	3.4796	-781.538917
-7.60711	-781.52521	-1.90424	-781.516517	3.7937	-781.539353
-7.29121	-781.525001	-1.58689	-781.515225	4.10553	-781.539602
-6.97557	-781.524792	-1.2695	-781.513792	4.41889	-781.53974
-6.65955	-781.524551	-0.95217	-781.512344	4.73187	-781.539825
-6.34312	-781.524274	-0.63475	-781.51102	5.0466	-781.539879
-6.02624	-781.523951	-0.31743	-781.510025		
-5.70977	-781.523586	<b>0</b>	<b>-781.5096</b>		

TS3-1\_A2\_Im1--> A2\_Im1\_1



Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.49733	-781.366957	-781.356747	-781.402738	
M06-2X/DG3/aug-cc-pVTZ		-781.504795	-781.3746	-781.364338	-781.410627	
MN15/cc-pVTZ		-781.131803	-781.002209	-780.991965	-781.037964	
MN15/aug-cc-pVTZ		-781.143373	-781.013987	-781.003707	-781.049885	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.054868	0.012425	-0.039009	<b>2098.2061i</b>	930.1748	1484.7381
C	-0.080291	0.024436	1.49051	46.1693	973.0946	1491.5586
C	1.261742	0.021051	2.192241	66.9123	981.8075	1747.3744
S	1.128264	-0.123159	3.998699	112.0052	999.533	3049.9575
C	1.429134	-1.901219	4.187809	162.9038	1031.1448	3054.871
H	0.922149	0.361099	-0.385509	205.5078	1071.4598	3074.8089
H	-0.299179	-0.961271	-0.461503	252.3785	1082.3164	3130.3308
H	-0.537713	1.2489	1.432372	285.5738	1195.2936	3140.4124
H	1.793821	0.941617	1.958227	343.129	1219.5589	3159.3377
H	1.873322	-0.814032	1.839344	368.6776	1254.1437	3172.6105
H	1.304108	-2.130793	5.242973	459.2721	1272.4682	3721.9887
H	0.718628	-2.484319	3.606531	577.0718	1328.4055	
H	2.445597	-2.144253	3.88755	594.9581	1355.8126	
O	-1.011699	-0.843913	1.983344	700.9629	1368.4361	
H	-0.963698	-0.813419	2.951297	725.5006	1392.1674	
O	-1.068302	0.917396	-0.416311	777.7182	1455.1203	
O	-0.851289	2.005131	0.423801	856.2422	1475.1822	

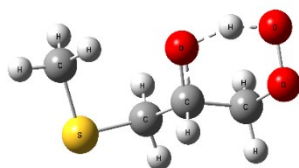




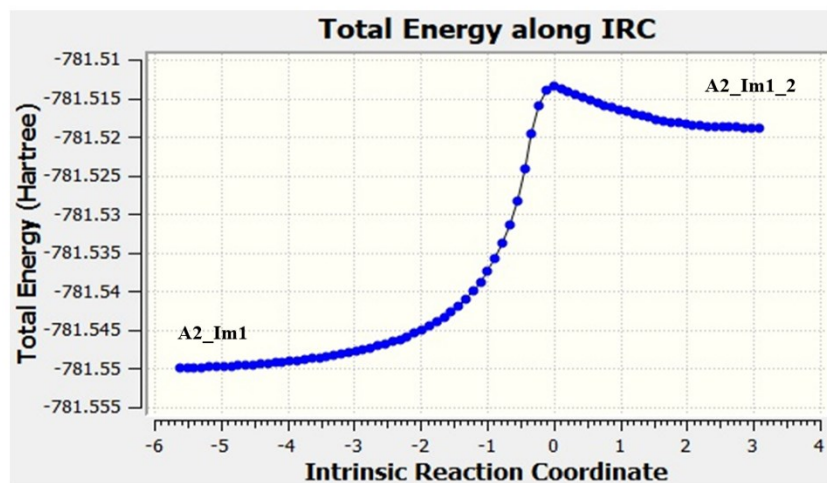
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-5.2676	-781.536286	-0.21088	-781.500934	4.8484	-781.547366
-5.16229	-781.536271	-0.10546	-781.498269	4.95384	-781.547507
-5.05694	-781.536251	<b>0</b>	<b>-781.4973</b>	5.05927	-781.547637
-4.95154	-781.536228	0.10545	-781.498246	5.1647	-781.547758
-4.84613	-781.536201	0.21085	-781.500817	5.27012	-781.547871
-4.74071	-781.53617	0.31623	-781.504512	5.37555	-781.547976
-4.63528	-781.536135	0.42154	-781.508507	5.48097	-781.548074
-4.52984	-781.536097	0.52669	-781.512208	5.58639	-781.548166
-4.42441	-781.536056	0.63183	-781.515414	5.69181	-781.548252
-4.31898	-781.536012	0.7371	-781.518214	5.79722	-781.548333
-4.21355	-781.535965	0.84241	-781.520662	5.90264	-781.54841
-4.10815	-781.535917	0.94771	-781.522808	6.00806	-781.548483
-4.00279	-781.535866	1.05302	-781.524701	6.11348	-781.548553
-3.89749	-781.535812	1.15833	-781.526392	6.2189	-781.54862
-3.79226	-781.535754	1.26368	-781.527926	6.32433	-781.548685
-3.68709	-781.535688	1.36906	-781.529337	6.42976	-781.548748
-3.5819	-781.53561	1.47447	-781.530647	6.53519	-781.548808
-3.47663	-781.535516	1.57989	-781.531871	6.64063	-781.548867
-3.3713	-781.535402	1.68532	-781.533015	6.74606	-781.548924
-3.26593	-781.535264	1.79076	-781.534086	6.8515	-781.54898
-3.16053	-781.535097	1.89619	-781.535089	6.95694	-781.549034
-3.05512	-781.534901	2.00163	-781.536027	7.06238	-781.549086
-2.9497	-781.53467	2.10707	-781.536904	7.16782	-781.549137
-2.84427	-781.534404	2.2125	-781.537725	7.27326	-781.549186
-2.73884	-781.534101	2.31794	-781.538491	7.3787	-781.549234
-2.63341	-781.53376	2.42337	-781.539208	7.48415	-781.549281
-2.52797	-781.533374	2.5288	-781.539878	7.58959	-781.549326

-2.42254	-781.532947	2.63424	-781.540503	7.69503	-781.54937
-2.3171	-781.532471	2.73967	-781.541088	7.80048	-781.549412
-2.21167	-781.531949	2.8451	-781.541636	7.90592	-781.549453
-2.10622	-781.531374	2.95054	-781.542149	8.01137	-781.549492
-2.00079	-781.530747	3.05597	-781.542629	8.11681	-781.54953
-1.89535	-781.530063	3.16141	-781.54308	8.22226	-781.549566
-1.78991	-781.529322	3.26684	-781.543502	8.3277	-781.549601
-1.68447	-781.52852	3.37228	-781.543898	8.43315	-781.549635
-1.57903	-781.527652	3.47771	-781.544268	8.53859	-781.549667
-1.47358	-781.526711	3.58315	-781.544614	8.64404	-781.549698
-1.36815	-781.525693	3.68859	-781.544938	8.74948	-781.549727
-1.26271	-781.524593	3.79403	-781.545242	8.85493	-781.549755
-1.15728	-781.523404	3.89946	-781.545526	8.96037	-781.549782
-1.05187	-781.522115	4.0049	-781.545792	9.06582	-781.549807
-0.94648	-781.520713	4.11034	-781.54604	9.17126	-781.549831
-0.84115	-781.519176	4.21578	-781.546272	9.27671	-781.549853
-0.73593	-781.517464	4.32122	-781.546488	9.38215	-781.549874
-0.6312	-781.515429	4.42666	-781.54669	9.4876	-781.549894
-0.52691	-781.512769	4.53209	-781.546878	9.59305	-781.549912
-0.42172	-781.509041	4.63753	-781.547053	9.6985	-781.549928
-0.31631	-781.504799	4.74297	-781.547215		

TS3-2\_A2\_Im1--> A2\_Im1\_2

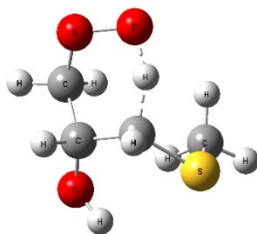


Method							Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ							-781.513527	-781.383692	-781.373856	-781.418871
M06-2X/DG3/aug-cc-pVTZ							-781.520387	-781.390684	-781.38084	-781.425862
MN15/cc-pVTZ							-781.146454	-781.017531	-781.007586	-781.052862
MN15/aug-cc-pVTZ							-781.157379	-781.02868	-781.018728	-781.064023
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )						
C	0.006893	0.003338	-0.000584	<b>1304.3605i</b>	915.8753	1475.4207				
C	-0.010996	-0.002387	1.612123	63.8718	942.4198	1479.6057				
C	1.472327	-0.008163	2.028975	92.2673	977.449	1832.3439				
S	1.697039	0.432725	3.75772	115.234	997.3366	3016.8922				
C	0.941754	-1.004439	4.544962	182.1355	1028.9733	3068.6605				
H	0.352131	0.971417	-0.355114	227.8081	1066.0606	3072.4773				
H	0.638841	-0.826104	-0.320604	239.0816	1160.8862	3077.5091				
H	-0.498484	0.93338	1.91501	314.0897	1178.3361	3135.2686				
H	2.027885	0.736773	1.459035	386.2451	1211.5116	3153.3739				
H	1.885363	-0.997087	1.828784	472.1253	1246.3411	3171.483				
H	1.031749	-0.855824	5.618105	508.4979	1278.7869	3174.07				
H	-0.107314	-1.082163	4.265826	573.5548	1301.2057					
H	1.464373	-1.913778	4.25682	711.8299	1322.8771					
O	-0.677504	-1.098802	2.003012	726.518	1359.1506					
H	-1.371912	-1.475187	0.9647	733.8975	1386.5989					
O	-1.294006	-0.162072	-0.415703	791.7049	1440.2213					
O	-1.688529	-1.439786	-0.09393	857.9316	1465.3246					

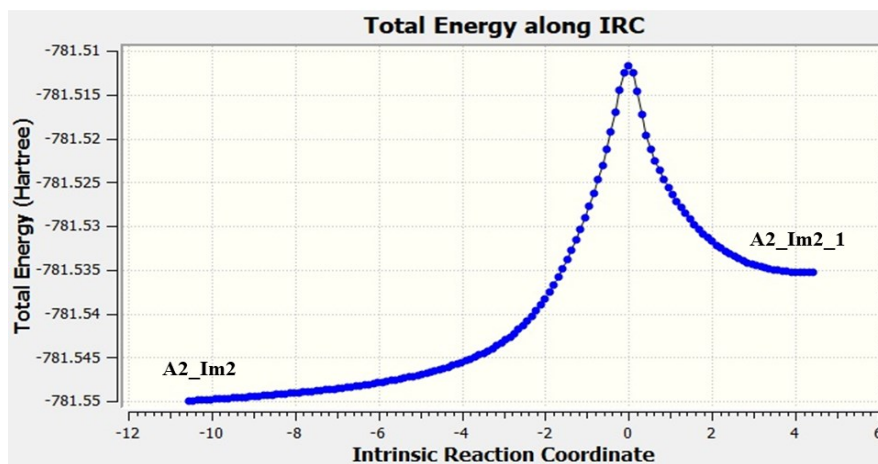


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-5.616	-781.550008	-2.64099	-781.547089	0.32687	-781.514535
-5.5058	-781.549965	-2.53082	-781.546823	0.43697	-781.514917
-5.39559	-781.549921	-2.42064	-781.546531	0.54714	-781.515279
-5.28539	-781.549875	-2.31047	-781.546209	0.65731	-781.515617
-5.1752	-781.549826	-2.2003	-781.545852	0.7675	-781.515933
-5.065	-781.549776	-2.09012	-781.545455	0.87769	-781.516233
-4.95481	-781.549723	-1.97995	-781.545013	0.98789	-781.516518
-4.84463	-781.549667	-1.86977	-781.544519	1.09809	-781.516791
-4.73444	-781.549608	-1.75959	-781.543967	1.20829	-781.517053
-4.62426	-781.549545	-1.64941	-781.543348	1.31849	-781.5173
-4.51409	-781.549479	-1.53924	-781.542655	1.4287	-781.517529
-4.40391	-781.549407	-1.42908	-781.541876	1.5389	-781.517738
-4.29374	-781.549331	-1.31897	-781.540994	1.64909	-781.517926
-4.18357	-781.549248	-1.20891	-781.539985	1.75928	-781.518093
-4.0734	-781.549159	-1.0989	-781.538811	1.86944	-781.518238
-3.96322	-781.549062	-0.98887	-781.537422	1.97959	-781.518362
-3.85304	-781.548958	-0.87881	-781.535767	2.08971	-781.518466
-3.74285	-781.548844	-0.76876	-781.53381	2.19983	-781.518551
-3.63266	-781.548721	-0.65928	-781.531419	2.30993	-781.518621
-3.52247	-781.548589	-0.55038	-781.528317	2.42	-781.518678
-3.41228	-781.548448	-0.44044	-781.524083	2.53001	-781.518723
-3.30208	-781.548295	-0.33029	-781.519603	2.63994	-781.518758
-3.19189	-781.548131	-0.22011	-781.516006	2.74985	-781.518788
-3.0817	-781.547953	-0.10997	-781.514026	2.85981	-781.518812
-2.97152	-781.547762	<b>0</b>	<b>-781.5135</b>	2.96988	-781.518832
-2.86133	-781.547556	0.10913	-781.513758	3.08001	-781.51885
-2.75116	-781.547332	0.21681	-781.514137		

TS3-3\_A2\_Im2--> A2\_Im2\_1



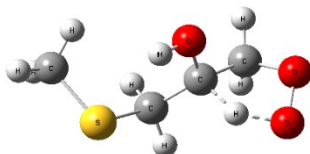
Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-781.511766	-781.38131	-781.371393	-781.415777
M06-2X/DG3/aug-cc-pVTZ				-781.518745	-781.388439	-781.378491	-781.42297
MN15/cc-pVTZ				-781.144343	-781.014512	-781.004639	-781.048795
MN15/aug-cc-pVTZ				-781.155603	-781.026059	-781.016137	-781.060434
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	0.068602	0.162314	-0.084998	<b>1941.9626i</b>	920.1433	1483.0108	
C	0.093103	-0.189648	1.414662	95.7857	981.0025	1500.1459	
C	1.477302	0.057799	2.014872	115.0601	984.7935	1586.1875	
S	2.565627	-1.292585	2.309794	159.042	1005.8091	3047.5124	
C	2.661344	-2.064275	0.674164	207.2335	1046.0645	3080.8582	
H	0.602849	-0.600213	-0.653692	215.9473	1088.9425	3086.1674	
H	-0.604349	0.485277	1.918651	249.6137	1128.3789	3147.6353	
H	1.467261	0.689195	2.899174	290.1255	1155.4175	3155.7369	
H	2.006053	0.799332	1.087057	325.7394	1217.2205	3173.775	
H	3.395672	-2.861218	0.756682	402.9029	1259.7407	3179.0176	
H	1.697898	-2.475996	0.38676	438.8812	1289.575	3828.18	
H	2.997713	-1.329823	-0.053495	532.0552	1296.7309		
O	-0.362797	-1.520825	1.513414	596.6535	1341.6659		
H	0.012394	-1.921413	2.304981	675.1734	1352.9573		
H	-0.957241	0.244076	-0.438783	712.5726	1383.834		
O	0.66086	1.424874	-0.273636	766.2381	1388.4193		
O	2.018163	1.292212	-0.053221	836.3047	1469.539		



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-10.54955	-781.549996	-5.48459	-781.547476	-0.42117	-781.519333
-10.44403	-781.549964	-5.37907	-781.547377	-0.3163	-781.517064
-10.33851	-781.549931	-5.27355	-781.547273	-0.21098	-781.514551
-10.23299	-781.549898	-5.16804	-781.547165	-0.10552	-781.512536
-10.12746	-781.549864	-5.06252	-781.547053	<b>0</b>	<b>-781.5118</b>
-10.02194	-781.549829	-4.95701	-781.546936	0.10553	-781.512535
-9.91642	-781.549794	-4.85149	-781.546814	0.21102	-781.514623
-9.8109	-781.549759	-4.74598	-781.546686	0.31646	-781.517335
-9.70538	-781.549724	-4.64047	-781.546552	0.42129	-781.519656
-9.59986	-781.549688	-4.53496	-781.546412	0.52501	-781.521279
-9.49433	-781.549651	-4.42945	-781.546265	0.63022	-781.522546
-9.38881	-781.549615	-4.32394	-781.54611	0.73565	-781.523664
-9.28329	-781.549578	-4.21843	-781.545947	0.8411	-781.524665
-9.17777	-781.54954	-4.11292	-781.545776	0.94656	-781.525574
-9.07225	-781.549502	-4.00741	-781.545596	1.05204	-781.52641
-8.96673	-781.549463	-3.9019	-781.545405	1.15753	-781.527185
-8.86121	-781.549424	-3.7964	-781.545204	1.26303	-781.527909
-8.75569	-781.549385	-3.6909	-781.544991	1.36853	-781.528586
-8.65017	-781.549344	-3.58539	-781.544764	1.47404	-781.52922
-8.54465	-781.549303	-3.47989	-781.544522	1.57955	-781.529812
-8.43913	-781.549261	-3.37439	-781.544264	1.68506	-781.530364
-8.33361	-781.549218	-3.26889	-781.543988	1.79058	-781.530875
-8.22809	-781.549174	-3.16339	-781.543693	1.89609	-781.531348
-8.12257	-781.54913	-3.05789	-781.543375	2.0016	-781.531785
-8.01706	-781.549085	-2.95239	-781.543032	2.10712	-781.532187
-7.91154	-781.549038	-2.84689	-781.542662	2.21263	-781.532558
-7.80602	-781.548991	-2.74139	-781.54226	2.31815	-781.532898
-7.7005	-781.548943	-2.63589	-781.541825	2.42367	-781.53321

-7.59498	-781.548893	-2.53038	-781.541352	2.52918	-781.533495
-7.48947	-781.548842	-2.42487	-781.540838	2.6347	-781.533752
-7.38395	-781.54879	-2.31937	-781.54028	2.74021	-781.533985
-7.27843	-781.548735	-2.21386	-781.539675	2.84571	-781.534192
-7.17291	-781.54868	-2.10835	-781.539019	2.95122	-781.534377
-7.06739	-781.548622	-2.00283	-781.538309	3.05672	-781.53454
-6.96187	-781.548562	-1.89732	-781.537541	3.16223	-781.534683
-6.85635	-781.548501	-1.79181	-781.536713	3.26773	-781.534808
-6.75083	-781.548438	-1.6863	-781.53582	3.37323	-781.534915
-6.64531	-781.548372	-1.58079	-781.534863	3.47873	-781.535007
-6.53979	-781.548304	-1.47527	-781.533838	3.5842	-781.535083
-6.43427	-781.548233	-1.36976	-781.532746	3.68965	-781.535145
-6.32875	-781.54816	-1.26426	-781.531586	3.79503	-781.535195
-6.22322	-781.548084	-1.15875	-781.530358	3.90032	-781.535234
-6.1177	-781.548005	-1.05326	-781.529061	4.00553	-781.535265
-6.01218	-781.547924	-0.94778	-781.527692	4.11075	-781.53529
-5.90666	-781.54784	-0.84232	-781.526244	4.21608	-781.535311
-5.80114	-781.547754	-0.73687	-781.524707	4.32151	-781.535329
-5.69562	-781.547664	-0.63145	-781.523066	4.427	-781.535345
-5.5901	-781.547572	-0.52611	-781.521307		

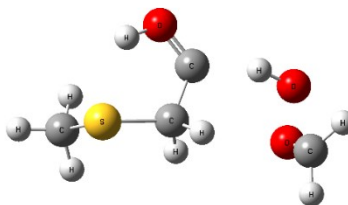
TS3-4\_A2\_Im1\_1--> Pw6



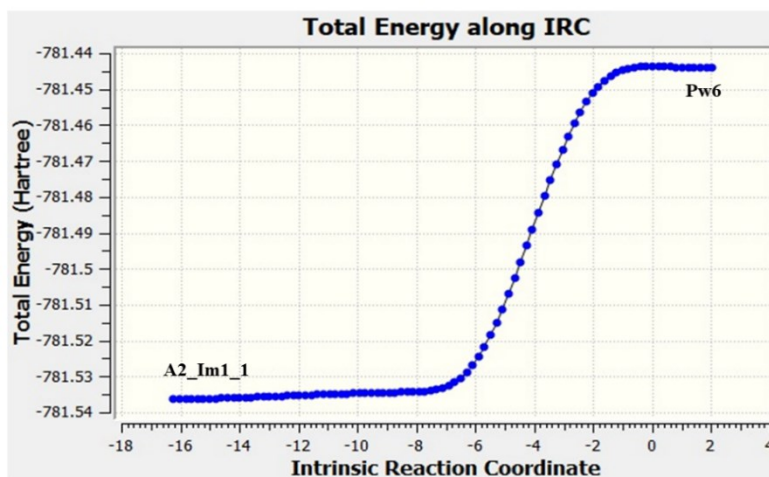
Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-781.443675	-781.31445	-781.303022	-781.352436
M06-2X/DG3/aug-cc-pVTZ				-781.450671	-781.321624	-781.31018	-781.359659
MN15/cc-pVTZ				-781.079426	-780.951019	-780.939275	-780.989147
MN15/aug-cc-pVTZ				-781.090369	-780.962175	-780.950436	-781.000275
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	0.065064	0.412556	-0.160924	<b>180.9258i</b>	784.9183	1489.6832	
C	-0.118421	1.102086	2.381339	42.4545	869.6275	1595.1756	
C	0.97534	0.220857	2.940961	50.0542	911.8867	2996.0313	
S	2.517738	1.046738	3.456188	73.4437	943.9301	3071.4612	
C	2.104752	1.401963	5.186869	114.76	961.0787	3077.2799	
H	-0.503825	1.271605	-0.488716	162.4998	982.788	3136.8569	
H	1.033731	0.178151	-0.580048	190.8373	1011.3515	3141.8599	
H	-1.50958	0.250347	1.504989	223.3591	1160.9497	3162.1795	
H	1.207896	-0.543918	2.201208	239.8249	1199.8657	3173.8691	
H	0.552552	-0.305814	3.800212	278.2633	1236.8258	3210.5687	
H	2.929817	1.974653	5.601997	315.4857	1255.3399	3276.0752	
H	1.190771	1.986607	5.260189	422.1667	1358.4897		
H	1.997711	0.47272	5.740935	515.8535	1377.7068		
O	0.139374	2.363309	2.439897	609.5142	1402.1672		
H	1.070791	2.520833	2.754075	722.6133	1440.2666		
O	-0.622449	-0.694132	0.166767	737.0131	1463.4328		
O	-1.857913	-0.316184	0.748743	778.1434	1477.206		



**Pw6**

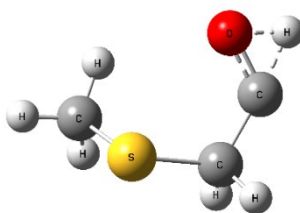


<b>Pw6</b>						
<b>Method</b>		<b>Ee</b>	<b>E+ZPE</b>	<b>ΔH</b>	<b>ΔG</b>	
M06-2X/GD3/cc-pVTZ		-781.445062	-781.316183	-781.303661	-781.356108	
M06-2X/DG3/aug-cc-pVTZ		-781.452155	-781.323461	-781.310909	-781.363555	
MN15/cc-pVTZ		-781.090689	-780.962602	-780.949892	-781.002848	
MN15/aug-cc-pVTZ		-781.079872	-780.951528	-780.938848	-780.991607	
<b>Coordinates (xyz)</b>				<b>Vibrations (cm<sup>-1</sup>)</b>		
C	0.415328	-0.694208	-0.137275	24.4859	793.6784	1489.518
C	-0.248569	0.688736	3.03111	49.169	861.5773	1597.1036
C	1.246208	0.753561	2.85713	69.1464	902.7519	3064.339
S	2.164112	1.830406	4.0009	99.4253	964.5069	3078.8833
C	2.327937	0.680738	5.394591	103.2736	964.881	3088.8481
H	-0.420028	-0.366992	-0.738093	144.7054	983.5195	3116.2004
H	1.386413	-0.898032	-0.565141	170.4005	1029.6341	3142.8705
H	-1.083414	-0.60289	1.971639	207.5431	1160.1547	3150.8257
H	1.403389	1.108716	1.833586	221.7294	1199.3507	3164.4116
H	1.642053	-0.262998	2.870655	266.8619	1243.8123	3177.5148
H	2.826496	1.217732	6.196918	302.8813	1254.3461	3285.4549
H	1.354005	0.342425	5.740146	305.1511	1359.6762	
H	2.934536	-0.171656	5.099328	511.4805	1374.3024	
O	-0.709495	1.526615	3.88133	618.8	1410.6638	
H	0.026223	2.073432	4.281557	681.5317	1450.3651	
O	0.137475	-1.522748	0.89324	711.1786	1475.5706	
O	-1.207154	-1.336986	1.302399	739.0881	1478.3057	

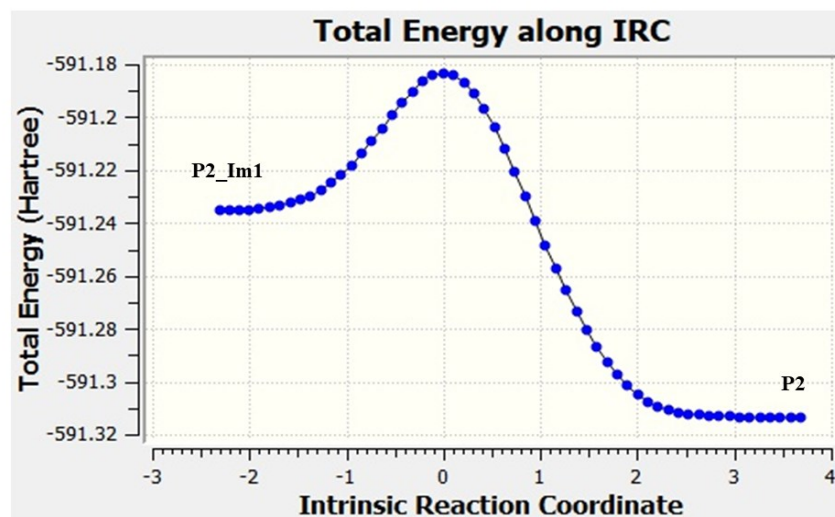


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-16.23216	-781.536428	-9.93545	-781.53472	-3.65594	-781.479824
-16.02908	-781.536397	-9.73233	-781.534675	-3.45282	-781.475361
-15.82599	-781.536364	-9.52922	-781.534633	-3.2497	-781.471055
-15.62288	-781.536327	-9.32611	-781.534591	-3.04659	-781.466955
-15.41977	-781.536287	-9.12302	-781.534552	-2.84347	-781.463113
-15.21665	-781.536244	-8.91992	-781.534513	-2.64035	-781.459582
-15.01353	-781.536198	-8.71687	-781.534475	-2.43723	-781.456407
-14.81041	-781.53615	-8.51394	-781.534438	-2.23412	-781.453628
-14.60728	-781.5361	-8.31174	-781.5344	-2.031	-781.451257
-14.40416	-781.536047	-8.1126	-781.534353	-1.82789	-781.449285
-14.20104	-781.535991	-7.91262	-781.534279	-1.62477	-781.447684
-13.99792	-781.535934	-7.71225	-781.534155	-1.42166	-781.446421
-13.79479	-781.535874	-7.51018	-781.533951	-1.21855	-781.44546
-13.59167	-781.535812	-7.30873	-781.533648	-1.01545	-781.444766
-13.38854	-781.535749	-7.10688	-781.533218	-0.81235	-781.444288
-13.18542	-781.535684	-6.90435	-781.532566	-0.60927	-781.443979
-12.98229	-781.535619	-6.70162	-781.531652	-0.40617	-781.443794
-12.77917	-781.535554	-6.49874	-781.530424	-0.20312	-781.443701
-12.57604	-781.535488	-6.29584	-781.528851	<b>0</b>	<b>-781.4437</b>
-12.37292	-781.535422	-6.0929	-781.526896	0.20311	-781.443695
-12.16979	-781.535356	-5.88993	-781.524539	0.40614	-781.443746
-11.96667	-781.535291	-5.68692	-781.521772	0.60924	-781.443814
-11.76354	-781.535227	-5.48387	-781.518608	0.8123	-781.443888
-11.56042	-781.535163	-5.2808	-781.515074	1.01538	-781.443962
-11.35729	-781.535101	-5.07771	-781.511217	1.21841	-781.44403
-11.15417	-781.53504	-4.87461	-781.507089	1.42141	-781.444088
-10.95105	-781.534981	-4.6715	-781.502749	1.6243	-781.444136
-10.74793	-781.534924	-4.46839	-781.498255	1.82703	-781.444175
-10.5448	-781.53487	-4.26528	-781.493662	2.02966	-781.444206
-10.34168	-781.534817	-4.06217	-781.489024		
-10.13856	-781.534767	-3.85905	-781.484395		

TS3-5\_P2\_Im1--> P2

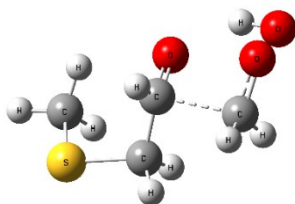


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-591.18334	-591.103316	-591.095738	-591.133819		
M06-2X/DG3/aug-cc-pVTZ	-591.187247	-591.107331	-591.099736	-591.137864		
MN15/cc-pVTZ	-590.940431	-590.860689	-590.853119	-590.891137		
MN15/aug-cc-pVTZ	-590.947207	-590.867597	-590.860008	-590.898089		
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.04427	-0.009687	0.007629	<b>2053.9103i</b>	923.5568	3061.4044
C	0.016115	0.005458	1.502655	95.0861	974.7935	3075.8847
S	1.617259	0.008869	2.341561	151.9526	993.8657	3109.3146
C	2.152751	1.692591	1.950127	163.7302	1153.5579	3159.2469
H	-0.528953	-0.886127	1.820121	216.1639	1257.5516	3177.4034
H	-0.596485	0.856524	1.812161	274.7561	1350.0731	
H	3.077142	1.860928	2.496811	516.463	1389.2166	
H	2.338443	1.80275	0.885895	629.692	1470.7117	
H	1.409435	2.413865	2.284649	729.6332	1492.5705	
O	1.182922	-0.007167	-0.595113	766.4823	1498.7389	
H	0.19931	0.00004	-1.238112	777.9019	2669.4671	



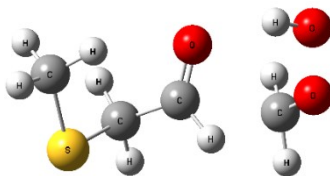
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-2.31053	-591.23519	-0.21102	-591.186632	1.89897	-591.301609
-2.20655	-591.235169	-0.10553	-591.184201	2.00442	-591.304972
-2.10754	-591.235101	<b>0</b>	<b>-591.1833</b>	2.10982	-591.307602
-2.0027	-591.234917	0.10553	-591.184223	2.21512	-591.309551
-1.89736	-591.234581	0.21102	-591.1868	2.32016	-591.310898
-1.79199	-591.234079	0.31652	-591.190975	2.42481	-591.311778
-1.68671	-591.233392	0.42202	-591.196669	2.52942	-591.312344
-1.58156	-591.232484	0.52752	-591.203729	2.63411	-591.312713
-1.47642	-591.231279	0.63303	-591.211868	2.73859	-591.312955
-1.37119	-591.229689	0.73853	-591.220724	2.84328	-591.313127
-1.26584	-591.227615	0.84404	-591.22995	2.94851	-591.313262
-1.16043	-591.225003	0.94954	-591.239262	3.05393	-591.313371
-1.05497	-591.221825	1.05504	-591.248424	3.15936	-591.313458
-0.94948	-591.2181	1.16055	-591.257256	3.26472	-591.313524
-0.84399	-591.213884	1.26605	-591.265612	3.36996	-591.313573
-0.73849	-591.209271	1.37155	-591.273391	3.47501	-591.313608
-0.63299	-591.204397	1.47704	-591.280514	3.57995	-591.313632
-0.5275	-591.199446	1.58253	-591.286926	3.68509	-591.313649
-0.42201	-591.194635	1.68802	-591.29259		
-0.31651	-591.190249	1.7935	-591.297485		

TS3-6\_A2\_Im1\_2--> Pw7

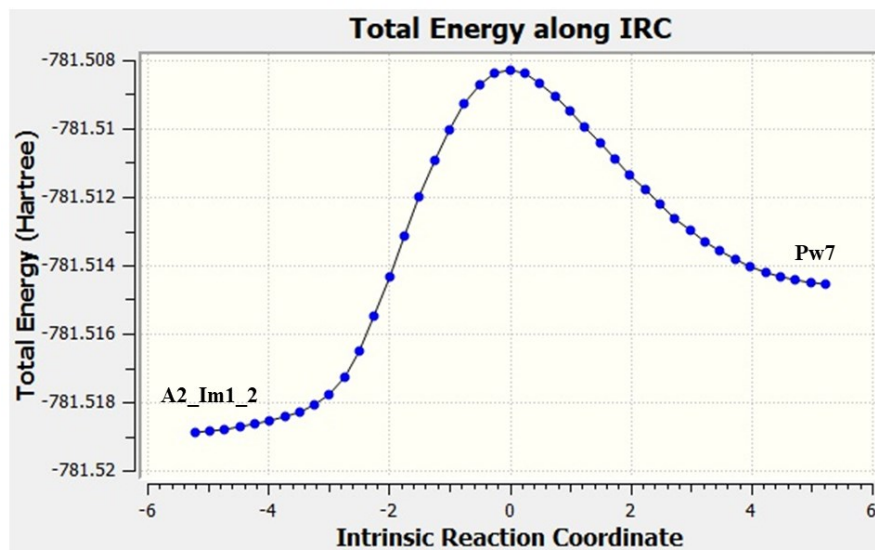


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-781.508278	-781.376897	-781.365907	-781.413858		
M06-2X/DG3/aug-cc-pVTZ	-781.515504	-781.384211	-781.373219	-781.421155		
MN15/cc-pVTZ	-781.14016	-781.009401	-780.998448	-781.046279		
MN15/aug-cc-pVTZ	-781.151133	-781.020634	-781.009664	-781.057543		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.009495	0.032905	0.035301	<b>307.0946i</b>	877.5953	1500.3737
C	-0.008876	-0.003603	2.193527	49.9467	926.6735	1613.5532
C	1.478753	-0.037642	2.437488	61.8852	964.936	2994.6446
S	1.789436	0.435026	4.163535	93.4356	982.4912	3075.2987
C	1.080262	-1.000724	5.001694	138.8585	986.216	3083.62
H	0.324482	1.031647	-0.2175	190.5252	1023.0127	3120.0373
H	0.629836	-0.824184	-0.141863	200.6341	1058.3877	3149.611
H	-0.4583	1.002062	2.201933	237.0064	1200.8151	3162.4599
H	2.002916	0.700336	1.832468	275.1756	1215.2993	3173.8409
H	1.873558	-1.034123	2.242382	293.0871	1240.5836	3254.7724
H	1.210493	-0.829143	6.067332	422.232	1263.5425	3498.3148
H	0.022992	-1.101936	4.770931	493.05	1358.7791	
H	1.609791	-1.906081	4.71331	519.8134	1383.2465	
O	-0.716576	-0.997038	2.413968	579.5776	1446.2448	
H	-1.632111	-1.534126	0.946403	638.5231	1461.4105	
O	-1.310221	-0.12712	-0.232782	710.7359	1468.4674	
O	-1.673355	-1.479358	-0.033909	756.1754	1485.9976	

Pw7

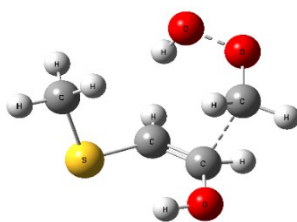


Method	Ee		E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ	-781.513851		-781.383506	-781.371604	-781.421779	
M06-2X/DG3/aug-cc-pVTZ	-781.521977		-781.391789	-781.379018	-781.432351	
MN15/cc-pVTZ	-781.146497		-781.017136	-781.004091	-781.058739	
MN15/aug-cc-pVTZ	-781.157261		-781.028198	-781.015117	-781.069941	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.080579	0.049684	-0.087631	24.2874	747.3467	1494.791
C	0.108762	-0.168541	2.90933	41.416	880.4753	1808.5128
C	1.568251	-0.014169	3.188077	55.1337	949.3544	3017.7033
S	1.693502	0.622138	4.887521	92.8592	967.0378	3076.8398
C	1.155274	-0.853851	5.783485	116.0551	983.8142	3096.089
H	0.17073	1.056875	-0.386477	125.2645	1041.9881	3155.9267
H	0.349679	-0.818427	-0.563739	161.1708	1069.6805	3162.5514
H	-0.447572	0.7661	2.738274	185.7299	1191.5905	3166.409
H	2.005928	0.743531	2.540672	209.7171	1198.7283	3174.0503
H	2.093465	-0.961509	3.087816	278.3535	1223.1326	3292.7846
H	1.151297	-0.589015	6.837762	290.9746	1246.7992	3644.807
H	0.154408	-1.153042	5.481613	347.0847	1361.7178	
H	1.85309	-1.671454	5.618302	500.1106	1421.1624	
O	-0.462284	-1.23378	2.947173	510.9304	1446.1956	
H	-1.52946	-1.540575	1.410499	556.8332	1451.3226	
O	-1.371895	-0.04468	0.305172	699.3423	1471.8925	
O	-1.72327	-1.407463	0.463828	721.8176	1486.1637	



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-5.21593	-781.51888	-1.49428	-781.511991	2.24127	-781.511802
-4.96749	-781.518848	-1.24526	-781.51095	2.49031	-781.512222
-4.71882	-781.518801	-0.9962	-781.510039	2.73938	-781.512618
-4.46998	-781.518739	-0.74717	-781.509291	2.98843	-781.512979
-4.22108	-781.518659	-0.49812	-781.508734	3.23749	-781.513305
-3.97226	-781.51856	-0.2491	-781.508392	3.48654	-781.513592
-3.7237	-781.51844	<b>0</b>	<b>-781.5083</b>	3.7356	-781.513839
-3.47581	-781.518293	0.24908	-781.508384	3.98464	-781.514045
-3.22957	-781.5181	0.498	-781.508662	4.23367	-781.514212
-2.98494	-781.517799	0.74703	-781.509048	4.48265	-781.514343
-2.73793	-781.51729	0.99602	-781.509488	4.73147	-781.514439
-2.48993	-781.51651	1.24507	-781.509955	4.97956	-781.514504
-2.24124	-781.515493	1.4941	-781.510429	5.2254	-781.514544
-1.9923	-781.514327	1.74316	-781.5109		
-1.74331	-781.513134	1.99221	-781.511359		

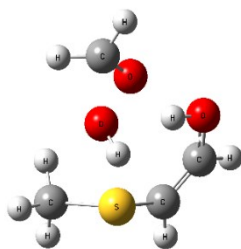
TS3-7\_A2\_Im2\_1--> Pw8



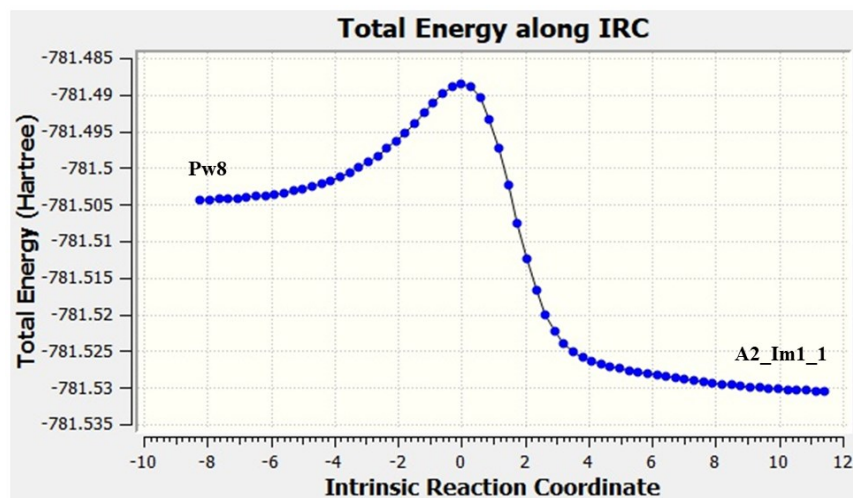
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.488469	-781.357529	-781.346223	-781.394533	
M06-2X/DG3/aug-cc-pVTZ		-781.49571	-781.36487	-781.353567	-781.401912	
MN15/cc-pVTZ		-781.122296	-780.992019	-780.980722	-781.028862	
MN15/aug-cc-pVTZ		-781.133421	-781.003342	-780.992044	-781.040216	
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	-0.231583	0.151109	0.06475	<b>511.6332i</b>	714.8887	1491.4306
C	-0.055267	0.115325	2.238219	43.5284	812.3523	1542.2434
C	1.248302	-0.196041	2.530451	76.6167	918.7931	3071.9261
S	1.696449	-1.823598	3.002752	97.5229	962.0121	3113.9707
C	2.636349	-2.425576	1.56351	143.266	966.9111	3157.6467
H	-0.218727	-0.914883	-0.134119	166.3061	982.1951	3174.0925
H	-0.367657	1.151637	2.231787	203.7106	1000.3121	3183.0011
H	1.982862	0.597926	2.574113	240.8061	1078.0131	3201.4015
H	2.17825	0.0222	0.443225	257.3119	1190.2522	3245.4202
H	2.954107	-3.437644	1.803723	278.0925	1206.266	3698
H	2.018942	-2.43744	0.669614	407.6592	1224.6654	3728.6255
H	3.518711	-1.8083	1.405292	456.3511	1334.0722	
O	-1.088835	-0.738659	2.435893	506.0019	1352.4904	
H	-0.717253	-1.608555	2.647194	549.8997	1354.3413	
H	-1.166699	0.688714	-0.034003	584.4872	1443.0985	
O	0.787062	0.868189	-0.473674	661.177	1447.0508	
O	1.950544	0.062448	-0.50125	688.303	1475.6365	



**Pw8**

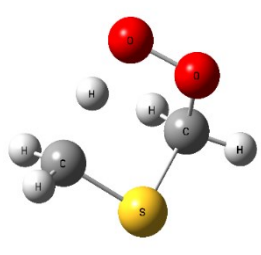


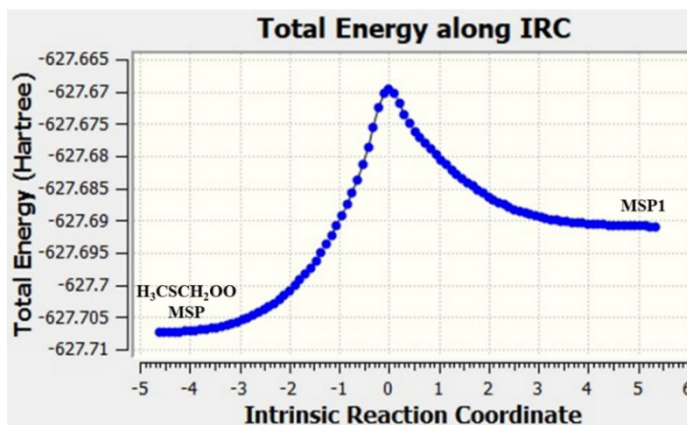
Method		Ee	E+ZPE	$\Delta H$	$\Delta G$	
M06-2X/GD3/cc-pVTZ		-781.506846	-781.375885	-781.363304	-781.414904	
M06-2X/DG3/aug-cc-pVTZ		-781.514065	-781.383267	-781.370677	-781.422299	
MN15/cc-pVTZ		-781.140269	-781.010279	-780.997517	-781.049694	
MN15/aug-cc-pVTZ		-781.151339	-781.021567	-781.008814	-781.060833	
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.290962	-0.535722	0.147738	41.3364	732.1286	1488.3965
C	0.036671	0.274642	3.462663	69.3845	769.2309	1685.4289
C	1.295231	-0.064288	3.765989	89.4733	821.0728	3077.9615
S	1.814527	-1.74994	3.727947	96.5557	960.6809	3151.3434
C	3.117775	-1.687427	2.466705	107.0693	970.945	3164.5386
H	1.098264	-0.95457	-0.436397	139.1545	988.169	3178.0545
H	-0.316274	1.293146	3.562441	166.0566	1000.495	3196.2626
H	1.966597	0.68392	4.165464	177.1656	1106.5193	3218.3371
H	1.801291	0.85535	1.716295	226.7066	1187.3334	3291.5178
H	3.566324	-2.677388	2.43327	246.5946	1228.7182	3680.3632
H	2.701847	-1.436983	1.494902	322.8396	1230.5058	3717.8824
H	3.876974	-0.96261	2.75224	447.7011	1346.4081	
O	-0.918167	-0.55406	3.027222	461.6771	1371.2682	
H	-0.519931	-1.428261	2.887953	514.8062	1390.8495	
H	-0.739341	-0.817996	-0.004308	616.9841	1446.0012	
O	0.399432	0.765997	0.496321	634.537	1452.4748	
O	1.762069	1.060891	0.765755	729.964	1472.8652	



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-8.21972	-781.504371	-1.46811	-781.493912	5.26758	-781.527651
-7.92716	-781.504326	-1.17444	-781.492552	5.5609	-781.527882
-7.63424	-781.504272	-0.88086	-781.491163	5.85456	-781.5281
-7.34098	-781.504208	-0.58724	-781.489849	6.14823	-781.528312
-7.04748	-781.504127	-0.29367	-781.488852	6.44193	-781.528512
-6.75389	-781.50403	<b>0</b>	<b>-781.4885</b>	6.73564	-781.528704
-6.46026	-781.503912	0.2937	-781.488929	7.02934	-781.528887
-6.16664	-781.503769	0.58729	-781.49048	7.32308	-781.529062
-5.87303	-781.503599	0.88099	-781.493316	7.61679	-781.529228
-5.57946	-781.503397	1.1747	-781.497402	7.91053	-781.529386
-5.28588	-781.503158	1.4684	-781.502341	8.20425	-781.529532
-4.99231	-781.502878	1.76203	-781.507533	8.49799	-781.52967
-4.6987	-781.502549	2.05556	-781.512467	8.7917	-781.529796
-4.40506	-781.502165	2.34891	-781.51672	9.08545	-781.529913
-4.11137	-781.501716	2.64152	-781.520028	9.37917	-781.53002
-3.81766	-781.501201	2.93287	-781.522345	9.67292	-781.530119
-3.52393	-781.500614	3.22457	-781.523945	9.96662	-781.530209
-3.23022	-781.49995	3.51694	-781.525083	10.26037	-781.53029
-2.93651	-781.499199	3.80878	-781.52587	10.55401	-781.53036
-2.64282	-781.498352	4.10016	-781.526436	10.8477	-781.530423
-2.34912	-781.497403	4.39127	-781.526839	11.14137	-781.530476
-2.05543	-781.496348	4.68278	-781.527151	11.43498	-781.530518
-1.76175	-781.495182	4.97462	-781.527414		

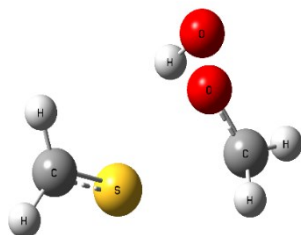
4. MSP decomposition

TS4-1_MSP-->MSP1						
						
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-627.669648	-627.601289	-627.595225	-627.630489		
M06-2X/DG3/aug-cc-pVTZ	-627.674394	-627.606103	-627.600038	-627.635299		
MN15/cc-pVTZ	-627.414333	-627.346277	-627.340178	-627.37549		
MN15/aug-cc-pVTZ	-627.42194	-627.354004	-627.3479	-627.383218		
SVECV-f12	-627.554261	-627.485971	-627.479906	-627.515167		
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.001485	-0.012139	-0.013498	<b>1836.5292i</b>	985.9391	3092.0438
S	-0.019768	0.211100	1.800631	187.3618	1015.9504	3108.4631
C	1.710700	0.084828	2.019286	363.5778	1031.2544	3180.3665
H	-1.027634	-0.018565	-0.361728	383.8515	1115.4696	3217.686
H	0.596141	0.763709	-0.493297	449.0052	1246.4396	
H	1.986288	-0.297183	2.994816	526.4722	1275.3136	
H	2.001157	-0.782823	1.026290	626.1916	1299.0041	
H	2.290466	0.941107	1.684253	703.0899	1427.9016	
O	1.912627	-1.209399	-0.103064	815.1256	1455.4505	
O	0.544718	-1.275812	-0.263628	920.2907	1549.8906	



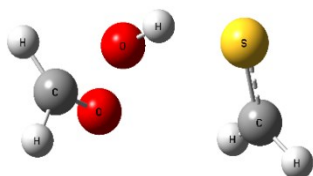
Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-4.61611	-627.707394	-1.25785	-627.693781	2.09676	-627.686768
-4.51123	-627.707377	-1.15292	-627.692405	2.20174	-627.687195
-4.40634	-627.707355	-1.04799	-627.690919	2.30671	-627.687587
-4.30147	-627.707324	-0.94307	-627.689316	2.41168	-627.687947
-4.19661	-627.707285	-0.83815	-627.687586	2.51665	-627.688274
-4.09173	-627.707235	-0.73325	-627.685718	2.62162	-627.688572
-3.98682	-627.707173	-0.62844	-627.683682	2.72658	-627.688841
-3.8819	-627.707097	-0.52404	-627.681412	2.83155	-627.689082
-3.77698	-627.707005	-0.41965	-627.678668	2.93651	-627.689299
-3.67203	-627.706896	-0.31486	-627.6755	3.04147	-627.689493
-3.56708	-627.706766	-0.20993	-627.672468	3.14642	-627.689666
-3.46212	-627.706615	-0.10498	-627.670368	3.25137	-627.689819
-3.35715	-627.706441	<b>0</b>	<b>-627.6696</b>	3.35631	-627.689955
-3.25219	-627.70624	0.10497	-627.670293	3.46124	-627.690075
-3.14722	-627.706011	0.20986	-627.671897	3.56617	-627.690182
-3.04225	-627.70575	0.31439	-627.673672	3.6711	-627.690276
-2.93728	-627.705457	0.41772	-627.675033	3.77602	-627.690359
-2.83231	-627.70513	0.52237	-627.676153	3.88094	-627.690433
-2.72734	-627.704763	0.62727	-627.677167	3.98586	-627.690499
-2.62237	-627.704356	0.73219	-627.678109	4.09078	-627.690559
-2.51739	-627.703906	0.83713	-627.678991	4.19571	-627.690612
-2.41242	-627.703409	0.94209	-627.679825	4.30065	-627.690661
-2.30745	-627.702861	1.04705	-627.680621	4.4056	-627.690705
-2.20248	-627.70226	1.15201	-627.681382	4.51056	-627.690745
-2.09751	-627.701602	1.25698	-627.682113	4.61552	-627.690782
-1.99254	-627.700883	1.36195	-627.682812	4.72049	-627.690816
-1.88758	-627.700099	1.46692	-627.683478	4.82546	-627.690846
-1.78261	-627.699247	1.57189	-627.684112	4.93044	-627.690873
-1.67765	-627.698322	1.67687	-627.684713	5.03542	-627.690897
-1.5727	-627.697319	1.78184	-627.685279	5.14039	-627.690918
-1.46774	-627.696231	1.88682	-627.685811	5.24537	-627.690937
-1.3628	-627.695055	1.99179	-627.686308	5.35035	-627.690952

TS4-2\_MSP1-->Pw9



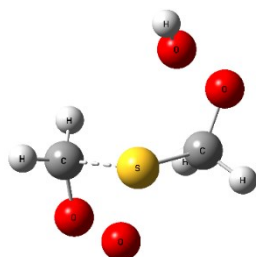
Method	E <sub>c</sub>	E+ZPE	ΔH	ΔG		
M06-2X/GD3/cc-pVTZ	-627.648034	-627.579198	-627.571201	-627.61161		
M06-2X/DG3/aug-cc-pVTZ	-627.652918	-627.584209	-627.576161	-627.616768		
MN15/cc-pVTZ	-627.395151	-627.326732	-627.317669	-627.361289		
MN15/aug-cc-pVTZ	-627.402679	-627.334414	-627.325278	-627.368825		
SVECV-f12	-627.531795	-627.463086	-627.455038	-627.495644		
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )		
C	0.000675	0.001792	-0.007309	<b>102.5325i</b>	957.4911	3159.6907
S	0.017094	0.022571	2.922901	52.3713	994.9849	3202.2957
C	1.601707	-0.017331	3.198661	87.4472	1004.8302	3303.836
H	0.329909	-0.979545	-0.310474	159.9874	1082.3346	3574.4659
H	-0.987442	0.383882	-0.217092	203.5002	1191.097	
H	2.091377	-0.914598	3.563037	285.0648	1235.3448	
H	2.241254	0.839236	3.009095	361.3667	1457.2957	
O	1.011950	0.884913	0.049604	512.4782	1481.5383	
O	0.523452	2.125293	0.532815	548.8712	1498.6038	
H	0.281305	1.888888	1.450584	692.7718	3112.1345	

Pw9



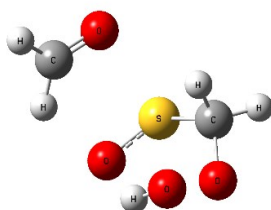
Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-627.648954	-627.580218	-627.571177	-627.614531
M06-2X/DG3/aug-cc-pVTZ				-627.653869	-627.585288	-627.576199	-627.619691
MN15/cc-pVTZ				-627.437079	-627.365868	-627.358086	-627.397086
MN15/aug-cc-pVTZ				-627.445	-627.373896	-627.366089	-627.405186
SVECV-f12				-627.534044	-627.465463	-627.456374	-627.499866
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	0.005528	0.002023	-0.005251	40.5892	960.7761	3157.6858	
S	0.007251	0.023756	3.672263	53.7619	1015.6163	3201.023	
C	1.600668	-0.010964	3.49161	130.2901	1048.2072	3298.5666	
H	0.396584	-0.907247	-0.434635	136.48	1119.9632	3562.2036	
H	-0.862663	0.50933	-0.399301	167.9295	1189.7658		
H	2.220915	-0.691986	4.066951	219.203	1235.678		
H	2.110641	0.634496	2.781617	293.0568	1450.2077		
O	0.988313	0.776231	0.510135	503.5115	1477.7222		
O	0.417003	1.938715	1.088761	555.1677	1505.5049		
H	0.038052	1.577315	1.915116	671.9182	3108.9207		

TS4-3\_MSP2-->Pw10



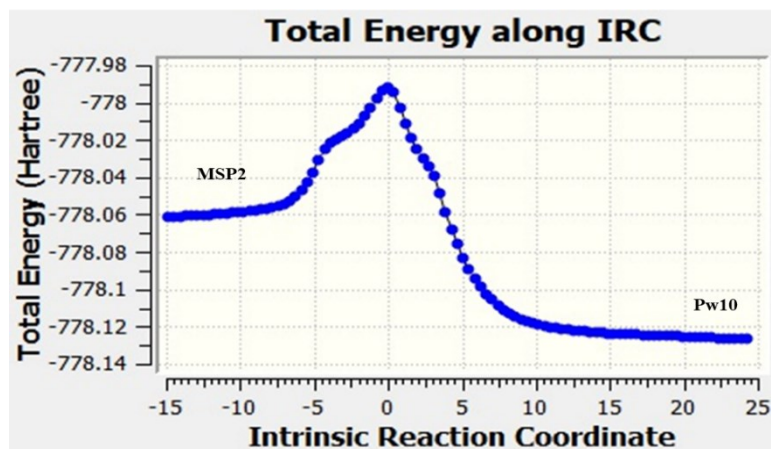
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-777.99177	-777.912301	-777.903124	-777.946227		
M06-2X/DG3/aug-cc-pVTZ	-778.000822	-777.921446	-777.912252	-777.955454		
MN15/cc-pVTZ	-777.648512	-777.569322	-777.56016	-777.603123		
MN15/aug-cc-pVTZ	-777.660763	-777.581658	-777.572516	-777.615448		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.016924	0.001630	-0.009237	<b>975.0376i</b>	744.0373	1503.4915
S	-0.054074	0.062050	1.819935	68.2111	855.2833	3069.4247
C	1.886866	0.030189	2.221771	119.8196	927.8848	3089.7928
H	-0.824696	0.628635	-0.379047	132.839	999.2984	3166.1933
H	0.952761	0.397504	-0.312409	191.8695	1120.0974	3170.16
H	1.958648	-0.189256	3.287905	194.0591	1129.2363	3823.3318
O	-0.259741	-1.271269	-0.514354	262.8213	1170.4936	
O	0.883862	-2.067647	-0.222438	319.2223	1214.7007	
H	0.496570	-2.758697	0.329652	364.4558	1261.1184	
H	2.395244	-0.684134	1.578817	500.2283	1315.8532	
O	2.086097	1.338735	1.891070	534.5001	1414.6594	
O	0.582435	1.713657	1.897645	721.0897	1457.8108	

**Pw10**



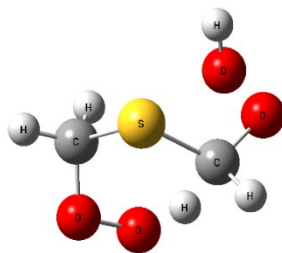
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-778.131921	-778.052609	-778.04161	-778.090575		
M06-2X/DG3/aug-cc-pVTZ	-778.139903	-778.060858	-778.049751	-778.099502		
MN15/cc-pVTZ	-777.794808	-777.716382	-777.705227	-777.754489		
MN15/aug-cc-pVTZ	-777.783678	-777.704988	-777.693885	-777.743035		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.112933	0.047346	-0.191413	17.1502	657.6133	1853.404
S	0.112184	0.455796	1.591255	55.0422	906.7562	2961.7233
C	3.601534	0.059493	0.76932	82.754	974.6835	3046.2054
H	-0.971808	0.621699	-0.539392	91.2729	1090.0456	3085.8745
H	0.797075	0.325046	-0.721042	111.6405	1135.4504	3158.7291
H	4.67936	-0.024601	0.555557	134.4935	1228.4035	3721.9414
O	-0.414444	-1.300825	-0.35305	159.0652	1268.2977	
O	0.804211	-2.033262	-0.32198	218.3134	1278.6738	
H	0.965882	-2.082104	0.634579	270.2201	1305.483	
H	3.164481	-0.667247	1.472296	395.5592	1446.8961	
O	2.93123	0.912604	0.25773	496.5468	1472.7111	
O	0.864126	-0.732605	2.143737	537.0832	1534.6625	



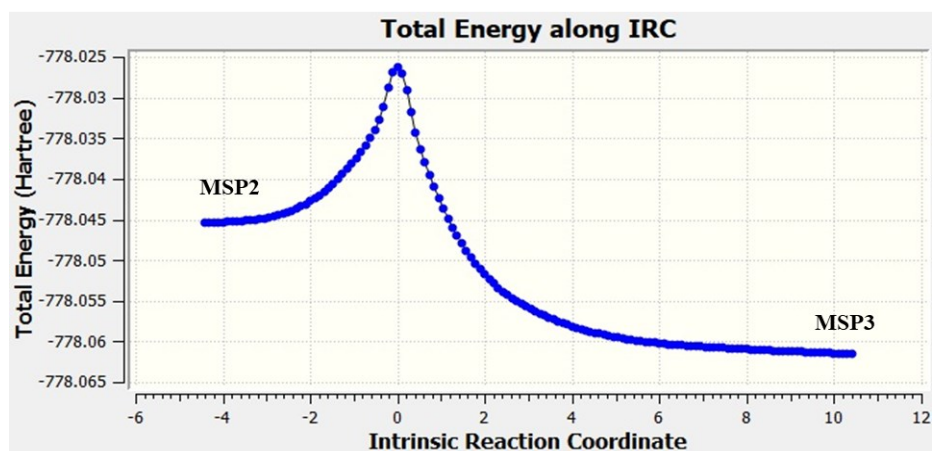


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-14.85381	-778.060988	-1.56326	-778.007126	11.73904	-778.121234
-14.46243	-778.060934	-1.17163	-778.002707	12.13064	-778.12162
-14.07106	-778.06086	-0.78044	-777.998021	12.52215	-778.12197
-13.67952	-778.060763	-0.39021	-777.993808	12.91375	-778.122289
-13.28789	-778.060642	<b>0</b>	<b>-777.9918</b>	13.30522	-778.122586
-12.89617	-778.060495	0.39086	-777.99468	13.69682	-778.122858
-12.50441	-778.060325	0.7823	-778.002548	14.0883	-778.123117
-12.11264	-778.060126	1.17382	-778.011607	14.47955	-778.123348
-11.72089	-778.059903	1.56519	-778.019308	14.87091	-778.123557
-11.32915	-778.059651	1.95626	-778.025172	15.26117	-778.123737
-10.93745	-778.059377	2.34692	-778.029684	15.65229	-778.123892
-10.54581	-778.059077	2.73652	-778.033786	16.04223	-778.124024
-10.1542	-778.058756	3.1238	-778.039286	16.43285	-778.12414
-9.76267	-778.058413	3.514	-778.048473	16.82314	-778.124247
-9.37111	-778.058057	3.90474	-778.058652	17.21439	-778.124357
-8.97987	-778.057686	4.29607	-778.067921	17.60594	-778.12447
-8.58911	-778.057304	4.68753	-778.075966	17.99753	-778.124593
-8.20051	-778.056891	5.07917	-778.08292	18.38912	-778.12472
-7.81319	-778.056357	5.47094	-778.088912	18.78079	-778.124852
-7.42405	-778.055549	5.86277	-778.094079	19.17253	-778.124986
-7.03318	-778.054306	6.25461	-778.098524	19.5642	-778.125129
-6.64176	-778.052506	6.64646	-778.102348	19.95575	-778.125273
-6.25014	-778.050035	7.0383	-778.105623	20.34752	-778.125413
-5.85848	-778.046785	7.43015	-778.10842	20.73931	-778.125547
-5.46687	-778.042645	7.822	-778.110804	21.131	-778.125681
-5.07639	-778.037475	8.21385	-778.112835	21.52271	-778.125814
-4.6866	-778.030954	8.60568	-778.114551	21.91438	-778.125943
-4.2963	-778.024505	8.9975	-778.115985	22.30608	-778.126058
-3.9102	-778.021491	9.38928	-778.117179	22.69772	-778.126167
-3.51937	-778.019756	9.78103	-778.118177	23.0893	-778.126265
-3.12803	-778.018133	10.17273	-778.119016	23.48073	-778.126357
-2.7373	-778.016289	10.56441	-778.119721	23.8721	-778.12644
-2.34634	-778.013947	10.95595	-778.120308	24.26353	-778.126523
-1.95494	-778.01092	11.34754	-778.120806		

TS4-4\_MSP2-->MSP3



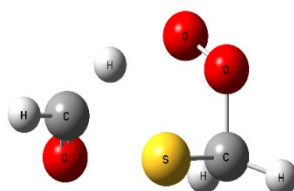
Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-778.026227	-777.949041	-777.940701	-777.981697		
M06-2X/DG3/aug-cc-pVTZ	-778.033797	-777.956874	-777.948458	-777.989676		
MN15/cc-pVTZ	-777.68226	-777.605574	-777.597136	-777.638358		
MN15/aug-cc-pVTZ	-777.693092	-777.616622	-777.608139	-777.6495		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.001309	-0.000405	0.001771	<b>1942.2075i</b>	759.8592	1460.0917
S	0.001540	0.007493	1.780325	101.9192	899.3292	1550.2099
C	1.834589	0.001522	2.011022	130.6415	962.8252	3110.3926
H	-0.740841	0.670242	-0.427230	188.7217	997.3354	3159.9239
H	1.210707	0.495154	-0.227092	219.6992	1017.8691	3189.9935
H	2.015726	0.179521	3.067460	305.0188	1123.2042	3785.3663
O	-0.132919	-1.199364	-0.666414	351.7358	1135.5261	
O	0.823633	-2.127017	-0.187751	398.9099	1194.8761	
H	0.306063	-2.621534	0.463635	504.3996	1281.2577	
H	2.249087	-0.940644	1.662975	557.7869	1301.5917	
O	2.372933	1.070692	1.301034	639.7867	1336.1927	
O	2.390254	0.738418	-0.037159	677.106	1423.8348	



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-4.41506	-778.045407	0.62934	-778.038008	5.67599	-778.060044
-4.30993	-778.045391	0.7345	-778.039572	5.7812	-778.060111
-4.20482	-778.045373	0.83968	-778.041029	5.88642	-778.060173
-4.09973	-778.045353	0.94487	-778.04239	5.99164	-778.060232
-3.99461	-778.04533	1.05007	-778.043663	6.09685	-778.060286
-3.88949	-778.045303	1.15528	-778.044855	6.20206	-778.060338
-3.78434	-778.045272	1.2605	-778.045968	6.30727	-778.060386
-3.6792	-778.045236	1.36572	-778.047004	6.41247	-778.060432
-3.57407	-778.045195	1.47094	-778.047966	6.51768	-778.060476
-3.46893	-778.045146	1.57616	-778.048857	6.6229	-778.060518
-3.36379	-778.045089	1.68138	-778.049678	6.72811	-778.060558
-3.25864	-778.045022	1.7866	-778.050434	6.83333	-778.060597
-3.15348	-778.044943	1.89182	-778.051129	6.93855	-778.060635
-3.04831	-778.044852	1.99704	-778.051768	7.04378	-778.060671
-2.94312	-778.044745	2.10226	-778.052356	7.14901	-778.060707
-2.83793	-778.044621	2.20748	-778.052897	7.25424	-778.060742
-2.73272	-778.044479	2.31269	-778.053396	7.35947	-778.060775
-2.62752	-778.044316	2.41791	-778.053857	7.4647	-778.060808
-2.52231	-778.04413	2.52313	-778.054285	7.56994	-778.060841
-2.4171	-778.043919	2.62834	-778.054681	7.67517	-778.060872
-2.31189	-778.04368	2.73356	-778.055051	7.78041	-778.060903
-2.20667	-778.04341	2.83878	-778.055397	7.88564	-778.060933
-2.10143	-778.043107	2.944	-778.055721	7.99088	-778.060963
-1.9962	-778.042773	3.04922	-778.056025	8.09612	-778.060992
-1.89097	-778.042406	3.15444	-778.056312	8.20135	-778.06102
-1.78574	-778.042004	3.25967	-778.056583	8.30659	-778.061048
-1.68051	-778.041565	3.36489	-778.05684	8.41182	-778.061076
-1.57527	-778.041089	3.47012	-778.057082	8.51706	-778.061102
-1.47004	-778.040576	3.57534	-778.057313	8.6223	-778.061129

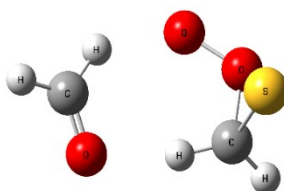
-1.36481	-778.040027	3.68057	-778.057532	8.72753	-778.061155
-1.25958	-778.03944	3.7858	-778.05774	8.83277	-778.061181
-1.15435	-778.038816	3.89103	-778.057938	8.938	-778.061206
-1.04913	-778.038152	3.99626	-778.058127	9.04324	-778.061231
-0.94392	-778.037445	4.10149	-778.058306	9.14847	-778.061256
-0.83871	-778.036688	4.20672	-778.058476	9.25371	-778.061281
-0.73353	-778.035868	4.31195	-778.058637	9.35894	-778.061305
-0.62837	-778.034964	4.41718	-778.05879	9.46418	-778.061329
-0.5233	-778.033956	4.52242	-778.058934	9.56941	-778.061353
-0.4188	-778.032719	4.62764	-778.05907	9.67465	-778.061376
-0.31547	-778.031099	4.73287	-778.059198	9.77989	-778.061399
-0.21043	-778.028859	4.8381	-778.059319	9.88512	-778.061422
-0.10524	-778.026958	4.94333	-778.059432	9.99036	-778.061444
0	-778.026227	5.04856	-778.059538	10.0956	-778.061466
0.10525	-778.027	5.15379	-778.059638	10.20083	-778.061488
0.21044	-778.029127	5.25901	-778.059731	10.30607	-778.06151
0.31556	-778.031872	5.363	-778.059818	10.4113	-778.061531
0.42024	-778.034344	5.46554	-778.059899		
0.5244	-778.036321	5.57077	-778.059973		

TS4-5\_MSP3a-->Pw11

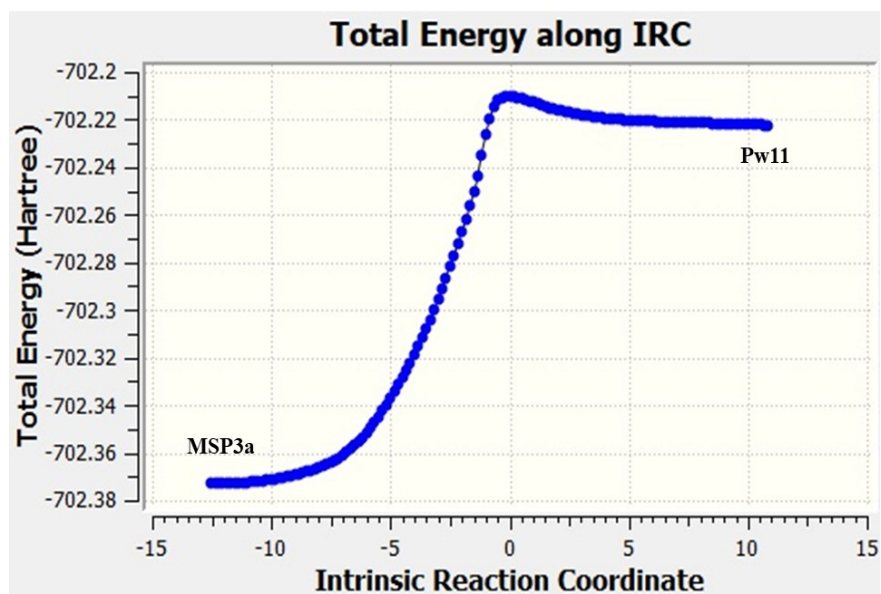


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-702.210294	-702.1478	-702.140405	-702.178674		
M06-2X/DG3/aug-cc-pVTZ	-702.216471	-702.154083	-702.146672	-702.185006		
MN15/cc-pVTZ	-701.919414	-701.857131	-701.849735	-701.88793		
MN15/aug-cc-pVTZ	-701.928172	-701.866019	-701.858612	-701.896839		
SVECV-f12	-702.102119	-702.039731	-702.03232	-702.070653		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	0.050199	-0.095753	-0.382678	<b>479.0372i</b>	917.6307	2105.5033
S	0.167193	0.689183	2.056623	97.6251	966.5764	2999.4367
C	1.771373	-0.071855	2.105243	155.9435	1077.2144	3110.5285
H	-0.947759	0.340982	-0.542904	241.8483	1128.9753	3208.0573
H	0.932474	0.661585	-0.285953	270.0252	1182.9956	
H	2.262496	-0.076743	3.071244	327.4978	1250.2076	
O	0.303916	-1.254412	-0.499524	411.596	1296.7779	
H	1.877627	-0.987179	1.526987	534.1015	1393.9249	
O	2.310463	1.033748	1.329523	701.0888	1469.5538	
O	2.471250	0.770384	0.085406	712.2222	1825.9207	

**Pw11**



<b>Method</b>							<b>Ee</b>			<b>E+ZPE</b>			<b><math>\Delta H</math></b>			<b><math>\Delta G</math></b>								
M06-2X/GD3/cc-pVTZ							-702.222321			-702.159395			-702.149993			-702.194179								
M06-2X/DG3/aug-cc-pVTZ							-702.229282			-702.166575			-702.157101			-702.201955								
MN15/cc-pVTZ							-701.924924			-701.862151			-701.85259			-701.897388								
MN15/aug-cc-pVTZ							-701.933715			-701.871213			-701.86156			-701.906748								
SVECV-f12							-702.100581			-702.037874			-702.0284			-702.073255								
<b>Coordinates (xyz)</b>							<b>Vibrations (cm<sup>-1</sup>)</b>																	
C	0.011474	0.008528	-0.073443	22.7406	861.4535	2958.9377	S	0.093853	0.061956	3.907621	67.726	952.3777	3064.9357	C	1.700553	-0.010143	3.157335	74.5299	1030.0847	3129.9693				
H	-0.603003	-0.080391	-0.984697	141.478	1164.755	3250.8687	H	-0.033438	0.949124	0.495016	152.2634	1210.6423	H	2.528024	-0.278763	3.801466	184.5447	1241.5948	O	0.712101	-0.901589	0.283504	234.306	1291.678
H	-0.033438	0.949124	0.495016	184.5447	1241.5948	H	1.734849	-0.268879	2.105463	442.7843	1481.5786	O	1.310033	1.354371	3.352636	478.4071	1537.3761	O	1.053778	2.026	2.194427	711.4431	1838.5148	

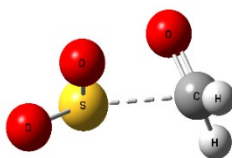


Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-12.52902	-702.372912	-4.67481	-702.331437	3.17549	-702.218284
-12.36187	-702.372888	-4.50765	-702.32844	3.34265	-702.218535
-12.19475	-702.372857	-4.34049	-702.325327	3.50981	-702.218769
-12.02765	-702.372819	-4.17334	-702.322099	3.67698	-702.218985
-11.86056	-702.372771	-4.00619	-702.318745	3.84414	-702.219187
-11.69345	-702.372713	-3.83905	-702.31526	4.0113	-702.219373
-11.52636	-702.372644	-3.6719	-702.311634	4.17846	-702.219546
-11.35927	-702.372564	-3.50476	-702.307863	4.34562	-702.219705
-11.19221	-702.372472	-3.33761	-702.303936	4.51277	-702.219851
-11.02516	-702.372368	-3.17047	-702.299849	4.67993	-702.219985
-10.85813	-702.372249	-3.00333	-702.295597	4.84709	-702.220109
-10.69108	-702.372112	-2.83619	-702.291184	5.01424	-702.220221
-10.52401	-702.371955	-2.66905	-702.286613	5.18139	-702.220324
-10.3569	-702.371772	-2.50191	-702.281893	5.34853	-702.220417
-10.18978	-702.371562	-2.33477	-702.277032	5.51567	-702.220502
-10.02263	-702.371322	-2.16764	-702.272033	5.6828	-702.22058
-9.85548	-702.371052	-2.00051	-702.266888	5.84993	-702.220652
-9.68832	-702.370751	-1.8334	-702.261589	6.01705	-702.220718
-9.52116	-702.370419	-1.66632	-702.256105	6.18418	-702.220779
-9.35399	-702.370055	-1.49981	-702.250339	6.35131	-702.220837
-9.18683	-702.36966	-1.33481	-702.24357	6.51845	-702.220891
-9.01966	-702.369235	-1.16814	-702.235107	6.68558	-702.220943
-8.85251	-702.368784	-1.00103	-702.226484	6.85274	-702.220994
-8.68534	-702.368306	-0.8339	-702.219411	7.01986	-702.221043
-8.5182	-702.367805	-0.66689	-702.214508	7.18702	-702.221093
-8.35106	-702.367276	-0.5004	-702.212011	7.35414	-702.221143

-8.18396	-702.366721	-0.33369	-702.210892	7.52129	-702.221195
-8.01689	-702.366134	-0.16707	-702.210423	7.68841	-702.221248
-7.8499	-702.365508	0	-702.210294	7.85555	-702.221306
-7.68295	-702.364827	0.16703	-702.210399	8.02268	-702.221365
-7.51602	-702.364073	0.33409	-702.210674	8.18984	-702.221428
-7.34907	-702.363222	0.50125	-702.211078	8.35698	-702.22149
-7.18205	-702.36225	0.66838	-702.211569	8.52415	-702.221555
-7.01498	-702.361141	0.83554	-702.21212	8.69128	-702.221618
-6.84787	-702.359887	1.00269	-702.212699	8.85845	-702.221684
-6.68074	-702.358484	1.16985	-702.213286	9.02559	-702.221747
-6.51359	-702.356936	1.33699	-702.213862	9.19275	-702.221812
-6.34644	-702.355243	1.50413	-702.214415	9.35989	-702.221873
-6.17928	-702.353409	1.67127	-702.214939	9.52706	-702.221935
-6.01212	-702.351439	1.8384	-702.215432	9.69421	-702.221992
-5.84495	-702.34934	2.00553	-702.215891	9.86136	-702.222049
-5.67779	-702.347119	2.17265	-702.216315	10.02851	-702.2221
-5.51062	-702.344783	2.33977	-702.216709	10.19566	-702.222147
-5.34346	-702.342334	2.5069	-702.217073	10.36281	-702.222188
-5.17629	-702.339774	2.67404	-702.21741	10.52995	-702.222224
-5.00913	-702.337102	2.84118	-702.217723	10.69711	-702.222254
-4.84197	-702.334323	3.00833	-702.218013	10.86422	-702.222279

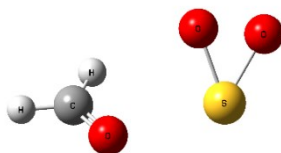


TS4-6\_Im1b\_Pw12

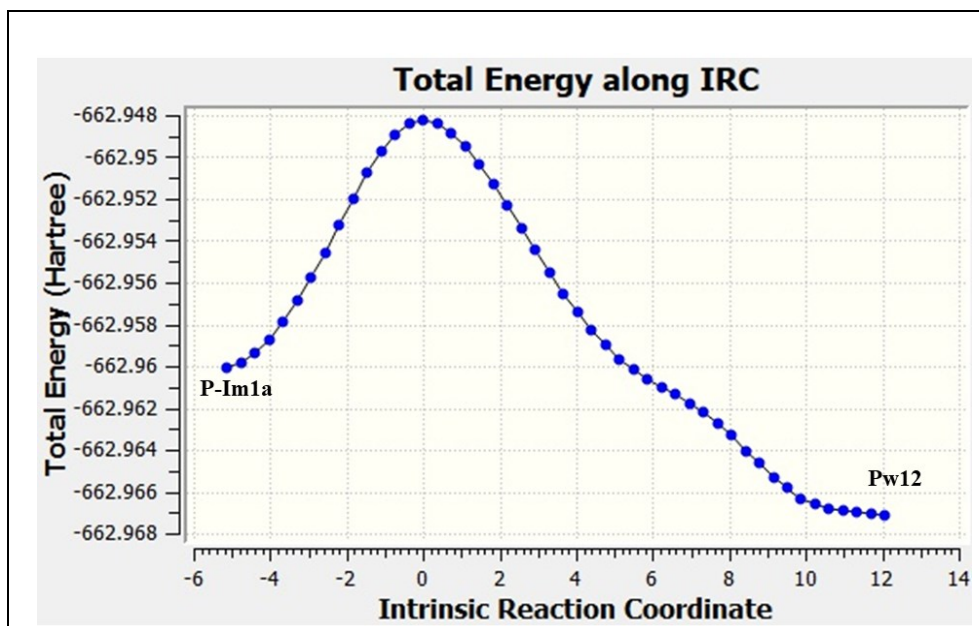


Method	Ee	E+ZPE	$\Delta H$	$\Delta G$		
M06-2X/GD3/cc-pVTZ	-662.948264	-662.911709	-662.905815	-662.940113		
M06-2X/DG3/aug-cc-pVTZ	-662.955562	-662.919071	-662.913158	-662.9475		
MN15/cc-pVTZ	-662.680055	-662.643744	-662.637845	-662.672125		
MN15/aug-cc-pVTZ	-662.68958	-662.653318	-662.647407	-662.681719		
Coordinates (xyz)			Vibrations (cm <sup>-1</sup> )			
C	-0.000934	0.000535	-0.002220	<b>248.5638i</b>	826.863	3117.574
S	-0.000161	-0.000815	2.077430	209.145	1072.437	
H	1.063157	0.000408	-0.258638	231.2508	1151.2541	
H	-0.587003	-0.855076	-0.351199	263.5475	1222.7973	
O	-0.577707	1.068423	0.369220	489.2853	1427.4478	
O	1.184992	-0.233754	3.244868	658.5295	1588.7117	
O	1.390945	0.815582	2.222249	731.1248	3027.8295	

Pw12



Method				Ee	E+ZPE	$\Delta H$	$\Delta G$
M06-2X/GD3/cc-pVTZ				-662.967128	-662.93193	-662.923976	-662.963984
M06-2X/DG3/aug-cc-pVTZ				-662.973399	-662.938212	-662.930274	-662.970242
MN15/cc-pVTZ				-662.698877	-662.663761	-662.655904	-662.695386
MN15/aug-cc-pVTZ				-662.707264	-662.6722	-662.664351	-662.703772
Coordinates (xyz)				Vibrations (cm <sup>-1</sup> )			
C	0.001027	0.001029	-0.000133	46.8705	791.8571	3064.071	
S	-0.019788	0.014551	3.180448	103.2135	1081.9433		
H	1.036037	0.014636	0.374685	140.6056	1226.3006		
H	-0.148115	0.035316	-1.089474	148.5107	1280.3898		
O	-0.934996	-0.047162	0.751017	197.725	1536.2419		
O	1.112346	0.911337	4.021142	248.0754	1847.5181		
O	0.808855	1.353247	2.667004	754.1331	2977.8317		



Rx Coord	Energy	Rx Coord	Energy	Rx Coord	Energy
-5.13335	-662.960052	0.73353	-662.948838	6.59998	-662.961368
-4.76669	-662.95984	1.10035	-662.949494	6.96618	-662.961785
-4.39984	-662.959383	1.46714	-662.950324	7.33156	-662.962179
-4.03307	-662.95872	1.83398	-662.951284	7.69726	-662.962784
-3.66628	-662.957876	2.20079	-662.952321	8.06273	-662.963298
-3.29966	-662.956887	2.56763	-662.953396	8.42785	-662.964057
-2.93316	-662.955772	2.93447	-662.95447	8.79341	-662.964619
-2.56675	-662.954562	3.30131	-662.95552	9.15773	-662.965369
-2.20028	-662.953282	3.66814	-662.95652	9.52328	-662.965822
-1.83372	-662.951997	4.03498	-662.95745	9.88233	-662.966355
-1.46703	-662.950777	4.40181	-662.958286	10.24624	-662.966559
-1.10032	-662.949726	4.76864	-662.959019	10.59899	-662.966809
-0.73355	-662.948923	5.13541	-662.959648	10.9641	-662.966908
-0.36683	-662.948431	5.5021	-662.960179	11.32992	-662.966993
0	-662.948264	5.86847	-662.960622	11.69646	-662.967053
0.36683	-662.948416	6.23462	-662.961016	12.0625	-662.967101

## II. Thermochemistry tables.

This section includes the thermochemical values ( $\Delta E$ ,  $\Delta E+ZPE$ ,  $\Delta G$  and  $\Delta H$ ) relative to reactants in kcal mol<sup>-1</sup> for barrier and final products for each calculated oxidation path. **TZ** stands for cc-pVTZ and **a-TZ** stands for aug-cc-pVTZ.

A. Table S2. Calculated relative energies (kcal mol<sup>-1</sup>) of the gas phase oxidation of AMS initiated by OH radicals in the absence of NO<sub>x</sub> radicals.

REACTION		ENERGY	M06-2X/GD3/TZ		M06-2X/GD3/a-TZ		MN15/TZ		MN15/a-TZ		SVECV-f12	
			Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products
AMS+OH (PRC) → A1	TS	$\Delta E$	-4.01	-34.69	-3.55	-34.06	-6.27	-35.36	-5.83	-34.89	-5.01	-32.12
		$\Delta(E+ZPE)$	-1.74	-30.34	-1.38	-29.76	-4.02	-31.04	-3.68	-30.61	-2.84	-27.82
		$\Delta H$	-2.88	-31.56	-2.46	-30.95	-5.16	-32.28	-4.77	-31.82	-3.92	-29.01
	1-C1	$\Delta G$	7.18	-21.16	7.33	-20.68	4.96	-21.80	5.16	-21.45	5.88	-18.74
A1+3/2O <sub>2</sub> → P1+MSP		$\Delta E$	-61.25	-94.92	-60.62	-94.61	-63.33	-101.38	-62.85	-101.11	-57.85	-92.91
		$\Delta(E+ZPE)$	-56.43	-88.28	-55.85	-80.00	-58.51	-94.67	-58.05	-94.41	-53.08	-80.00
		$\Delta H$	-58.41	-90.35	-57.80	-90.05	-60.55	-96.80	-60.07	-96.54	-55.04	-88.35
	1-1	$\Delta G$	-41.55	-75.85	-41.01	-75.52	-43.50	-82.16	-43.06	-81.87	-38.25	-73.84
A1O +3/2O <sub>2</sub> → P2+P3+HO <sub>2</sub>		$\Delta E$	-59.49	-73.85	-58.92	-73.85	-61.81	-80.19	-61.37	-79.64	-56.00	-75.41
		$\Delta(E+ZPE)$	-55.02	-72.10	-54.46	-72.10	-57.23	-78.44	-56.76	-77.90	-51.54	-70.00
		$\Delta H$	-56.75	-72.71	-56.18	-72.71	-59.04	-79.07	-58.56	-78.52	-53.26	-74.29
	1-2	$\Delta G$	-40.82	-69.92	-40.27	-69.92	-42.84	-76.23	-42.36	-75.27	-37.35	-71.13
A1 → A2 → A2O		$\Delta E$	-1.05	-70.90	-0.69	-70.15	-3.11	-74.83	-2.93	-74.39	-3.27	-68.66
		$\Delta(E+ZPE)$	0.34	-64.65	0.69	-63.95	-1.63	-68.31	-1.40	-67.89	-1.89	-62.47
		$\Delta H$	-0.42	-66.62	-0.06	-65.89	-2.47	-70.44	-2.25	-70.01	-2.65	-64.40
	1-3	$\Delta G$	8.27	-49.77	8.71	-49.19	6.84	-53.07	7.15	-52.66	6.13	-47.70
A1O+3/2O <sub>2</sub> →A2O +3/2O <sub>2</sub> → P2+P3+HO <sub>2</sub>		$\Delta E$	-48.78	-73.85	-48.16	-73.49	-54.54	-80.19	-54.10	-79.64	-46.66	-75.41
		$\Delta(E+ZPE)$	-45.53	-72.10	-44.89	-71.77	-51.02	-78.44	-50.57	-77.90	-43.39	-73.69
		$\Delta H$	-47.98	-72.71	-47.32	-72.37	-53.55	-79.07	-53.09	-78.52	-45.82	-74.29
	1-4	$\Delta G$	-30.08	-69.92	-29.52	-69.21	-35.40	-76.23	-34.96	-75.27	-28.03	-71.13

REACTION	ENERGY	M06-2X/GD3/TZ		M06-2X/GD3/a-TZ		MN15/TZ		MN15/a-TZ		SVECV-fl2	
		Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products
AMS+OH (PRC) → A2 <b>1-C2</b>	$\Delta E$	-1.20	-33.65	-0.67	-32.93	-3.67	-34.26	-3.24	-33.67	-2.13	-31.05
	$\Delta(E+ZPE)$	0.94	-30.70	1.37	-30.06	-1.55	-31.16	-1.16	-30.60	-0.09	-28.18
	$\Delta H$	-0.22	-31.61	0.26	-30.90	-2.74	-32.15	-2.32	-31.55	-1.19	-29.03
	$\Delta G$	10.02	-21.97	10.36	-21.55	7.62	-22.27	7.99	-21.83	8.91	-19.67
A2O +2O <sub>2</sub> → P3+P4+MSP <b>1-5</b>	$\Delta E$	-59.81	-128.48	-59.09	-128.13	-62.23	-136.53	-61.64	-136.12	-56.11	-128.13
	$\Delta(E+ZPE)$	-55.69	-123.63	-55.00	-123.33	-58.10	-131.68	-57.51	-131.26	-52.02	-123.33
	$\Delta H$	-57.37	-125.10	-56.66	-124.80	-59.83	-133.17	-59.22	-132.76	-53.67	-124.80
	$\Delta G$	-41.42	-116.95	-40.84	-116.23	-43.78	-124.98	-43.36	-124.12	-37.86	-116.25
A2O +2O <sub>2</sub> → 2P3+P5+P6+OH <b>1-7</b>	$\Delta E$	-54.29	-149.42	-53.87	-150.75	-55.79	-159.09	-54.98	-160.10	-53.12	-170.37
	$\Delta(E+ZPE)$	-56.69	-151.20	-55.40	-152.57	-57.03	-160.79	-56.21	-161.84	-54.65	-100.00
	$\Delta H$	-56.74	-150.90	-55.24	-143.80	-56.99	-160.52	-56.17	-161.57	-54.49	-171.90
	$\Delta G$	-64.92	-158.57	-63.33	-150.19	-65.24	-168.53	-63.99	-168.33	-62.58	-178.77
A2O + O <sub>2</sub> → 2P3+MSP <b>1-8</b>	$\Delta E$	10.25	-65.19	10.72	-64.62	5.17	-71.51	5.70	-70.91	11.20	-65.38
	$\Delta(E+ZPE)$	8.57	-63.49	9.01	-62.93	3.58	-69.76	4.15	-69.14	9.50	-63.70
	$\Delta H$	8.51	-64.16	8.98	-63.60	3.48	-70.45	4.06	-69.83	9.47	-64.37
	$\Delta G$	10.80	-61.55	11.61	-60.16	5.92	-67.80	6.88	-66.32	12.09	-60.94

B. Table S3. Calculated relative energies (kcal mol<sup>-1</sup>) for the gas phase decomposition of the A1O2 intermediate: C1 addition.

REACTION	ENERGY	M06-2X/GD3/TZ		M06-2X/GD3/a-TZ		MN15/TZ		MN15/a-TZ		
		Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products	
A1O2(Im1) + O <sub>2</sub> → P3+P6+P9+OH	TS	ΔE	-25.84	-118.53	-24.92	-119.83	-31.82	-126.62	-31.10	-127.87
		Δ(E+ZPE)	-20.71	-117.12	-19.85	-85.00	-26.64	-125.22	-26.00	-126.53
		ΔH	-22.63	-117.63	-21.73	-119.03	-28.59	-125.72	-27.90	-127.01
	2-6	ΔG	-1.81	-118.35	-1.07	-119.42	-7.60	-126.84	-7.19	-127.34
A1O2(Im1) → P2+P3+OH		ΔE	-43.29	-65.81	-41.78	-66.03	-49.83	-68.89	-48.62	-69.04
		Δ(E+ZPE)	-38.70	-66.58	-37.24	-66.82	-45.34	-69.62	-44.17	-69.76
		ΔH	-41.72	-66.46	-40.24	-66.69	-48.35	-69.51	-47.16	-69.66
	2-2	ΔG	-17.56	-67.37	-16.14	-67.23	-24.20	-70.39	-23.05	-70.12
A1O2(Im2) → P2+P3+OH		ΔE	-14.63	-65.81	-15.23	-66.03	-18.92	-68.89	-19.42	-69.04
		Δ(E+ZPE)	-15.35	-66.58	-15.97	-66.82	-19.62	-69.62	-20.10	-69.76
		ΔH	-15.22	-66.46	-15.83	-66.69	-19.50	-69.51	-19.98	-69.66
	P3	ΔG	-16.18	-67.37	-16.83	-67.23	-20.42	-70.39	-20.89	-70.12
A1O2(Im3) → P10+OH		ΔE	-19.40	-95.51	-18.98	-95.89	-43.62	-98.20	-44.22	-98.68
		Δ(E+ZPE)	-15.63	-91.53	-15.39	-75.00	-39.37	-94.28	-39.93	-94.79
		ΔH	-17.59	-92.41	-17.28	-92.84	-41.54	-95.14	-42.06	-95.62
	2-7	ΔG	3.98	-81.05	4.11	-81.73	-19.25	-83.87	-19.87	-84.59
Im3_1 → P11+HO <sub>2</sub>		ΔE	-46.26	-48.57	-45.46	-48.36	-52.37	-53.63	-51.92	-53.61
		Δ(E+ZPE)	-39.82	-43.75	-39.13	-43.59	-45.96	-48.79	-45.59	-48.78
		ΔH	-41.85	-44.96	-41.11	-44.79	-48.03	-50.03	-47.62	-50.02
	2-8	ΔG	-20.31	-35.32	-19.77	-35.16	-26.26	-40.30	-25.97	-40.27
A1O2(Im3) → P1+P12+OH		ΔE	-50.44	-26.00	-49.25	-27.20	-55.51	-31.44	-54.63	-32.68
		Δ(E+ZPE)	-45.13	-26.60	-43.99	-27.81	-50.26	-31.89	-49.43	-33.05
		ΔH	-48.27	-26.94	-47.12	-28.16	-53.41	-32.30	-52.56	-33.49
	2-5	ΔG	-23.84	-27.13	-22.75	-28.76	-28.92	-32.75	-28.10	-33.89
A1O2+NO <sub>2</sub> → P1+MSP+NO <sub>3</sub>		ΔE	--	-80.26	--	-79.96	--	-91.48	-	-91.11
		Δ(E+ZPE)	--	-72.47	--	-72.12	--	-84.28	-	-84.01
		ΔH	--	-75.20	--	-74.89	--	-87.00	-	-86.70
	NO <sub>x</sub>	ΔG	--	-55.66	--	-54.88	--	-66.98	-	-66.72

C. Table S4. Calculated relative energies (kcal mol<sup>-1</sup>) for the gas phase decomposition of the A2O2 intermediate: C2 addition.

REACTION	ENERGY	M06-2X/GD3/TZ		M06-2X/GD3/a-TZ		MN15/TZ		MN15/a-TZ	
		Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products
TS A2O2(Im1) → P2+P3+OH	$\Delta E$	15.97	-65.81	15.42	-66.03	11.20	-68.89	10.73	-69.04
	$\Delta(E+ZPE)$	-33.81	11.49	-33.10	10.89	-40.55	6.84	-40.01	6.37
	$\Delta H$	11.72	-66.46	11.13	-66.69	7.04	-69.51	6.58	-69.66
	$\Delta G$	10.59	-67.37	10.36	-67.23	6.02	-70.39	5.94	-70.12
3-5 A2O2(Im1) → P2+P3+OH	$\Delta E$	-45.42	-65.81	-44.49	-66.03	-50.45	-68.89	-49.54	-69.04
	$\Delta(E+ZPE)$	-44.31	-40.05	-43.19	-39.13	-50.16	-45.06	-49.23	-44.18
	$\Delta H$	-42.14	-66.46	-41.21	-66.69	-47.21	-69.51	-46.32	-69.66
	$\Delta G$	-20.80	-67.37	-19.88	-67.23	-25.71	-70.39	-24.84	-70.12
A2O2(Im2) → P3+P13+OH	$\Delta E$	-47.61	-64.26	-46.52	-64.78	-53.07	-68.55	-52.34	-69.00
	$\Delta(E+ZPE)$	-42.81	-64.12	-41.78	-64.68	-48.27	-68.32	-47.58	-68.75
	$\Delta H$	-45.58	-64.09	-44.52	-64.64	-51.09	-68.32	-50.38	-68.75
	$\Delta G$	-22.00	-65.05	-21.02	-65.29	-27.29	-69.24	-26.65	-69.21
3-7 A2O2+NO <sub>2</sub> → P7+P8	$\Delta E$	-57.80	-146.21	-56.46	-145.45	-65.70	-150.49	-64.67	-149.76
	$\Delta(E+ZPE)$	-49.87	-136.72	-48.62	-136.09	-57.98	-141.17	-56.99	-140.52
	$\Delta H$	-53.14	-139.23	-51.86	-138.55	-61.20	-143.69	-60.18	-143.00
	$\Delta G$	-17.92	-117.48	-16.38	-116.66	-25.60	-121.40	-24.70	-120.95
NO <sub>x</sub>									



D. Table S5. Calculated relative energies (kcal mol<sup>-1</sup>) for the gas phase decomposition of the MSP intermediate.

REACTION	ENERGY	M06-2X/GD3/TZ		M06-2X/GD3/a-TZ		MN15/TZ		MN15/a-TZ	
		Barrier	Products	Barrier	Products	Barrier	Products	Barrier	Products
2MSP→2P3+DMDS	$\Delta E$	--	-125.86	--	-125.79	--	-129.20	--	-129.46
	$\Delta(E+ZPE)$	--	-122.64	--	-122.59	--	-125.96	--	-126.20
	$\Delta H$	--	-123.54	--	-123.50	--	-126.93	--	-127.17
	$\Delta G$	--	-119.78	--	-119.33	--	-122.57	--	-123.43
MSP+O <sub>2</sub> →2P3+P6+OH	$\Delta E$	--	-188.08	--	-189.99	--	-199.57	--	-201.27
	$\Delta(E+ZPE)$	--	-187.37	--	-189.33	--	-198.73	--	-200.50
	$\Delta H$	--	-187.76	--	-189.72	--	-199.20	--	-200.96
	$\Delta G$	--	-189.51	--	-190.66	--	-201.20	--	-201.72
MSP→MSP1→P3+P14+OH	$\Delta E$	-57.65	-78.48	-57.51	-79.56	-66.37	-84.07	-66.21	-85.01
	$\Delta(E+ZPE)$	-53.90	-79.89	-53.82	-80.98	-62.64	-85.33	-62.53	-86.27
	$\Delta H$	-55.53	-79.64	-55.42	-80.74	-63.66	-85.15	-63.50	-86.08
	$\Delta G$	-42.22	-86.06	-42.24	-86.75	-52.20	-91.41	-51.99	-91.93
MSP1+O <sub>2</sub> →MSP2→2P3+P15+OH	$\Delta E$	-39.46	-129.09	-40.30	-130.85	-55.44	-135.32	-56.14	-137.07
	$\Delta(E+ZPE)$	-36.81	-129.97	-37.70	-131.76	-52.63	-136.09	-53.38	-137.89
	$\Delta H$	-38.81	-129.75	-39.69	-131.54	-54.70	-135.94	-55.44	-137.73
	$\Delta G$	-22.26	-136.93	-23.19	-137.90	-37.93	-142.96	-38.69	-143.92
MSP2+1/2O <sub>2</sub> →2P3+P6+OH	$\Delta E$	-47.88	-188.08	-50.28	-189.99	-58.42	-199.57	-60.70	-201.27
	$\Delta(E+ZPE)$	-44.87	-187.37	-47.28	-189.33	-55.32	-198.73	-57.60	-200.50
	$\Delta H$	-46.32	-187.76	-48.72	-189.72	-56.81	-199.20	-59.09	-200.96
	$\Delta G$	-41.76	-189.51	-44.17	-190.66	-52.11	-201.20	-54.38	-201.72
MSP2→MSP3+O <sub>2</sub> →P3+P16+HO <sub>2</sub> +2OH	$\Delta E$	-89.76	-127.30	-92.32	-129.62	-96.80	-139.15	-99.07	-141.05
	$\Delta(E+ZPE)$	-92.39	-128.94	-94.96	-131.29	-99.34	-140.59	-101.64	-142.55
	$\Delta H$	-91.86	-128.45	-94.43	-130.81	-98.85	-140.18	-101.15	-142.13
	$\Delta G$	-98.90	-134.71	-101.05	-136.66	-105.78	-146.27	-107.66	-147.81
MSP3→MSP3-b+2OH+O <sub>2</sub> →P17+2OH+HO <sub>2</sub>	$\Delta E$	-92.32	-124.08	-94.45	-126.41	-100.62	-136.39	-102.74	-138.51
	$\Delta(E+ZPE)$	-92.69	-123.84	-94.93	-126.22	-100.74	-135.90	-102.93	-138.09
	$\Delta H$	-93.07	-124.05	-95.30	-126.42	-101.26	-136.19	-103.43	-138.37
	$\Delta G$	-88.95	-120.40	-91.18	-122.81	-96.48	-132.34	-98.69	-134.55
MSP3→MSP3-a+OH+O <sub>2</sub> →2P3+P15+OH	$\Delta E$	-71.46	-129.09	-72.01	-130.85	-83.91	-135.32	-84.59	-137.07
	$\Delta(E+ZPE)$	-63.55	-129.97	-64.14	-131.76	-75.88	-136.09	-76.57	-137.89
	$\Delta H$	-66.51	-129.75	-67.09	-131.54	-78.92	-135.94	-79.62	-137.73
	$\Delta G$	-40.30	-136.93	-40.95	-137.90	-52.45	-142.96	-53.12	-143.92