

## Supplementary Material

# Theoretical Investigation of Oxidative Cleavage of Cholesterol by Dual O<sub>2</sub> Activation and Sulfide Reduction

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## Detailed Computational methods

Density functional theory (DFT) calculations were carried out with Gaussian 09<sup>1</sup> suite of programs. The minimum crossing point energy (MECP) was located with a FORTRAN script written by Harvey *et al.*<sup>2</sup> evoking iterative calculations with Gaussian 09. Mulliken population analyses<sup>3</sup> were performed with AOMix program<sup>4</sup> to derive the local site reactivity descriptor, the Fukui condensed function<sup>5</sup>. Electronic structural and geometry graphics were rendered with CYLview<sup>6</sup>. The reduced density gradient based non-covalent interactions were calculated with NCIPLOT program<sup>7</sup> and 3-D volumes were plotted with VMD<sup>8</sup>.

To properly describe the energy of the broken symmetry <sup>1</sup>O<sub>2</sub> and singlet diradical peroxy complexes with density functional theory, the spin-projection technique developed by Yamaguchi and co-workers is adapted in our computations for accuracy.<sup>9</sup> The singlet spin-projected energy,  $E_{BS}^{SP}$  is estimated from equations (1) and (2):

$$E_{BS}^{SP} = \alpha E_{BS} + (1 - \alpha) E_{HS} \quad (1)$$

$$\alpha = \frac{HS \langle S^2 \rangle - \langle S^2 \rangle_{exact}^{LS}}{HS \langle S^2 \rangle - BS \langle S^2 \rangle} \quad (2)$$

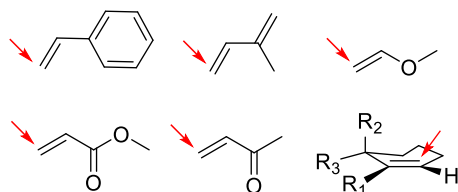
The spin-projection method is a cost effective and reliable technique that can reproduce energy trends that are comparable to multi-reference methods such as CASSCF and CAS-PT2<sup>10</sup>. A survey of DFT methods was carried out to select an appropriate functional (see Table S1). On this basis, we selected the Minnesota meta hybrid functional M11 (an improved version of the Minnesota 06 functional series)<sup>11</sup> with Pople's basis set 6-31+G(d,p)<sup>12</sup>. This level of theory produced a value for the energy gap between the desired triplet ground state (<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) and lowest excited singlet oxygen (<sup>1</sup>Δ<sub>g</sub>) of 21.7 kcal mol<sup>-1</sup>, which is close to the experimental value of 22.5 kcal mol<sup>-1</sup><sup>13</sup>. This chosen level of theory is thus used for all the geometry optimizations, frequency calculations and electronic energies reported in this study.

Solvation Gibbs free energies were calculated on optimized geometries with Cramer and Truhlar's SMD polarizable continuum solvation model<sup>14</sup> at the M11/6-31+G(d,p) level of theory. The calculations were performed in water. The Gibbs free energy of solvation  $\Delta G_{solv}$  was combined with the gas phase free energy so as to obtain free energy of solution  $G_{sol}$  as follows:  $G_{sol} = G_{gas} + \Delta G_{solv} + \Delta nRT \ln(RT/P^\circ)$ . The term  $\Delta nRT \ln(RT/P^\circ)$  is the correction term that accounts for passage of molecules from 1 atm to 1 mol/L in solution. The gas-phase Gibbs free energies at 298 K were calculated using the M11 geometries and frequencies in conjunction with the harmonic oscillator approximation. The enthalpy in the solution phase was obtained from the temperature dependence of  $G_{sol}$ . The single imaginary frequency of transition states were visually inspected to ensure they were first order saddle-point structures and had the features required for bond breaking or forming. Intrinsic reaction coordinate (IRC) calculations were also performed at this level to confirm the connectivity of the transition state structures with their intermediates.

**Table S1. Summary of DFT methods and the spin-projected energies<sup>a</sup>**

Functional/ 6-31+G(d,p)	$E_{BS}$	$E_{HS}$	$E_{BS}^{SP}$	$^{HS}\langle S^2 \rangle$	$^{BS}\langle S^2 \rangle$	$\Delta E_{S-T}$
B3LYP	-150.3110038	-150.327576	-150.294430	2.0000	1.0000	20.8
M06-2X	-150.2639480	-150.279856	-150.219285	1.9969	0.9969	28.0
M11	-150.2495452	-150.266872	-150.232213	2.0000	1.0000	21.7
M11-L	-150.2238629	-150.244360	-150.203372	1.9997	0.9997	25.7

<sup>a</sup>  $E_{BS}$  and  $E_{HS}$  both corresponds to electronic energies of the broken symmetry and high spin states respectively.  $E_{BS}^{SP}$  is the spin-projected approximate energy derived by using equations (1) and (2).  $^{HS}\langle S^2 \rangle$  is the spin squared expectant value for the high spin state and  $^{BS}\langle S^2 \rangle$  for the broken symmetry singlet diradical.  $\Delta E_{S-T}$  is the singlet-triplet energy gap between  $E_{BS}^{SP}$  and  $E_T$ .

**Table S2. Summary of Global Nucleophilicity Indices**

Entry	Molecule	HOMO (eV)	$N^\circ$ <sup>a</sup>
1	<b>chol</b>	-0.33264	0.102
2	styrene	-0.32453	0.110
3	isoprene	-0.33083	0.104
4	acrylate	-0.39804	0.037
5	butenone	-0.37131	0.063
6	vinyl methyl ether	-0.33695	0.098
Cyclohexene & derivatives			
7	R <sub>1</sub> = H, R <sub>2</sub> = H, R <sub>3</sub> = H ( <b>ch1</b> )	-0.3396	0.095
8	R <sub>1</sub> = CH <sub>3</sub> , R <sub>2</sub> = H, R <sub>3</sub> = H ( <b>ch2</b> )	-0.32817	0.107
9	R <sub>1</sub> = H, R <sub>2</sub> = CH <sub>3</sub> , R <sub>3</sub> = H ( <b>ch3</b> )	-0.34078	0.094
10	R <sub>1</sub> = H, R <sub>2</sub> = H, R <sub>3</sub> = CH <sub>3</sub> ( <b>ch4</b> )	-0.34029	0.094
11	R <sub>1</sub> =CH <sub>3</sub> , R <sub>2</sub> = CH <sub>3</sub> , R <sub>3</sub> = H ( <b>ch5</b> )	-0.32882	0.106
12	R <sub>1</sub> =CH <sub>3</sub> , R <sub>2</sub> = H, R <sub>3</sub> = CH <sub>3</sub> ( <b>ch6</b> )	-0.32794	0.107

<sup>a</sup> The  $N^\circ$  index<sup>15</sup> is derived simply by subtracting the  $E_{HOMO}$  of the alkene nucleophile by  $E_{HOMO}$  of electrophile which is  $^3O_2$  in our context.  $N^\circ = E_{HOMO}[\text{alkene}] - E_{HOMO}[^3O_2]$ ;  $E_{HOMO}[^3O_2] = -0.43475$  eV

**Table S3. Summary of energies and corrections at M11/6-31+G(d,p) level of theory<sup>a</sup>**

Molecules	M11/6-31+G(d,p)	E(approx. proj.)	$\Delta G_{\text{solv}}$	$G_{\text{correction}}$	$H_{\text{correction}}$	$G_{\text{gas}}$	$H_{\text{gas}}$	$S_{\text{gas}}$	$G_{\text{soln}}$	$H_{\text{soln}}$
<b>1O2</b>	-150.266872	-150.2322131	-0.000685248	-0.014913	0.007308	-150.2471261	-150.2249051	7.45671E-05	-150.2478114	-150.2255904
<b>3O2</b>	-150.266872		-0.000685248	-0.015923	0.007334	-150.282795	-150.259538	7.80436E-05	-150.2834802	-150.2602232
<b>chol</b>	-504.9550739		-0.010007809	0.235864	0.283803	-504.7192099	-504.6712709	0.000160869	-504.7292177	-504.6812787
<b>Me2S</b>	-477.9241041		-0.0015936	0.048425	0.081419	-477.8756791	-477.8426851	0.000110718	-477.8772727	-477.8442787
<b>DMSO</b>	-553.082549		-0.020206849	0.050755	0.085886	-553.031794	-552.996663	0.000117889	-553.0520008	-553.0168698
<b>1a-S</b>	-655.2266386	-655.192227	-0.010454017	0.234721	0.292641	-654.957506	-654.899586	0.000194362	-654.96796	-654.91004
<b>1b-S</b>	-655.2270333	-655.1925438	-0.010597441	0.234307	0.292477	-654.9582368	-654.9000668	0.000195201	-654.9688342	-654.9106642
<b>TS1a-S</b>	-655.181902	-655.1714304	-0.016669057	0.237006	0.290134	-654.9344244	-654.8812964	0.000178282	-654.9510935	-654.8979655
<b>TS1b-S</b>	-655.1822498	-655.1729236	-0.017370241	0.236811	0.290828	-654.9361126	-654.8820956	0.000181265	-654.9534828	-654.8994658
<b>TS1c-S</b>	-655.1748304	-655.1673529	-0.018262657	0.23645	0.290028	-654.9309029	-654.8773249	0.000179792	-654.9491656	-654.8955876
<b>TS1d-S</b>	-655.1844641	-655.1725253	-0.018103297	0.23646	0.290586	-654.9360653	-654.8819393	0.000181631	-654.9541686	-654.9000426
<b>TS1e-S</b>	-655.1739737		-0.019904065	0.239451	0.291072	-654.9345227	-654.8829017	0.000173225	-654.9544267	-654.9028057
<b>TS1f-S</b>	-655.170687		-0.023266561	0.238714	0.291413	-654.931973	-654.879274	0.000176842	-654.9552396	-654.9025406
<b>TS1g-S</b>	-655.168801		-0.022724737	0.237846	0.290141	-654.930955	-654.87866	0.000175487	-654.9536798	-654.9013848
<b>TS1h-S</b>	-655.1639019		-0.027521474	0.23888	0.291153	-654.9250219	-654.8727489	0.000175413	-654.9525434	-654.9002704
<b>TS1i-S</b>	-655.1682013		-0.017832385	0.238004	0.290435	-654.9301973	-654.8777663	0.000175943	-654.9480297	-654.8955987
<b>2-S</b>	-655.2648415		-0.019298497	0.241939	0.294204	-655.0229025	-654.9706375	0.000175386	-655.042201	-654.989936
<b>2a-S</b>	-655.1992754		-0.035059202	0.242455	0.293891	-654.9568204	-654.9053844	0.000172604	-654.9918796	-654.9404436
<b>2b-S</b>	-655.2527064		-0.021880129	0.240425	0.294654	-655.0122814	-654.9580524	0.000181977	-655.0341616	-654.9799326
<b>1a-T</b>	-655.2266386		-0.010438081	0.232523	0.29263	-654.9941156	-654.9340086	0.000201701	-655.0045537	-654.9444467
<b>1b-T</b>	-655.2270333		-0.010597441	0.233457	0.292503	-654.9935763	-654.9345303	0.000198141	-655.0041737	-654.9451277
<b>TS1a-T</b>	-655.181902		-0.016206913	0.236175	0.290075	-654.945727	-654.891827	0.000180872	-654.9619339	-654.9080339
<b>TS1b-T</b>	-655.1822498		-0.016621249	0.235792	0.290937	-654.9464578	-654.8913128	0.00018505	-654.9630791	-654.9079341
<b>TS1c-T</b>	-655.1748304		-0.017083393	0.23564	0.289942	-654.9391904	-654.8848884	0.000182221	-654.9562738	-654.9019718
<b>TS1d-T</b>	-655.1844641		-0.017912065	0.236056	0.290638	-654.9484081	-654.8938261	0.000183161	-654.9663202	-654.9117382
<b>2-T</b>	-655.1920012		-0.016939969	0.237668	0.292427	-654.9543332	-654.8995742	0.000183755	-654.9712732	-654.9165142
<b>2-Q</b>	-805.4649159		-0.017752705	0.236888	0.301313	-805.2280279	-805.1636029	0.000216191	-805.2457806	-805.1813556

<b>1-Q</b>	-805.4986817		-0.011043649	0.231598	0.301358	-805.2670837	-805.1973237	0.000234094	-805.2781273	-805.2083673
<b>TS2a-Q</b>	-805.4528085		-0.017354305	0.234633	0.299038	-805.2181755	-805.1537705	0.000216124	-805.2355298	-805.1711248
<b>TS2-Q</b>	-805.4571419		-0.018900097	0.234613	0.299363	-805.2225289	-805.1577789	0.000217282	-805.241429	-805.176679
<b>1-T</b>	-805.4986817	-805.4756753	-0.011027713	0.232635	0.301386	-805.2430403	-805.1742893	0.000230708	-805.254068	-805.185317
<b>TS2a-T</b>	-805.4528085	-805.4461325	-0.017943937	0.234887	0.299178	-805.2112455	-805.1469545	0.000215742	-805.2291894	-805.1648984
<b>TS2-T</b>	-805.4571419	-805.4489668	-0.018931969	0.233367	0.299188	-805.2155998	-805.1497788	0.000220876	-805.2345318	-805.1687108
<b>MECP1</b>	-805.4644083									
<b>3-T</b>	-805.520192		-0.019346305	0.246679	0.304293	-805.273513	-805.215899	0.000193336	-805.2928593	-805.2352453
<b>MECP2</b>	-1283.393463									
<b>1c-Q</b>	-1283.426946		-0.014358337	0.297811	0.385204	-1283.129135	-1283.041742	0.000293265	-1283.143493	-1283.0561
<b>TS1-Q</b>	-1283.386586		-0.021465793	0.29935	0.382514	-1283.087236	-1283.004072	0.000279074	-1283.108702	-1283.025538
<b>3-Q</b>	-1283.394183		-0.020525569	0.302318	0.384667	-1283.091865	-1283.009516	0.000276339	-1283.11239	-1283.030041
<b>1c-T</b>	-1283.426946	-1283.392466	-0.014358337	0.298091	0.385172	-1283.094375	-1283.007294	0.000292218	-1283.108734	-1283.021653
<b>TS1-T</b>	-1283.386586	-1283.374216	-0.021481729	0.298575	0.382522	-1283.075641	-1282.991694	0.000281701	-1283.097122	-1283.013175
<b>4-T</b>	-1283.448255		-0.021370177	0.310624	0.387641	-1283.137631	-1283.060614	0.000258446	-1283.159001	-1283.081984
<b>5-T</b>	-1283.4493		-0.021386113	0.311076	0.387994	-1283.138224	-1283.061306	0.000258114	-1283.15961	-1283.082692
<b>TS3a-T</b>	-1283.405352		-0.025035458	0.314053	0.385267	-1283.091299	-1283.020085	0.000238973	-1283.116334	-1283.04512
<b>TS3-T</b>	-1283.407523		-0.027999554	0.314619	0.385386	-1283.092904	-1283.022137	0.000237473	-1283.120903	-1283.050136
<b>6-T</b>	-1283.472812		-0.035441666	0.312083	0.385937	-1283.160729	-1283.086875	0.000247832	-1283.19617	-1283.122316
<b>MECP3</b>	-1283.471624									
<b>6-S</b>	-1283.472812	-1283.474793	-0.035377922	0.313138	0.385869	-1283.161655	-1283.088924	0.000244064	-1283.197032	-1283.124301
<b>TS4-S</b>	-1283.467596	-1283.479558	-0.03861293	0.311157	0.384377	-1283.168401	-1283.095181	0.000245705	-1283.207013	-1283.133793
<b>TS4-T</b>	-1283.450408		-0.038995394	0.310593	0.383092	-1283.139815	-1283.067316	0.000243285	-1283.17881	-1283.106311
<b>7-S</b>	-1283.530179		-0.035999426	0.312328	0.386666	-1283.217851	-1283.143513	0.000249456	-1283.25385	-1283.179512
<b>TS5-S</b>	-1283.513015		-0.03160109	0.314079	0.385571	-1283.198936	-1283.127444	0.000239906	-1283.230537	-1283.159045
<b>8-S</b>	-730.4908306		-0.019155073	0.249451	0.300805	-730.2413796	-730.1900256	0.000172329	-730.2605347	-730.2091807
<b>Reactivity studies <sup>b</sup></b>										
<b>isoprene</b>	-195.1790934		0.000685248	0.084386	0.119791	-195.0947074	-195.0593024	0.000118809	-195.0940221	-195.0586171
<b>TS1_isoprene</b>	-345.4086332		-0.006724992	0.083414	0.126519	-345.3252192	-345.2821142	0.000144648	-345.3319442	-345.2888392
<b>styrene</b>	-309.4508255		-0.003235008	0.101744	0.140881	-309.3490815	-309.3099445	0.000131332	-309.3523165	-309.3131795

<b>TS1_styrene</b>	-459.6803681	-0.010501825	0.101999	0.147852	-459.5783691	-459.5325161	0.000153869	-459.5888709	-459.5430179
<b>butenone</b>	-231.111729	-0.008382337	0.060605	0.096059	-231.051124	-231.01567	0.000118973	-231.0595063	-231.0240523
<b>TS1_butenone</b>	-381.334214	-0.013991809	0.059924	0.102929	-381.27429	-381.231285	0.000144312	-381.2882818	-381.2452768
<b>acrylate</b>	-306.3266772	-0.005832576	0.065173	0.103034	-306.2615042	-306.2236432	0.00012705	-306.2673368	-306.2294758
<b>TS1_acrylate</b>	-456.547612	-0.012541633	0.067953	0.110809	-456.479659	-456.436803	0.000143812	-456.4922006	-456.4493446
<b>ether</b>	-193.0160641	-0.00191232	0.058718	0.090954	-192.9573461	-192.9251101	0.000108174	-192.9592585	-192.9270225
<b>TS1_ehter</b>	-343.2383354	-0.010294657	0.057996	0.098226	-343.1803394	-343.1401094	0.000135	-343.1906341	-343.1504041
<b>ch1</b>	-234.497643	0.000175296	0.117021	0.152148	-234.380622	-234.345495	0.000117876	-234.3804467	-234.3453197
<b>TS1_ch1</b>	-384.7220722	-0.007968001	0.11573	0.158637	-384.6063422	-384.5634352	0.000143983	-384.6143102	-384.5714032
<b>ch2</b>	-273.7910509	0.000844608	0.142455	0.181256	-273.6485959	-273.6097949	0.000130205	-273.6477513	-273.6089503
<b>TS1_ch2</b>	-424.0199048	-0.007282752	0.141986	0.188014	-423.8779188	-423.8318908	0.000154456	-423.8852015	-423.8391735
<b>ch3</b>	-273.7868757	0.000733056	0.143076	0.181492	-273.6437997	-273.6053837	0.000128913	-273.6430667	-273.6046507
<b>TS1_ch3</b>	-424.0118975	-0.00725088	0.142768	0.188216	-423.8691295	-423.8236815	0.00015251	-423.8763804	-423.8309324
<b>ch4</b>	-273.7876109	0.000844608	0.142866	0.181314	-273.6447449	-273.6062969	0.00012902	-273.6439003	-273.6054523
<b>TS1_ch4</b>	-424.0120552	-0.0071712	0.141621	0.187807	-423.8704342	-423.8242482	0.000154987	-423.8776054	-423.8314194
<b>ch5</b>	-313.0797572	0.00135456	0.168665	0.210717	-312.9110922	-312.8690402	0.000141114	-312.9097377	-312.8676857
<b>TS1_ch5</b>	-463.3100341	-0.006342528	0.169405	0.217686	-463.1406291	-463.0923481	0.000162017	-463.1469716	-463.0986906
<b>ch6</b>	-313.0801592	0.001386432	0.169168	0.210642	-312.9109912	-312.8695172	0.000139174	-312.9096047	-312.8681307
<b>TS1_ch6</b>	-463.30913	-0.006900288	0.168324	0.21733	-463.140806	-463.0918	0.00016445	-463.1477063	-463.0987003

<sup>a</sup> All values are in Hatrees. <sup>b</sup> See table S4 for nomenclature.

## References

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## Cartesian coordinates

### Chol

C	0.794531	2.87425	-0.21765
C	1.566382	2.48047	-1.47409
C	1.02805	2.513012	-2.69872
C	-0.36393	3.002824	-3.01119
H	-1.01286	2.140885	-3.24455
H	-0.33825	3.618846	-3.92272
C	-0.94754	3.794728	-1.83932
H	-0.46608	4.784024	-1.7916
H	-2.0222	3.970506	-1.98966
C	-0.70476	3.031284	-0.53663
H	-1.15308	2.027475	-0.63269
H	-1.20274	3.524404	0.313631
C	2.994057	2.029479	-1.25156
H	3.610646	2.865291	-0.87927
H	3.434951	1.701446	-2.20624
C	1.34769	4.197971	0.34792
H	2.42424	4.143297	0.556544
H	0.835024	4.446785	1.289772
H	1.192149	5.024256	-0.35923
C	0.959333	1.748877	0.832003
H	0.408499	0.862517	0.473399
H	0.474955	2.064654	1.770228
C	2.414596	1.349323	1.089301
H	2.99605	2.186046	1.507833
H	2.469256	0.528555	1.818239
C	3.078047	0.909873	-0.20801
H	1.639675	2.178052	-3.54345
H	2.548432	0.017494	-0.59463
O	4.43018	0.578225	0.094742
H	4.879931	0.288715	-0.70701

### Me<sub>2</sub>S

S	0.528311	0.367504	-0.58746
C	0.085508	1.713187	-1.72178
H	0.976174	2.275547	-2.03031
H	-0.63907	2.394392	-1.25728
H	-0.373	1.263176	-2.60945
C	1.22525	1.378673	0.749003
H	1.559785	0.699466	1.541058
H	0.468303	2.057779	1.161914
H	2.086946	1.957873	0.39299

### DMSO

S	0.000046	0.229779	-0.45164
C	-1.35292	-0.80404	0.186931
H	-2.29117	-0.29351	-0.05457
H	-1.24571	-0.88366	1.275733
H	-1.32824	-1.79178	-0.28995
C	1.352432	-0.80481	0.1869
H	2.290978	-0.295	-0.05499
H	1.326965	-1.79275	-0.2895
H	1.245334	-0.8838	1.275758
O	0.0005	1.489641	0.390095

### TS1a-S

Imaginary frequency = 549.6196i cm<sup>-1</sup>

C	-1.55337	-0.49221	-1.45039
C	-2.68857	-0.31576	-0.44435
O	-1.92248	-1.26139	1.062079
O	-2.79318	-1.67108	1.869524
C	-2.80873	0.915906	0.217204
H	-3.7259	1.10285	0.782202
C	-1.64293	1.824671	0.454474
H	-1.98267	2.869419	0.512842
H	-1.25504	1.581655	1.463004
C	-3.91988	-1.15755	-0.6726
H	-4.46761	-0.76125	-1.54375
C	-1.28493	-1.98952	-1.70584
H	-0.55266	-2.07491	-2.5245
H	-0.81455	-2.42478	-0.81047
C	-2.55269	-2.77902	-2.0494
H	-2.32001	-3.84527	-2.17588
C	-1.98967	0.181834	-2.77116
H	-1.15078	0.168465	-3.48371
H	-2.29453	1.225022	-2.61385
H	-2.83609	-0.33752	-3.23781
C	-0.281	0.190982	-0.91467
H	0.513623	0.094297	-1.67177
H	0.060458	-0.34854	-0.01704
C	-0.5112	1.665934	-0.57115
H	-0.75249	2.230703	-1.48337
H	0.411313	2.108075	-0.17008
H	-4.58322	-1.07016	0.201854
H	-2.99595	-2.44029	-2.99853



C	-3.60125	-2.63432	-0.95459
H	-3.22347	-3.10589	-0.03281
O	-4.77305	-3.31598	-1.39792
H	-5.39542	-3.39525	-0.66633

**TS1b-S**

597.4269i cm<sup>-1</sup>

C	0.694728	0.144507	-1.03768
C	-0.49805	0.469899	-0.16207
O	0.18177	0.524248	2.269417
O	-0.75043	-0.0905	2.849873
C	-0.46475	1.501842	0.784793
H	-1.4075	1.720841	1.295768
C	0.541179	2.628771	0.710298
H	0.004068	3.587822	0.722755
H	1.148949	2.60024	1.629535
C	-1.63722	-0.50727	-0.16204
H	-2.1378	-0.52797	-1.14618
C	1.110238	-1.32473	-0.76887
H	1.919879	-1.59217	-1.46666
H	1.530907	-1.37823	0.249696
C	-0.04763	-2.31899	-0.87416
H	0.296808	-3.33868	-0.65329
C	0.312001	0.311627	-2.52469
H	1.154847	0.001303	-3.16033
H	0.070276	1.357179	-2.75941
H	-0.55884	-0.29833	-2.79748
C	1.883099	1.06513	-0.69694
H	2.646157	0.968084	-1.48494
H	2.343565	0.71875	0.244486
C	1.447714	2.519098	-0.51894
H	0.910791	2.866744	-1.41507
H	2.320961	3.175104	-0.40003
H	-2.38776	-0.21445	0.587207
H	-0.47708	-2.33902	-1.88841
C	-1.14332	-1.94256	0.112359
H	-0.73325	-1.98946	1.137149
O	-2.20544	-2.87757	-0.03465
H	-2.83	-2.77604	0.692296

**TS1c-S**

538.7912i cm<sup>-1</sup>

C	-1.55976	-0.5412	-1.53158
C	-2.90797	-0.015	-1.00155
O	-3.52386	1.058376	-2.43283
O	-4.50917	0.580307	-3.05143
C	-2.89802	1.044587	-0.06395
H	-3.77544	1.181899	0.572409
C	-1.85375	2.115898	-0.09508
H	-2.35118	3.097777	-0.15033
H	-1.29496	2.116031	0.859036
C	-4.01966	-1.03149	-0.90919
H	-4.32106	-1.30955	-1.93374
C	-1.2372	-1.83899	-0.74644
H	-0.29023	-2.24486	-1.13559
H	-1.05541	-1.57041	0.308811
C	-2.34569	-2.88893	-0.79193
H	-2.05052	-3.79561	-0.24581
C	-1.63378	-0.8466	-3.03967
H	-0.78319	-1.48308	-3.32571
H	-1.58639	0.079956	-3.62671
H	-2.56275	-1.36144	-3.32096
C	-0.41127	0.462323	-1.26305
H	0.379923	0.298036	-2.01033
H	0.036973	0.249831	-0.2775
C	-0.88487	1.914538	-1.26534
H	-1.38969	2.150124	-2.21374
H	-0.03092	2.599224	-1.17066
H	-4.90319	-0.58412	-0.43296
H	-2.56005	-3.18916	-1.83239
C	-3.60799	-2.30743	-0.16351
H	-3.40427	-2.06828	0.892329
O	-4.68022	-3.23872	-0.12746
H	-4.95437	-3.44062	-1.03071

**TS1d-S**

640.3961i cm<sup>-1</sup>

C	0.665873	0.106078	-0.95398
C	-0.52615	0.386488	-0.06261
O	-1.62144	2.630596	-0.7588
O	-2.67064	2.073746	-1.16529
C	-0.70472	1.628278	0.558893
C	0.439484	2.592068	0.75073
H	0.035009	3.612129	0.821404
H	0.923643	2.370433	1.716206
C	-1.65174	-0.60348	-0.0902

H	-2.17366	-0.53364	-1.06436
C	1.08801	-1.37275	-0.79537
H	1.879158	-1.59399	-1.52928
H	1.538613	-1.49955	0.203907
C	-0.0721	-2.35962	-0.94376
H	0.273394	-3.39219	-0.79574
C	0.252062	0.377245	-2.4214
H	1.096089	0.148951	-3.09009
H	-0.03766	1.426283	-2.56586
H	-0.60221	-0.24054	-2.72768
C	1.856074	1.010672	-0.57683
H	2.632701	0.91312	-1.35189
H	2.296802	0.640113	0.364859
C	1.454239	2.474505	-0.38782
H	1.010259	2.875352	-1.31144
H	2.339358	3.087762	-0.16843
H	-2.39993	-0.35035	0.677049
H	-0.51554	-2.31229	-1.95038
C	-1.16229	-2.0503	0.072302
H	-0.74632	-2.17737	1.090453
O	-2.2189	-2.97906	-0.13729
H	-2.94112	-2.79696	0.474675
H	-1.52235	1.691758	1.284622

**TS1e-S**

253.1646i cm<sup>-1</sup>

C	1.007001	0.125523	-0.53288
C	1.743544	0.867156	-1.44676
O	2.279393	1.623237	0.288742
O	1.506536	2.449356	0.856363
C	-0.29984	0.591434	-0.05425
H	-0.01394	1.317633	0.767458
H	-0.88234	-0.21322	0.41096
H	1.465316	-0.76121	-0.08953
C	1.116133	1.977107	-2.27753
C	-0.19349	2.506391	-1.65234
H	-0.72741	3.085856	-2.42228
H	0.053302	3.197501	-0.83492
C	-1.08426	1.390972	-1.10005
H	-1.98273	1.825059	-0.64023
H	-1.42914	0.723773	-1.90507
C	3.117833	0.407041	-1.86145
H	3.520988	-0.29062	-1.11415
H	3.061793	-0.13734	-2.81804

C	4.090083	1.576406	-2.04487
H	4.314776	2.002945	-1.05301
C	2.133803	3.129747	-2.40293
H	2.258152	3.579165	-1.40442
H	1.706995	3.903736	-3.06055
C	0.793063	1.386671	-3.67004
H	1.673576	0.969987	-4.17403
H	0.38342	2.182313	-4.31014
H	0.042787	0.587066	-3.59402
O	5.270913	1.014418	-2.61463
H	5.966791	1.68052	-2.63526
C	3.492899	2.665654	-2.93672
H	4.187061	3.519254	-2.98637
H	3.40802	2.267339	-3.95989

**TS1f-S**

334.4990i cm<sup>-1</sup>

C	1.054675	0.029074	-0.56345
C	1.751175	0.671931	-1.57843
O	2.404925	1.119135	0.310723
O	3.442274	0.450731	0.60819
C	-0.26387	0.486975	-0.01143
H	-0.07413	0.810309	1.026111
H	-0.94303	-0.37571	0.055367
H	1.438999	-0.93122	-0.20917
C	1.2329	1.958142	-2.19378
C	0.192636	2.611361	-1.26419
H	-0.24855	3.475801	-1.78477
H	0.716125	2.999365	-0.37469
C	-0.89209	1.630024	-0.81659
H	-1.6452	2.145095	-0.2049
H	-1.42374	1.227683	-1.69156
C	3.003718	0.073432	-2.13589
H	3.35201	-0.72333	-1.45939
H	2.80198	-0.38936	-3.11672
C	4.109486	1.128559	-2.31651
C	2.402539	2.94277	-2.41184
H	2.024452	3.810775	-2.97494
C	0.589378	1.604427	-3.55378
H	1.320726	1.17413	-4.25
H	0.178401	2.51611	-4.01294
H	-0.22579	0.876863	-3.4422
H	4.413435	1.473595	-1.31437
H	2.726573	3.310075	-1.42454

C	3.603757	2.316168	-3.1213
H	4.417197	3.047891	-3.22024
H	3.352498	1.980615	-4.14002
O	5.220663	0.566373	-3.00649
H	5.701866	-0.01969	-2.41162

**TS1g-S**

384.8150i cm<sup>-1</sup>

C	1.079457	0.047173	-0.8956
C	1.931255	0.852719	-1.63012
O	0.575764	-0.78764	-2.56804
O	1.486398	-1.36931	-3.23813
C	-0.25976	0.50478	-0.39559
H	-0.15199	0.725812	0.679497
H	-0.96493	-0.33606	-0.47224
H	1.506697	-0.839	-0.41782
C	1.467335	2.155187	-2.25303
C	0.329798	2.752346	-1.40571
H	-0.0711	3.639353	-1.92151
H	0.745951	3.099417	-0.44402
C	-0.78779	1.736903	-1.14139
H	-1.59293	2.204094	-0.55758
H	-1.23771	1.417603	-2.09177
C	3.196327	0.270317	-2.04935
H	3.557081	-0.49608	-1.35094
H	2.824517	-0.36978	-2.94798
C	4.333772	1.224005	-2.44001
C	2.676994	3.112365	-2.30212
H	2.355859	4.068797	-2.74339
C	0.97535	1.89863	-3.70107
H	1.613054	1.181102	-4.234
H	0.970055	2.849166	-4.25666
H	-0.0328	1.473072	-3.71288
H	4.856087	1.50112	-1.51111
H	3.010824	3.33073	-1.2726
C	3.836732	2.510716	-3.10096
H	4.678639	3.213455	-3.16813
H	3.520035	2.297855	-4.13423
O	5.321539	0.563156	-3.21685
H	4.911661	0.206909	-4.01489

**TS1h-S**

420.3388i cm<sup>-1</sup>

C	0.947274	0.058332	-0.98401
C	1.68607	0.725594	-1.97274
O	0.137237	-0.33828	-2.59387
O	-1.05875	0.126752	-2.63533
C	-0.1138	0.72224	-0.16861
H	0.189147	0.678139	0.889437
H	-1.01973	0.10228	-0.27969
H	1.277803	-0.93381	-0.66746
C	1.574801	2.219592	-2.20428
C	0.85814	2.892666	-1.01603
H	0.641493	3.938029	-1.28606
H	1.552021	2.922234	-0.1586
C	-0.4179	2.163624	-0.60716
H	-0.91477	2.698381	0.214067
H	-1.12015	2.138387	-1.44957
C	2.718227	-0.03995	-2.75766
H	2.795335	-1.07329	-2.39366
H	2.360359	-0.09289	-3.8024
C	4.098729	0.630635	-2.76388
C	3.00441	2.818828	-2.28743
H	2.905379	3.874666	-2.58392
C	0.818849	2.47504	-3.52624
H	1.349921	2.02893	-4.37881
H	0.745862	3.559504	-3.69672
H	-0.18733	2.037809	-3.50196
H	4.521654	0.617009	-1.74709
H	3.44572	2.817326	-1.27609
C	3.957188	2.07771	-3.22504
H	4.94548	2.558052	-3.23137
H	3.580467	2.093132	-4.26231
O	5.016728	-0.11133	-3.5516
H	4.716967	-0.11903	-4.46919

**TS1i-S**

263.8109i cm<sup>-1</sup>

C	0.055819	-0.19344	0.990349
C	-0.38651	-0.11894	-0.48686
H	-0.20714	-1.07175	-1.00211
H	0.15574	0.659615	-1.03588
H	-1.46611	0.095743	-0.53109
C	1.566917	-0.28253	1.078435
C	2.351662	0.954018	1.093787
H	2.54506	1.075103	2.224504
H	3.352538	0.836609	0.659278

C	1.690269	2.234521	0.600494	H	0.557123	1.895338	1.552225
H	2.274888	3.08222	0.993197	C	2.541168	1.247996	0.950524
C	0.215025	2.363678	1.061943	H	3.021552	2.149726	1.361187
H	0.113264	3.211696	1.753532	H	2.651711	0.464261	1.71271
H	-0.38892	2.605382	0.1742	C	3.322733	0.836674	-0.29436
C	-0.33751	1.098169	1.734953	H	2.095642	2.85626	-3.75276
H	0.044649	1.021906	2.766742	H	2.982373	-0.1596	-0.62469
H	-1.43582	1.158811	1.797345	O	4.698608	0.778043	0.083442
C	2.207966	-1.44665	1.444186	H	5.213739	0.407725	-0.64184
H	3.301613	-1.43958	1.479115	O	1.065747	0.650951	-1.97179
C	-0.59258	-1.41088	1.675321	O	1.718938	0.073955	-3.091
H	-1.67231	-1.40165	1.45709	H	1.082317	0.240886	-3.80336
H	-0.47272	-1.30943	2.765664				
C	0.038301	-2.72933	1.220351				
H	-0.0712	-2.84207	0.131496	<b>2a-S</b>			
H	-0.48598	-3.58123	1.674727	C	-0.95094	-1.16357	1.167531
C	1.523703	-2.77419	1.59962	C	-0.18682	-0.49098	0.099904
H	2.060258	-3.53271	1.01087	O	0.091471	-0.18756	1.558106
H	1.640123	-3.0641	2.657888	O	1.253157	-0.80106	2.115771
O	1.812458	2.234714	-0.82914	C	-2.33965	-0.74798	1.591153
H	1.579477	3.105594	-1.16996	H	-2.26415	-0.45393	2.649024
O	1.957506	-0.78503	3.35286	H	-2.99002	-1.63285	1.557716
O	2.570984	0.26881	3.674902	H	-0.59421	-2.15263	1.464018
				C	-0.77649	0.733	-0.58996
<b>2-S</b>				C	-1.84572	1.387954	0.308081
C	0.838075	2.491906	-0.5074	H	-2.29786	2.22123	-0.2514
C	1.620079	1.983729	-1.74604	H	-1.35501	1.821979	1.193034
C	1.334459	2.830016	-2.96773	C	-2.92756	0.396415	0.748921
C	0.188068	3.498952	-3.1081	H	-3.70069	0.915647	1.330879
H	0.020577	4.0865	-4.0159	H	-3.43297	-0.01403	-0.13745
C	-0.88895	3.550068	-2.05285	C	0.979648	-1.15066	-0.58306
H	-0.93856	4.586736	-1.67633	H	1.344841	-1.98113	0.032076
H	-1.86769	3.360308	-2.51846	H	0.653388	-1.53793	-1.56012
C	-0.64994	2.570879	-0.89405	C	2.094361	-0.11207	-0.7869
H	-0.99618	1.566315	-1.17533	C	0.375643	1.72824	-0.84198
H	-1.2334	2.882725	-0.01334	H	-0.014	2.582308	-1.41819
C	3.11068	1.82991	-1.44284	C	-1.4123	0.275176	-1.91731
H	3.542245	2.804614	-1.17012	H	-0.6573	-0.02573	-2.65356
H	3.6277	1.479772	-2.34944	H	-1.9939	1.102396	-2.34966
C	1.32388	3.891941	-0.08843	H	-2.08965	-0.57904	-1.77407
H	2.333456	3.875475	0.338798	H	2.436432	0.196283	0.215763
H	0.645459	4.287491	0.682729	H	0.700864	2.120636	0.136225
H	1.332052	4.595643	-0.93137	C	1.580547	1.102294	-1.55306
C	1.054983	1.498833	0.652647	H	2.394315	1.835141	-1.63849
H	0.561922	0.546984	0.404468	H	1.331077	0.789558	-2.5794
				O	3.168078	-0.67122	-1.53548

H	3.668893	-1.27216	-0.97246
<b>2b-S</b>			
C	0.007388	-0.1441	0.995309
C	-0.39513	-0.56293	-0.43589
H	-0.07018	-1.58224	-0.67688
H	0.044012	0.10318	-1.18903
H	-1.49175	-0.53173	-0.53474
C	1.524143	-0.07573	1.146233
C	2.216047	1.055708	0.997042
H	3.302366	1.049632	1.124913
C	1.598403	2.411982	0.790071
H	1.731995	2.961652	1.742998
C	0.10584	2.335645	0.463745
H	-0.36685	3.314142	0.641819
H	0.004301	2.121745	-0.60978
C	-0.57522	1.247938	1.299921
H	-0.42959	1.462239	2.372368
H	-1.6614	1.241668	1.114614
C	2.234633	-1.33472	1.606202
C	-0.52319	-1.17786	2.004316
H	-1.62467	-1.19026	1.966626
H	-0.23395	-0.84913	3.013867
C	0.02668	-2.59683	1.753265
H	-0.61302	-3.12908	1.034116
H	-0.02633	-3.16261	2.692929
C	1.484011	-2.60609	1.230318
H	1.512641	-2.6865	0.134655
H	2.030913	-3.47284	1.625602
O	2.340812	3.079039	-0.23313
H	2.047136	3.995163	-0.29165
O	2.28508	-1.39039	3.050291
H	3.272309	-1.3472	1.234609
O	3.115707	-0.33089	3.510211
H	3.826104	-0.82631	3.94391

**TS1a-T**

580.3767i cm<sup>-1</sup>

C	-1.54995	-0.49979	-1.44503
C	-2.67512	-0.33815	-0.41985
O	-1.92944	-1.27184	1.000365
O	-2.78163	-1.50527	1.898018
C	-2.82427	0.929569	0.19328

H	-3.75935	1.138458	0.718299
C	-1.64567	1.811299	0.462219
H	-1.96352	2.860298	0.550435
H	-1.26388	1.52885	1.463893
C	-3.91385	-1.16956	-0.66677
H	-4.45266	-0.7624	-1.53782
C	-1.27961	-1.99492	-1.71364
H	-0.55723	-2.0725	-2.54181
H	-0.7967	-2.43613	-0.82812
C	-2.54901	-2.7861	-2.05012
H	-2.31512	-3.85166	-2.18005
C	-2.00085	0.182851	-2.75531
H	-1.16598	0.185952	-3.47263
H	-2.31566	1.221113	-2.58529
H	-2.84403	-0.3403	-3.22354
C	-0.27656	0.186774	-0.91563
H	0.512424	0.098481	-1.67968
H	0.076124	-0.35593	-0.02422
C	-0.51068	1.659304	-0.56209
H	-0.75118	2.230348	-1.47071
H	0.410501	2.099472	-0.15563
H	-4.58036	-1.08242	0.205648
H	-2.99729	-2.44639	-2.99653
C	-3.59752	-2.64533	-0.95369
H	-3.21978	-3.12173	-0.0332
O	-4.76782	-3.32619	-1.4013
H	-5.40226	-3.38703	-0.6783

**TS1b-T**

603.0607i cm<sup>-1</sup>

C	0.69101	0.139439	-1.01086
C	-0.4981	0.463124	-0.13142
O	0.303845	0.670046	2.282384
O	-0.45756	-0.21978	2.753921
C	-0.43018	1.482882	0.84953
H	-1.37751	1.705324	1.351774
C	0.516069	2.658779	0.692849
H	-0.07467	3.58393	0.637018
H	1.119361	2.729207	1.612094
C	-1.64676	-0.50156	-0.1544
H	-2.14399	-0.49174	-1.1409
C	1.10106	-1.3298	-0.73068
H	1.930168	-1.59726	-1.40537
H	1.492505	-1.38563	0.299957

C	-0.0566	-2.31957	-0.87598
H	0.27853	-3.3429	-0.65739
C	0.315098	0.295571	-2.50067
H	1.154136	-0.03646	-3.13059
H	0.091972	1.341984	-2.74862
H	-0.56542	-0.30136	-2.77001
C	1.876568	1.064467	-0.67314
H	2.646743	0.957007	-1.45278
H	2.329126	0.734959	0.277966
C	1.432527	2.519956	-0.52769
H	0.901161	2.843002	-1.43593
H	2.300887	3.184074	-0.41946
H	-2.3976	-0.22	0.598882
H	-0.45619	-2.32753	-1.90232
C	-1.18091	-1.95445	0.082868
H	-0.81106	-2.04162	1.118891
O	-2.252	-2.86672	-0.13575
H	-2.89334	-2.79215	0.579628

**TS1c-T**

542.0487i cm<sup>-1</sup>

C	-1.57952	-0.52827	-1.56496
C	-2.93554	0.008409	-1.04199
O	-3.52125	1.058977	-2.39679
O	-4.28845	0.481199	-3.21663
C	-2.87201	0.998896	-0.01437
H	-3.71358	1.086331	0.676661
C	-1.83915	2.080745	-0.04022
H	-2.34592	3.06039	-0.04686
H	-1.25185	2.056397	0.896343
C	-4.0418	-1.01881	-0.94055
H	-4.32703	-1.32554	-1.96055
C	-1.25736	-1.80658	-0.74753
H	-0.30818	-2.2186	-1.12476
H	-1.07823	-1.51032	0.300755
C	-2.36047	-2.86288	-0.76614
H	-2.06074	-3.75218	-0.19446
C	-1.6416	-0.87033	-3.06456
H	-0.76486	-1.47864	-3.33161
H	-1.62765	0.042747	-3.67452
H	-2.54708	-1.42891	-3.33699
C	-0.42761	0.480625	-1.31407
H	0.331663	0.349148	-2.0996
H	0.065877	0.239762	-0.35728

C	-0.90342	1.930432	-1.2445
H	-1.43181	2.203965	-2.16914
H	-0.04647	2.610626	-1.14387
H	-4.93216	-0.5663	-0.48172
H	-2.57081	-3.19293	-1.79838
C	-3.62701	-2.27019	-0.15749
H	-3.42751	-2.00029	0.891944
O	-4.695	-3.20564	-0.09798
H	-4.94341	-3.45883	-0.99577

**TS1d-T**

641.7359i cm<sup>-1</sup>

C	0.654783	0.109954	-0.95598
C	-0.5381	0.386337	-0.06527
O	-1.59352	2.647918	-0.72127
O	-2.52778	2.040951	-1.3082
C	-0.73656	1.654916	0.526244
C	0.428368	2.589509	0.755945
H	0.045636	3.616201	0.848916
H	0.898332	2.330994	1.718733
C	-1.65532	-0.61323	-0.07439
H	-2.19317	-0.54816	-1.03999
C	1.081358	-1.36826	-0.80515
H	1.868055	-1.58512	-1.54508
H	1.539005	-1.49752	0.190612
C	-0.07721	-2.35743	-0.94796
H	0.272449	-3.39011	-0.81099
C	0.241386	0.385935	-2.42334
H	1.07562	0.130948	-3.09471
H	-0.01875	1.441875	-2.57269
H	-0.63326	-0.20728	-2.72097
C	1.846207	1.013597	-0.5774
H	2.619906	0.91991	-1.35596
H	2.290267	0.637008	0.360235
C	1.448962	2.477265	-0.37759
H	1.012083	2.889599	-1.29971
H	2.335798	3.084174	-0.14769
H	-2.39332	-0.36478	0.704836
H	-0.53259	-2.30326	-1.94901
C	-1.15445	-2.05609	0.083823
H	-0.7221	-2.17979	1.095537
O	-2.20775	-2.99241	-0.10913
H	-2.92375	-2.81171	0.510495
H	-1.53661	1.701541	1.273703

**2-T**

C	-0.27284	-0.5559	-1.17962
C	-0.12979	-0.09811	0.255135
C	-1.34729	0.283619	1.022499
C	-2.38294	1.069878	0.229338
H	-1.98779	2.084153	0.064989
H	-3.29748	1.16336	0.83201
C	1.119245	-0.45692	1.002958
H	1.10143	-1.53291	1.266995
H	1.156023	0.088428	1.960643
H	-1.07847	0.777353	1.968279
O	-2.098	-0.94549	1.454147
O	-1.36268	-1.73425	2.174511
C	-0.65609	-2.0591	-1.18676
H	-1.63775	-2.22856	-0.72546
H	0.073622	-2.66317	-0.63033
H	-0.6884	-2.42658	-2.22398
C	1.064564	-0.36276	-1.93032
H	0.985822	-0.83989	-2.92008
H	1.209334	0.716355	-2.10982
C	2.389886	-0.20954	0.180933
H	2.51073	0.878672	0.015963
C	2.278584	-0.89879	-1.17052
H	2.204189	-1.9846	-1.00078
H	3.202523	-0.72614	-1.73989
C	-1.36344	0.257269	-1.91111
H	-1.55253	-0.21136	-2.89023
H	-0.96924	1.268284	-2.112
C	-2.66218	0.392517	-1.11469
H	-3.39395	0.98167	-1.68509
H	-3.11815	-0.59388	-0.94002
O	3.540309	-0.72948	0.837877
H	3.60469	-0.35696	1.724668

**2-Q**

C	-0.27443	-0.56327	-1.18148
C	-0.13471	-0.11724	0.256165
C	-1.34706	0.27645	1.02387
C	-2.38253	1.064494	0.231931
H	-1.99018	2.080771	0.071339
H	-3.29713	1.155512	0.834875
C	1.121032	-0.44899	1.004867

H	1.115114	-1.51926	1.292253
H	1.153306	0.118854	1.950605
H	-1.06985	0.777062	1.964562
O	-2.10386	-0.9445	1.468895
O	-1.36421	-1.7417	2.175419
O	0.65579	2.887065	-0.40693
O	0.67572	2.858595	0.789442
C	-0.66298	-2.06474	-1.19935
H	-1.64389	-2.23356	-0.73605
H	0.066141	-2.67365	-0.64714
H	-0.69913	-2.42643	-2.23852
C	1.064649	-0.36838	-1.92886
H	0.987489	-0.84258	-2.92012
H	1.210189	0.711552	-2.10504
C	2.389824	-0.20675	0.178261
H	2.512017	0.88016	0.003155
C	2.277164	-0.90553	-1.16783
H	2.199299	-1.9901	-0.99164
H	3.20143	-0.73875	-1.73839
C	-1.35897	0.262309	-1.90845
H	-1.54536	-0.19382	-2.89398
H	-0.95906	1.274505	-2.09509
C	-2.66003	0.393715	-1.11545
H	-3.39008	0.986384	-1.68437
H	-3.11694	-0.5933	-0.9466
O	3.541642	-0.71911	0.83846
H	3.603042	-0.34296	1.723976

**1-Q**

C	0.200152	0.022467	1.139974
C	0.146821	-0.10913	-0.37969
C	0.895326	0.636831	-1.19929
C	1.937667	1.62688	-0.74567
H	1.569391	2.654455	-0.91486
H	2.836764	1.519294	-1.37242
C	-0.81747	-1.14264	-0.91952
H	-0.48289	-2.1596	-0.64962
H	-0.85498	-1.0998	-2.01685
H	0.765874	0.507422	-2.27973
O	3.13778	-1.64331	-0.88408
O	2.260018	-2.44374	-1.02663
O	-1.14184	3.145709	-0.59837
O	-1.86581	2.47286	-1.2727
C	0.850052	-1.23063	1.763162
H	0.403187	-2.164	1.394909

H	0.73541	-1.20874	2.857997
H	1.923718	-1.26959	1.533765
C	-1.24956	0.172764	1.657663
H	-1.23375	0.218768	2.758756
H	-1.64462	1.141798	1.303782
C	-2.18014	-0.94452	1.177735
H	-1.83971	-1.92984	1.533814
H	-3.19438	-0.79009	1.580372
C	-2.2233	-0.97165	-0.34992
H	-2.64134	-0.01373	-0.71345
C	1.001615	1.273065	1.547972
H	0.373876	2.16661	1.390679
H	1.220648	1.22178	2.62696
C	2.285727	1.430914	0.731759
H	2.912999	0.53166	0.839745
H	2.87865	2.278326	1.104152
O	-3.00304	-2.05786	-0.84377
H	-3.90707	-1.98014	-0.51865

**TS2a-Q**

575.7280i cm<sup>-1</sup>

C	-0.09221	-0.58843	1.039549
C	0.013287	-0.12589	-0.4165
C	-1.17823	-0.08758	-1.18228
C	-2.29499	-1.05423	-0.94742
H	-2.09488	-1.93461	-1.59037
H	-3.24567	-0.63268	-1.30644
C	-2.41458	-1.51774	0.511869
H	-2.93789	-0.74963	1.1006
H	-3.03923	-2.42053	0.560762
C	-1.03701	-1.80272	1.121925
H	-0.57048	-2.6518	0.597896
H	-1.14102	-2.09512	2.179231
C	1.081968	0.905429	-0.70402
H	0.775202	1.87182	-0.27146
H	1.1582	1.042268	-1.79394
C	-0.66791	0.571728	1.880147
H	-0.03532	1.467707	1.839509
H	-0.73911	0.256076	2.932204
H	-1.67037	0.86252	1.542805
C	1.306905	-0.95435	1.577719
H	1.652386	-1.87665	1.086251
H	1.217118	-1.1794	2.652261
C	2.339878	0.158092	1.359537

H	2.079011	1.066258	1.924511
H	3.329443	-0.15886	1.716339
C	2.449711	0.530284	-0.11402
H	-1.16941	0.478873	-2.11712
H	2.85848	-0.33025	-0.67007
O	3.349528	1.632834	-0.20739
H	3.573773	1.788067	-1.13179
O	-3.10915	2.165942	-0.24878
O	-2.11324	2.828634	-0.2869
O	0.792014	-1.62869	-1.15289
O	1.220979	-1.4067	-2.31773

**TS2-Q**

632.9414i cm<sup>-1</sup>

C	-0.2634	-0.51625	-1.14234
C	-0.13357	-0.05972	0.295711
C	-1.23604	0.476797	0.996893
C	-2.38614	1.116369	0.25527
H	-2.13272	2.174021	0.069147
H	-3.27456	1.108814	0.903264
C	1.104851	-0.44371	1.048157
H	1.060451	-1.52316	1.292928
H	1.139392	0.090303	2.012031
H	-0.99706	0.92112	1.970284
O	-2.13658	-0.95019	1.665322
O	-1.39137	-1.83561	2.161141
O	0.613612	2.939269	-0.43586
O	0.775171	2.962705	0.749758
C	-0.63094	-2.02107	-1.1418
H	-1.60184	-2.19532	-0.66067
H	0.110901	-2.62102	-0.59813
H	-0.67949	-2.3888	-2.17822
C	1.078474	-0.31173	-1.88231
H	1.00329	-0.77435	-2.87911
H	1.225719	0.76984	-2.04612
C	2.388114	-0.19959	0.241435
H	2.523909	0.890282	0.095667
C	2.28679	-0.86265	-1.12367
H	2.21268	-1.95146	-0.9766
H	3.215011	-0.67769	-1.68199
C	-1.35869	0.287129	-1.87276
H	-1.54381	-0.18073	-2.85285
H	-0.97567	1.303661	-2.07125
C	-2.65499	0.39943	-1.06888



H	-3.41404	0.946631	-1.6452
H	-3.07054	-0.59869	-0.86313
O	3.524543	-0.74115	0.903177
H	3.586562	-0.3788	1.794386

**1-T**

C	0.198661	0.026124	1.138145
C	0.146296	-0.1106	-0.38114
C	0.897267	0.630639	-1.20277
C	1.941373	1.619897	-0.75162
H	1.575163	2.647791	-0.92375
H	2.840472	1.508885	-1.37777
C	-0.8202	-1.14349	-0.91817
H	-0.48886	-2.16036	-0.64401
H	-0.85635	-1.10468	-2.01569
H	0.768447	0.49769	-2.28286
O	3.131419	-1.65834	-0.87489
O	2.250142	-2.45533	-1.01501
O	-1.13015	3.150025	-0.59649
O	-1.84585	2.470208	-1.27399
C	0.844323	-1.22672	1.76629
H	0.396312	-2.16013	1.39955
H	0.727321	-1.20152	2.860794
H	1.918429	-1.26878	1.539323
C	-1.25113	0.182586	1.653714
H	-1.23636	0.232536	2.754651
H	-1.64277	1.151494	1.295915
C	-2.18457	-0.93356	1.176789
H	-1.84756	-1.91861	1.536858
H	-3.19877	-0.77458	1.577697
C	-2.2261	-0.96623	-0.35082
H	-2.64063	-0.00838	-0.71847
C	1.003528	1.275686	1.542696
H	0.378482	2.170603	1.382544
H	1.222021	1.226941	2.621909
C	2.288399	1.427305	0.72649
H	2.912722	0.526347	0.837241
H	2.883834	2.273953	1.096582
O	-3.00862	-2.05192	-0.84144
H	-3.9145	-1.96622	-0.52367

**TS2a-T**

612.9384i cm<sup>-1</sup>

C	-0.11057	-0.23457	1.588612
C	-0.45886	-0.2834	0.12139
C	0.077454	0.690969	-0.73442
C	0.68524	1.961315	-0.23981
H	-0.07083	2.574087	0.281276
H	1.096442	2.559998	-1.0601
C	-0.80483	-1.63008	-0.45121
H	0.095752	-2.26277	-0.46292
H	-1.18465	-1.53842	-1.47613
H	-0.06464	0.554855	-1.80862
O	3.224566	-0.15875	0.228223
O	2.555661	-0.76279	-0.56164
O	-2.22733	0.448443	0.338893
O	-3.06156	-0.01279	-0.4704
H	-0.72105	-0.94949	2.153742
H	-1.57056	-2.12692	0.158784
H	0.95069	-0.48712	1.739119
H	-0.28386	0.768933	1.999431
H	1.491345	1.768524	0.487439

**TS2-T**

614.9215i cm<sup>-1</sup>

C	-0.27028	-0.51293	-1.15707
C	-0.14186	-0.02913	0.27216
C	-1.2259	0.535059	0.952852
C	-2.41143	1.112748	0.221884
H	-2.20627	2.178632	0.022607
H	-3.28983	1.074431	0.882518
C	1.09524	-0.4036	1.031665
H	1.036147	-1.47617	1.303196
H	1.134139	0.152398	1.982874
H	-1.00155	0.975885	1.930828
O	-2.13072	-0.96979	1.685159
O	-1.36846	-1.8228	2.199826
O	0.62648	2.818128	-0.19237
O	1.007901	2.996429	0.928597
C	-0.62634	-2.01963	-1.13004
H	-1.59499	-2.19197	-0.64408
H	0.120191	-2.60587	-0.57806
H	-0.67367	-2.40527	-2.15997
C	1.070702	-0.31008	-1.89799
H	0.994787	-0.77337	-2.89441
H	1.218757	0.771715	-2.06175
C	2.385116	-0.1956	0.223759

H	2.547257	0.888658	0.070761
C	2.276795	-0.86429	-1.138
H	2.196872	-1.95193	-0.98693
H	3.205667	-0.68718	-1.69776
C	-1.37207	0.271992	-1.89557
H	-1.55061	-0.20435	-2.87274
H	-0.99976	1.291759	-2.09931
C	-2.66957	0.373523	-1.09207
H	-3.43871	0.899592	-1.67461
H	-3.06688	-0.62897	-0.87283
O	3.506877	-0.75716	0.894153
H	3.584014	-0.37621	1.776417

**MECP 1**

C	0.204175	-0.5093	1.177601
C	0.119793	-0.10805	-0.27728
C	1.364506	0.203121	-1.03315
C	2.424692	0.953927	-0.24033
H	2.082028	1.993903	-0.12188
H	3.355754	0.978691	-0.82418
C	-1.12033	-0.43739	-1.05023
H	-1.14218	-1.5199	-1.29023
H	-1.10661	0.086071	-2.02126
H	1.131838	0.691204	-1.99187
O	2.036713	-1.07646	-1.43088
O	1.354167	-1.71688	-2.33032
O	-0.54924	2.932868	0.183194
O	-0.56546	2.919539	-1.01356
C	0.518699	-2.02599	1.257672
H	1.50631	-2.25383	0.836015
H	-0.21874	-2.61893	0.69932
H	0.501568	-2.35381	2.30869
C	-1.14419	-0.22538	1.878005
H	-1.11335	-0.65786	2.890616
H	-1.24949	0.866546	2.003024
C	-2.40404	-0.11571	-0.27479
H	-2.49174	0.982177	-0.15628
C	-2.35613	-0.75013	1.106735
H	-2.31824	-1.84452	0.986108
H	-3.28833	-0.5194	1.640592
C	1.311002	0.286703	1.902189
H	1.45059	-0.14176	2.907749
H	0.960921	1.324469	2.043075
C	2.635365	0.319652	1.136458
H	3.382428	0.89517	1.70068

H	3.043514	-0.69554	1.017244
O	-3.55338	-0.62089	-0.94404
H	-3.59003	-0.26682	-1.83988

**3-T**

C	-0.15186	1.188008	-0.36334
C	-0.07802	-0.20887	0.302205
O	0.061536	0.10343	1.751825
O	0.211137	-0.96043	2.48309
C	-1.39204	-1.01583	0.24264
C	-2.5918	-0.20502	0.715629
H	-2.48556	-0.0729	1.802944
H	-3.50155	-0.79728	0.545959
C	-2.68151	1.164051	0.030907
H	-2.92038	1.027962	-1.03457
H	-3.51475	1.733628	0.465106
C	-1.37389	1.95018	0.191759
H	-1.2084	2.172025	1.25823
H	-1.44293	2.918034	-0.32926
C	1.153151	-1.00466	-0.11762
H	1.104663	-1.21561	-1.19488
H	1.147448	-1.97341	0.404378
C	-0.27407	1.085926	-1.89746
H	0.537873	0.504418	-2.34975
H	-0.22209	2.103941	-2.31139
H	-1.21671	0.634337	-2.22304
C	1.152738	1.940058	-0.016
H	1.17864	2.138568	1.066897
H	1.129999	2.919852	-0.5178
C	2.411597	1.167276	-0.4293
H	2.469054	1.054963	-1.52256
H	3.316028	1.709111	-0.12075
C	2.441123	-0.22711	0.189073
H	-1.26075	-1.94075	0.82109
O	-1.64796	-1.42944	-1.12771
O	-1.07826	-2.56703	-1.41267
H	2.548811	-0.13085	1.284797
O	3.57503	-0.90047	-0.34669
H	3.676152	-1.75863	0.08086

**MECP 2**

C	-2.34679	-0.47504	-0.11431
C	-0.87689	-0.12818	-0.14684

C	0.139337	-1.20737	-0.01081	C	3.022866	1.312655	-1.04047
C	-0.21311	-2.29229	0.997051	C	3.825513	2.467162	-0.49904
H	-0.09241	-1.86739	2.006161	H	3.19054	3.370819	-0.47445
H	0.50507	-3.11875	0.898687	H	4.650669	2.693327	-1.19201
C	-0.45079	1.167561	-0.76488	C	1.823098	-0.864	-0.95741
H	-0.51537	1.097865	-1.87015	H	2.424314	-1.79093	-0.92534
H	0.613822	1.356962	-0.5384	H	1.640434	-0.63568	-2.01965
H	1.141947	-0.78342	0.157981	H	2.79202	1.335501	-2.11225
O	0.258353	-1.93921	-1.31224	O	5.724971	-0.44058	-1.37418
O	0.730619	-1.18221	-2.25613	O	5.131991	-1.4798	-1.38737
O	-0.60451	0.768285	2.868653	O	0.067035	2.530498	-0.5235
O	0.50604	0.878968	2.435957	O	-0.03978	2.104317	-1.63646
C	-2.77943	-0.95195	-1.52574	C	3.796458	-0.90392	1.549261
H	-2.28976	-1.89511	-1.79934	H	3.56633	-1.86233	1.064447
H	-2.51747	-0.21552	-2.29817	H	3.809246	-1.07032	2.637393
H	-3.86956	-1.10299	-1.54872	H	4.808008	-0.61213	1.236839
C	-3.16597	0.774571	0.280359	C	1.40781	-0.14957	1.845046
H	-4.23706	0.544615	0.165308	H	1.55459	-0.2794	2.929344
H	-2.99852	0.977963	1.352399	H	0.737116	0.717815	1.71693
C	-1.32226	2.350566	-0.32464	C	0.734152	-1.38288	1.241389
H	-1.14633	2.5506	0.750607	H	1.353304	-2.28529	1.367701
C	-2.79489	2.022256	-0.52249	H	-0.22792	-1.58319	1.733211
H	-2.97631	1.877268	-1.59901	C	0.498571	-1.16262	-0.24498
H	-3.40024	2.883826	-0.20904	H	-0.18208	-0.29805	-0.36788
C	-2.62041	-1.59078	0.917144	C	3.248099	1.54786	1.750901
H	-3.66359	-1.92675	0.804009	H	2.391816	2.245282	1.762988
H	-2.53091	-1.15923	1.92956	H	3.570519	1.415691	2.79634
C	-1.65411	-2.77234	0.803947	C	4.361072	2.163377	0.901258
H	-1.89832	-3.53275	1.558778	H	5.206758	1.462139	0.821661
H	-1.74859	-3.26046	-0.17786	H	4.749412	3.077027	1.372749
O	-1.03537	3.516974	-1.08596	O	-0.11683	-2.3374	-0.76516
H	-0.09984	3.736921	-1.00973	H	-0.29804	-2.21996	-1.70467
S	4.813275	0.330048	-0.0553	S	2.787113	-0.29411	-5.62447
C	3.733383	-0.43679	-1.29511	C	1.186716	0.023787	-4.83191
H	2.897664	0.225027	-1.55951	H	1.281246	0.7536	-4.0161
H	3.337268	-1.39786	-0.93873	H	0.749375	-0.9078	-4.44697
H	4.331966	-0.61965	-2.19446	H	0.516076	0.436328	-5.59415
C	3.57258	0.563751	1.245106	C	3.662874	-0.98989	-4.19462
H	2.751742	1.202204	0.88941	H	3.159263	-1.89294	-3.82284
H	4.05923	1.059253	2.093027	H	3.741922	-0.25524	-3.38303
H	3.168197	-0.39971	1.586982	H	4.672432	-1.26067	-4.52514

**1c-Q**

C	2.770831	0.192367	1.197576
C	2.578916	0.280163	-0.31476

**TS1-Q**

624.9601i cm<sup>-1</sup>

C	-0.50359	-0.19975	-0.75481	C	-0.18494	-0.80143	-2.20574
C	-0.36066	0.293864	0.668928	C	-0.00222	-0.39325	-0.763
C	-1.45107	0.86367	1.361773	C	-1.18391	0.006869	0.044669
C	-2.60348	1.488882	0.612286	C	-2.22996	0.827217	-0.69864
H	-2.34472	2.539018	0.393042	H	-1.8299	1.842675	-0.84498
H	-3.48632	1.506843	1.267947	H	-3.12644	0.914502	-0.06811
C	0.87929	-0.0791	1.424099	C	1.268649	-0.75419	-0.05514
H	0.826269	-1.15013	1.702699	H	1.257167	-1.83017	0.209607
H	0.925998	0.48444	2.371079	H	1.332759	-0.20659	0.902047
H	-1.19536	1.338822	2.316296	H	-0.86625	0.48946	0.98237
O	-2.36035	-0.53022	2.093121	O	-1.95759	-1.20304	0.500898
O	-1.62313	-1.4379	2.561084	O	-1.19793	-2.09748	1.053293
O	0.430823	3.279054	-0.08841	O	0.804841	2.619631	-1.34636
O	0.497637	3.321304	1.105885	O	0.816755	2.551683	-0.15134
C	-0.879	-1.70206	-0.71336	C	-0.59701	-2.29598	-2.24926
H	-1.85025	-1.85878	-0.22679	H	-1.5696	-2.46094	-1.76739
H	-0.13976	-2.29171	-0.15514	H	0.134642	-2.92865	-1.72787
H	-0.93092	-2.0962	-1.73978	H	-0.66291	-2.63238	-3.29536
C	0.83497	-0.02051	-1.50733	C	1.137733	-0.6075	-2.98248
H	0.750583	-0.50421	-2.49325	H	1.029288	-1.05762	-3.98186
H	0.987907	1.056392	-1.69523	H	1.293689	0.474302	-3.13734
C	2.160908	0.13104	0.604692	C	2.519253	-0.50797	-0.90781
H	2.306408	1.215927	0.432489	H	2.650064	0.5809	-1.06383
C	2.044068	-0.56288	-0.7439	C	2.362335	-1.17692	-2.2647
H	1.962514	-1.6473	-0.57089	H	2.273634	-2.26378	-2.10886
H	2.969897	-0.39839	-1.31236	H	3.27372	-1.01048	-2.85555
C	-1.59922	0.591164	-1.49823	C	-1.27516	0.05909	-2.8828
H	-1.79529	0.098255	-2.46368	H	-1.49473	-0.36824	-3.87434
H	-1.21041	1.599122	-1.72714	H	-0.86351	1.069315	-3.0541
C	-2.88825	0.735249	-0.68782	C	-2.55322	0.192225	-2.05312
H	-3.64852	1.270359	-1.27365	H	-3.28806	0.80894	-2.58917
H	-3.30849	-0.25368	-0.4496	H	-3.02145	-0.79118	-1.89428
O	3.294249	-0.4076	1.272358	O	3.680445	-1.04822	-0.28877
H	3.380164	-0.01069	2.146856	H	3.782752	-0.67783	0.595509
H	-1.38083	-0.19133	5.87601	S	-0.19491	1.127412	4.589186
C	-1.12305	0.5411	5.102843	C	-0.85314	-0.33135	3.733268
H	-0.44143	0.061541	4.38728	H	-0.11422	-0.75257	3.037888
H	-2.04549	0.840345	4.586418	H	-1.77631	-0.0916	3.187534
S	-0.33711	1.956337	5.921672	H	-1.08535	-1.08746	4.491515
C	-0.01864	2.965675	4.448935	C	0.143526	2.149934	3.130467
H	0.647978	2.442438	3.749447	H	0.867906	1.657328	2.46682
H	0.473301	3.889315	4.774491	H	0.573717	3.097104	3.475242
H	-0.9554	3.228686	3.937591	H	-0.77958	2.366202	2.573973

3-Q

1c-T

C	2.77052	0.192771	1.197696
C	2.578881	0.280529	-0.31464
C	3.023465	1.312739	-1.0404
C	3.825948	2.467307	-0.49896
H	3.191045	3.371033	-0.47514
H	4.651604	2.693057	-1.19147
C	1.822835	-0.86331	-0.9576
H	2.423727	-1.79048	-0.92589
H	1.6404	-0.6344	-2.01975
H	2.792793	1.335245	-2.11224
O	5.724934	-0.44131	-1.37434
O	5.131416	-1.48024	-1.38789
O	0.072573	2.52587	-0.52331
O	-0.03723	2.097993	-1.63605
C	3.796549	-0.90323	1.549197
H	3.566301	-1.86174	1.06464
H	3.809985	-1.06938	2.637347
H	4.807805	-0.61131	1.235956
C	1.407667	-0.14976	1.845159
H	1.554623	-0.28004	2.92938
H	0.736583	0.717437	1.71755
C	0.734201	-1.38298	1.241054
H	1.353529	-2.28532	1.366983
H	-0.22779	-1.58365	1.732865
C	0.498355	-1.16198	-0.24518
H	-0.18235	-0.29737	-0.36731
C	3.247395	1.548389	1.751019
H	2.390987	2.245661	1.762792
H	3.569494	1.416402	2.796585
C	4.360621	2.164033	0.901798
H	5.206631	1.463113	0.822983
H	4.748334	3.077956	1.373278
O	-0.11722	-2.33642	-0.76585
H	-0.29932	-2.21819	-1.70507
S	2.78664	-0.29391	-5.62433
C	1.186274	0.023826	-4.83169
H	1.280869	0.75306	-4.01541
H	0.748595	-0.90793	-4.44749
H	0.515861	0.437102	-5.59376
C	3.662561	-0.99006	-4.19469
H	3.158821	-1.89305	-3.82297
H	3.741938	-0.2555	-3.38306
H	4.67199	-1.26094	-4.52553

608.4017i cm<sup>-1</sup>

C	-0.50787	-0.20051	-0.76356
C	-0.36619	0.314548	0.652898
C	-1.43658	0.914978	1.324051
C	-2.61906	1.489847	0.586393
H	-2.40201	2.547487	0.357323
H	-3.49333	1.481507	1.253843
C	0.871669	-0.05239	1.414591
H	0.807699	-1.11811	1.711217
H	0.920931	0.526968	2.351776
H	-1.1941	1.383643	2.284899
O	-2.36483	-0.54547	2.11566
O	-1.62112	-1.44902	2.569582
O	0.410348	3.17907	0.012763
O	0.623181	3.410085	1.168065
C	-0.87819	-1.70282	-0.70103
H	-1.84863	-1.85553	-0.21192
H	-0.13727	-2.28341	-0.13567
H	-0.92912	-2.11071	-1.7221
C	0.831083	-0.02727	-1.51635
H	0.746289	-0.51641	-2.49953
H	0.985975	1.048429	-1.70994
C	2.158132	0.132363	0.595577
H	2.319823	1.213195	0.416072
C	2.03774	-0.56932	-0.74868
H	1.951852	-1.65225	-0.56935
H	2.964596	-0.41225	-1.31753
C	-1.60589	0.578598	-1.51443
H	-1.79774	0.078495	-2.477
H	-1.22235	1.587621	-1.74829
C	-2.89614	0.718678	-0.70508
H	-3.66261	1.238651	-1.29641
H	-3.30486	-0.27217	-0.45572
O	3.281504	-0.41688	1.271428
H	3.380965	-0.00176	2.135985
H	-1.37966	-0.21297	5.842826
C	-1.11681	0.536114	5.087449
H	-0.42774	0.073112	4.368081
H	-2.03495	0.844191	4.568784
S	-0.34045	1.936266	5.940484
C	-0.01012	2.970908	4.48837
H	0.662827	2.460162	3.785898
H	0.477875	3.889555	4.833415
H	-0.94261	3.241189	3.973145

TS1-T

## 4-T

C	-2.36565	-0.35167	0.009667
C	-0.85395	-0.06423	0.192783
C	0.058375	-1.27602	-0.09435
C	-0.37571	-2.51581	0.677947
H	-0.16859	-2.33171	1.742309
H	0.252001	-3.36057	0.362594
C	-0.40314	1.229733	-0.47833
H	-0.52822	1.146728	-1.5661
H	0.672017	1.375359	-0.28686
H	1.101239	-0.99095	0.112219
O	-0.0022	-1.62091	-1.50602
O	0.760273	-0.85904	-2.23785
O	-0.71778	0.127657	1.663857
O	0.492848	0.433419	2.020843
C	-2.73529	-0.57034	-1.47243
H	-2.37001	-1.52479	-1.86514
H	-2.35328	0.219056	-2.13128
H	-3.83229	-0.56733	-1.55405
C	-3.14226	0.874011	0.541322
H	-4.21657	0.697027	0.378352
H	-2.99638	0.954072	1.629812
C	-1.21806	2.427869	0.028759
H	-0.99543	2.589378	1.099337
C	-2.71457	2.182363	-0.13399
H	-2.94178	2.166411	-1.21114
H	-3.26104	3.034789	0.291933
C	-2.74078	-1.61249	0.819207
H	-3.80051	-1.84246	0.626983
H	-2.65169	-1.38996	1.894408
C	-1.86521	-2.82512	0.477045
H	-2.14709	-3.67702	1.110851
H	-2.03444	-3.14275	-0.56255
O	-0.90197	3.600693	-0.71175
H	0.019591	3.843374	-0.56618
H	4.426771	-0.37663	-2.14991
C	3.8363	-0.3017	-1.22989
H	3.019682	0.414468	-1.39271
H	3.410583	-1.28985	-1.00679
S	4.936606	0.252978	0.100675
C	3.691713	0.365317	1.41408
H	2.899399	1.076359	1.145668
H	4.18976	0.718625	2.324009
H	3.240537	-0.61533	1.619914

## 5-T

C	-1.15288	2.017091	3.781758
C	-1.47988	1.121474	5.002902
O	-2.34196	1.989342	5.850313
O	-2.66598	1.431798	6.978474
C	-2.38839	-0.07785	4.684334
C	-3.63795	0.319316	3.907006
H	-4.28843	0.869197	4.604031
H	-4.1676	-0.59976	3.621423
C	-3.31848	1.192809	2.688377
H	-2.79993	0.588658	1.928894
H	-4.25804	1.526023	2.226697
C	-2.46959	2.410364	3.078868
H	-3.05393	3.065022	3.745038
H	-2.22004	3.00359	2.185175
C	-0.24805	0.758202	5.825728
H	0.422488	0.128408	5.224048
H	-0.56778	0.167502	6.697752
C	-0.23415	1.301046	2.769992
H	0.670481	0.888779	3.231953
H	0.082938	2.039654	2.018905
H	-0.73242	0.47906	2.246504
C	-0.42604	3.27697	4.303371
H	-1.11874	3.8669	4.923719
H	-0.1621	3.905052	3.438606
C	0.831149	2.93703	5.112097
H	1.586207	2.440003	4.484323
H	1.299245	3.850458	5.503292
C	0.50624	2.016003	6.283269
H	-2.64564	-0.58989	5.624035
O	-1.57602	-1.0192	3.922646
O	-2.17356	-2.17017	3.803499
H	-0.12675	2.567134	7.002735
O	1.741425	1.665431	6.895943
H	1.579503	1.177305	7.711262
S	-0.27305	-4.5243	6.793735
C	-0.44267	-4.88358	5.022649
H	-0.00892	-5.87313	4.839785
H	0.092716	-4.13834	4.420532
H	-1.49954	-4.89291	4.72705
C	-1.04921	-2.88441	6.777234
H	-2.09653	-2.95515	6.452579
H	-0.5025	-2.21318	6.100995
H	-1.01389	-2.48149	7.796422

**TS3a-T**

1098.5233i cm<sup>-1</sup>

C	0.118855	2.844569	-0.86866
C	0.493502	2.149761	-2.21999
O	0.15002	0.780793	-2.01069
O	0.654581	-0.05992	-3.31927
C	-0.37698	2.607782	-3.40437
C	-1.86692	2.50074	-3.10528
H	-2.09877	1.4258	-3.05758
H	-2.42328	2.926448	-3.95226
C	-2.24709	3.177945	-1.78361
H	-2.13009	4.267982	-1.88449
H	-3.31193	3.001407	-1.57452
C	-1.39219	2.657148	-0.62019
H	-1.59776	1.585593	-0.46783
H	-1.66182	3.176722	0.313864
C	1.993653	2.277129	-2.50698
H	2.285221	3.334349	-2.58126
H	2.208889	1.798163	-3.47469
C	0.444947	4.352072	-0.85181
H	1.501401	4.559042	-1.05754
H	0.221648	4.737633	0.155011
H	-0.14175	4.927932	-1.57425
C	0.936437	2.153227	0.244945
H	0.595208	1.111157	0.34309
H	0.720177	2.655474	1.201614
C	2.447565	2.178111	-0.02551
H	2.835871	3.207706	0.007318
H	2.98866	1.615368	0.74858
C	2.792525	1.596691	-1.39369
H	-0.10596	2.014003	-4.28818
O	-0.01929	3.987753	-3.72344
O	-0.50794	4.35221	-4.87398
H	2.54752	0.51928	-1.40627
O	4.197776	1.77231	-1.57959
H	4.436039	1.487389	-2.46916
S	0.459635	-1.86197	-3.37093
C	1.194174	-2.12753	-1.74243
H	0.898083	-1.2833	-1.10471
H	2.281997	-2.13795	-1.86987
H	0.853779	-3.08586	-1.33352
C	-1.28898	-1.81971	-2.92006
H	-1.42447	-0.99696	-2.20542
H	-1.58624	-2.78422	-2.4924
H	-1.85779	-1.62099	-3.83458

**TS3-T**

1059.3299i cm<sup>-1</sup>

C	0.361174	2.360897	-0.48252
C	0.774004	2.272561	-1.97218
O	1.636628	1.055073	-2.0192
O	2.194268	0.872743	-3.17732
C	-0.39054	1.960789	-2.93869
C	-1.17316	0.72392	-2.49079
H	-0.53688	-0.16475	-2.62986
H	-2.03845	0.626119	-3.16088
C	-1.61367	0.826645	-1.02667
H	-2.35098	1.637259	-0.92891
H	-2.12373	-0.0996	-0.72573
C	-0.41381	1.0815	-0.10311
H	0.270876	0.218904	-0.14665
H	-0.74432	1.176203	0.943928
C	1.632391	3.450916	-2.41566
H	1.034336	4.370667	-2.35367
H	1.919931	3.302607	-3.46887
C	-0.53281	3.587963	-0.2137
H	-0.04364	4.532207	-0.48305
H	-0.75098	3.622293	0.864788
H	-1.47671	3.543558	-0.76573
C	1.647778	2.485068	0.36483
H	2.22363	1.549178	0.288107
H	1.357529	2.593597	1.421672
C	2.528937	3.666955	-0.06052
H	2.021707	4.626703	0.120257
H	3.458337	3.68703	0.525314
C	2.885594	3.591935	-1.54138
H	0.064328	1.775545	-3.92977
O	-1.20349	3.113794	-3.00853
O	-2.1313	2.896852	-4.33151
H	3.535979	2.713742	-1.70547
O	3.599176	4.783266	-1.86827
H	3.971327	4.702672	-2.75351
S	-2.03462	3.967722	-5.79919
C	-0.2348	3.915141	-5.91305
H	0.157317	3.9895	-4.88974
H	0.126861	4.737446	-6.54101
H	0.041693	2.950794	-6.35325
C	-2.22556	5.496404	-4.85695
H	-1.82258	6.342365	-5.42579

H	-1.69803	5.355424	-3.90415
H	-3.29546	5.637965	-4.67351

H	-1.48195	1.316671	-6.90564
H	-2.39059	1.234588	-5.36428

**6-T**

**MECP 3**

C	0.42832	2.475277	-0.27316
C	0.469711	3.237119	-1.61792
O	0.829551	2.19069	-2.61422
O	0.875211	2.6504	-3.82582
C	-0.92529	3.755196	-2.03951
C	-1.96634	2.625291	-2.08292
H	-1.6874	1.931689	-2.89245
H	-2.93881	3.066841	-2.33902
C	-2.01685	1.865791	-0.75214
H	-2.41723	2.526294	0.031869
H	-2.71692	1.022767	-0.83437
C	-0.62535	1.349375	-0.3597
H	-0.29256	0.599546	-1.09565
H	-0.66687	0.840602	0.61619
C	1.55574	4.304106	-1.66758
H	1.322834	5.082546	-0.92853
H	1.540921	4.778013	-2.66213
C	0.049639	3.431999	0.87337
H	0.777006	4.24092	1.007601
H	0.013018	2.854592	1.809146
H	-0.93135	3.902351	0.729429
C	1.829694	1.883527	-0.00803
H	2.033794	1.098506	-0.75398
H	1.818602	1.389054	0.975746
C	2.942021	2.939251	-0.05386
H	2.833759	3.66976	0.761834
H	3.925617	2.467781	0.076468
C	2.936819	3.703321	-1.37382
H	-0.81747	4.17604	-3.06867
O	-1.30187	4.842129	-1.30198
O	-2.68487	3.864397	-6.62998
H	3.20529	3.006001	-2.18917
O	3.923669	4.723763	-1.2711
H	3.997944	5.19395	-2.10926
S	-1.52945	3.421125	-5.75382
C	-0.01993	3.707426	-6.72355
H	-0.17582	3.281104	-7.72217
H	0.838807	3.249325	-6.2188
H	0.115291	4.791441	-6.80264
C	-1.48081	1.607691	-5.84787
H	-0.58726	1.239309	-5.32782

C	-2.02269	0.955977	-0.46257
C	-0.99555	0.066079	0.278267
O	-0.12162	-0.45886	-0.80994
O	0.705297	-1.37151	-0.39654
C	-0.03074	0.844554	1.201082
C	0.640975	2.021483	0.428458
H	1.295019	1.549251	-0.31985
H	1.274113	2.574322	1.132995
C	-0.38409	2.915132	-0.27099
H	-0.98873	3.449336	0.476504
H	0.148845	3.683189	-0.84936
C	-1.27845	2.087703	-1.20372
H	-0.66103	1.65395	-2.00755
H	-2.02705	2.733603	-1.68884
C	-1.64049	-1.12543	0.976816
H	-2.30566	-0.74684	1.76586
H	-0.85491	-1.72414	1.462836
C	-3.03395	1.591899	0.513726
H	-3.59205	0.848809	1.09425
H	-3.76246	2.168457	-0.07626
H	-2.56257	2.268222	1.233706
C	-2.78352	0.061691	-1.46605
H	-2.08629	-0.28099	-2.24723
H	-3.54669	0.675584	-1.9696
C	-3.44417	-1.15148	-0.79847
H	-4.23988	-0.84046	-0.10508
H	-3.91933	-1.79342	-1.55274
C	-2.43771	-1.98625	-0.0125
H	0.796462	0.172566	1.513174
O	-0.63408	1.350467	2.311644
O	4.938097	0.335578	0.540064
H	-1.73106	-2.45598	-0.72172
O	-3.17562	-2.99523	0.668741
H	-2.57305	-3.58979	1.129572
S	3.583416	-0.23911	0.173354
C	3.795168	-2.04094	0.101272
H	4.691988	-2.25219	-0.49424
H	2.90005	-2.49829	-0.33634
H	3.943276	-2.39226	1.127987
C	3.393902	0.012202	-1.6165
H	2.468097	-0.46803	-1.95738



H	4.275291	-0.40243	-2.1214
H	3.354282	1.094021	-1.78772

H	-4.54686	0.109593	-1.96893
H	-3.64297	-1.36956	-1.51835

**6-S**

C	2.14846	-0.94557	-0.32005
C	0.989555	-0.05248	0.178507
O	0.271726	0.3392	-1.05941
O	-0.72781	1.130135	-0.8227
C	-0.05409	-0.8539	1.004688
C	-0.58745	-2.06739	0.230981
H	-1.16558	-1.70406	-0.63384
H	-1.27646	-2.61436	0.888692
C	0.560529	-2.9588	-0.25706
H	1.059485	-3.41869	0.609528
H	0.158467	-3.7858	-0.85855
C	1.566981	-2.15197	-1.08935
H	1.076154	-1.79181	-2.00803
H	2.40403	-2.79353	-1.40658
C	1.467617	1.217571	0.868786
H	2.016659	0.941456	1.77884
H	0.591993	1.808629	1.179084
C	2.977308	-1.45982	0.872027
H	3.463159	-0.65109	1.429945
H	3.766529	-2.12233	0.486652
H	2.378111	-2.03343	1.59105
C	3.04652	-0.09646	-1.24596
H	2.484026	0.147887	-2.1617
H	3.905857	-0.71035	-1.55755
C	3.536807	1.197293	-0.58242
H	4.208729	0.983762	0.262366
H	4.113715	1.800677	-1.29645
C	2.375517	2.036334	-0.0589
H	-0.8925	-0.13876	1.193794
O	0.418574	-1.13471	2.251755
O	-4.94456	-0.17512	0.821126
H	1.779366	2.394995	-0.91865
O	2.938552	3.146537	0.630715
H	2.238093	3.740398	0.923601
S	-3.60898	0.241292	0.236056
C	-3.73196	2.025013	-0.08669
H	-4.67089	2.205829	-0.62429
H	-2.86392	2.358419	-0.66758
H	-3.76038	2.530096	0.884761
C	-3.62928	-0.27396	-1.50576
H	-2.73208	0.107832	-2.00948

**TS4-S**

424.1565i cm<sup>-1</sup>

C	0.022987	2.125388	-0.37478
C	0.536698	2.303294	-1.80628
O	0.744662	1.017375	-2.34329
O	1.395935	0.991632	-3.46798
C	-0.79313	2.862487	-2.88406
C	-1.91891	1.840618	-2.71408
H	-1.59372	0.872457	-3.12294
H	-2.75919	2.196514	-3.32935
C	-2.34858	1.692159	-1.25067
H	-2.71366	2.663086	-0.88461
H	-3.19315	0.992362	-1.18763
C	-1.19944	1.184449	-0.36804
H	-0.89195	0.181959	-0.70584
H	-1.53896	1.08002	0.673983
C	1.738091	3.198929	-1.96358
H	1.496838	4.193254	-1.56729
H	2.002779	3.304966	-3.02428
C	-0.34898	3.470285	0.271604
H	0.514289	4.137618	0.377635
H	-0.73722	3.268609	1.280696
H	-1.1125	4.007947	-0.30071
C	1.210821	1.494069	0.401571
H	1.378265	0.472882	0.022407
H	0.918628	1.399687	1.458589
C	2.505727	2.311392	0.286336
H	2.40923	3.284037	0.790928
H	3.331924	1.784556	0.78246
C	2.904057	2.574523	-1.16535
H	-0.16804	2.717976	-3.8016
O	-1.01521	4.077874	-2.53836
O	-0.18299	5.82546	-7.52151
H	3.183193	1.61737	-1.64224
O	4.020489	3.45046	-1.14285
H	4.428654	3.490868	-2.01508
S	-0.56927	6.033193	-6.07015
C	0.748936	5.276125	-5.07494
H	0.960701	4.284454	-5.49828
H	0.420868	5.209797	-4.0283
H	1.635237	5.913184	-5.16947

C	-1.83581	4.786225	-5.69115	H	0.238314	5.09333	-3.85612
H	-2.07642	4.826707	-4.62091	H	1.67319	5.836685	-4.67333
H	-1.45189	3.79852	-5.97992	C	-1.69785	5.003463	-5.888
H	-2.71593	5.030453	-6.29581	H	-2.07445	4.908218	-4.86138

H	-1.31768	4.045333	-6.26637
H	-2.47857	5.380611	-6.55717

**TS4-T**

179.2016i cm<sup>-1</sup>

C	0.050686	2.13355	-0.37398
C	0.551276	2.214243	-1.7956
O	0.794167	0.870412	-2.27113
O	1.091092	0.837035	-3.54591
C	-1.14066	2.792303	-3.00959
C	-2.03398	1.620677	-2.61416
H	-1.58767	0.676732	-2.9582
H	-2.96307	1.765539	-3.18918
C	-2.35047	1.570728	-1.11493
H	-2.72927	2.554434	-0.80068
H	-3.16225	0.84995	-0.94519
C	-1.1396	1.160492	-0.26504
H	-0.81321	0.149425	-0.55613
H	-1.43066	1.107877	0.795718
C	1.70836	3.109604	-2.0767
H	1.463626	4.137849	-1.77788
H	1.947735	3.098963	-3.15105
C	-0.3429	3.514762	0.177267
H	0.505789	4.207854	0.216184
H	-0.70959	3.382346	1.205737
H	-1.12778	3.985015	-0.42409
C	1.276083	1.58846	0.427622
H	1.463018	0.545955	0.124673
H	1.000525	1.570574	1.493327
C	2.544248	2.430122	0.225346
H	2.428001	3.435847	0.655049
H	3.393347	1.9671	0.746164
C	2.915705	2.593152	-1.2483
H	-0.50175	2.641555	-3.91033
O	-1.39153	3.951697	-2.63921
O	0.280736	6.130171	-7.29839
H	3.216628	1.610524	-1.65626
O	4.000403	3.503148	-1.31202
H	4.38653	3.502807	-2.19519
S	-0.33453	6.20441	-5.91398
C	0.75439	5.256043	-4.81272
H	0.987686	4.306226	-5.31399

**7-S**

C	-0.32491	2.791802	-1.30816
C	-0.54959	4.2197	-0.9013
O	-1.55993	4.77842	-1.40803
O	-1.76667	6.126966	-1.17622
C	-3.14158	3.827475	0.659741
C	-3.64406	3.016609	-0.50762
H	-3.81921	3.717445	-1.33989
H	-4.64345	2.655853	-0.20864
C	-2.75146	1.836508	-0.91829
H	-2.36401	1.351761	-0.00996
H	-3.39521	1.095518	-1.413
C	-1.5947	2.14038	-1.89165
H	-1.96984	2.756152	-2.72371
H	-1.26539	1.186013	-2.33324
C	0.536992	4.991899	-0.28409
H	1.050145	4.41342	0.492659
H	0.196593	5.963165	0.085644
C	0.246179	1.947504	-0.15469
H	1.272228	2.239137	0.09987
H	0.269163	0.89451	-0.47226
H	-0.37241	2.036187	0.746315
C	0.7506	2.952285	-2.43605
H	0.253302	3.388981	-3.31826
H	1.091405	1.94441	-2.71924
C	1.947281	3.831085	-2.03589
H	2.564162	3.342003	-1.2663
H	2.600388	3.989928	-2.90482
C	1.514628	5.193985	-1.49368
H	-3.77413	4.690045	0.964506
O	-2.11785	3.58133	1.264194
O	1.009191	8.100316	-0.73033
H	0.948566	5.744699	-2.27233
O	2.64579	5.917762	-1.10102
H	2.333736	6.825219	-0.91374
S	-0.06561	8.590395	-1.70764
C	0.425072	10.29953	-2.07798

H	0.615851	10.82015	-1.13175
H	-0.36653	10.79621	-2.65289
H	1.345984	10.25434	-2.66921
C	-1.49297	8.99193	-0.67395
H	-2.26342	9.46747	-1.29337
H	-1.15571	9.657172	0.130458
H	-1.86208	8.041278	-0.27486

**TS5-S**

367.6694i cm<sup>-1</sup>

C	-1.56946	0.512327	0.961626
C	-0.91475	0.291371	-0.37165
O	-0.07525	-0.6904	-0.34357
O	0.233109	-1.23207	-1.59411
C	-1.87917	-1.81324	-1.55164
C	-1.84166	-2.63594	-0.27577
H	-0.80642	-2.95125	-0.0842
H	-2.40893	-3.55522	-0.4991
C	-2.48109	-1.9487	0.951389
H	-3.46451	-1.55454	0.653432
H	-2.68207	-2.74109	1.687166
C	-1.6853	-0.8457	1.688392
H	-0.67413	-1.21208	1.924497
H	-2.18428	-0.6518	2.651172
C	-0.7056	1.428314	-1.30213
H	-1.64367	1.965171	-1.48504
H	-0.29053	1.06405	-2.2484
C	-2.95038	1.16937	0.807003
H	-2.88326	2.182791	0.392887
H	-3.41037	1.249011	1.802647
H	-3.60533	0.580572	0.154898
C	-0.59145	1.477786	1.693287
H	0.335407	0.930914	1.920819
H	-1.0562	1.78606	2.642734
C	-0.24322	2.714877	0.846971
H	-1.11457	3.375006	0.7108
H	0.526991	3.305266	1.360774
C	0.29107	2.34733	-0.53814
H	-1.75869	-2.32868	-2.51836
O	-2.32383	-0.65268	-1.52398
H	1.242222	1.801881	-0.40902
O	0.485941	3.558503	-1.25618
H	1.014528	3.389816	-2.04381
S	3.373917	-0.60755	0.630425

C	3.369621	-0.37466	-1.17023
H	2.332937	-0.4629	-1.52905
H	4.007044	-1.13826	-1.63448
H	3.781996	0.622094	-1.36463
C	2.54374	-2.22608	0.628255
H	1.683824	-2.19284	-0.05253
H	2.226973	-2.4134	1.660649
H	3.26652	-2.99035	0.314688
O	2.370994	0.401418	1.180399

**8-S**

C	-0.0057	1.14905	0.075828
C	0.006825	-0.38316	0.207955
O	0.349546	-0.91009	-1.10394
O	1.229703	-1.99183	-0.81528
C	2.030931	-1.38437	0.188353
C	2.980051	-0.32003	-0.39288
H	2.973152	-0.44133	-1.48632
H	4.001624	-0.53494	-0.04854
C	2.619716	1.127083	-0.02182
H	2.624432	1.235365	1.072712
H	3.426626	1.77154	-0.40067
C	1.291662	1.636865	-0.60734
H	1.253365	1.372008	-1.67525
H	1.281061	2.737766	-0.5543
C	-1.30471	-0.99732	0.674054
H	-1.51014	-0.69361	1.710766
H	-1.17215	-2.09008	0.659047
C	-0.12308	1.771936	1.475832
H	-1.05103	1.485259	1.986732
H	-0.11559	2.868309	1.388331
H	0.714815	1.465151	2.114871
C	-1.21462	1.541221	-0.80248
H	-1.02643	1.186324	-1.83011
H	-1.27164	2.639907	-0.85088
C	-2.54327	0.957915	-0.30776
H	-2.80835	1.344706	0.688367
H	-3.3623	1.236596	-0.98487
C	-2.46327	-0.56151	-0.22824
O	1.063302	-0.8257	1.052714
H	-2.28836	-0.96033	-1.24444
O	-3.7108	-1.0305	0.273953
H	-3.71981	-1.99431	0.270982
H	2.53889	-2.20454	0.709844

Product			
C	1.100125	-1.1859	0.014432
C	1.007829	0.282942	0.418923
O	-0.05084	0.884913	0.475708
C	2.325998	1.014082	0.559049
H	2.996125	0.496589	1.2604
H	2.126209	2.029642	0.924036
C	1.941829	-2.012	1.005583
H	1.577355	-1.90213	2.033747
H	1.875825	-3.0736	0.721171
H	3.002045	-1.73172	0.98544
C	-0.29636	-1.80832	-0.17889
H	-0.89307	-1.13522	-0.81496
H	-0.13863	-2.73423	-0.75656
C	-1.11689	-2.1791	1.071907
H	-1.87536	-2.90795	0.752285
H	-0.48551	-2.69509	1.810187
C	-1.84852	-1.02344	1.762302
H	-2.2552	-0.30605	1.035248
H	-2.70952	-1.40435	2.340489
C	2.991244	1.033973	-0.83217
H	2.342128	1.60797	-1.52069
C	1.81528	-1.14237	-1.3706
H	1.129756	-0.67685	-2.09973
H	1.974642	-2.18006	-1.70272
C	3.149426	-0.38468	-1.36603
H	3.898904	-0.89837	-0.74568
H	3.562878	-0.33757	-2.38286
C	-1.0202	-0.25004	2.756665
H	-1.4432	0.726886	3.083539
O	0.028866	-0.64132	3.224333
O	4.28479	1.618454	-0.78492
H	4.217653	2.542946	-0.52069

**isoprene**

C	-2.6378	-0.24489	-0.47375
H	-3.50844	-0.90097	-0.48609
C	-2.66981	0.932139	0.157134
H	-3.58603	1.241539	0.669361
H	-1.74651	-0.59572	-0.99761
C	-1.54483	1.8863	0.229241
C	-1.69389	3.040074	0.892111
H	-2.63567	3.292005	1.383847
H	-0.88173	3.765392	0.963515

C	-0.2551	1.515818	-0.45687
H	0.152473	0.581959	-0.04266
H	-0.41817	1.355035	-1.53262
H	0.495509	2.305591	-0.33471

**TS1\_isoprene**

739.9543i cm<sup>-1</sup>

C	-2.67527	-0.30714	-0.29373
H	-3.6296	-0.83065	-0.35966
O	-1.95991	-1.41754	0.993812
O	-0.96676	-0.92761	1.568197
C	-2.655	0.993264	0.232748
H	-3.50879	1.333526	0.82231
H	-1.95261	-0.5704	-1.0692
C	-1.50694	1.846384	0.181512
C	-1.51942	3.022469	0.867591
H	-2.38584	3.317547	1.461146
H	-0.66523	3.699686	0.851966
C	-0.30562	1.434454	-0.63885
H	0.11362	0.490822	-0.26594
H	-0.58156	1.293727	-1.69425
H	0.477563	2.200128	-0.59202

**styrene**

C	-2.75115	-0.20553	-0.5597
H	-3.63317	-0.84412	-0.51144
C	-2.65618	0.888134	0.199021
H	-3.48905	1.142197	0.862029
H	-1.9675	-0.49994	-1.26029
C	-1.51916	1.835772	0.230275
C	-1.68444	3.076056	0.857048
C	-0.27507	1.537493	-0.34009
C	-0.64623	4.003668	0.898209
H	-2.6474	3.316662	1.313549
C	0.763973	2.460943	-0.30014
H	-0.11282	0.565722	-0.80891
C	0.582358	3.699272	0.31709
H	-0.79799	4.966439	1.388366
H	1.727249	2.210361	-0.74705
H	1.399627	4.420985	0.349759

**TS1\_styrene**745.4297i cm<sup>-1</sup>

C	-2.65132	-0.33626	-0.37495
H	-3.60212	-0.86	-0.48153
O	-1.9278	-1.49404	0.833754
O	-0.76573	-1.16462	1.151355
C	-2.66797	0.941789	0.202643
H	-3.56236	1.248405	0.748546
H	-1.92534	-0.55289	-1.1616
C	-1.55165	1.851714	0.224067
C	-1.70651	3.11451	0.837314
C	-0.2967	1.536841	-0.33934
C	-0.66126	4.024843	0.8764
H	-2.6705	3.368816	1.283272
C	0.747919	2.450303	-0.29523
H	-0.13578	0.560476	-0.79585
C	0.572695	3.696629	0.309029
H	-0.8036	4.9953	1.353569
H	1.712674	2.186734	-0.73043
H	1.397056	4.409964	0.341451

**acrylate**

C	-0.89891	-0.84541	-0.7814
H	-1.7224	-1.4938	-1.08261
C	-1.12748	0.363614	-0.27381
H	-2.13036	0.76679	-0.13314
H	0.119725	-1.21475	-0.90749
C	-0.04023	1.287598	0.151585
O	-0.23729	2.392664	0.611168
O	1.192632	0.781609	-0.02146
C	2.26397	1.64535	0.378425
H	3.185842	1.094278	0.173648
H	2.227905	2.578425	-0.19749
H	2.176455	1.881666	1.44619

**TS1\_acrylate**820.1729i cm<sup>-1</sup>

C	-0.74948	-0.97851	-0.69665
H	-1.5584	-1.5665	-1.13344
O	-0.51007	-1.99046	0.723466
O	0.469681	-1.63806	1.410634

C	-1.05909	0.316173	-0.2364
H	-2.07812	0.616795	-0.00165
H	0.235599	-1.12321	-1.1443
C	-0.01959	1.297995	0.103873
O	-0.2466	2.369629	0.631505
O	1.217343	0.893142	-0.23541
C	2.27019	1.798012	0.120597
H	3.198586	1.319081	-0.20168
H	2.125315	2.759495	-0.3876
H	2.268904	1.961131	1.205421

**butenone**

C	-0.92872	-0.9104	-0.62232
H	-1.76714	-1.60508	-0.68702
C	-1.10809	0.356725	-0.24985
H	-2.09532	0.7483	0.004131
H	0.057864	-1.30329	-0.87738
C	-0.00432	1.360176	-0.14224
C	1.412735	0.933	-0.46441
H	1.728291	0.117793	0.201289
H	1.478909	0.568026	-1.49858
H	2.076918	1.792328	-0.33398
O	-0.26196	2.499041	0.202073

**TS1\_butenone**819.1639i cm<sup>-1</sup>

C	-0.841	-1.0052	-0.64853
H	-1.71436	-1.58108	-0.95982
O	-0.48136	-1.99019	0.79092
O	0.644674	-1.74764	1.267777
C	-1.04876	0.318436	-0.21393
H	-2.03145	0.642195	0.129786
H	0.075269	-1.23082	-1.19966
C	0.020607	1.324236	-0.09519
C	1.425934	0.970454	-0.5343
H	1.792594	0.092035	0.014784
H	1.443036	0.733517	-1.60813
H	2.077355	1.828387	-0.3437
O	-0.25671	2.433388	0.341937

**ether**

C	-0.90683	-0.51377	-0.67346
H	-1.77625	-1.15688	-0.78686
C	-1.08666	0.736116	-0.23834
H	0.067827	-0.92825	-0.92283
H	-2.07325	1.132823	0.006386
O	-0.13472	1.677026	-0.036
C	1.198613	1.291751	-0.31608
H	1.828209	2.161511	-0.10492
H	1.303213	1.001803	-1.37406
H	1.499677	0.447165	0.324451

**TS1\_ether**

617.2820i cm<sup>-1</sup>

C	-0.81538	-0.59682	-0.56448
H	-1.68198	-1.20917	-0.81638
O	-0.29682	-1.45396	0.922535
O	0.86662	-1.92916	0.773398
C	-1.10499	0.743605	-0.2648
H	0.094128	-0.83812	-1.11867
H	-2.10544	1.085857	-0.00682
O	-0.18581	1.702577	-0.10222
C	1.181095	1.363827	-0.33958
H	1.765015	2.243492	-0.05523
H	1.338205	1.144219	-1.40638
H	1.475358	0.497384	0.26937

**ch1**

C	0.651426	0.147853	-0.96754
C	-0.54989	0.451078	-0.10365
C	-0.63321	1.521455	0.690883
C	0.442962	2.578072	0.779165
H	-0.02216	3.575486	0.786186
H	0.96909	2.482179	1.744814
C	1.861261	0.99815	-0.56458
H	2.657931	0.911367	-1.31706
H	2.27066	0.617821	0.385836
C	1.441779	2.45929	-0.37636
H	0.966488	2.817915	-1.30428
H	2.316434	3.099578	-0.19297
H	-1.52498	1.65808	1.308983
H	0.395747	0.33228	-2.02537
H	0.893002	-0.92353	-0.89743
H	-1.38366	-0.25579	-0.13523

**TS1\_ch1**

695.3347i cm<sup>-1</sup>

C	0.695363	0.124928	-0.94077
C	-0.51789	0.397895	-0.10729
O	-1.60901	2.629319	-0.76011
O	-2.7262	2.14436	-1.07017
C	-0.74583	1.652513	0.495502
C	0.419485	2.58879	0.729939
H	0.039654	3.618196	0.799524
H	0.872911	2.345091	1.70442
C	1.893042	0.996658	-0.53948
H	2.691819	0.902543	-1.28819
H	2.303975	0.635013	0.417173
C	1.463125	2.458233	-0.38326
H	1.027062	2.817509	-1.3296
H	2.329022	3.097795	-0.16242
H	-1.55529	1.6946	1.23021
H	0.435702	0.32726	-1.99825
H	0.948446	-0.94461	-0.89639
H	-1.33381	-0.32595	-0.1189

**ch2**

C	0.695363	0.124928	-0.94077
C	-0.51789	0.397895	-0.10729
O	-1.60901	2.629319	-0.76011
O	-2.7262	2.14436	-1.07017
C	-0.74583	1.652513	0.495502
C	0.419485	2.58879	0.729939
H	0.039654	3.618196	0.799524
H	0.872911	2.345091	1.70442
C	1.893042	0.996658	-0.53948
H	2.691819	0.902543	-1.28819
H	2.303975	0.635013	0.417173
C	1.463125	2.458233	-0.38326
H	1.027062	2.817509	-1.3296
H	2.329022	3.097795	-0.16242
H	-1.55529	1.6946	1.23021
H	0.435702	0.32726	-1.99825
H	0.948446	-0.94461	-0.89639
H	-1.33381	-0.32595	-0.1189

**TS1\_ch2**

628.1241i cm<sup>-1</sup>

C	0.632277	0.173819	-0.98644
C	-0.53771	0.383138	-0.068
O	-1.60489	2.656131	-0.64701
O	-2.5333	2.055015	-1.25013
C	-0.72475	1.63377	0.562713
C	0.448791	2.562012	0.784208
H	0.069555	3.587884	0.899292
H	0.936322	2.2901	1.734476
C	1.856981	1.015283	-0.60625
H	2.617119	0.946266	-1.39695
H	2.309813	0.60811	0.312599
C	1.45118	2.471939	-0.36902
H	0.985416	2.87771	-1.28157
H	2.331879	3.091945	-0.15056
H	-1.50654	1.663411	1.329626
H	0.305019	0.447537	-2.00955
H	0.882695	-0.89741	-1.02838
C	-1.63853	-0.62497	-0.09002
H	-2.3901	-0.42955	0.685086
H	-2.15664	-0.58551	-1.06465
H	-1.24888	-1.64678	0.035227

ch3

C	0.689132	0.168977	-0.99084
C	-0.52687	0.458449	-0.13915
C	-0.64004	1.512404	0.673087
C	0.429004	2.568766	0.818619
H	-0.04024	3.563122	0.864095
H	0.947248	2.43259	1.783695
C	1.874727	1.051891	-0.56472
H	2.668206	0.999873	-1.32587
H	2.300084	0.658164	0.372947
C	1.436751	2.501381	-0.33227
H	0.967551	2.897345	-1.24691
H	2.306424	3.139042	-0.11884
H	-1.55116	1.63247	1.265995
H	0.966841	-0.88554	-0.82644
H	-1.35849	-0.24948	-0.2142
C	0.35336	0.326583	-2.48326
H	1.205272	0.027302	-3.11066
H	-0.51035	-0.29354	-2.76201
H	0.099994	1.36995	-2.71915

TS1\_ch3

687.4620i cm<sup>-1</sup>

C	0.705871	0.149804	-0.96141
C	-0.49592	0.396351	-0.09803
O	-1.58615	2.635107	-0.73985
O	-2.6245	2.092019	-1.19487
C	-0.74449	1.641152	0.517228
C	0.408494	2.583888	0.780854
H	0.016534	3.605875	0.884742
H	0.867421	2.313479	1.745672
C	1.886855	1.050248	-0.5556
H	2.670582	0.992237	-1.32565
H	2.327192	0.669421	0.380391
C	1.448134	2.502377	-0.34043
H	1.011825	2.909605	-1.26575
H	2.315175	3.131228	-0.09474
H	-1.56307	1.664934	1.242807
H	1.004961	-0.9044	-0.84359
H	-1.3053	-0.33568	-0.12875
C	0.310435	0.351114	-2.44271
H	1.15889	0.111821	-3.09959
H	-0.53357	-0.29625	-2.71676
H	0.002873	1.389101	-2.63015

ch4

C	0.694576	0.127273	-0.97311
C	-0.52486	0.446389	-0.13541
C	-0.63443	1.523655	0.646213
C	0.429576	2.590826	0.746361
H	-0.04357	3.584286	0.723365
H	0.929045	2.515153	1.727616
C	1.881906	0.995309	-0.5378
H	2.704179	0.895488	-1.26247
H	2.257204	0.618067	0.42977
C	1.460337	2.458141	-0.37901
H	1.012634	2.807009	-1.32405
H	2.330808	3.098944	-0.17844
H	-1.53888	1.65643	1.246576
H	0.457824	0.365456	-2.02635
H	-1.34899	-0.27384	-0.17296
C	1.032792	-1.36583	-0.89183
H	0.195605	-1.98644	-1.24195
H	1.913032	-1.60339	-1.50632

H 1.254493 -1.65212 0.146998

**TS1\_ch4**

700.1098i cm<sup>-1</sup>

C 0.694936 0.114005 -0.92913  
C -0.5129 0.404208 -0.08811  
O -1.60834 2.622357 -0.77733  
O -2.72543 2.133967 -1.08093  
C -0.74782 1.665593 0.496979  
C 0.412936 2.60881 0.724823  
H 0.030571 3.638461 0.7743  
H 0.858616 2.381652 1.7068  
C 1.884494 0.994981 -0.51742  
H 2.692995 0.886288 -1.25547  
H 2.279328 0.630463 0.44691  
C 1.465274 2.460359 -0.37731  
H 1.041513 2.815123 -1.33081  
H 2.334506 3.094714 -0.15444  
H -1.56049 1.71409 1.227786  
H 0.425136 0.384789 -1.97065  
H -1.32184 -0.32978 -0.08273  
C 1.050807 -1.37665 -0.90768  
H 0.205545 -1.99481 -1.24074  
H 1.904782 -1.58203 -1.56795  
H 1.323452 -1.69211 0.110017

**ch5**

C 0.666881 0.180883 -1.00377  
C -0.52751 0.418399 -0.09326  
C -0.59927 1.473932 0.726275  
C 0.451185 2.552815 0.831747  
H -0.03743 3.537942 0.878977  
H 0.993428 2.43775 1.786653  
C 1.864592 1.049247 -0.58611  
H 2.646762 0.996975 -1.3589  
H 2.298748 0.644148 0.342704  
C 1.437506 2.497637 -0.33685  
H 0.955923 2.902684 -1.24073  
H 2.31209 3.13136 -0.13154  
H -1.4757 1.570179 1.375818  
H 0.953571 -0.87942 -0.89132  
C -1.62824 -0.61219 -0.15387  
H -2.42367 -0.39095 0.569193

H -2.08368 -0.65296 -1.15472

H -1.23446 -1.6176 0.061545

C 0.295027 0.397466 -2.4816

H 1.155863 0.184506 -3.13167

H -0.5289 -0.25865 -2.79307

H -0.02114 1.435309 -2.65863

**TS1\_ch5**

616.7325i cm<sup>-1</sup>

C 0.681698 0.165957 -0.97781  
C -0.51167 0.377028 -0.08063  
O -1.59802 2.645686 -0.6805  
O -2.52729 2.047236 -1.2861  
C -0.73389 1.626934 0.542125  
C 0.419155 2.570876 0.797998  
H 0.022916 3.589616 0.917814  
H 0.891993 2.293372 1.754155  
C 1.871492 1.054995 -0.57463  
H 2.645157 1.001262 -1.35526  
H 2.321127 0.660365 0.351323  
C 1.443193 2.505534 -0.33666  
H 0.995252 2.926248 -1.25024  
H 2.315487 3.128084 -0.09328  
H -1.5351 1.642676 1.289443  
H 0.984385 -0.89089 -0.88642  
C -1.60611 -0.64062 -0.10706  
H -2.23227 -0.5882 0.793572  
H -2.27159 -0.44812 -0.96789  
H -1.20754 -1.66049 -0.20857  
C 0.269966 0.397985 -2.44956  
H 1.114837 0.182413 -3.11898  
H -0.56866 -0.25169 -2.73476  
H -0.04816 1.436886 -2.61147

**ch6**

C 0.682028 0.101945 -0.93433  
C -0.5463 0.420674 -0.09296  
C -0.6244 1.522767 0.663166  
C 0.444999 2.58482 0.747311  
H -0.02667 3.579245 0.742579  
H 0.973405 2.503372 1.713136  
C 1.86873 0.995698 -0.55194  
H 2.666798 0.88679 -1.30214



H	2.281424	0.640176	0.408795
C	1.443183	2.455721	-0.40476
H	0.965159	2.789316	-1.3405
H	2.31431	3.104991	-0.23585
H	-1.53297	1.684063	1.25283
H	0.416309	0.308686	-1.98872
C	1.079779	-1.37792	-0.83672
H	0.308598	-2.04454	-1.24513
H	2.009269	-1.55868	-1.39535
H	1.255443	-1.6604	0.212653
C	-1.69194	-0.55918	-0.17049
H	-1.96556	-0.75614	-1.21935
H	-1.42595	-1.5275	0.278969
H	-2.57823	-0.17339	0.348777

### TS1\_ch6

631.2369i cm<sup>-1</sup>

C	0.660216	0.115882	-0.90294
C	-0.54589	0.38756	-0.03619
O	-1.57186	2.62099	-0.81128
O	-2.4737	1.984265	-1.41749
C	-0.75308	1.677109	0.505437
C	0.405578	2.620831	0.729222
H	0.020596	3.650422	0.765438
H	0.846466	2.405628	1.716105
C	1.857883	0.991938	-0.50308
H	2.657318	0.87114	-1.24933
H	2.259951	0.626188	0.45802
C	1.460364	2.461741	-0.36687
H	1.044479	2.820953	-1.32179
H	2.337621	3.083914	-0.14073
H	-1.57294	1.755341	1.227757
H	0.361664	0.4094	-1.9318
C	1.052816	-1.36633	-0.93442
H	0.257522	-1.99717	-1.35246
H	1.951059	-1.5055	-1.55176
H	1.280535	-1.72782	0.079902
C	-1.66577	-0.60251	-0.02588
H	-2.03656	-0.76148	-1.05371
H	-1.3424	-1.5816	0.360315
H	-2.50968	-0.24669	0.577224