Electronic Supplementary Information

Theoretical study on formation mechanism of peroxovanadate and the origin of its high activity for oxidation of sulfide

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Content

1. Benchmark calculations of functionals for geometry optimization

The crystal structure of a $\{V_5O_9Cl\}$-based metal-organic polyhedra is shown in Figure S1. Several functionals (See Table S1) have been tested for geometry optimization compared with the experimental results. The V–O1, V–O2, V–O3, V–O4, V–O5, and V–Cl distances were considered as parameters. As shown in Table S1, the RMSE of B3LYP-D3(BJ) functional is the minimum. In this work, all geometry optimizations were performed by B3LYP-D3(BJ) functional because dispersion correction should be considered and the optimization by B3LYP-D3(BJ) functional reproduced other crystal structures well, in which the SDD basis sets were employed for valence electrons of V atom with corresponding effective core potentials presenting their core electrons and 6-31G(d) basis sets were employed for other atoms.

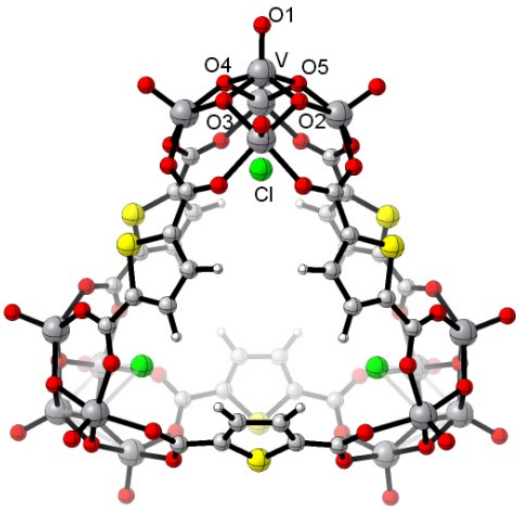


Fig. S1 Crystal structure of $\{V_5O_9Cl\}$-based metal-organic polyhedra[1]. (distance [Å]).

Table S1 Benchmark of functionals for geometry optimization. Angstrom unit was used. Basis set: SDD for V, 6-31G(d) basis sets for other atoms.

	V–O1	V–O2	V–O3	V–O4	V–O5	V–Cl	RMSE
Experiment[1]	1.570	1.874	1.874	1.874	1.874	3.261	
B3LYP-D3(BJ)	1.594	1.866	1.866	1.866	1.866	3.296	0.019
B3LYP-D3	1.594	1.867	1.867	1.867	1.867	3.357	0.041
B3LYP	1.595	1.869	1.869	1.869	1.869	3.317	0.025
ωB97XD	1.578	1.857	1.857	1.857	1.857	1.857	0.030
B3PW91-D3(DJ)	1.586	1.859	1.859	1.859	1.859	3.227	0.020

2. Benchmark calculations for selecting basis sets for evaluation of energy changes

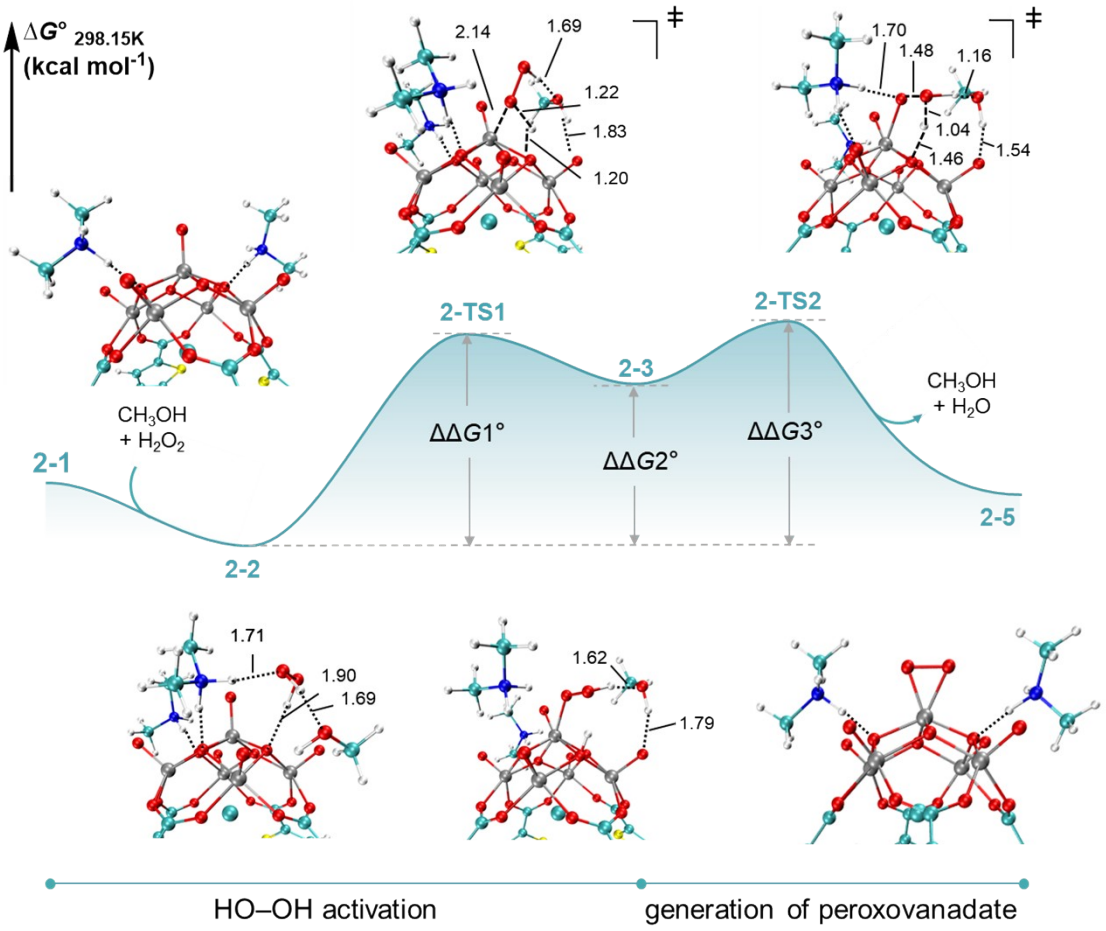


Fig. S2 Gibbs energy profile (in kcal mol^{-1}) of H_2O_2 activation via H–OOH bond cleavage (methanol participation). The bond length is given in Å. Long dashed lines represent the transition state, while short dashed lines indicate hydrogen bonding interactions.

Table S2 Benchmark of basis set for potential energy change. Values are in kcal mol^{-1} unit.

	ΔΔ*G*1°	ΔΔ*G*2°	ΔΔ*G*3°
6-311G(d)	23.0	17.3	24.0
6-311++G(d,p)	23.3	19.5	25.0
def2-TZVP	24.4	20.6	25.8

We have performed test calculation on basis sets as shown in Table S2. The

relative energy barrier is slightly dependent on the basis sets and such a small difference does not change the understanding of the reaction mechanism.

3. Spin density distribution and SOMO orbital of polyoxovanadate

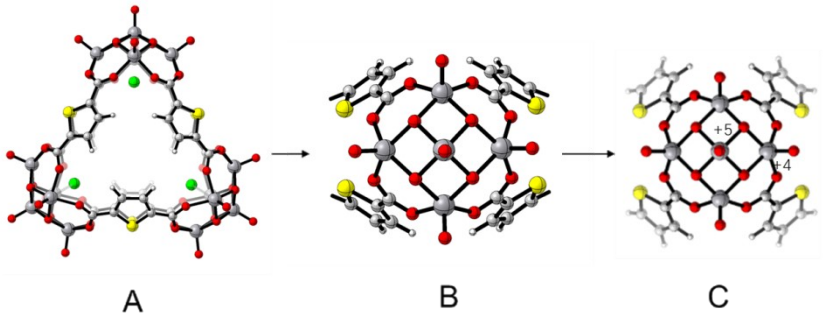


Fig. S3 Model selection process (**C** is structure 1 of the Gibbs energy profile).

Considering the periodic structure of the clusters, their structural complexity renders direct calculations computationally expensive. Therefore, we propose extracting a representative cluster model with the active site was extracted, which typically includes the active site, from the macromolecular cluster. This simplified model can then be utilized for computational simulations and analyses. Based on established research, the critical components of the reaction and the active sites are generally localized at the metal centers. This study specifically selects segment **B**, which encompasses the $\{V_5O_9Cl\}$ cluster, for detailed investigation, as shown in Fig. S3. And the ends are sealed by hydrogen atom to preserve the electronic properties, resulting in the construction of cluster model **C**.

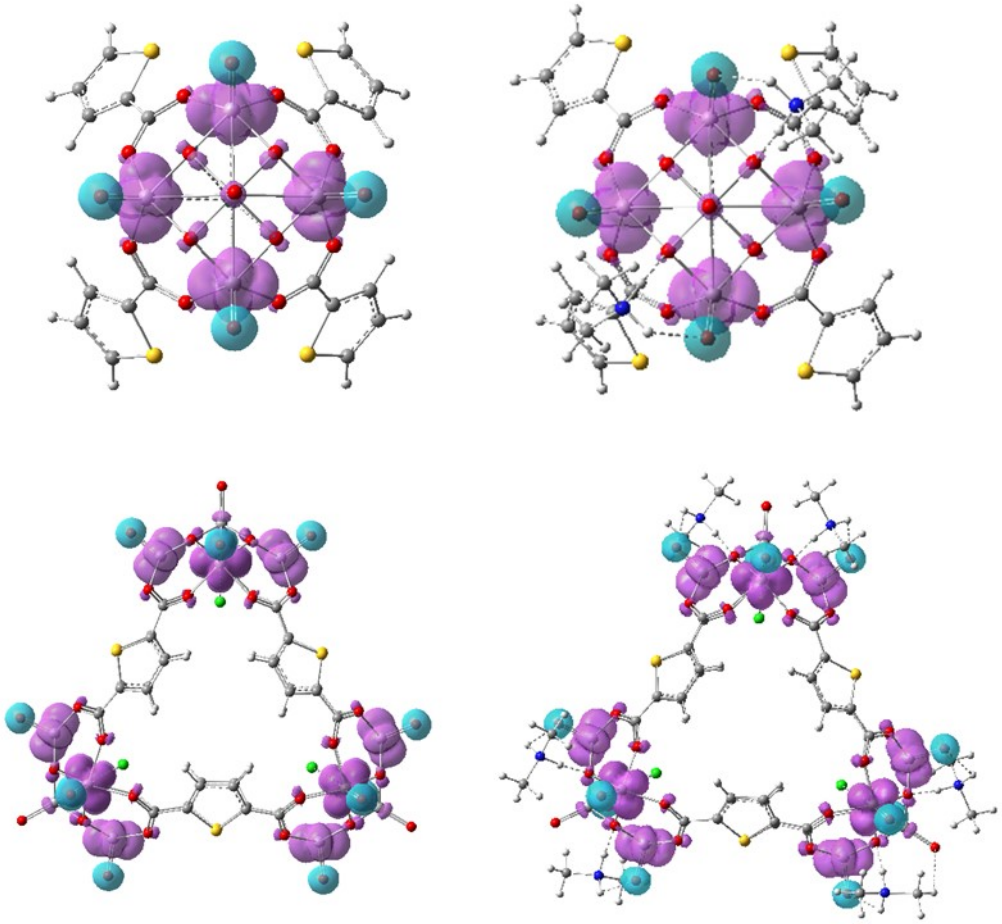


Fig. S4 Model **C**, Model **C** with counterions, Structure **A**, Structure **A** with counterions Self-selected density distributions without coupling interactions between electrons.

Table S3 Gibbs energy corresponding to different multiple of Model **C**, Model **C** with counterions, Structure **A**, Structure **A** with counterions.

Model **C**		Model **C** with counterions		Structure **A**		Structure **A** with counterions	
charge/ multiplicity	ΔG (kcal/mol)	charge/ multiplicity	ΔG (kcal/mol)	charge/ multiplicity	ΔG (kcal/mol)	charge/ multiplicity	ΔG (kcal/mol)
-2/5	0.0	0/5	0.0	-6/13	0.0	0/13	0.0
-2/3	0.2	0/3	0.2	-6/11	0.2	0/11	Convergence failure
-2/1	73.9	0/1	75.4	-6/9	0.4	0/9	0.15
				-6/7	0.6	0/7	0.3
				-6/1	Convergence failure	0/1	Convergence failure

In the current work, all the possible electronic states of the clusters were evaluated, as shown in Fig. S4 and Table S3, the electronic structure of the quintuplet state is more stable than the triplet and singlet states. The model features four single electrons whose spins are evenly distributed around the surrounding V^{IV} atoms. Addition of the counterions $(NH_2Me_2)^+$ has very little effect on the electronic structure, with minimal difference observed. The 13th multiplicity state electronic structure of the entire cluster is the most stable, containing 12 single electrons. The calculation results showed that there is no electronic coupling between the four unpaired electrons for $\{V_5O_9Cl\}$. Model **C** and its variants with the addition of the counterion $(NH_2Me_2)^+$ have the lowest energy and most stable electronic structure in the quintet state, indicating no coupling between the four electrons and a minimal effect of the counterion on the electronic structure. The spin density distribution shows that the electrons are uniformly distributed on the surrounding V^{IV} atoms. Structure A and its counterion $(NH_2Me_2)^+$ variant have the lowest energy and the most stable electronic structure in the 13th multiplet state, containing 12 isolated single electrons and no electronic interactions

between the metal units.

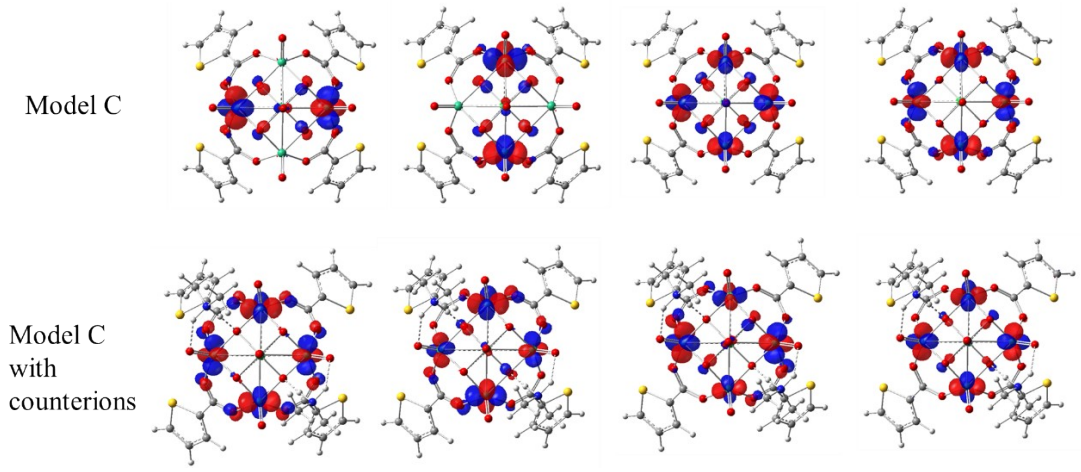


Fig. S5 SOMO orbital of Model **C** and Model **C** with counterions

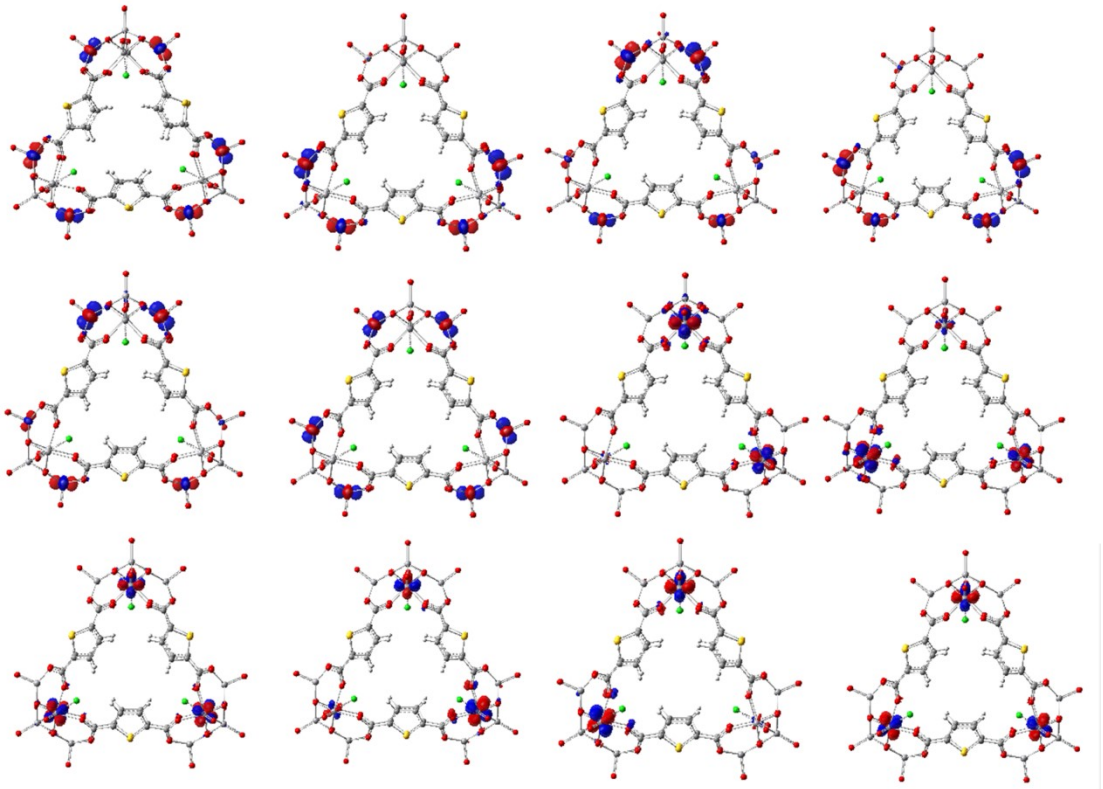


Fig. S6 SOMO orbital of Structure **A**

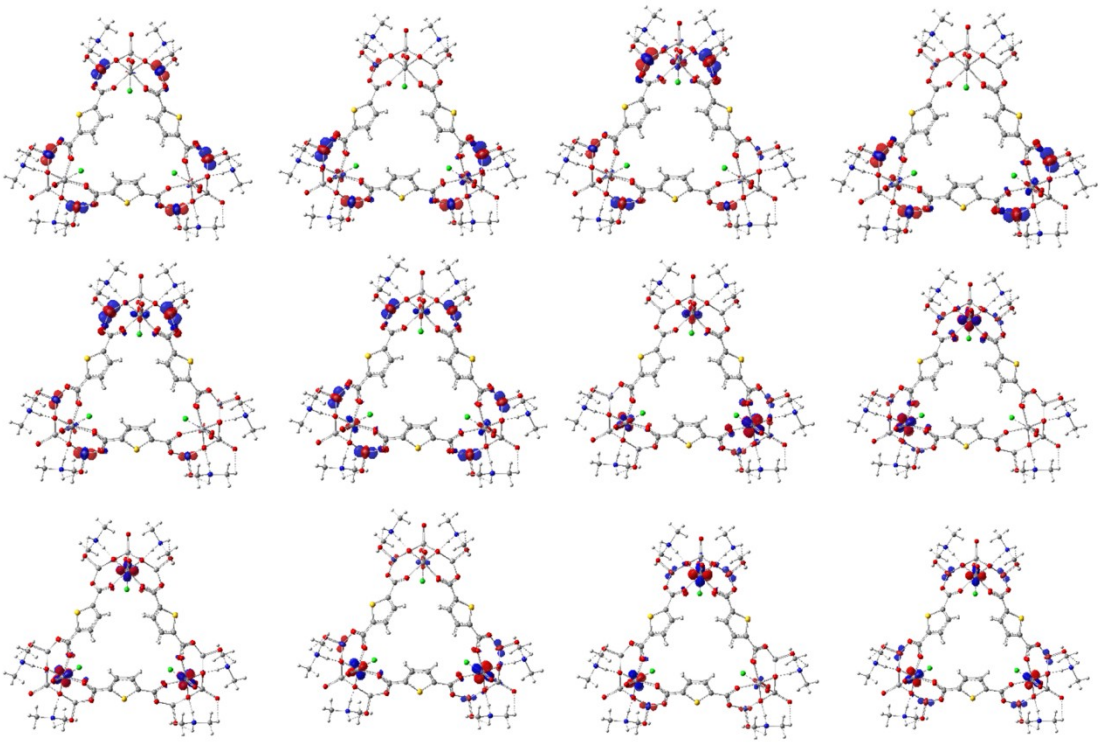


Fig. S7 SOMO orbital of Structure **A** with counterions

The SOMO orbital analyses reveal that individual electrons are not restricted to the d-orbitals of a single vanadium atom but are distributed across the d-orbitals of at least two vanadium atoms. This distribution likely contributes to the very small energy level differences observed between the multiplet states. When electrons are spread uniformly over several atoms, the electronic interactions that typically influence energy levels are averaged out, leading to significantly minimized differences between the multiplet states and resulting in the extremely small observed energy level variations.

4 H_2O_2 oxidizing methyl phenyl sulfoxide

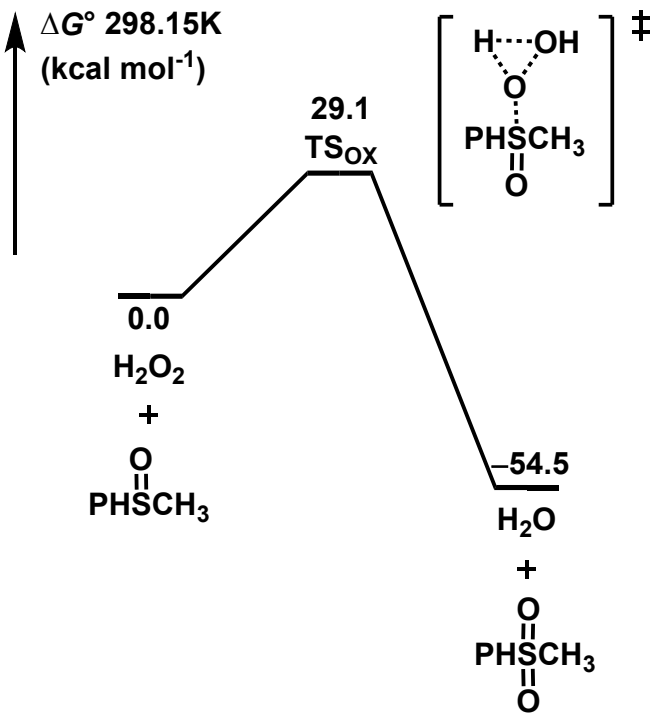


Fig. S8 Gibbs energy profile (in kcal mol^{-1}) of H_2O_2 oxidizing methyl phenyl sulfoxide.

5 V-peroxo intermediates Prediction

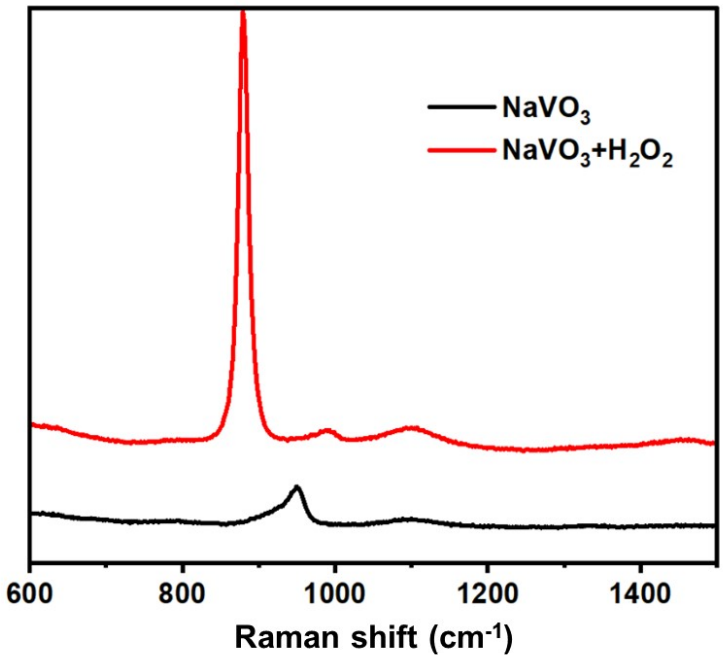


Fig. S9 Raman spectra of $NaVO_3$ (black line) and $NaVO_3$ treated with 30% H_2O_2(red line).

The peroxovanadate intermediates were proposed in several experimental works.[2-3] Especially, Liu's group shows that a new peak belonging to the O–O stretching vibration, located at 870 cm^{-1} of Raman spectroscopy was found in H_2O_2-handled $\{V_6\}$-MOF.[5] We tested the Raman spectrum of a relevant $NaVO_3$ treated with 30% H_2O_2. results clearly shows that a new peak appeared at 870 cm^{-1}, which should be attributed as O–O stretching vibrations.[6] (Fig. S9) In this context, the proposed peroxovanadate intermediates is reasonable.

6 $VOSO_4$-catalyzed decomposition

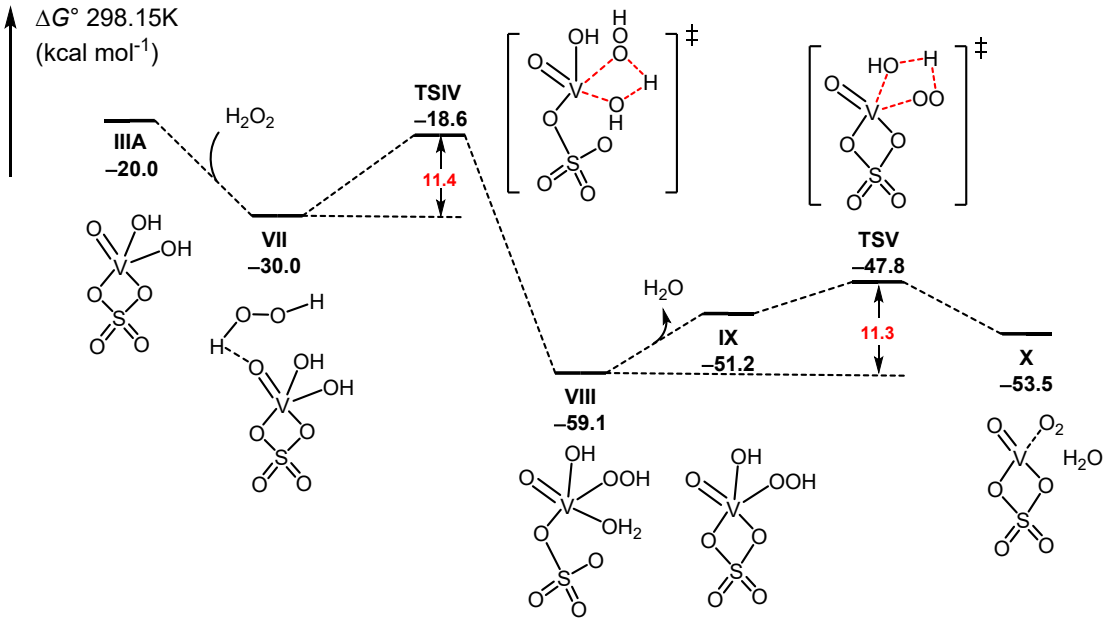


Fig. S10 Gibbs energy profile (in kcal mol^{-1}) of $VOSO_4$-catalyzed decomposition of H_2O_2. The red dashed line represents the transition state part.

$VOSO_4$ may encounter the challenge of competitive decomposition of H_2O_2 in the catalytic oxidation of sulfide substrate, as shown in Fig.S10. The results show that H_2O_2 interacts with intermediate **IIIA** generating a stable adduct **VII** (−10.0 kcal/mol). Following this, the proton transfer from H_2O_2 to the hydroxyl group to produce H_2O via transition state **TSIV**, generating intermediate **VIII**. This process overcomes an energy barrier of 11.4 kcal mol^{-1} and is exothermic (-29.1 kcal mol^{-1}). Later, the proton of the OOH group transfers to another hydroxyl group to produce H_2O (**TSV**), with an energy barrier of 11.3 kcal mol^{-1}. The energy barrier for this side reaction pathway is relatively lower than that for the oxidized sulfide substrate.

7 $VOSO_4$ Catalysed the reaction

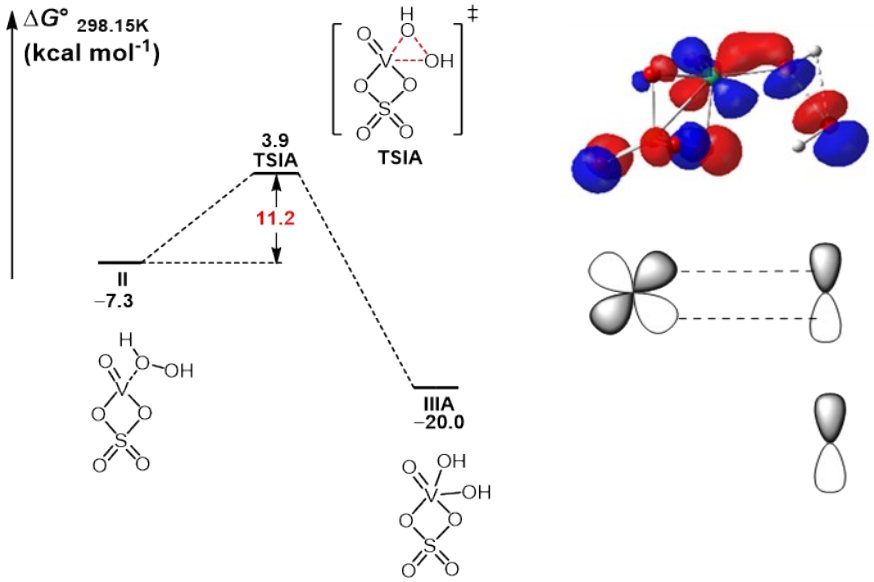


Fig. S11 dπ orbital activation of V between two oxygens of hydrogen peroxide σ* orbitals

The activation of H_2O_2 by the $VOSO_4$ complex essentially involves both the activation of the O–O bond and the activation of the H–O bond. The addition of H_2O_2 to **I** result in the formation of the intermediate **II**, which is characterized by the free energy of the process is -7.3 kcal mol^{-1}, which is then followed by a rapid oxidative addition of the O–O bond to V via the three-centred transition state **TSIA**, with a barrier of 11.2 kcal mol^{-1}, leading to the formation of **IIIA**. Next, from **IIIA**, the hydrogen atom is transferred through **TSII** to form the H_2O molecule. the Gibbs free energy of **TSII** is 23.0 kcal/mol higher than that of **IIIA**, and the ΔG value for **IIIA** → **IV** is -4.4 kcal mol^{-1}. Then, a benzene sulfoxide approaches **IV**, displacing the H_2O molecule to form the pre-reactive adduct **V**, Gibbs free energy of this process decreases to -39.0 kcal mol^{-1}. From **V**, the oxygen atom is transferred via **TSIII**. **TSIII** lies above **V** by 4.8 kcal mol^{-1} in Gibbs free energy, and the ΔG value of **V** → **VI** is -33.8 kcal mol^{-1}. In other way, H–O bond activation via **TSIB** or **TSIC**, which has a higher energy barrier of 26.5 kcal mol^{-1} and 14.6 kcal mol^{-1}. The results show that $VOSO_4$ achieves its

activation by breaking the O–O bond in H_2O_2 to generate two hydroxyl groups. Fig. S11 illustrates the molecular orbitals of the transition state **TSIA**, in which the dπ orbitals of vanadium interact with the σ* orbitals of H_2O_2 to facilitate the breaking of O–O bonds.

8 Effects of counterions $(H_2Me_2N)^+$

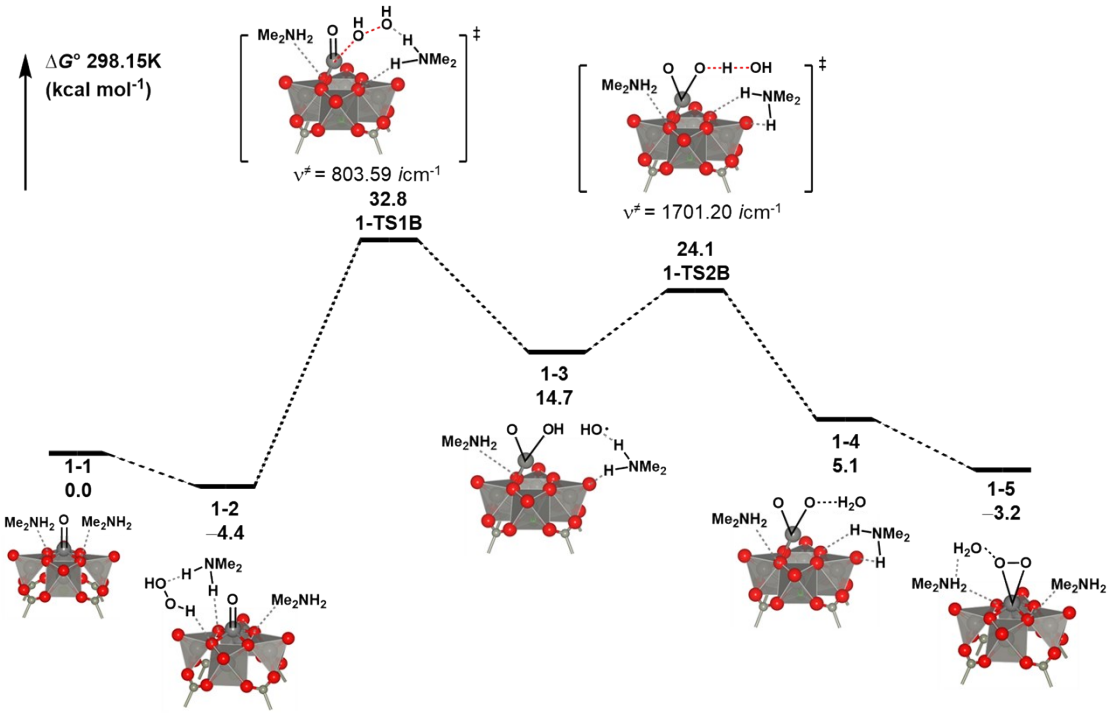
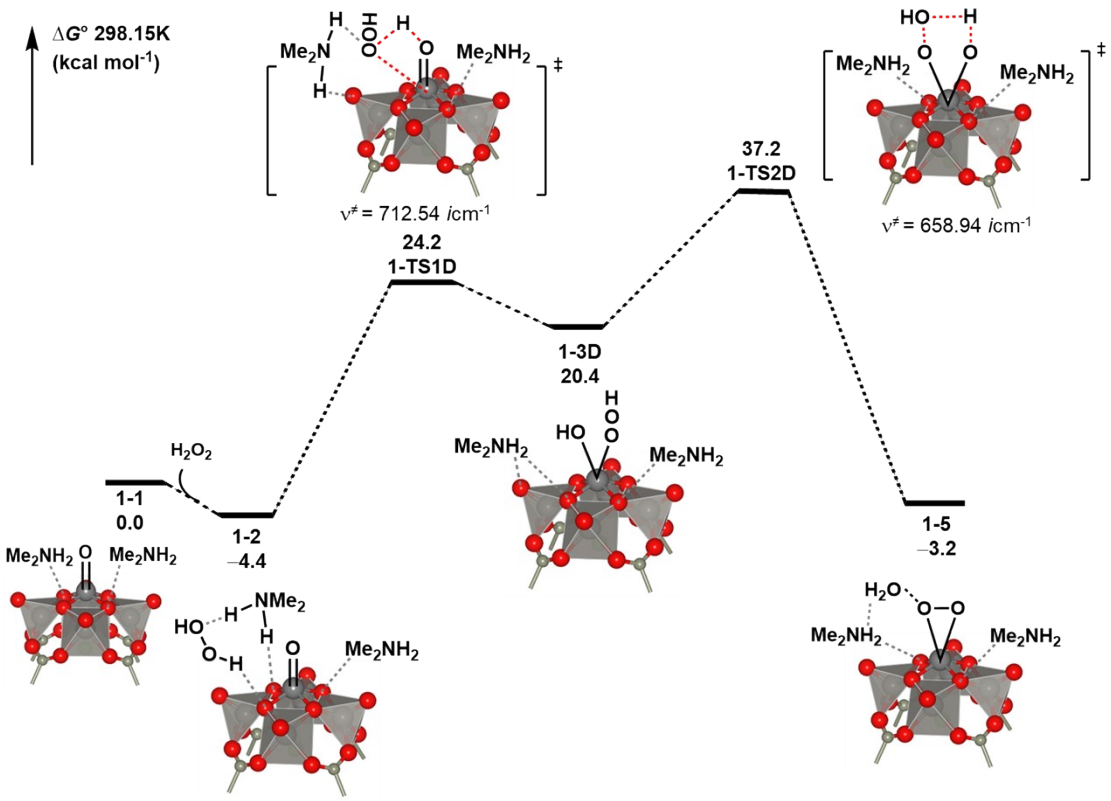


Fig. S12 Gibbs energy profile of $[(V_5O_9Cl)(TDA)_4](H_2Me_2N)_2$-catalysed oxidation of methyl phenyl sulfoxide by O−O bond breaking in H_2O_2. The red dashed line represents the transition state part.



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175 **Fig. S13** Gibbs energy profile of $[(V_5O_9Cl)(TDA)_4](H_2Me_2N)_2$-catalysed oxidation of
176 methyl phenyl sulfoxide by O−H bond breaking in H_2O_2(terminal oxygen
177 participation). The red dashed line represents the transition state part.

178

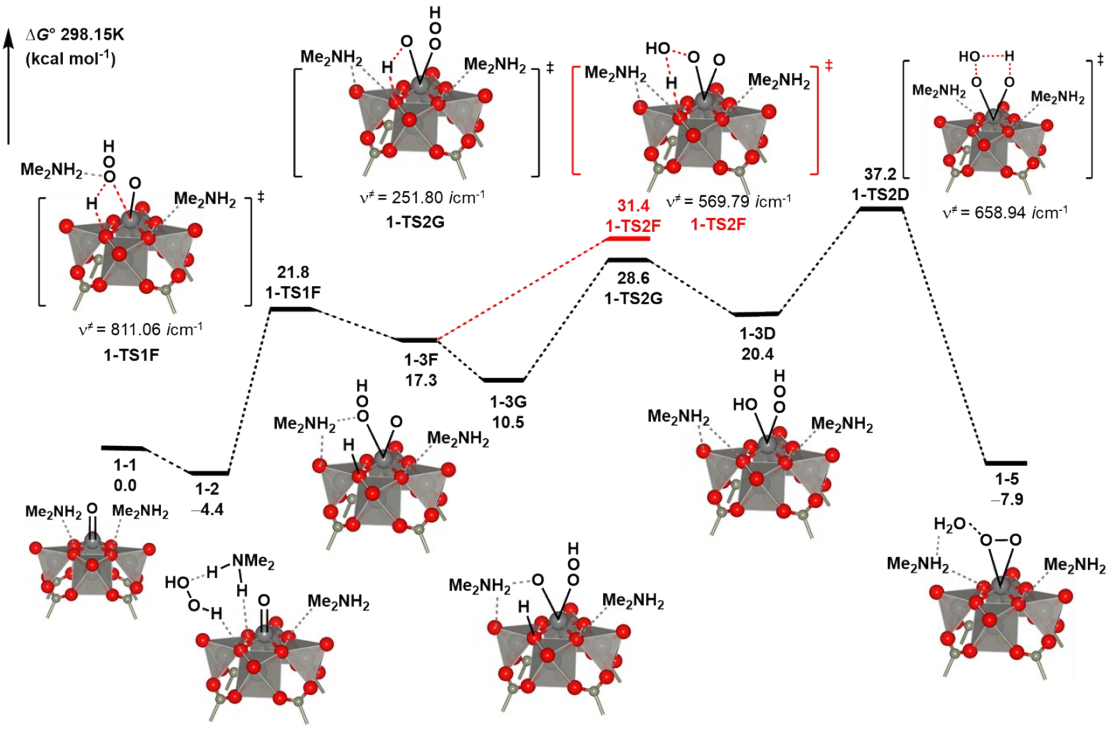

Fig. S14 Gibbs energy profile of $[(V_5O_9Cl)•(TDA)_4](H_2Me_2N)_2$-catalysed oxidation of methyl phenyl sulfoxide by O−H bond breaking in H_2O_2(bridging oxygen participation). The red dashed line represents the transition state part.

Since the charge of the whole system just calculated is -2, we next considered the effect of the presence of electrostatic interactions by adding the counterbalancing ion dimethylammonium root for the simulation, and the addition of the dimethylammonium heel had little effect on the decisive velocity step and energy barrier when activating the oxygen-oxygen bond and, the end-oxygen is involved in the process. When the hydrogen atom is transferred to the bridging oxygen, in addition to the equilibrium valence, the possibility of isomerization was also considered, and the results showed that the activation mode of the decisive step are consistent with the unincorporated $(NH_2Me_2)^+$ the energy of the overall structure of the reaction process does not change much the counterbalance ions have almost no effect on the reaction.

9 Effects of solvent

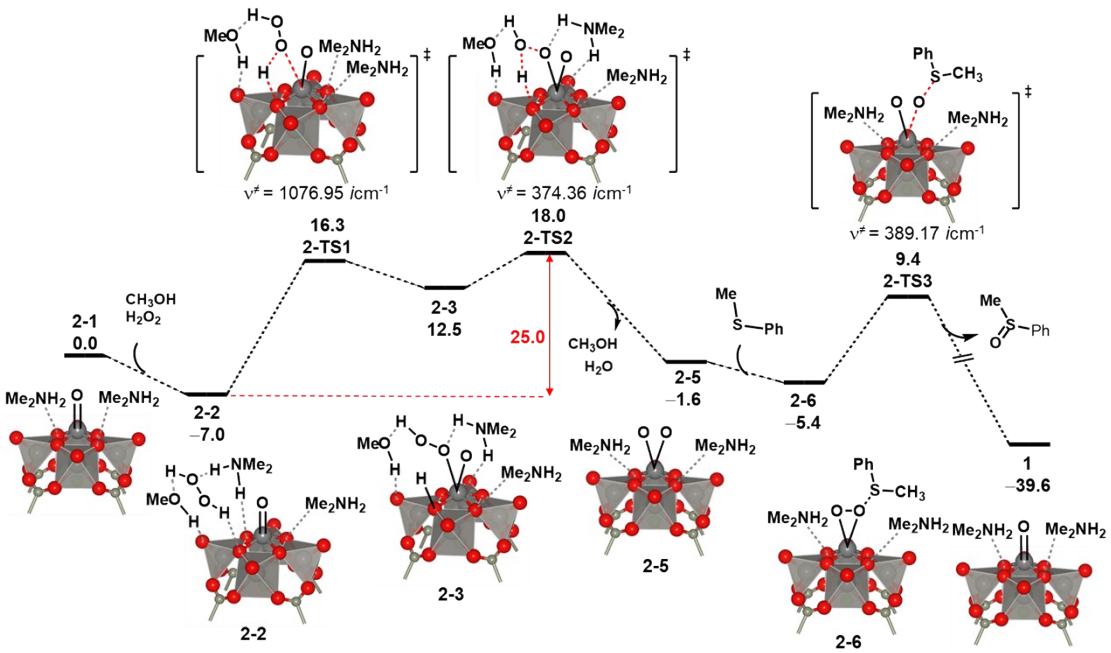

Fig. S15 Gibbs energy profile (in kcal mol^{-1}) of H_2O_2 activation via H–OOH bond cleavage (methanol participation). The red dashed line represents the transition state part.

10 Molecular orbitals for oxygen atom transfer processes

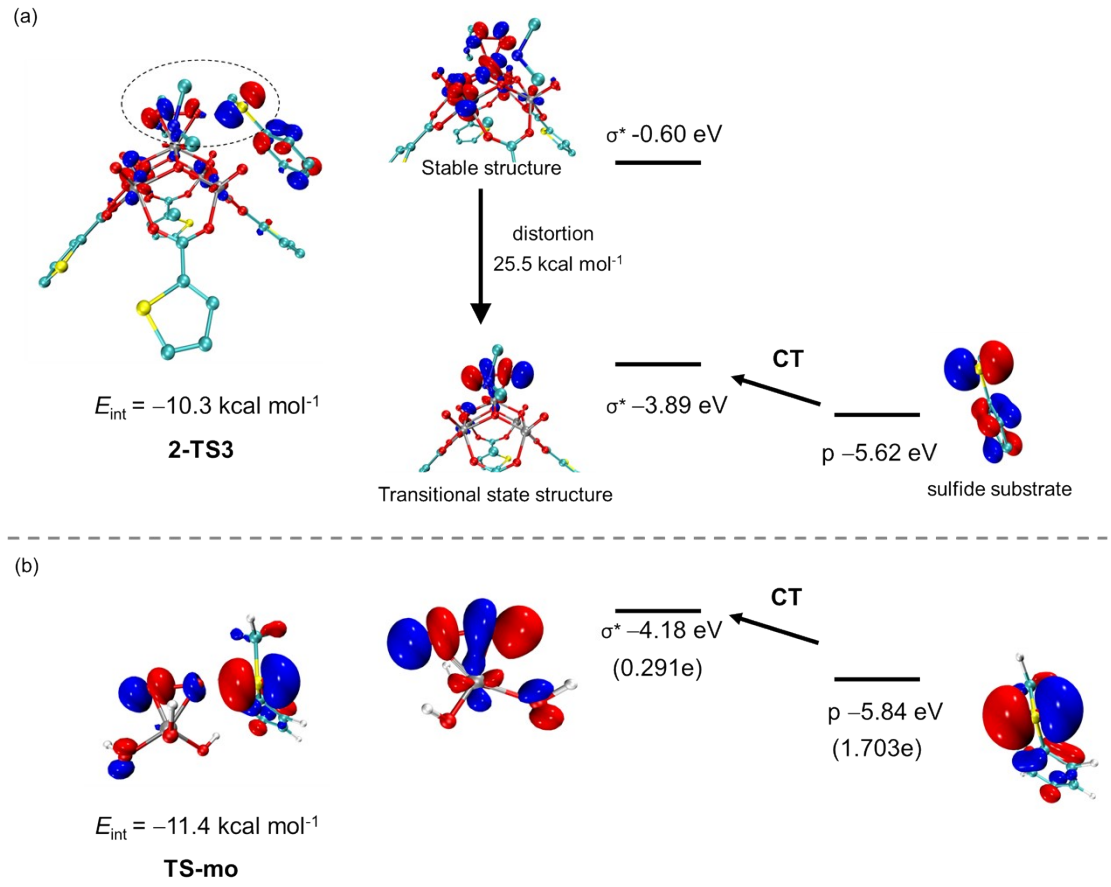

Fig. S16 (a) Orbital interactions in the transition state of the oxygen atom transfer. (b) Mos and charge transfer analysis on a simplified transition state model.

The transition state of oxygen atom transfer and confirmed that the antibonding orbital (σ*) of the O–O bond in peroxovanadate intermediate and p orbital of sulfide substrate are corresponded in the orbital symmetry, as shown in Fig. S16 (a). Results show that the σ* orbital energy level of equilibrium structure of peroxovanadate intermediate is -0.60 eV while that of lone pair orbital of S atom in equilibrium structure of the sulfide is -5.62eV. Such a large energy gap is not favorable for the charge transfer from the lone pair (p) orbital of sulfur to the antibonding orbital (σ*) of the O–O bond of peroxovanadate intermediate. However, the structure of peroxovanadate intermediate distorted a lot (25.5 kcal mol^{-1}) in transition state and corresponding σ* orbital energy of O–O bond decrease to -3.89 eV, which is favorable for the charge transfer. The transition state is stabilized by such a CT interaction about 10.3 kcal mol^{-1}.

In order to evaluate the stabilization in transition state by such a CT interaction, we employed linear combination of fragment MOs analysis on a model (**TS-mo)** as shown in Fig. S16 (b) (this analysis is unavailable for POVs because their electronic structures are open-shell). Results show the amount of charge transfer from the lone pair (p) orbital of sulfur to the antibonding orbital (σ*) of the O–O bond is 0.291 e. Such a CT interaction stabilize the model (**TS-mo)** by –11.4 kcal mol^{-1}, which is only slightly more negative than that in **2-TS3**. These results clearly show that the charge transfer from the lone pair (p-orbital) of sulfur to the antibonding orbital (σ*) of the O–O bond is crucial for the oxidation of sulfide.

11 POV catalyzes the decomposition of H_2O_2

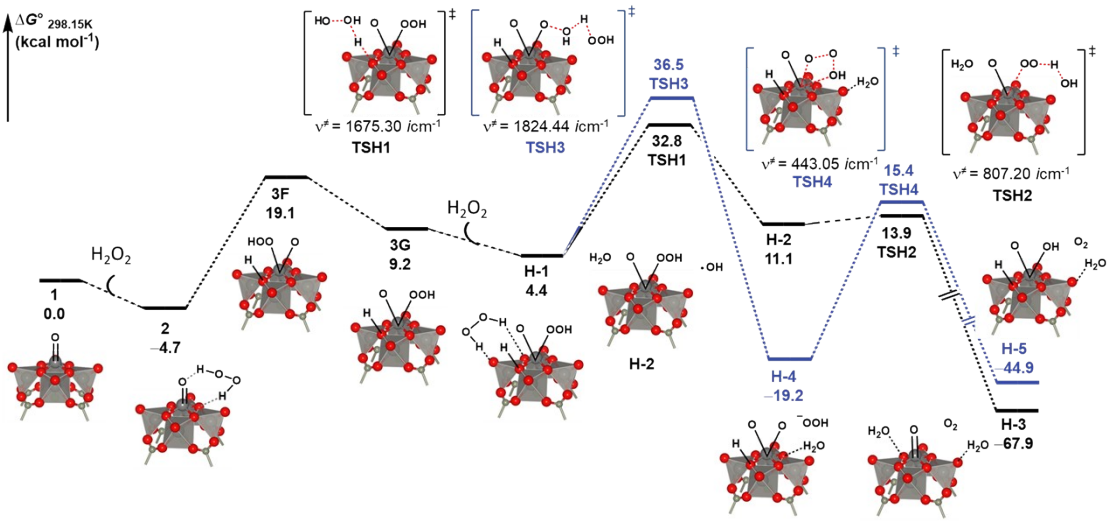

Fig. S17 Gibbs energy profile (in kcal mol^{-1}) of POV's selectivity towards H_2O_2 decomposition. The red dashed line represents the transition state part.

There are two possible paths for the decomposition of H_2O_2, as shown in Fig.S17. The black path involves H transfer from the bridge oxygen atom to the OH group of the second adsorbed H_2O_2 via **TSH1**, concomitant with O–O bond cleavage to form hydroxyl radical (·OH) and then generate intermediate **H-2**. The $\Delta G^{\circ\ddagger}$ is 28.4 kcal mol^{-1} and the ΔG° value is 6.7 kcal mol^{-1}. Subsequently, H transfer from OOH to the hydroxyl radical (·OH) to form H_2O via transition state **TSH2**, concurrent with V–O bond cleavage yielding molecular oxygen (O_2). This step exhibits an energy barrier of 2.8 kcal/mol. The rate determining step is the H of bridge oxygen atom transfer with a relatively high activation energy (37.5 kcal mol^{-1}). Other pathways for H_2O_2 decomposition (blue line) proceeds via hydrogen transfer from the second H_2O_2 to the OOH group through **TSH3** ($\Delta G^{\circ\ddagger}$ = 32.1 kcal mol^{-1} relative to **H–1**), forming H_2O and intermediate **H-4** (ΔG° = -23.6 kcal mol^{-1}). The OOH group subsequently forms a four-membered ring transition state (**TSH4**) with the V–O bond, leading to molecular oxygen (O_2) formation. The $\Delta G^{\circ\ddagger}$ is 34.6 kcal mol^{-1} and the ΔG° value is -25.7 kcal mol^{-1}. The rate determining step is the hydrogen transfer of H_2O_2, which has a relatively high activation energy (41.2 kcal mol^{-1}). The results show that the energy barriers of both pathways for H_2O_2 decomposition is difficult to be overcome in the presence of

POVs as catalyst.

12 Distortion of $[V_5O_9Cl(TDA)_4]^{2-}$

Fig. S18 Distortion of $[V_5O_9Cl(TDA)_4]^{2-}$ structure in a radical pathway. The bond length is given in Å.

One of the O–V bond breaks during the POV distortion process and the bond length is stretched from 1.87 Å to 2.84 Å. This substantial structural distortion in the POV framework incurs a high energy penalty of 24.5 kcal mol^{-1}.

13 V–OOH intermediates catalyzes the oxidation of sulfide

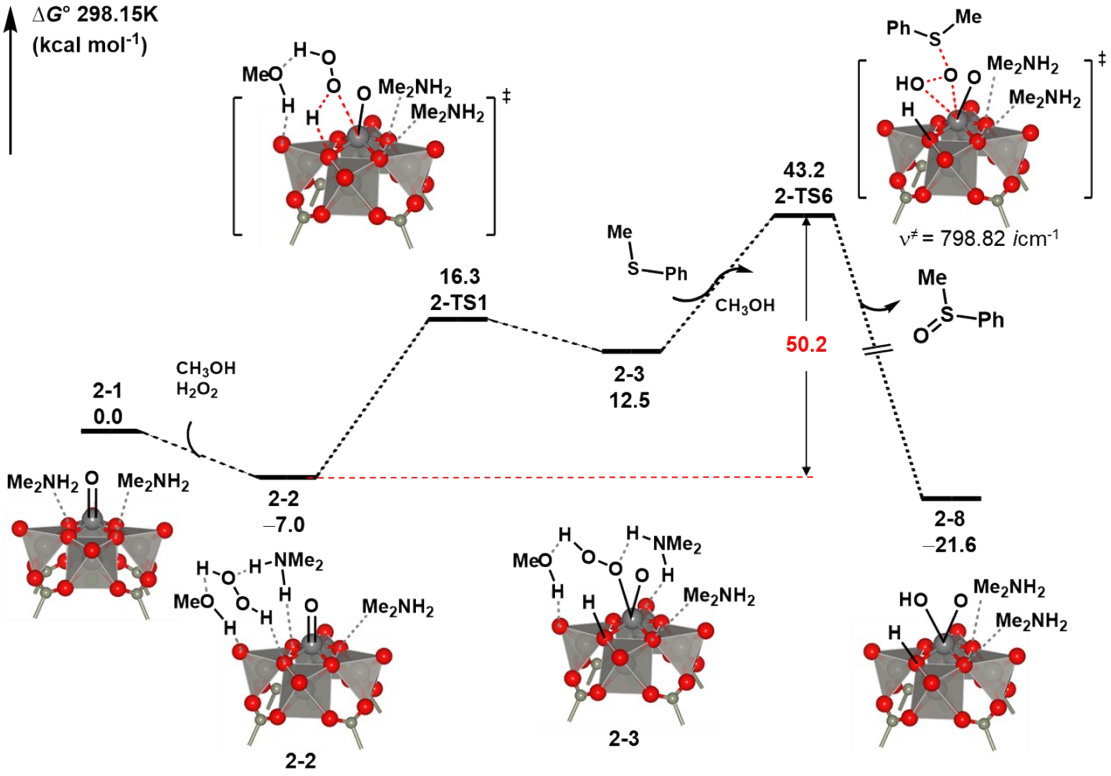

Fig. S19 The Gibbs activation energy (in kcal mol^{-1}) and associated structures for intermediate **2-3** direct oxidized sulfide substrate. The red dashed line represents the transition state part.

According to previous reports, intermediates **2-3** (V-OOH) might also catalyzes the oxidation of alkenes.[7] As shown in Fig. S19, the barrier for intermediate **2-3** directly oxidizes sulfide via **2-TS6** is significantly higher (50.2 kcal mol^{-1}). This result clearly shows that intermediate **2-3** directly oxidizes sulfide is kinetically less favorable than the peroxovanadate intermediate catalyzed ones.

14 Spin density distribution and SOMO orbital of peroxovanadate

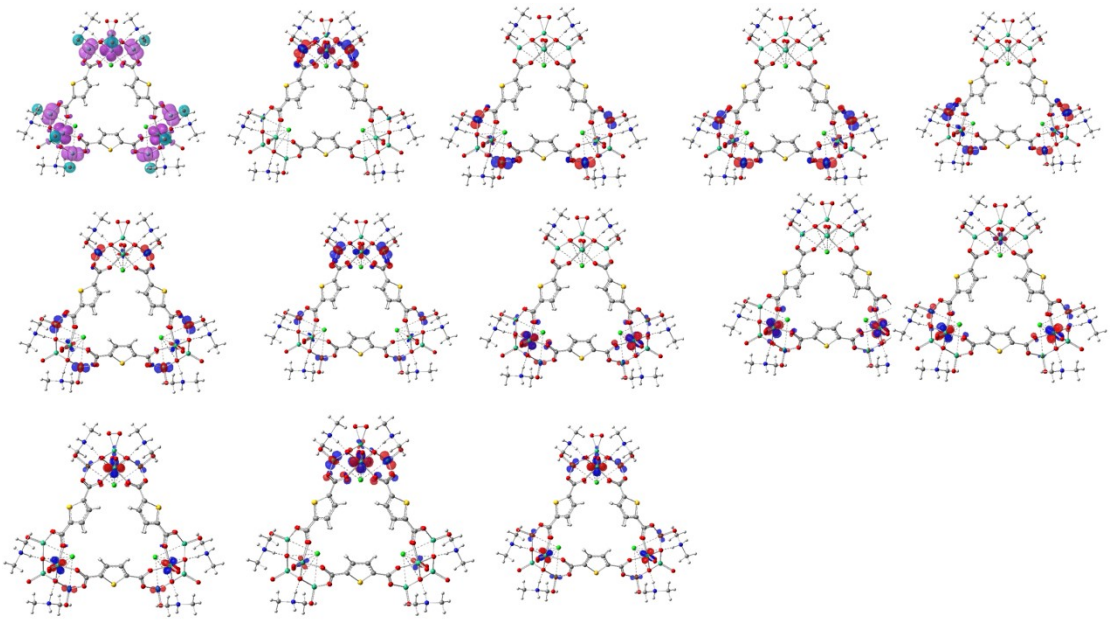

Fig. S20 Spin density distribution and SOMO orbital of peroxovanadate

15 Reference

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285 **16 Cartesian coordinates**

Cartesian coordinates

59

1，B3LYP/6-311++G(d,p) =-4461.962538

C	4.386035	8.491624	7.501009
C	2.983171	10.485867	7.951886
C	2.384791	11.713576	8.531366
C	2.550598	9.768188	6.864065
H	1.677961	10.071040	6.298350
C	3.355818	8.623731	6.602341
H	3.175447	7.928020	5.788804
O	3.811353	14.492763	10.898323
O	1.357920	12.153222	7.945311
O	2.972345	12.180493	9.548292
O	1.231013	14.431976	9.663093
O	-0.003415	16.683108	10.898150
O	-0.002784	14.442211	7.083209
S	4.387155	9.757510	8.681672
V	2.497738	13.613652	10.898238
V	-0.002690	13.585712	8.412167
V	-0.003112	15.099097	10.898125
C	-4.389658	8.489758	14.294920
C	-2.987603	10.484599	13.844171
C	-2.389715	11.712582	13.264762
C	-2.554737	9.767024	14.931944
H	-1.682220	10.070191	15.497675
C	-3.359494	8.622226	15.193597
H	-3.178840	7.926535	16.007088
O	-3.817349	14.491320	10.897909
O	-1.363017	12.152603	13.850839
O	-2.977458	12.179323	12.247864
O	-1.236984	14.431465	12.133137
O	-0.003198	14.442091	14.713021
S	-4.391296	9.755723	13.114343
V	-2.503401	13.612707	10.897966
V	-0.002959	13.585634	13.384037
C	4.385682	8.491530	14.295522
C	2.982853	10.485776	13.844546
C	2.384534	11.713503	13.265038
C	2.550160	9.768059	14.932293
H	1.677459	10.070889	15.497921
C	3.355362	8.623603	15.194077
H	3.174907	7.927869	16.007576
O	1.357599	12.153129	13.850995
O	2.972199	12.180452	12.248191
O	1.230879	14.431937	12.133271
S	4.386913	9.757440	13.114884
C	-4.389330	8.489903	7.500610
C	-2.987296	10.484704	7.951599
C	-2.389461	11.712659	8.531120
C	-2.554314	9.767163	6.863850
H	-1.681730	10.070341	6.298229
C	-3.359067	8.622394	6.602052
H	-3.178336	7.926739	5.788547
O	-1.362697	12.152695	7.945171
O	-2.977311	12.179366	9.547972
O	-1.236850	14.431504	9.662959
S	-4.391068	9.755805	8.681254
Cl	-0.002462	11.743201	10.898072
H	-5.140438	7.710896	7.534857
H	-5.140747	7.710739	14.260553
H	5.137441	7.712908	7.535326
H	5.137099	7.712823	14.261269

63

2A，B3LYP/6-311++G(d,p) =-4613.598549

C	2.648481	-5.543151	-2.827063
C	0.942795	-3.772824	-2.509542
C	0.214117	-2.483467	-2.448337
C	0.503258	-5.010419	-2.107962
H	-0.487005	-5.151491	-1.692362
C	1.480683	-6.028738	-2.291284
H	1.326532	-7.071529	-2.032559
O	0.704990	0.927492	-4.325673
O	-0.954560	-2.533143	-1.974696
O	0.846412	-1.476019	-2.876808
O	-1.394245	0.236676	-2.508076
O	-2.706110	2.738418	-2.257135
O	-3.579565	-1.580541	-2.211715
S	2.575729	-3.837754	-3.112398
V	0.515743	0.516630	-2.813089
V	-2.293315	-1.117603	-1.421088
V	-1.749622	1.733757	-1.472084
C	1.762738	0.725801	6.367736
C	1.081881	1.449787	4.096889

C	0.344649	1.693587	2.834546				
C	2.374230	1.801760	4.400140				
H	2.997503	2.331521	3.690116	63			
C	2.766502	1.388420	5.704444	2B，B3LYP/6-311++G(d,p) =-4613.585287			
H	3.748793	1.570292	6.128882	C	2.607067	-3.662139	-5.234022
O	-3.464998	1.790506	1.994280	C	2.735793	-2.204555	-3.232866
O	0.984036	2.297000	1.929787	C	2.668293	-1.656160	-1.856570
O	-0.845156	1.267083	2.802377	C	3.104242	-1.555801	-4.385835
O	-1.328862	2.440670	0.224270	H	3.404693	-0.515144	-4.378076
O	0.883293	4.230421	-0.070448	C	3.032840	-2.391661	-5.535926
S	0.326124	0.593184	5.411827	H	3.281242	-2.064212	-6.540595
V	-2.220725	1.081786	1.334469	O	2.681957	-3.376602	1.689322
V	0.609208	2.679690	-0.024462	O	2.979292	-0.436641	-1.735443
C	6.597789	-0.369415	-0.947272	O	2.304219	-2.463502	-0.959178
C	4.369592	0.714333	-0.871128	O	2.738863	-0.572444	1.113695
C	2.967843	1.122162	-1.127770	O	2.528421	0.428723	3.906535
C	5.198996	1.136223	0.138860	O	4.343995	1.404012	-0.153778
H	4.870795	1.859736	0.875101	S	2.284551	-3.857775	-3.544854
C	6.479617	0.516424	0.095712	V	1.795028	-2.261709	1.001568
H	7.273997	0.714742	0.808273	V	2.870674	0.830904	-0.173904
O	2.481522	1.961339	-0.321576	V	1.734930	0.255625	2.540499
O	2.413949	0.580993	-2.127752	C	-5.804984	3.057969	-0.779318
O	0.036450	2.120945	-1.808435	C	-3.958698	1.836456	0.333495
S	5.149283	-0.464138	-1.889760	C	-2.661207	1.429268	0.916756
C	-2.218914	-4.556908	4.422650	C	-5.110062	1.092744	0.248738
C	-2.362118	-3.098855	2.423176	H	-5.161327	0.082985	0.637127
C	-2.416523	-1.942548	1.497290	C	-6.171941	1.793147	-0.388924
C	-2.348205	-4.434807	2.105081	H	-7.161147	1.377475	-0.552058
H	-2.387589	-4.771802	1.076415	O	0.212372	3.633722	2.259239
C	-2.267895	-5.273807	3.252067	O	-2.588692	0.258335	1.363882
H	-2.242459	-6.358131	3.210268	O	-1.752953	2.320310	0.887718
O	-2.457448	-2.223490	0.267397	O	-0.154094	0.990978	2.566379
O	-2.414196	-0.802427	2.042770	O	-1.782902	-1.066078	3.654553
O	-2.738765	0.525596	-0.463103	S	-4.160668	3.414012	-0.375780
S	-2.266322	-2.849451	4.144375	V	0.185766	2.320751	1.394316
Cl	0.239482	-0.353720	0.177287	V	-1.060858	-0.766667	2.265776
H	-2.149875	-4.943030	5.431713	C	-2.723609	-5.929379	-1.781011
H	1.795416	0.303644	7.364121	C	-1.908643	-4.145151	-0.265016
H	3.548855	-6.097008	-3.060813	C	-1.067803	-3.201369	0.509920
H	7.456765	-0.975724	-1.205390	C	-3.279336	-4.212014	-0.316251
O	-2.491920	5.287593	-1.042255	H	-3.900792	-3.532868	0.254558
H	-2.712175	4.512576	-1.603571	C	-3.749277	-5.237266	-1.184881
O	-2.923907	4.803017	0.264436	H	-4.799162	-5.448145	-1.362321
H	-2.265455	4.089993	0.427878	O	-1.695439	-2.351330	1.205665

O	0.178503	-3.343563	0.388325	C	3.520380	14.121967	18.670225
O	0.729672	-1.386260	2.370657	C	2.852831	14.867562	16.401797
S	-1.170335	-5.340438	-1.294947	C	2.119724	15.128227	15.139246
C	-0.687351	4.781617	-4.441367	C	4.149973	15.198065	16.708234
C	0.538708	3.495163	-2.715658	H	4.782089	15.720924	16.000912
C	0.979900	2.847813	-1.459962	C	4.534676	14.772415	18.011021
C	1.104371	3.381010	-3.962196	H	5.519457	14.936845	18.437002
H	1.985179	2.773589	-4.130842	O	-1.694686	15.260906	14.271708
C	0.402539	4.121020	-4.954306	O	2.770223	15.728434	14.239577
H	0.688896	4.156760	-6.000534	O	0.924532	14.716897	15.105411
O	1.989471	2.106346	-1.531304	O	0.490391	15.897446	12.587429
O	0.275676	3.127113	-0.435062	O	2.670551	17.663492	12.224367
O	1.881299	1.807604	1.250349	S	2.082999	14.015663	17.711746
S	-0.877258	4.508972	-2.743615	V	-0.435064	14.575546	13.612616
Cl	-0.034397	-0.098432	-0.422237	V	2.366230	16.115787	12.288952
H	-1.392496	5.406373	-4.974691	C	8.318048	12.987362	11.345380
H	-6.414144	3.796564	-1.284701	C	6.110692	14.113225	11.423633
H	2.459801	-4.489453	-5.916643	C	4.717973	14.550661	11.165222
H	-2.800322	-6.748929	-2.484263	C	6.941005	14.503042	12.445534
O	-1.448287	1.897488	4.926692	H	6.620903	15.220456	13.191271
H	-0.888196	1.775597	4.127221	C	8.209731	13.859091	12.401269
O	-2.744119	1.465961	4.415852	H	9.002653	14.030405	13.122506
H	-2.577689	0.503703	4.296344	O	4.240812	15.388273	11.976340
				O	4.158636	14.036035	10.155022
				O	1.733859	15.580876	10.485318
63, $\nu^{\neq}$ = 243.82 *i*cm^{-1}				S	6.874140	12.935326	10.392315
TS1A，B3LYP/6-311++G(d,p) =-4613.514299				C	-0.441202	8.899330	16.643882
C	4.350523	7.884834	9.453464	C	-0.607878	10.379347	14.662264
C	2.666236	9.675993	9.771465	C	-0.670051	11.546220	13.749970
C	1.953380	10.974783	9.834125	C	-0.600996	9.047039	14.329564
C	2.209349	8.442569	10.166047	H	-0.653669	8.721880	13.297669
H	1.215669	8.312889	10.577151	C	-0.507267	8.195367	15.466302
C	3.174372	7.412352	9.982533	H	-0.484189	7.111465	15.412326
H	3.005653	6.370590	10.236530	O	-0.732663	11.281211	12.517933
O	2.456531	14.379890	7.970980	O	-0.655538	12.680429	14.303700
O	0.781629	10.936654	10.301440	O	-0.949822	14.076033	11.763695
O	2.601872	11.975387	9.413325	S	-0.488216	10.609959	16.384482
O	0.400266	13.664233	9.773069	Cl	2.009900	13.082179	12.466477
O	-0.911885	15.620088	9.326229	H	-0.359027	8.502024	17.647638
O	-1.820990	11.941369	10.042947	H	3.545839	13.694109	19.664422
S	4.300743	9.592427	9.175168	H	5.244683	7.320313	9.221260
V	2.253236	13.968771	9.482381	H	9.166764	12.368138	11.083878
V	-0.529677	12.391404	10.834109	O	-0.911908	17.014221	10.948686
V	-0.053026	15.314623	10.762680	H	-1.441700	17.352542	10.203613

O	-0.892662	18.377495	12.533652	H	-3.644218	-5.403087	-2.309563
H	-0.334213	17.625333	12.839178	O	-0.445038	-2.326609	0.162736
				O	1.395649	-3.316301	-0.710062
				O	2.027714	-1.266303	1.370544
63, $\nu^{\neq}$ = 733.24 *i*cm^{-1}				S	-0.013931	-5.335660	-2.333890
TS1B, B3LYP/6-311++G(d,p) =-4613.514299				C	0.783545	4.660505	-5.631218
C	4.489360	-3.659173	-6.212734	C	1.975867	3.416521	-3.851234
C	4.340613	-2.199575	-4.212727	C	2.387415	2.800192	-2.569957
C	4.092425	-1.648140	-2.856381	C	2.562725	3.268576	-5.084217
C	4.863670	-1.551951	-5.304753	H	3.443927	2.653809	-5.221527
H	5.161797	-0.511752	-5.255018	C	1.880323	3.984110	-6.107666
C	4.951151	-2.388444	-6.453609	H	2.184791	3.991467	-7.149444
H	5.335892	-2.061290	-7.414549	O	3.396318	2.051569	-2.597745
O	3.813379	-3.393577	0.616698	O	1.682116	3.096217	-1.561259
O	4.397922	-0.433326	-2.698180	O	3.104482	1.631723	0.389050
O	3.595798	-2.455143	-2.020664	S	0.563188	4.431500	-3.930592
O	4.047178	-0.638502	0.026970	Cl	1.320680	-0.169652	-1.504929
O	4.577168	-0.332724	2.559787	H	0.089479	5.272616	-6.193058
O	5.605407	1.474543	-1.009557	H	-5.038765	3.315800	-3.226478
S	3.939494	-3.854007	-4.582679	H	4.439153	-4.487410	-6.908204
V	3.006570	-2.232714	-0.088185	H	-1.688590	-6.739238	-3.465758
V	4.160900	0.841351	-1.135881	O	2.521463	1.031722	3.152577
V	3.327430	0.049312	1.676976	H	1.711201	1.473785	2.810216
C	-4.451889	2.658137	-2.597840	O	1.623600	0.131740	4.390505
C	-2.663970	1.626487	-1.223414	H	1.120648	-0.431512	3.760597
C	-1.399552	1.332664	-0.503272				
C	-3.785209	0.838898	-1.313449				
H	-3.837848	-0.127283	-0.826784	63, $\nu^{\neq}$ = 1284.10 *i*cm^{-1}			
C	-4.813413	1.429998	-2.100934	TS1C, B3LYP/6-311++G(d,p) =-4613.519652			
H	-5.774419	0.963323	-2.293126	C	0.704351	-0.063577	-6.790535
O	1.355893	3.625304	1.046449	C	1.315992	0.410902	-4.434827
O	-1.361118	0.224386	0.101594	C	1.872304	0.349617	-3.061007
O	-0.507392	2.230987	-0.595641	C	0.476964	1.359198	-4.966135
O	0.727518	1.143636	1.379365	H	0.135935	2.203959	-4.380125
O	-0.472812	-1.002260	2.564517	C	0.125884	1.089541	-6.319284
S	-2.851689	3.110469	-2.116737	H	-0.529180	1.719200	-6.913335
V	1.381935	2.256854	0.257365	O	4.963526	-1.487917	-1.557895
V	0.168219	-0.673745	1.149620	O	1.534198	1.287879	-2.286133
C	-1.585374	-5.912576	-2.774334	O	2.622281	-0.631115	-2.810024
C	-0.712688	-4.120454	-1.300175	O	3.281258	0.348682	-0.129910
C	0.153820	-3.176806	-0.554114	O	4.959443	-0.555716	2.140642
C	-2.084853	-4.172731	-1.315920	O	2.357505	3.026699	-0.304404
H	-2.683377	-3.480198	-0.736711	S	1.682491	-0.839120	-5.591168
C	-2.587934	-5.202088	-2.160829	V	3.456515	-1.351722	-1.095340

V	1.772552	1.553607	-0.295730	O	3.413905	0.923507	3.562455
V	3.465692	-0.302804	1.655209	H	4.326553	0.667104	3.797331
C	-4.766260	-3.523993	2.447958	O	3.944366	1.883429	2.220560
C	-2.320321	-3.156195	2.293702	H	3.044518	2.250999	2.076267
C	-0.960021	-2.568391	2.288492				
C	-2.684309	-4.439881	1.968616				
H	-1.949401	-5.177570	1.670303	63			
C	-4.088607	-4.653577	2.058210	3A, B3LYP/6-311++G(d,p) =-4613.560896			
H	-4.573824	-5.599190	1.837718	C	2.829538	-5.466587	-2.921668
O	0.371044	0.675911	3.898837	C	1.122478	-3.715325	-2.516240
O	-0.019615	-3.332439	1.953818	C	0.379967	-2.436902	-2.403582
O	-0.888730	-1.351363	2.632564	C	0.692247	-4.969013	-2.156059
O	1.855291	-1.173071	2.540671	H	-0.292580	-5.129592	-1.734895
O	2.627106	-3.921638	2.644403	C	1.670536	-5.976007	-2.389202
S	-3.703967	-2.182623	2.706302	H	1.522929	-7.028138	-2.167265
V	0.540725	0.078373	2.449944	O	0.631419	0.990165	-4.276150
V	1.955906	-2.926836	1.611082	O	-0.789952	-2.521442	-1.940606
C	0.899792	-6.474513	-4.077783	O	1.022666	-1.405209	-2.782260
C	1.477969	-5.079663	-2.109908	O	-1.190765	-0.089705	-2.807483
C	1.992700	-4.017042	-1.208950	O	-2.604502	2.191880	-2.948248
C	0.725758	-6.179377	-1.778238	O	-3.472298	-1.517214	-2.234549
H	0.432099	-6.374408	-0.753998	S	2.748076	-3.751936	-3.141312
C	0.394046	-6.982465	-2.906287	V	0.373690	0.531567	-2.790815
H	-0.195977	-7.892109	-2.851179	V	-2.163628	-1.053808	-1.487465
O	1.693121	-4.144101	0.011379	V	-1.975712	2.195642	-1.487351
O	2.666260	-3.106951	-1.766120	C	1.570624	1.247993	6.608814
O	3.311411	-1.965299	0.708924	C	1.023096	1.694434	4.231296
S	1.785325	-5.008689	-3.823166	C	0.363838	1.775104	2.903764
C	-5.003322	2.293794	-0.056021	C	2.268150	2.153505	4.584386
C	-2.546339	1.982221	0.069967	H	2.910919	2.650523	3.868045
C	-1.169222	1.594719	0.466108	C	2.583869	1.899387	5.949200
C	-2.936171	2.677734	-1.047925	H	3.519882	2.185438	6.418799
H	-2.214483	3.026192	-1.776565	O	-3.443707	1.705396	1.907791
C	-4.346330	2.858853	-1.121512	O	1.046418	2.314172	1.987618
H	-4.849724	3.379398	-1.930213	O	-0.798551	1.281069	2.838953
O	-0.249545	1.956663	-0.313641	O	-1.199182	2.557082	0.447199
O	-1.087630	0.938806	1.550600	O	1.037690	4.145109	-0.172147
O	1.528425	1.206760	1.592185	S	0.216969	0.935061	5.575967
S	-3.913310	1.528596	1.049889	V	-2.106868	1.131421	1.296358
Cl	0.455037	-1.111120	-0.348484	V	0.633856	2.630895	0.027527
H	-6.069574	2.280001	0.131370	C	6.394794	-0.744435	-1.298445
H	-5.833761	-3.408778	2.586947	C	4.279605	0.510774	-0.998304
H	0.600541	-0.500368	-7.775743	C	2.917515	1.071159	-1.148226
H	0.792348	-6.881092	-5.075485	C	5.155696	0.693105	0.043687

H	4.903268	1.316800	0.892558	S	1.022803	-2.697861	-4.875714
C	6.371795	-0.025861	-0.127697	V	2.027632	-1.799077	-0.171313
H	7.188627	-0.015616	0.586999	V	2.248583	1.585005	-1.045812
O	2.506830	1.820562	-0.229396	V	3.269799	-0.208193	1.680201
O	2.297578	0.748119	-2.205285	C	-6.248282	1.454763	2.032091
O	-0.134760	2.080076	-1.789936	C	-3.861241	0.806562	2.193867
S	4.933244	-0.560106	-2.205591	C	-2.380218	0.776080	2.126526
C	-2.225311	-4.613992	4.270892	C	-4.708515	-0.176119	2.642682
C	-2.330983	-3.093454	2.315651	H	-4.331806	-1.119760	3.017840
C	-2.355840	-1.908056	1.425015	C	-6.080006	0.194691	2.551892
C	-2.361210	-4.419105	1.958520	H	-6.902826	-0.444483	2.856440
H	-2.417584	-4.723530	0.920491	O	0.167577	3.645480	2.309436
C	-2.302020	-5.294002	3.080026	O	-1.836452	-0.299238	2.513011
H	-2.311350	-6.376987	3.006245	O	-1.830987	1.818111	1.675288
O	-2.426241	-2.150745	0.187098	O	0.531594	1.032598	2.621008
O	-2.306909	-0.784701	1.988693	O	0.250037	-1.280655	4.099630
O	-2.559416	0.702314	-0.642723	S	-4.738358	2.207834	1.645993
S	-2.220807	-2.898130	4.042716	V	0.168521	2.321247	1.441668
Cl	0.248464	-0.330145	0.134332	V	0.108054	-0.840155	2.592549
H	-2.164236	-5.031617	5.267882	C	-2.573004	-6.332280	-0.399623
H	1.550400	0.934410	7.644884	C	-1.352809	-4.386289	0.535415
H	3.728744	-6.007772	-3.187385	C	-0.400724	-3.277740	0.787472
H	7.190188	-1.378625	-1.668931	C	-2.460937	-4.722310	1.273709
O	-2.779802	3.761124	-1.028261	H	-2.738884	-4.165523	2.160321
H	-3.328042	4.049029	-1.775967	C	-3.162140	-5.839756	0.738881
O	-1.998328	4.989618	1.571334	H	-4.063489	-6.256481	1.177024
H	-1.799240	4.153391	1.065953	O	-0.625620	-2.579676	1.810183
				O	0.534388	-3.149939	-0.056953
				O	1.911129	-1.348759	1.812429
63				S	-1.156198	-5.439474	-0.838283
3B, B3LYP/6-311++G(d,p) =-4613.576517				C	-3.295794	4.610206	-3.549339
C	0.792636	-2.179208	-6.511124	C	-1.325805	3.595823	-2.438604
C	1.423023	-1.076201	-4.381579	C	-0.374598	3.026582	-1.452593
C	1.747912	-0.768043	-2.968166	C	-1.173118	3.696756	-3.799622
C	1.369808	-0.199755	-5.437610	H	-0.275452	3.348767	-4.295915
H	1.582616	0.854361	-5.307443	C	-2.302834	4.280785	-4.439263
C	1.008935	-0.831356	-6.661150	H	-2.376938	4.444076	-5.509808
H	0.911030	-0.309271	-7.607678	O	0.711561	2.588726	-1.928189
O	3.215874	-2.830324	-0.221627	O	-0.767879	3.035341	-0.251360
O	2.033938	0.431198	-2.716418	O	1.649143	2.333374	0.578813
O	1.699644	-1.742474	-2.162189	S	-2.870838	4.210610	-1.919790
O	2.990102	-0.001438	-0.084956	Cl	-0.146108	-0.141061	-0.268487
O	4.662115	-0.923616	1.913459	H	-4.256226	5.059717	-3.767523
O	3.511894	2.426215	-1.479694	H	-7.179607	1.977335	1.854081

H	0.505340	-2.891999	-7.273617	C	-0.392547	-3.320945	0.799021
H	-2.899541	-7.168357	-1.004922	C	-2.498603	-4.702525	1.282641
O	3.199202	1.121330	2.819220	H	-2.750187	-4.149038	2.179159
H	2.236938	1.385457	2.854051	C	-3.241734	-5.787880	0.737842
O	-0.616697	1.893969	5.007479	H	-4.153631	-6.179929	1.177300
H	-0.172184	1.596541	4.166324	O	-0.588647	-2.627211	1.830772
				O	0.541933	-3.217392	-0.046292
				O	1.976771	-1.405139	1.789410
63				S	-1.235718	-5.432307	-0.849758
3C, B3LYP/6-311++G(d,p) =-4613.578737				C	-3.145855	4.905841	-3.295169
C	0.704300	-2.442338	-6.464847	C	-1.211838	3.709510	-2.305334
C	1.364274	-1.267725	-4.381842	C	-0.262604	3.043259	-1.376052
C	1.723270	-0.917967	-2.984549	C	-1.115416	3.836752	-3.668918
C	1.255042	-0.420792	-5.457047	H	-0.271184	3.434777	-4.215672
H	1.440528	0.641901	-5.358869	C	-2.224095	4.524855	-4.239224
C	0.877073	-1.093184	-6.653821	H	-2.334115	4.723332	-5.300873
H	0.736470	-0.597828	-7.609474	O	0.757364	2.527602	-1.917395
O	3.231354	-2.966531	-0.209445	O	-0.592459	3.059907	-0.158894
O	1.975505	0.295427	-2.768085	O	1.832585	2.275113	0.561834
O	1.734738	-1.877175	-2.160802	S	-2.677710	4.428673	-1.697974
O	3.023557	-0.138458	-0.134362	Cl	-0.090488	-0.184571	-0.316725
O	4.723392	-1.137748	1.783599	H	-4.076909	5.434531	-3.456069
O	3.549430	2.233321	-1.606850	H	-7.021956	1.968372	1.550639
S	0.996942	-2.912143	-4.824194	H	0.415453	-3.181855	-7.200951
V	2.074454	-1.897007	-0.162449	H	-3.038676	-7.098700	-1.027277
V	2.274584	1.448361	-1.101728	O	3.240953	0.468584	3.431520
V	3.394432	-0.299768	1.641466	H	4.149087	0.458365	3.784864
C	-6.103910	1.442679	1.781070	O	3.991857	1.538224	1.754024
C	-3.731266	0.791362	2.091739	H	3.160442	2.050028	1.469703
C	-2.245999	0.761423	2.120795				
C	-4.605820	-0.204494	2.450015				
H	-4.253589	-1.161306	2.815636	63, $\nu^{\neq} = 1623.08$ *i*cm^{-1}			
C	-5.968901	0.167977	2.274041	TS2B, B3LYP/6-311++G(d,p)=-4613.555679			
H	-6.809219	-0.481833	2.498079	C	-3.728583	12.607925	1.568656
O	0.411078	3.529973	2.436078	C	-3.145611	13.720872	3.707001
O	-1.731367	-0.317974	2.529975	C	-2.851019	14.034134	5.126809
O	-1.676318	1.815643	1.723140	C	-3.177256	14.592618	2.646388
O	0.671071	0.906517	2.539340	H	-2.968595	15.647521	2.776867
O	0.346208	-1.375028	4.120002	C	-3.510885	13.955431	1.417834
S	-4.571960	2.206260	1.520672	H	-3.588960	14.473585	0.467224
V	0.347071	2.240303	1.514695	O	-1.461235	11.957420	7.894752
V	0.214756	-0.918536	2.613443	O	-2.573007	15.235700	5.379039
C	-2.678621	-6.283555	-0.412420	O	-2.914341	13.062303	5.933324
C	-1.385539	-4.393301	0.540377	O	-1.663946	14.797349	8.016228

O	-0.035710	13.721502	9.886725	H	-8.862600	19.855159	4.252627
O	-1.118187	17.236608	6.645503	H	-11.881164	16.535678	9.452312
S	-3.532844	12.096588	3.211060	H	-3.998348	11.891611	0.803018
V	-2.629447	13.010693	7.936198	H	-7.543381	7.632252	6.988644
V	-2.383927	16.385662	7.055386	O	-1.021188	15.952936	10.822712
V	-1.353971	14.594337	9.780076	H	-1.751711	16.707570	11.468124
C	-10.950428	16.042669	9.703052	O	-2.516878	16.777836	12.306692
C	-8.562915	15.469736	10.051772	H	-3.338272	16.436105	11.805139
C	-7.078009	15.486964	10.096856				
C	-9.411299	14.456587	10.424332				
H	-9.035218	13.519450	10.816217	63, $\nu^{\neq}$ = 1411.47 *i*cm^{-1}			
C	-10.782889	14.784093	10.226424	TS2C, B3LYP/6-311++G(d,p)=-4613.544672			
H	-11.605901	14.114989	10.457565	C	1.070266	-5.428017	-5.051788
O	-4.541871	18.380354	10.395602	C	1.819765	-3.596555	-3.556273
O	-6.535438	14.430416	10.534248	C	2.151586	-2.746040	-2.386068
O	-6.533839	16.546284	9.682662	C	1.952505	-3.283384	-4.886601
O	-4.189437	15.771090	10.668681	H	2.342177	-2.323857	-5.204106
O	-4.460897	13.486017	12.201087	C	1.523646	-4.333754	-5.746726
S	-9.439244	16.845852	9.440771	H	1.547193	-4.278175	-6.830576
V	-4.515257	17.066632	9.506879	O	3.013937	-3.617000	1.205189
V	-4.575701	13.914502	10.685750	O	2.621870	-1.608301	-2.650223
C	-7.217037	8.454974	7.612114	O	1.923178	-3.255764	-1.251845
C	-6.000485	10.384101	8.586663	O	3.358611	-1.063111	0.033907
C	-5.051110	11.491193	8.858272	O	4.687555	-1.142101	2.405667
C	-7.102702	10.025020	9.322840	O	4.497779	0.354822	-2.158508
H	-7.377856	10.559074	10.224202	S	1.156753	-5.192657	-3.338675
C	-7.801893	8.917234	8.765424	V	2.091857	-2.484219	0.613030
H	-8.698833	8.485760	9.198514	V	3.063529	0.064474	-1.569022
O	-5.272049	12.163907	9.899516	V	3.494111	-0.376111	1.704576
O	-4.122711	11.644277	8.013799	C	-5.365284	2.528050	-0.348594
O	-2.757924	13.490953	9.928919	C	-3.219513	1.736616	0.608879
S	-5.806918	9.365041	7.187217	C	-1.784034	1.510037	0.912777
C	-7.903175	19.409546	4.483046	C	-4.309373	1.109518	1.160408
C	-5.947076	18.392465	5.617126	H	-4.197615	0.348139	1.922647
C	-5.010593	17.815390	6.613907	C	-5.542770	1.563855	0.613231
C	-5.769166	18.514805	4.261108	H	-6.515483	1.188513	0.915520
H	-4.859451	18.180529	3.777487	O	1.359680	3.718117	0.563767
C	-6.890678	19.100335	3.608136	O	-1.542077	0.637479	1.792071
H	-6.945137	19.278797	2.538779	O	-0.973859	2.215842	0.244495
O	-3.913977	17.389632	6.152846	O	1.034572	1.392601	1.738049
O	-5.426944	17.807001	7.807213	O	0.102142	0.008821	3.993999
O	-3.017745	17.113715	8.674978	S	-3.692605	2.893438	-0.604562
S	-7.506566	18.988492	6.114626	V	1.085098	2.192376	0.237459
Cl	-4.804076	14.636377	7.778814	V	0.221329	-0.171448	2.431449

C	-3.426616	-5.793561	1.277841	O	1.830024	-1.857064	-2.182805
C	-1.861027	-3.903872	1.638200	O	3.109386	-0.098894	-0.335688
C	-0.692786	-2.988949	1.632553	O	4.555771	-0.551200	1.943072
C	-3.082898	-3.701121	2.231039	O	3.464763	2.363305	-1.669124
H	-3.298549	-2.794247	2.782821	S	1.208773	-3.004099	-4.823738
C	-3.982742	-4.785204	2.026096	V	2.123592	-1.843630	-0.186325
H	-4.996627	-4.813556	2.412859	V	2.252638	1.466584	-1.200268
O	-0.838503	-1.906709	2.258704	V	3.196759	0.118635	1.451048
O	0.323240	-3.393332	0.998544	C	-6.118053	1.617129	2.038579
O	1.921553	-1.168019	2.123381	C	-3.763628	0.859779	2.189130
S	-1.798857	-5.434817	0.809584	C	-2.286163	0.766767	2.131372
C	-1.458288	3.010072	-5.687938	C	-4.656125	-0.102723	2.592521
C	0.164649	2.109668	-4.043821	H	-4.324414	-1.076904	2.930184
C	0.917854	1.786149	-2.805495	C	-6.009145	0.330887	2.508069
C	0.363952	1.616892	-5.309768	H	-6.861368	-0.283523	2.780821
H	1.152031	0.904653	-5.521620	O	0.439904	3.518213	2.386889
C	-0.565884	2.134084	-6.255906	O	-1.786932	-0.337286	2.491982
H	-0.575018	1.864469	-7.307427	O	-1.695521	1.803979	1.707891
O	1.857821	0.951987	-2.940349	O	0.541552	0.928898	2.694079
O	0.526763	2.375494	-1.761165	O	0.323028	-1.445414	4.065533
O	2.620638	1.541314	-0.415113	S	-4.574564	2.318376	1.691756
S	-1.180955	3.214552	-3.991451	V	0.315292	2.176114	1.545462
Cl	0.298742	-0.684166	-0.557678	V	0.157852	-0.925119	2.583880
H	-2.267393	3.538497	-6.176133	C	-2.613909	-6.214589	-0.650685
H	-6.128869	3.035379	-0.924583	C	-1.340839	-4.361402	0.395299
H	0.685455	-6.355630	-5.456272	C	-0.351166	-3.304723	0.714245
H	-3.889521	-6.723575	0.972998	C	-2.484284	-4.676325	1.087513
O	3.295461	1.062740	3.218596	H	-2.765811	-4.141294	1.986295
H	4.027078	0.867748	3.826251	C	-3.215946	-5.740746	0.489053
O	4.119544	1.315610	1.111383	H	-4.147584	-6.133585	0.883821
H	3.693020	1.633730	2.180440	O	-0.577004	-2.631807	1.754457
				O	0.616589	-3.190086	-0.090429
				O	1.907649	-1.137056	1.694530
63				S	-1.148029	-5.368124	-1.013160
4, B3LYP/6-311++G(d,p)=-4613.58404				C	-3.360435	4.740327	-3.125334
C	0.938394	-2.600859	-6.485157	C	-1.326030	3.641615	-2.233530
C	1.475898	-1.329501	-4.425344	C	-0.302423	3.028547	-1.352705
C	1.778425	-0.920692	-3.032510	C	-1.314137	3.746479	-3.602699
C	1.352710	-0.522583	-5.529826	H	-0.488429	3.367536	-4.192518
H	1.479630	0.551039	-5.462411	C	-2.481175	4.379044	-4.116892
C	1.045093	-1.250837	-6.713560	H	-2.661929	4.553018	-5.172999
H	0.906368	-0.793816	-7.688238	O	0.703701	2.533412	-1.936678
O	3.289694	-2.897447	-0.090539	O	-0.547585	3.067924	-0.117739
O	1.945315	0.315119	-2.846117	O	1.813373	1.956808	0.608252

S	-2.781498	4.312300	-1.551639	V	-2.516746	13.651490	10.752131
Cl	-0.159867	-0.192549	-0.377910	V	-0.015958	13.695901	13.283825
H	-4.320347	5.227941	-3.239027	C	4.405904	8.685301	14.427046
H	-7.024385	2.186542	1.875985	C	2.981218	10.641214	13.888698
H	0.710323	-3.377288	-7.204306	C	2.370723	11.835791	13.258333
H	-2.957882	-7.011088	-1.298246	C	2.554297	9.965835	15.005670
O	3.416182	1.639505	2.268101	H	1.677645	10.282593	15.557381
H	-0.218368	3.064954	4.271033	C	3.372264	8.843481	15.317567
O	-0.425853	2.423764	4.974055	H	3.198696	8.181562	16.160101
H	-0.088214	1.609265	4.560416	O	1.334475	12.286489	13.820325
				O	2.955726	12.269382	12.224425
				O	1.222698	14.500762	12.050270
63				S	4.395711	9.899323	13.193623
5, B3LYP/6-311++G(d,p)=-4613.594327				C	-4.383466	8.456418	7.455329
C	4.311514	8.430897	7.616246	C	-2.994305	10.465101	7.878688
C	2.935311	10.459035	7.987463	C	-2.404495	11.702988	8.441083
C	2.349453	11.712111	8.520599	C	-2.556286	9.735387	6.800838
C	2.499698	9.710738	6.921552	H	-1.685861	10.035903	6.230482
H	1.635342	10.005971	6.339335	C	-3.353912	8.582456	6.554904
C	3.289831	8.546622	6.705557	H	-3.169159	7.876839	5.751080
H	3.105175	7.825849	5.915247	O	-1.377526	12.141475	7.851993
O	3.781287	14.548169	10.802733	O	-2.994623	12.182426	9.450788
O	1.334614	12.148793	7.911845	O	-1.275008	14.443258	9.515797
O	2.933295	12.205823	9.526969	S	-4.393991	9.738301	8.617926
O	1.168247	14.469729	9.603085	Cl	-0.031355	11.798836	10.855479
O	0.487416	16.849955	11.234683	H	-5.130086	7.673713	7.500158
O	0.004544	14.420817	6.975836	H	-5.139414	7.821435	14.231511
S	4.323098	9.736239	8.752670	H	5.051236	7.643205	7.683027
V	2.471813	13.666776	10.849596	H	5.166790	7.915152	14.427649
V	-0.039620	13.586550	8.316513	O	-0.555591	16.841292	10.239797
V	-0.019651	15.201548	10.762387	H	-2.100252	17.307610	11.685478
C	-4.393418	8.605638	14.256557	O	-2.496527	17.208598	12.568002
C	-3.001937	10.600782	13.779244	H	-2.251418	16.290693	12.776564
C	-2.407687	11.820071	13.181399				
C	-2.572291	9.906896	14.883700				
H	-1.706572	10.226687	15.450709	76			
C	-3.371216	8.761852	15.160604	6, B3LYP/6-311++G(d,p)=-5207.022353			
H	-3.192638	8.083058	15.988587	C	5.766819	-2.794142	-2.275125
O	-3.829928	14.524722	10.742697	C	4.266298	-1.137601	-1.202398
O	-1.387071	12.279155	13.763988	C	3.381444	-0.403360	-0.266054
O	-2.989681	12.267247	12.152832	C	4.576602	-0.809916	-2.499416
O	-1.227203	14.536741	11.967153	H	4.176004	0.080690	-2.968041
O	-0.070965	14.593133	14.581897	C	5.439630	-1.758969	-3.116466
S	-4.395118	9.849073	13.052747	H	5.795950	-1.680451	-4.138782

O	3.008675	-0.445330	3.625305	O	-1.523071	1.260556	-1.811923
O	2.867792	0.657850	-0.712915	O	-0.379303	2.184893	0.630989
O	3.241283	-0.922476	0.877774	S	-1.979699	0.879878	-4.693612
O	1.559701	1.227256	1.784684	Cl	0.097538	-0.941565	-0.032921
O	-0.138463	2.060181	4.083186	H	-1.772376	0.720824	-7.141684
O	2.153334	3.283865	-0.133213	H	-5.839158	-3.874930	-3.293227
S	5.024779	-2.629394	-0.719950	H	6.397330	-3.647411	-2.490815
V	1.984955	-0.588363	2.430727	H	2.632626	-7.758539	1.280083
V	1.398668	1.900789	-0.064732	O	-0.377548	3.075545	3.094696
V	-0.132134	1.437385	2.403639	C	-0.510223	5.287566	-1.289740
C	-5.281129	-3.635080	-2.397007	C	0.509334	5.473740	-2.239020
C	-3.960149	-2.501462	-0.631269	C	0.323086	5.079366	-3.560198
C	-3.189591	-1.521862	0.172303	C	-0.877100	4.485751	-3.962010
C	-4.218091	-3.817823	-0.337791	C	-1.878348	4.278123	-3.014351
H	-3.856436	-4.274808	0.575278	C	-1.705161	4.673392	-1.686913
C	-4.977570	-4.470263	-1.349772	H	1.458824	5.896429	-1.923297
H	-5.280158	-5.511754	-1.304791	H	1.131630	5.213773	-4.275742
O	-3.148910	2.375579	0.183270	H	-1.010080	4.146884	-4.985733
O	-2.718838	-1.951332	1.260712	H	-2.795303	3.765839	-3.291762
O	-3.091293	-0.362919	-0.321712	H	-2.483224	4.445780	-0.969455
O	-1.725501	0.656849	1.990213	S	-0.194222	5.869046	0.354456
O	-2.289248	-1.372971	3.950081	C	-1.622064	5.249091	1.293909
S	-4.641315	-2.043197	-2.167745	H	-2.546871	5.766651	1.018463
V	-2.001955	1.281361	0.145098	H	-1.731396	4.174246	1.156744
V	-1.431991	-1.185523	2.635697	H	-1.390015	5.436281	2.344340
C	1.946550	-6.953461	1.510869				
C	0.924766	-4.757169	2.037811				
C	0.685381	-3.320677	2.314950	76, $\nu^{\neq}$ = 496.33 *i*cm^{-1}			
C	-0.004032	-5.763932	1.939172	TS3, B3LYP/6-311++G(d,p)=-5206.99828			
H	-1.061628	-5.572738	2.074029	C	6.023949	10.762317	8.341488
C	0.580925	-7.026305	1.638496	C	4.500977	12.507053	9.227383
H	0.014340	-7.944131	1.516914	C	3.607027	13.326314	10.082127
O	-0.519640	-2.985992	2.485756	C	4.812757	12.697884	7.903827
O	1.716083	-2.589362	2.347131	H	4.404073	13.528577	7.341451
O	0.212208	-0.318232	3.121716	C	5.688679	11.698163	7.393699
S	2.539201	-5.345275	1.751496	H	6.047977	11.671369	6.369645
C	-1.202980	0.911332	-6.240845	O	3.219756	13.615876	13.988809
C	-0.475926	1.233048	-3.892979	O	3.080290	14.329128	9.526903
C	-0.427452	1.416245	-2.424450	O	3.471599	12.931072	11.273292
C	0.556875	1.356587	-4.788080	O	1.798866	15.161860	12.013610
H	1.562070	1.590049	-4.460076	O	0.081968	16.113049	14.173694
C	0.141738	1.172672	-6.137222	O	2.392351	16.989591	9.961996
H	0.809436	1.230091	-6.991139	S	5.273083	11.083102	9.867874
O	0.701207	1.708632	-1.945147	V	2.207135	13.404750	12.791642

V	1.621244	15.612909	10.111315	O	-0.089939	17.367733	12.843699
V	0.090671	15.483636	12.625653	C	-0.389367	18.805412	9.756182
C	-5.156447	9.832961	8.422408	C	0.800289	19.260776	9.173013
C	-3.791647	11.176840	9.999176	C	0.949448	19.237237	7.788954
C	-2.991853	12.241380	10.655195	C	-0.082932	18.763183	6.977705
C	-4.086332	9.926623	10.484324	C	-1.265853	18.308873	7.563049
H	-3.733498	9.600965	11.455312	C	-1.423487	18.319099	8.948007
C	-4.870234	9.153886	9.581194	H	1.616497	19.591581	9.805512
H	-5.202282	8.139765	9.780628	H	1.887532	19.564880	7.348415
O	-2.963941	16.032808	10.327280	H	0.043081	18.715211	5.899350
O	-2.545749	11.965525	11.800660	H	-2.058323	17.896166	6.945621
O	-2.846476	13.309327	9.996447	H	-2.312839	17.885669	9.385279
O	-1.519846	14.632649	12.277851	S	-0.459156	18.871306	11.538090
O	-2.047689	12.782618	14.427928	C	-2.239501	18.750290	11.864109
S	-4.470748	11.422911	8.414051	H	-2.775165	19.553017	11.348104
V	-1.758327	14.986074	10.365882	H	-2.605618	17.768453	11.555678
V	-1.228720	12.856087	13.075407	H	-2.339821	18.853142	12.945587
C	2.075746	6.996464	12.199509				
C	1.088604	9.229602	12.633201				
C	0.871328	10.682556	12.844284	76			
C	0.145539	8.232606	12.587834	7, B3LYP/6-311++G(d,p)=-5207.086616			
H	-0.908148	8.445751	12.720270	C	5.947294	-3.061005	-2.287795
C	0.710381	6.949332	12.340817	C	4.451972	-1.389535	-1.231681
H	0.129809	6.035148	12.265347	C	3.564842	-0.647953	-0.304193
O	-0.326979	11.037317	13.018433	C	4.792817	-1.056991	-2.519836
O	1.912370	11.398735	12.823922	H	4.417604	-0.155942	-2.989499
O	0.433389	13.713264	13.399213	C	5.652906	-2.014649	-3.127399
S	2.692130	8.606125	12.360474	H	6.031066	-1.933607	-4.141559
C	-1.179680	15.311457	3.936531	O	3.203775	-0.689271	3.587336
C	-0.350024	15.250862	6.274883	O	3.071032	0.423517	-0.753017
C	-0.238018	15.191392	7.754820	O	3.399687	-1.172140	0.833957
C	0.639509	15.536411	5.367800	O	1.862394	1.047667	1.750394
H	1.657715	15.723298	5.686092	O	0.063901	2.397537	3.498605
C	0.166058	15.570110	4.024802	O	2.366899	3.079496	-0.205988
H	0.795377	15.776419	3.164578	S	5.177963	-2.896693	-0.746229
O	0.917725	15.384926	8.218617	V	2.174635	-0.772264	2.392459
O	-1.313513	14.961002	8.377505	V	1.634503	1.680317	-0.076378
O	-0.158508	15.951875	10.720952	V	0.121130	1.275266	2.381324
S	-1.887840	15.020004	5.490567	C	-5.410401	-3.444986	-2.292841
Cl	0.280529	12.872362	10.282706	C	-3.977685	-2.397242	-0.562273
H	-1.788082	15.267753	3.042075	C	-3.135692	-1.466538	0.226484
H	-5.726438	9.479890	7.572326	C	-4.286244	-3.704286	-0.274927
H	6.664529	9.898030	8.219384	H	-3.915183	-4.189475	0.619593
H	2.748517	6.171811	12.000586	C	-5.110057	-4.307211	-1.266763

H	-5.459683	-5.333843	-1.223168	H	1.346089	4.264870	-2.505709
O	-2.898698	2.449914	0.314325	H	-0.115545	4.256760	-4.532442
O	-2.649081	-1.933721	1.292417	H	-2.539590	4.749045	-4.301526
O	-2.997564	-0.306623	-0.259041	H	-3.486574	5.274200	-2.062446
O	-1.584355	0.605020	2.036067	S	-2.414577	5.616648	0.494883
O	-2.134473	-1.410206	3.988543	C	-1.199740	4.968532	1.683932
S	-4.691135	-1.887101	-2.067228	H	-1.657928	5.044432	2.672063
V	-1.841938	1.276694	0.224540	H	-0.961136	3.929165	1.462141
V	-1.317515	-1.229506	2.648740	H	-0.303197	5.593736	1.645810
C	1.828543	-7.118864	1.451531				
C	0.905412	-4.884214	1.998956				
C	0.729453	-3.440596	2.286417	63, $\nu^{\neq}$ = 714.09 *i*cm^{-1}			
C	-0.066244	-5.849863	1.901602	TS1D, B3LYP/6-311++G(d,p)=-4613.54608			
H	-1.113665	-5.614780	2.046137	C	3.904867	8.113758	9.967333
C	0.462049	-7.134139	1.589142	C	3.312786	10.493977	10.327035
H	-0.143993	-8.026269	1.466897	C	2.878030	11.788361	10.903908
O	-0.458657	-3.055812	2.466884	C	3.667495	10.226548	9.027599
O	1.791390	-2.754979	2.317362	H	3.664790	11.000828	8.270139
O	0.396261	-0.408110	3.116706	C	4.009678	8.860644	8.819408
S	2.491134	-5.538962	1.697033	H	4.313914	8.450440	7.861613
C	-1.261230	1.165090	-6.185834	O	2.732829	13.123662	14.574314
C	-0.420103	1.260309	-3.857777	O	2.836067	12.763427	10.105185
C	-0.300903	1.349306	-2.384494	O	2.596844	11.773659	12.136359
C	0.589604	1.308071	-4.787375	O	2.109176	14.610334	12.204679
H	1.628278	1.387882	-4.490878	O	1.459830	16.718672	13.876468
C	0.108599	1.253920	-6.126084	O	3.333929	15.496739	9.782975
H	0.748062	1.277587	-7.002776	S	3.383860	9.062972	11.317548
O	0.871850	1.479561	-1.935989	V	1.703051	13.093895	13.379354
O	-1.385285	1.291561	-1.739604	V	2.086657	14.644900	10.250091
O	-0.120711	2.060950	0.687867	V	0.728342	15.744411	12.658672
S	-1.982119	1.142791	-4.612953	C	-6.403891	12.254566	9.081391
Cl	0.219037	-1.033463	-0.013301	C	-4.657040	13.187848	10.572069
H	-1.881179	1.102289	-7.071124	C	-3.507680	13.936105	11.134660
H	-6.010375	-3.646215	-3.171231	C	-5.440225	12.248475	11.196660
H	6.568968	-3.922105	-2.497748	H	-5.271217	11.967372	12.228973
H	2.477963	-7.951096	1.211291	C	-6.445273	11.712693	10.342866
O	-2.357087	7.140417	0.589257	H	-7.161664	10.956732	10.648733
C	-1.593487	5.115342	-1.052480	O	-1.718662	17.223498	9.984451
C	-0.232452	4.835155	-1.178450	O	-3.218467	13.681879	12.336809
C	0.296910	4.532172	-2.434482	O	-2.941953	14.747449	10.350001
C	-0.525866	4.519272	-3.561457	O	-1.127799	15.670117	12.369831
C	-1.889664	4.791462	-3.431123	O	-2.368904	14.770203	14.772895
C	-2.422272	5.085828	-2.177674	S	-5.137461	13.422303	8.914420
H	0.422676	4.796376	-0.317860	V	-1.210221	15.796651	10.419466

V	-1.639921	14.182502	13.499475	O	2.161437	13.497579	9.035089
C	-1.227694	7.461705	14.359555	O	3.435087	12.723170	10.745331
C	-1.134071	9.929870	14.146384	O	1.975990	15.149426	11.452131
C	-0.693953	11.335666	13.978226	O	1.558716	16.685730	14.001984
C	-2.417734	9.456205	14.263250	O	1.321209	16.138053	8.847141
H	-3.270205	10.124281	14.248441	S	4.655507	10.469005	9.301609
C	-2.473535	8.039294	14.387614	V	2.897666	13.702820	12.436894
H	-3.395216	7.474733	14.487612	V	0.939293	14.930638	9.791422
O	-1.611079	12.200486	13.944418	V	0.737187	15.752707	12.668219
O	0.555315	11.510959	13.887493	C	-5.144628	9.258732	12.977691
O	0.270455	14.340581	13.784428	C	-3.407473	10.975195	13.403722
S	0.031148	8.635486	14.177151	C	-2.538403	12.174731	13.349424
C	-1.380189	12.799715	4.730752	C	-3.296621	9.890383	14.238395
C	-0.264193	13.688850	6.757771	H	-2.512110	9.827740	14.982651
C	0.038536	14.349263	8.050081	C	-4.294438	8.904404	13.996613
C	0.583131	12.953779	5.965565	H	-4.374186	7.973470	14.549094
H	1.618784	12.795122	6.240318	O	-3.060043	15.752041	11.888376
C	-0.055353	12.443844	4.800000	O	-1.584980	12.206885	14.173359
H	0.443536	11.836747	4.051126	O	-2.846506	13.039914	12.481841
O	1.224328	14.226436	8.467406	O	-0.740902	14.881374	13.327441
O	-0.922514	14.963330	8.591403	O	-0.084967	13.801878	15.906528
O	0.707373	15.900602	10.734762	S	-4.739407	10.797003	12.295622
S	-1.869915	13.757651	6.086490	V	-1.908311	14.679757	11.755958
Cl	-0.294225	12.871156	11.020108	V	0.045687	13.402101	14.381073
H	-2.094236	12.541878	3.958881	C	3.382835	7.500074	14.092997
H	-7.045712	12.022330	8.241003	C	2.386758	9.769750	14.157035
H	4.098591	7.055361	10.087217	C	2.088306	11.207957	13.950704
H	-0.985664	6.408700	14.428273	C	1.660078	8.851294	14.874051
O	0.271930	17.907006	12.308076	H	0.748635	9.129514	15.388928
H	1.053514	17.614859	13.425766	C	2.231291	7.547827	14.840024
O	1.283385	18.388172	11.387270	H	1.804594	6.684999	15.341753
H	1.166595	17.719580	10.675838	O	1.041961	11.637569	14.510614
				O	2.916038	11.840728	13.233999
				O	1.589362	14.266686	13.692259
63				S	3.785518	9.041731	13.416790
3D, B3LYP/6-311++G(d,p)=-4613.564403				C	-3.896462	11.421626	6.569630
C	4.706542	9.661811	7.771372	C	-2.316265	12.818155	7.873441
C	3.522047	11.638814	8.684680	C	-1.658446	13.635977	8.921102
C	2.994076	12.710697	9.561934	C	-1.802263	12.426389	6.661802
C	3.208792	11.393696	7.370315	H	-0.804321	12.711958	6.352262
H	2.505757	12.016853	6.831156	C	-2.708712	11.625834	5.910889
C	3.889405	10.259936	6.843439	H	-2.487734	11.216608	4.930095
H	3.773801	9.901778	5.825308	O	-0.483702	14.018571	8.663938
O	4.293985	14.276184	12.910215	O	-2.348936	13.858098	9.956755

O	-0.380558	15.579288	11.023359	S	-6.791669	16.805933	16.281201
S	-3.926233	12.198790	8.115969	V	-2.693082	17.360232	13.782186
Cl	0.213784	12.475223	11.439102	V	-1.159956	15.275943	16.171011
H	-4.750685	10.849572	6.230254	C	-2.957858	8.811277	17.180793
H	-5.981363	8.692859	12.588110	C	-2.092140	11.081893	16.686009
H	5.328324	8.785702	7.637451	C	-1.427403	12.258205	16.071715
H	4.009449	6.638831	13.898716	C	-2.873935	11.046510	17.814236
O	0.359359	17.554817	12.364308	H	-3.074255	11.941364	18.390729
H	1.986647	15.982589	14.526743	C	-3.370523	9.743450	18.101180
O	-0.416608	18.047286	11.287178	H	-4.008802	9.510122	18.947709
H	-0.651330	17.195285	10.833344	O	-1.599215	13.356880	16.668222
				O	-0.766545	12.023307	15.020147
				O	0.079965	14.685380	14.852764
63, $\nu^{\neq}$ = 776.69 *i*cm^{-1}				S	-1.961752	9.508979	15.948798
TS2D, B3LYP/6-311++G(d,p)=-4613.528969				C	-8.164799	16.138958	10.618371
C	-3.310182	8.765517	10.502135	C	-5.712657	16.041420	10.975988
C	-2.399157	11.042727	10.863819	C	-4.334801	16.203572	11.503564
C	-1.668971	12.226284	11.378194	C	-6.121069	15.299489	9.895186
C	-3.320211	10.995734	9.846426	H	-5.414358	14.738877	9.295576
H	-3.598709	11.885463	9.294992	C	-7.528354	15.355441	9.687072
C	-3.843178	9.688591	9.635870	H	-8.044600	14.834384	8.886793
H	-4.584751	9.445984	8.881183	O	-3.433041	15.583411	10.875835
O	1.574723	12.633930	13.557748	O	-4.226694	16.944064	12.523234
O	-1.914508	13.320510	10.800747	O	-1.454764	16.752470	12.443613
O	-0.877497	12.012248	12.338239	S	-7.058549	16.816831	11.764499
O	0.031365	14.770744	12.430947	Cl	-2.870571	14.280996	13.778264
O	1.603825	16.632250	14.091123	H	-9.224762	16.345951	10.694771
O	-0.821479	15.688691	9.863277	H	-8.825793	16.286936	17.565669
S	-2.167170	9.476723	11.590173	H	-3.536553	7.708537	10.563098
V	0.107357	13.221898	13.635250	H	-3.194249	7.754947	17.158308
V	-1.459019	15.245521	11.240537	O	0.261146	17.571215	12.280384
V	0.055784	16.189622	13.653936	H	2.013317	17.462910	13.182531
C	-7.760277	16.098484	17.529230	O	1.939448	18.072743	12.240074
C	-5.358132	16.048249	16.917315	H	2.140761	17.445029	11.523713
C	-4.046933	16.235791	16.250657				
C	-5.638623	15.288956	18.026554				
H	-4.863893	14.734451	18.541941	63, $\nu^{\neq}$ = 500.45 *i*cm^{-1}			
C	-7.017115	15.317906	18.380653	TS1F, B3LYP/6-311++G(d,p)=-4613.553797			
H	-7.438386	14.780036	19.224196	C	1.710187	9.947865	6.308883
O	-2.708149	18.938616	13.777713	C	1.096725	11.844214	7.783886
O	-3.070524	15.633071	16.770865	C	1.090048	12.914319	8.811013
O	-4.050060	16.983405	15.231399	C	0.071062	11.465101	6.953421
O	-1.158763	16.796423	14.892621	H	-0.891205	11.961575	6.981618
O	-0.366222	15.749119	17.453952	C	0.421787	10.377575	6.104368

H	-0.252433	9.931276	5.380059	O	-2.341154	13.719502	10.241809
O	3.928166	14.900701	10.629704	O	-2.982551	13.325798	12.384393
O	0.013843	13.562732	8.921550	O	-1.009163	15.429717	12.142355
O	2.165482	13.057866	9.459154	S	-5.042632	11.312845	11.782377
O	1.095341	15.217122	10.955673	Cl	0.160226	12.360810	11.972768
O	1.546351	16.780767	14.325662	H	-6.586229	9.727489	10.705256
O	-1.121885	16.078910	9.353773	H	-3.337489	7.844478	16.559553
S	2.512893	10.859250	7.542406	H	2.224922	9.139067	5.805811
V	2.656382	14.102798	11.124791	H	5.621312	7.437790	11.385825
V	-0.683106	14.887896	10.293858	O	0.471798	17.489021	12.219180
V	0.758057	15.771948	12.713699	H	2.138080	16.152394	14.776455
C	-2.543717	8.553852	16.362350	O	1.909701	17.487079	12.177957
C	-1.218221	10.530751	15.666561	H	2.053937	17.396751	13.305066
C	-0.775326	11.836352	15.118743				
C	-0.444531	9.542993	16.224484				
H	0.628669	9.653072	16.321212	63			
C	-1.203798	8.407713	16.626163	3F, B3LYP/6-311++G(d,p)=-4613.56269			
H	-0.774912	7.521954	17.084279	C	4.909256	9.931850	7.610995
O	-2.647725	15.187861	14.454456	C	3.528253	11.729090	8.619449
O	0.463671	12.068948	15.188907	C	2.898248	12.703469	9.546590
O	-1.687880	12.569556	14.644383	C	3.244136	11.522683	7.292008
O	0.136684	14.670872	14.094191	H	2.484450	12.101173	6.780647
O	2.397136	14.057565	15.661979	C	4.036526	10.492312	6.710931
S	-2.898749	10.075219	15.616798	H	3.959415	10.179209	5.674390
V	-1.675729	14.299697	13.579451	O	4.209440	14.267457	12.886890
V	1.648156	13.504340	14.374437	O	1.996351	13.428630	9.044917
C	5.104039	8.203565	11.949869	O	3.340902	12.685229	10.734036
C	3.981272	10.288867	12.682570	O	2.062513	15.075467	11.288442
C	3.380206	11.642413	12.748205	O	0.148680	16.795042	14.062711
C	4.002483	9.326065	13.661565	O	1.052997	16.052714	8.901843
H	3.554322	9.497372	14.632666	S	4.775518	10.649829	9.180763
C	4.648402	8.128476	13.243425	V	2.817992	13.679368	12.432161
H	4.764179	7.250458	13.871078	V	0.709515	14.820729	9.852084
O	2.831727	11.950059	13.843512	V	0.531226	15.822313	12.880224
O	3.481665	12.341892	11.701856	C	-5.146346	9.117207	12.885055
O	2.294815	14.629161	12.943433	C	-3.436120	10.856414	13.333208
S	4.748655	9.732743	11.221179	C	-2.592599	12.077865	13.298494
C	-5.814159	10.455752	10.491548	C	-3.295360	9.753855	14.139364
C	-4.037995	12.177899	10.652759	H	-2.501487	9.688601	14.873388
C	-3.034393	13.157825	11.132636	C	-4.277382	8.754847	13.884976
C	-4.296154	11.802214	9.357392	H	-4.333042	7.809589	14.415853
H	-3.750687	12.230946	8.525550	O	-3.222748	15.760681	11.977335
C	-5.316979	10.814700	9.262544	O	-1.628897	12.098424	14.113640
H	-5.662213	10.386751	8.326626	O	-2.933726	12.951454	12.451699

O	-0.990780	14.686250	13.360675	H	2.279839	11.695299	7.047382
O	-0.206686	13.729987	15.914032	C	3.919393	10.176334	6.969145
S	-4.778458	10.679795	12.236848	H	3.743832	9.736670	5.992294
V	-2.073245	14.682834	11.814931	O	4.470969	14.658950	12.644850
V	-0.079247	13.383772	14.376936	O	1.971778	13.261298	9.189383
C	3.459426	7.567264	14.333852	O	3.539676	12.792950	10.775986
C	2.398054	9.807416	14.276699	O	2.021222	15.070026	11.339193
C	2.062737	11.226859	14.011323	O	0.327090	17.046825	13.715896
C	1.675718	8.896882	15.008132	O	0.836785	15.821215	8.985132
H	0.742327	9.169366	15.485533	S	4.926271	10.667938	9.296471
C	2.284230	7.610521	15.043308	V	3.096238	13.910468	12.421291
H	1.867006	6.756080	15.566765	V	0.692698	14.610296	10.021612
O	0.992688	11.649635	14.517078	V	0.716530	15.751994	12.814172
O	2.892168	11.866305	13.299187	C	-4.138361	8.657936	14.405954
O	1.473411	14.426949	13.654428	C	-2.617505	10.616331	14.449047
S	3.839775	9.092765	13.609667	C	-1.936599	11.906844	14.177160
C	-4.223606	11.453068	6.660589	C	-2.260507	9.647425	15.354129
C	-2.580585	12.803869	7.933391	H	-1.392970	9.762988	15.992308
C	-1.887160	13.611562	8.964182	C	-3.133372	8.522926	15.332259
C	-2.085361	12.361986	6.731082	H	-3.017576	7.652381	15.970344
H	-1.075179	12.593320	6.415973	O	-3.115731	15.270015	12.526556
C	-3.028142	11.587590	5.997776	O	-0.909309	12.139944	14.871801
H	-2.826845	11.146666	5.026561	O	-2.462718	12.622706	13.278061
O	-0.694856	13.940033	8.702983	O	-0.611345	14.671156	13.733005
O	-2.551242	13.888106	9.997872	O	0.527327	14.113212	16.283084
O	-0.457417	15.581052	11.185550	S	-4.033069	10.155701	13.544216
S	-4.216855	12.264508	8.189268	V	-1.863285	14.320630	12.345404
Cl	0.263022	12.508192	11.417623	V	0.521495	13.580036	14.794400
H	-5.103578	10.913788	6.333622	C	4.492018	8.067294	14.746187
H	-5.977200	8.545108	12.491883	C	3.261086	10.218014	14.659722
H	5.617481	9.132043	7.435261	C	2.778577	11.578974	14.322197
H	4.116304	6.718200	14.193574	C	2.733368	9.341400	15.575561
O	1.389032	17.446662	12.246574	H	1.864932	9.599889	16.169149
O	2.146541	17.549621	10.997995	C	3.439634	8.106542	15.627828
H	1.459605	17.421212	10.307862	H	3.175891	7.284026	16.285228
H	2.528736	15.938041	11.124703	O	1.770547	11.982182	14.960053
				O	3.431489	12.190767	13.429105
				O	1.844665	14.639932	13.765736
63, $v^{\neq}$ = 475.01 *i*cm^{-1}				S	4.634962	9.533177	13.836637
TS2F, B3LYP/6-311++G(d,p)=-4613.539865				C	-4.122529	10.446046	7.704740
C	4.925988	9.775559	7.813088	C	-2.541519	12.085593	8.683795
C	3.553571	11.604496	8.773566	C	-1.846458	13.046591	9.573439
C	2.970821	12.644939	9.657214	C	-2.141200	11.634633	7.449978
C	3.131990	11.225269	7.522929	H	-1.220199	11.977229	6.994265

C	-3.048606	10.694334	6.885287	O	-1.248067	12.338465	13.982245
H	-2.908208	10.220443	5.918849	O	-2.937858	12.359799	12.466597
O	-0.758486	13.517412	9.134593	O	-1.164126	14.540486	12.203154
O	-2.410947	13.292650	10.673041	O	0.337446	14.603739	14.645747
O	-0.466947	15.328155	11.406053	S	-4.548975	10.211889	13.684563
S	-4.041733	11.351266	9.177787	V	-2.498615	13.673570	11.060769
Cl	0.543738	12.344716	11.867045	V	0.117211	13.652239	13.398675
H	-4.951204	9.773510	7.522776	C	4.514591	8.566082	14.003481
H	-4.928565	7.953017	14.180427	C	3.096886	10.557555	13.634835
H	5.661058	8.998996	7.643462	C	2.476855	11.776491	13.107904
H	5.184289	7.251887	14.578855	C	2.713289	9.831267	14.740427
O	1.437359	17.423035	12.126378	H	1.870728	10.124476	15.354749
O	2.371816	17.363561	10.706044	C	3.528182	8.688361	14.953142
H	1.651201	17.278708	10.037031	H	3.390378	7.985993	15.767342
H	2.524528	16.337438	10.898545	O	1.479807	12.233683	13.746159
				O	3.005487	12.273978	12.062693
				O	1.300381	14.531449	12.078209
81				S	4.466230	9.835344	12.833966
1-1, B3LYP/6-311++G(d,p)=-4733.406882				C	-4.516193	8.574471	7.777157
C	4.607695	9.148832	6.768402	C	-3.101483	10.565877	8.157476
C	3.035853	10.894335	7.539808	C	-2.483358	11.782698	8.691516
C	2.352350	11.955793	8.283222	C	-2.717051	9.846882	7.047415
C	2.622613	10.285791	6.375520	H	-1.875141	10.145140	6.434631
H	1.701620	10.564613	5.878247	C	-3.530219	8.704012	6.828006
C	3.525667	9.284524	5.931474	H	-3.391552	8.006797	6.009536
H	3.382913	8.690374	5.036014	O	-1.487210	12.245337	8.055802
O	3.730140	14.665441	10.849379	O	-3.012580	12.273039	9.739785
O	1.240321	12.356478	7.821034	O	-1.312769	14.534641	9.735676
O	2.930577	12.374813	9.336171	S	-4.469481	9.836701	8.954318
O	1.151846	14.549961	9.610823	Cl	-0.003203	11.975122	10.900389
O	-0.008763	16.771166	10.912711	H	-5.265370	7.796782	7.848010
O	-0.349384	14.622253	7.168624	H	-5.438707	8.431503	15.118606
S	4.545656	10.235375	8.108527	H	5.438550	8.463004	6.666551
V	2.488256	13.680091	10.748885	H	5.264997	7.790002	13.928122
V	-0.127497	13.664765	8.410809	N	2.968517	16.113374	13.269424
V	-0.006903	15.184012	10.908615	H	3.619100	16.340857	12.511033
C	-4.609206	9.119436	15.019962	C	2.280518	17.318234	13.803135
C	-3.040626	10.871369	14.256520	H	1.787275	17.825846	12.972294
C	-2.359083	11.937462	13.517920	H	1.527912	16.977264	14.515642
C	-2.626535	10.258694	15.418334	H	3.004888	17.977232	14.287177
H	-1.706268	10.537249	15.917101	C	3.652801	15.269989	14.287366
C	-3.527718	9.253726	15.857810	H	2.895860	14.915469	14.988117
H	-3.384048	8.656040	16.750767	H	4.105624	14.423556	13.769253
O	-3.742812	14.656437	10.965345	H	4.415977	15.859121	14.800821

H	2.236294	15.500186	12.792495	O	0.368941	14.483317	14.730319
N	-2.983373	16.120396	8.552977	S	-4.407799	9.969563	13.788234
H	-3.634579	16.345692	9.311429	V	-2.531245	13.540762	11.202918
C	-2.295223	17.326993	8.023266	V	0.154348	13.534123	13.481865
H	-1.802985	17.832471	8.855997	C	4.720715	8.588963	13.944229
H	-1.541802	16.988166	7.310600	C	3.235157	10.539020	13.628270
H	-3.019362	17.987061	7.540334	C	2.567074	11.742516	13.128648
C	-3.666773	15.279990	7.531952	C	2.896796	9.788561	14.732874
H	-2.909261	14.928040	6.830517	H	2.058509	10.048072	15.367868
H	-4.119619	14.431764	8.047093	C	3.750789	8.669583	14.915300
H	-4.429778	15.870524	7.019855	H	3.651781	7.954092	15.723617
H	-2.251156	15.505804	9.028244	O	1.567085	12.160518	13.789784
				O	3.059565	12.270377	12.080051
				O	1.278018	14.466678	12.143792
85				S	4.609495	9.868967	12.791227
1-2, B3LYP/6-311++G(d,p)=-4885.045344				C	-4.683086	8.539568	7.885814
C	4.627584	9.186722	6.776039	C	-3.208830	10.484133	8.278377
C	3.018962	10.883640	7.578427	C	-2.548713	11.672174	8.823448
C	2.321767	11.928507	8.330557	C	-2.868137	9.781451	7.143519
C	2.588536	10.242657	6.437724	H	-2.034118	10.072951	6.516874
H	1.640647	10.478780	5.969759	C	-3.715637	8.665647	6.917088
C	3.512685	9.269347	5.975996	H	-3.614490	7.984911	6.079530
H	3.361387	8.656719	5.094568	O	-1.543786	12.114485	8.187552
O	3.675432	14.694608	10.868256	O	-3.046548	12.156031	9.891175
O	1.180078	12.281431	7.902914	O	-1.385694	14.423575	9.859216
O	2.919465	12.384697	9.357939	S	-4.578185	9.772922	9.088910
O	1.074981	14.496543	9.683001	Cl	0.034213	11.894213	10.974682
O	-0.143377	16.674256	11.014754	H	-5.451200	7.780509	7.955854
O	-0.452640	14.508300	7.274986	H	-5.228547	8.145003	15.206592
S	4.571570	10.289881	8.102553	H	5.479746	8.530962	6.654197
V	2.470539	13.664051	10.788019	H	5.493035	7.837542	13.844402
V	-0.209444	13.554079	8.514447	N	2.911308	16.097042	13.337994
V	-0.070344	15.070688	11.001561	H	3.543777	16.375202	12.581452
C	-4.418944	8.856087	15.106837	C	2.183080	17.257683	13.917246
C	-2.909197	10.660091	14.349042	H	1.664983	17.775295	13.107996
C	-2.268830	11.755049	13.618799	H	1.450358	16.865630	14.624123
C	-2.461730	10.041198	15.495573	H	2.887272	17.926700	14.416614
H	-1.542490	10.336874	15.986313	C	3.642972	15.253277	14.323518
C	-3.329330	9.006290	15.931794	H	2.910789	14.852972	15.025741
H	-3.157445	8.399374	16.813396	H	4.119523	14.438623	13.776609
O	-3.795152	14.507823	11.252611	H	4.390676	15.858408	14.840789
O	-1.160892	12.179901	14.071418	H	2.199384	15.469950	12.854030
O	-2.875142	12.178308	12.583329	N	-2.473053	16.553925	8.645894
O	-1.175924	14.406812	12.316337	H	-2.875182	16.994962	9.502274

C	-1.487895	17.459293	7.997128	O	2.135351	2.421511	1.117602
H	-0.748738	17.742375	8.747708	O	-0.407336	1.612916	1.566555
H	-0.999339	16.911189	7.191347	S	1.867723	6.466561	-2.383469
H	-2.007538	18.341859	7.617504	V	3.604575	2.886546	0.386654
C	-3.552951	16.055180	7.756131	V	0.631376	1.478174	0.364907
H	-3.092408	15.489162	6.944842	C	-2.862021	-1.320324	-4.671277
H	-4.201681	15.402879	8.343838	C	-1.487955	-0.531857	-2.773996
H	-4.121909	16.900140	7.362656	C	-0.480749	-0.384147	-1.720877
H	-1.975245	15.714907	9.028242	C	-2.503565	0.342527	-3.092060
O	-2.501365	17.728186	12.156286	H	-2.653192	1.268956	-2.551072
H	-1.649528	17.376996	11.809298	C	-3.293600	-0.110687	-4.180974
O	-3.446990	17.232463	11.172017	H	-4.140413	0.431868	-4.585642
H	-3.633062	16.313236	11.484841	O	-0.542031	0.666492	-1.008604
				O	0.369765	-1.315944	-1.601107
				O	1.493715	-0.227505	0.888228
85, $\nu^{\neq} = 803.59\ i\text{cm}^{-1}$				S	-1.488463	-1.926480	-3.818969
1-TS1B, B3LYP/6-311++G(d,p)=-4884.988116				C	5.873310	5.121405	-4.892240
C	4.110538	-4.311002	-5.867335	C	5.693426	3.323935	-3.208873
C	4.239635	-2.812266	-3.904618	C	5.428095	2.537932	-2.009894
C	3.964598	-2.053630	-2.680140	C	6.144565	2.863795	-4.427761
C	5.390324	-2.795964	-4.660883	H	6.372283	1.818584	-4.598084
H	6.242325	-2.181842	-4.395616	C	6.249561	3.896642	-5.393712
C	5.316952	-3.657215	-5.787354	H	6.581873	3.744055	-6.414082
H	6.118109	-3.788403	-6.505883	O	5.659698	1.300123	-2.032150
O	1.545441	-2.906802	0.362402	O	4.994493	3.170311	-0.980998
O	4.875539	-1.263755	-2.280993	O	4.413010	1.179460	0.803738
O	2.827405	-2.240709	-2.140353	S	5.380166	5.037780	-3.241773
O	3.712355	-1.118913	0.163590	Cl	2.576047	1.080168	-1.694909
O	3.561475	-1.204146	2.761260	H	5.854782	6.069253	-5.414077
O	6.459325	-0.460188	-0.044080	H	0.736518	8.172427	-3.734553
S	3.045761	-3.890631	-4.574725	H	3.792203	-5.018803	-6.621488
V	1.980894	-1.609116	-0.465618	H	-3.279812	-1.885529	-5.494115
V	5.053799	-0.094118	-0.687774	O	2.634690	1.095241	3.164242
V	3.176558	-0.106622	1.681955	H	2.382302	1.958832	2.748375
C	0.565264	7.242020	-3.209124	O	1.061719	0.655308	3.776792
C	0.812537	5.176135	-1.873464	H	0.518745	1.083569	3.064287
C	1.305587	4.065035	-1.057563	N	6.533027	1.857967	2.137261
C	-0.472385	5.358918	-2.335886	H	6.211881	2.636439	2.718439
H	-1.264758	4.652766	-2.120249	C	6.939654	0.692273	2.969453
C	-0.614549	6.544659	-3.102296	H	6.100729	0.415658	3.611150
H	-1.544718	6.868172	-3.555191	H	7.160446	-0.130868	2.289005
O	4.298867	3.789505	1.485366	H	7.814207	0.952406	3.570190
O	0.467251	3.179291	-0.723014	C	7.568736	2.336419	1.180110
O	2.559365	4.098145	-0.769219	H	7.806247	1.506655	0.513837

H	7.141180	3.159969	0.606844	O	-1.828065	2.057877	1.658874
H	8.453772	2.663727	1.730678	O	0.408540	1.111489	2.703889
H	5.664091	1.565572	1.571087	O	-0.083610	-1.140348	4.175736
N	0.583346	-1.999845	2.861682	S	-4.702159	2.666470	1.454825
H	1.080111	-2.239440	1.979285	V	0.145648	2.392708	1.433088
C	0.942488	-3.000015	3.897145	V	-0.189373	-0.732599	2.629426
H	2.024142	-2.960104	4.030752	C	-3.021371	-6.210203	-0.122845
H	0.434324	-2.748550	4.830281	C	-1.745714	-4.271081	0.727400
H	0.639374	-3.991228	3.554664	C	-0.757404	-3.212363	0.950552
C	-0.864513	-1.903011	2.538195	C	-2.911873	-4.486707	1.427861
H	-1.419965	-1.664870	3.447485	H	-3.208789	-3.853669	2.255157
H	-0.988194	-1.106958	1.803352	C	-3.644300	-5.600736	0.940321
H	-1.199076	-2.855291	2.123556	H	-4.588370	-5.936651	1.354088
H	0.910688	-1.054752	3.162550	O	-0.984611	-2.407644	1.904034
				O	0.240096	-3.184538	0.163810
				O	1.646078	-1.395424	2.047937
85				S	-1.536438	-5.439314	-0.548152
1-3, B3LYP/6-311++G(d,p)=-4885.011303				C	-2.913069	4.719883	-3.722190
C	1.251825	-2.632326	-6.305019	C	-1.086829	3.582476	-2.506312
C	1.628189	-1.427225	-4.180400	C	-0.225384	2.982540	-1.484793
C	1.778320	-1.049831	-2.773443	C	-0.892131	3.587934	-3.869866
C	1.760063	-0.611654	-5.282756	H	-0.025526	3.126965	-4.327779
H	2.003765	0.439924	-5.192252	C	-1.940115	4.242900	-4.568228
C	1.544664	-1.303719	-6.503073	H	-1.976380	4.353888	-5.645958
H	1.602941	-0.842822	-7.482565	O	0.828719	2.401629	-1.892127
O	2.963855	-3.056246	0.177516	O	-0.622439	3.090956	-0.280051
O	2.069806	0.161328	-2.530831	O	1.663492	2.202501	0.640471
O	1.592723	-1.962575	-1.909595	S	-2.572820	4.379143	-2.064362
O	2.912961	-0.227503	0.103240	Cl	-0.197360	-0.118629	-0.112598
O	4.402207	-1.106531	2.259942	H	-3.816601	5.251907	-3.989863
O	3.581171	2.151746	-1.205324	H	-7.153557	2.597997	1.500585
S	1.233765	-3.062670	-4.633554	H	1.044439	-3.381577	-7.057790
V	1.815665	-1.998744	0.052366	H	-3.360739	-7.073505	-0.680147
V	2.225258	1.341860	-0.947083	O	2.998227	1.107702	2.871979
V	3.060837	-0.373376	1.858286	H	2.004077	1.308615	2.851812
C	-6.274695	2.011150	1.733533	O	0.419897	2.050294	5.170868
C	-3.959756	1.204222	2.044470	H	0.272145	1.768164	4.203879
C	-2.501933	1.065197	2.072320	N	4.125230	3.198999	1.319155
C	-4.900582	0.273035	2.424892	H	3.652187	2.494496	1.922572
H	-4.622015	-0.700930	2.808301	C	5.594789	3.087720	1.495172
C	-6.230445	0.737012	2.247894	H	5.893729	2.064503	1.260036
H	-7.114192	0.156123	2.486077	H	6.090714	3.782913	0.815299
O	0.326883	3.727421	2.261221	H	5.852747	3.323927	2.529428
O	-2.039253	-0.041479	2.497863	C	3.548239	4.542540	1.597055

H	3.941482	5.253079	0.867498	O	-6.497557	14.186820	10.937106
H	2.463298	4.466910	1.519315	O	-6.191909	15.527930	9.125222
H	3.830563	4.847044	2.607155	O	-4.213392	15.559609	10.804442
H	3.881928	2.911012	0.343963	O	-4.724133	14.295680	13.210077
N	1.795654	-0.277792	5.863710	S	-9.008830	15.675224	8.292356
H	1.488870	0.707366	5.680408	V	-4.217611	15.886253	9.080146
C	1.208833	-0.727002	7.153450	V	-4.667119	13.917482	11.661617
H	0.125956	-0.613272	7.091568	C	-7.151505	7.655247	11.372200
H	1.461400	-1.776962	7.312416	C	-5.921768	9.793625	11.532249
H	1.609936	-0.116535	7.964812	C	-4.922793	10.863008	11.461062
C	3.272142	-0.424600	5.762286	C	-7.214888	9.889804	11.997260
H	3.526660	-1.485653	5.789336	H	-7.619198	10.820467	12.376556
H	3.597914	0.013375	4.819186	C	-7.920930	8.661505	11.906322
H	3.737695	0.094206	6.603383	H	-8.950766	8.527034	12.217085
H	1.295086	-0.796051	5.102803	O	-5.254736	11.997967	11.919446
				O	-3.791166	10.563018	10.969537
				O	-2.734573	13.347712	11.570789

85, $\nu^{\neq}$ = 1701.20 *i*cm^{-1}

1-TS2B, B3LYP/6-311++G(d,p)=-4884.994543

S	-5.558777	8.185363	10.967875	C	-6.706148	14.639829	3.280542
C	-1.561095	7.443878	5.746671	C	-4.958587	14.571704	5.027156
C	-1.659101	9.701839	6.748691	C	-4.177604	14.746226	6.255513
C	-1.788087	10.844795	7.655970	C	-4.634349	13.813718	3.923960
C	-1.405273	9.732960	5.395395	H	-3.710037	13.252007	3.865099
H	-1.268100	10.663916	4.858872	C	-5.637310	13.854252	2.919744
C	-1.347957	8.436494	4.819942	H	-5.575002	13.324152	1.976169
H	-1.158137	8.244802	3.769963	O	-3.062950	14.137940	6.317377
O	-1.222544	11.043405	11.503989	O	-4.682683	15.502154	7.141808
O	-1.667562	12.000721	7.149457	O	-2.578578	15.340662	8.741498
O	-2.024816	10.582072	8.878004	S	-6.512894	15.339875	4.847048
O	-1.114396	13.205164	9.615944	Cl	-4.250909	12.856250	9.014712
O	-0.126312	13.735033	12.069535	H	-7.601834	14.838395	2.706598
O	-0.479422	14.570254	7.224833	H	-11.443631	15.450506	8.095602
S	-1.834126	8.069316	7.332464	H	-1.572254	6.375002	5.578112
V	-2.226562	11.705805	10.485115	H	-7.441606	6.628702	11.190226
V	-1.772605	13.869187	7.822152	O	-0.528531	15.941867	10.499228
V	-1.202606	14.240406	11.039192	H	-1.075503	16.432276	11.407521
C	-10.602235	15.158850	8.710443	O	-2.005610	15.919095	12.009155
C	-8.347296	14.840055	9.671545	H	-2.912633	16.026111	11.547364
C	-6.906496	14.857025	9.937199	N	-1.123021	17.279055	7.773755
C	-9.327677	14.200380	10.396848	H	-0.253404	16.758348	7.619611
H	-9.100817	13.625323	11.286204	C	-1.798092	17.512927	6.468379
C	-10.623123	14.384851	9.846261	H	-1.871606	16.555921	5.952484
H	-11.528924	13.964299	10.267999	H	-2.795265	17.904865	6.670741
O	-4.083836	17.461583	8.968495	H	-1.213897	18.222024	5.877346

C	-0.903970	18.502657	8.582959	O	0.895367	3.601258	2.286168
H	-1.881003	18.923877	8.822642	O	-1.509332	-0.113861	2.662510
H	-0.388665	18.214544	9.498452	O	-1.353872	1.976208	1.777815
H	-0.305522	19.218060	8.013511	O	0.863377	1.025795	2.710686
H	-1.715795	16.572106	8.313224	O	0.696911	-1.400373	4.063868
N	-2.597202	12.752916	14.161190	S	-4.178002	2.722021	2.069274
H	-2.448062	12.877495	13.126589	V	0.590348	2.234930	1.539898
C	-1.507960	13.439694	14.902627	V	0.361326	-0.803758	2.629425
H	-1.486860	14.482561	14.584509	C	-2.945067	-5.643998	-0.695103
H	-1.702109	13.368507	15.975131	C	-1.443926	-4.020127	0.408329
H	-0.560669	12.965351	14.646527	C	-0.339129	-3.128881	0.763720
C	-2.753801	11.304864	14.457786	C	-2.635687	-4.181794	1.080727
H	-2.887175	11.167858	15.533035	H	-2.861890	-3.632585	1.986615
H	-3.628222	10.941788	13.918625	C	-3.497275	-5.115261	0.447599
H	-1.866068	10.782004	14.101034	H	-4.481367	-5.381854	0.815773
H	-3.492395	13.257103	14.281784	O	-0.459576	-2.456161	1.833816
				O	0.667083	-3.118615	-0.010649
				O	2.107954	-1.113285	1.739383
85				S	-1.371721	-5.013124	-1.022103
1-4, B3LYP/6-311++G(d,p)=-4885.027526				C	-3.306469	4.252704	-3.046211
C	1.558674	-2.908525	-6.426388	C	-1.148765	3.373472	-2.226104
C	1.895132	-1.553511	-4.386525	C	-0.036301	2.916806	-1.394141
C	2.060426	-1.085258	-3.009517	C	-1.260030	3.306620	-3.597842
C	1.904808	-0.793513	-5.535484	H	-0.473213	2.895938	-4.218828
H	2.047410	0.280040	-5.512652	C	-2.498699	3.813940	-4.069148
C	1.712784	-1.571554	-6.706877	H	-2.783680	3.849137	-5.114433
H	1.689375	-1.163728	-7.710984	O	0.964821	2.403952	-1.986956
O	3.339143	-3.009144	0.176811	O	-0.146928	3.093131	-0.142080
O	2.210778	0.163493	-2.838451	O	2.131626	1.911221	0.576555
O	2.021959	-1.971389	-2.095498	S	-2.577535	4.053205	-1.494754
O	3.346106	-0.217051	-0.351533	Cl	0.117673	-0.119385	-0.273523
O	4.747371	-0.671195	1.955715	H	-4.298405	4.677844	-3.126363
O	3.700826	2.286986	-1.626604	H	-6.576449	2.796622	2.574705
S	1.645163	-3.242664	-4.735139	H	1.397833	-3.715792	-7.128868
V	2.249200	-1.909971	-0.141730	H	-3.385919	-6.369834	-1.365834
V	2.485574	1.333391	-1.261117	O	3.781238	1.657614	2.063524
V	3.462189	0.083313	1.401903	H	-0.116111	3.268092	4.297056
C	-5.703073	2.162303	2.651308	O	-0.231199	2.545829	4.934297
C	-3.419504	1.226027	2.541342	H	0.247180	1.821019	4.497330
C	-1.991328	1.009797	2.323079	N	3.461804	4.215059	0.493250
C	-4.320643	0.357339	3.116415	H	2.936907	3.311736	0.670691
H	-4.026271	-0.620693	3.476719	C	3.981022	4.755635	1.777085
C	-5.632105	0.895152	3.180254	H	4.611783	3.994899	2.234978
H	-6.484306	0.372270	3.598982	H	4.543022	5.672453	1.584680

H	3.125951	4.951875	2.424274	H	-3.433384	8.385511	16.574160
C	2.554044	5.134495	-0.246329	O	-3.774138	14.380936	10.899714
H	3.072986	6.075489	-0.441443	O	-1.331585	12.170764	13.917198
H	2.275190	4.650937	-1.182215	O	-2.926208	12.100203	12.307151
H	1.668378	5.298355	0.367557	O	-1.183939	14.355944	12.071993
H	4.218327	3.913223	-0.129849	O	0.158927	14.469863	14.624448
N	2.878200	-3.132796	3.334389	S	-4.496505	9.876693	13.439457
H	2.708330	-2.389412	2.608876	V	-2.496904	13.432553	10.913749
C	4.340464	-3.375041	3.470580	V	0.041253	13.495405	13.383646
H	4.825993	-2.436701	3.735512	C	4.460279	8.479709	14.281082
H	4.508350	-4.137492	4.234300	C	3.034637	10.445308	13.820425
H	4.712072	-3.705366	2.500423	C	2.422515	11.645862	13.248397
C	2.088260	-4.341518	2.963489	C	2.613235	9.731348	14.920756
H	2.279198	-5.129679	3.694675	H	1.741466	10.022367	15.494008
H	1.034165	-4.066730	2.962420	C	3.432836	8.603411	15.186277
H	2.398583	-4.650798	1.965218	H	3.269739	7.912085	16.005146
H	2.470627	-2.711783	4.178406	O	1.392643	12.101623	13.834415
				O	2.988780	12.135960	12.218565
				O	1.258483	14.354759	12.124260
85				S	4.445907	9.728932	13.089841
1-5, B3LYP/6-311++G(d,p)=-4885.044764				C	-4.574337	8.436975	7.517481
C	4.741061	8.807233	7.186209	C	-3.087764	10.353345	7.993996
C	3.145854	10.592985	7.800896	C	-2.439854	11.532132	8.572985
C	2.437928	11.693499	8.458237	C	-2.690450	9.637076	6.886374
C	2.769663	9.914928	6.662663	H	-1.812194	9.907478	6.312921
H	1.864621	10.161318	6.120977	C	-3.544894	8.537376	6.611805
C	3.686253	8.890529	6.308585	H	-3.404760	7.849533	5.785759
H	3.572013	8.243308	5.446482	O	-1.391043	11.954175	7.997354
O	3.712164	14.510283	10.962198	O	-2.992138	12.033934	9.604611
O	1.341837	12.065770	7.940486	O	-1.311631	14.289185	9.627516
O	2.982403	12.177231	9.501879	S	-4.520140	9.674912	8.719387
O	1.138641	14.342625	9.679422	Cl	0.008772	11.758624	10.913949
O	0.469578	16.690817	11.347002	H	-5.360841	7.694101	7.542294
O	-0.177883	14.291884	7.129210	H	-5.376469	8.055874	14.827309
S	4.636656	9.971923	8.456124	H	5.574694	8.118075	7.152047
V	2.486022	13.508058	10.870376	H	5.223109	7.712756	14.250295
V	-0.067135	13.381110	8.416883	O	-0.564902	16.690647	10.353418
V	-0.031880	15.032589	10.857535	H	-2.457200	17.193694	10.843918
C	-4.578247	8.784573	14.773617	O	-3.388269	17.120522	10.558030
C	-3.058641	10.611802	14.094395	H	-3.669380	16.249100	10.914266
C	-2.390605	11.708770	13.391485	N	2.892812	15.919743	13.402365
C	-2.681606	10.022390	15.280866	H	3.545822	16.184739	12.658613
H	-1.807040	10.347861	15.830854	C	2.236793	17.103253	14.018076
C	-3.554893	8.974036	15.671914	H	1.751453	17.676314	13.227213

H	1.481464	16.735162	14.713652	C	-6.567035	11.240012	11.989141
H	2.982424	17.709994	14.536858	H	-7.228366	10.560887	12.515154
C	3.571888	15.009505	14.365094	O	-2.270379	16.657602	10.388335
H	2.815398	14.625820	15.050712	O	-3.015971	13.341946	13.095694
H	4.012437	14.188771	13.798225	O	-3.076125	14.116623	10.967451
H	4.343940	15.559483	14.907741	O	-1.130370	15.406854	12.632352
H	2.154807	15.339596	12.890437	O	-1.661816	14.568450	15.286539
N	-2.675600	16.043439	8.130818	S	-5.526226	12.701718	10.127711
H	-3.092408	16.570716	8.940156	V	-1.503886	15.303998	10.734478
C	-1.898590	16.958006	7.256999	V	-1.287851	13.924307	13.883479
H	-1.163979	17.473491	7.877590	C	-0.393179	7.272184	14.651023
H	-1.380984	16.364139	6.503830	C	-0.435549	9.731353	14.397971
H	-2.578196	17.678073	6.795348	C	-0.103337	11.134564	14.136222
C	-3.707246	15.232776	7.437322	C	-1.651885	9.217586	14.790090
H	-3.212199	14.601303	6.697044	H	-2.515677	9.850592	14.952804
H	-4.206975	14.611712	8.182668	C	-1.627460	7.805706	14.936649
H	-4.427213	15.895321	6.951879	H	-2.482455	7.210149	15.235791
H	-2.026301	15.373684	8.611093	O	-1.028307	11.984883	14.310745
				O	1.091098	11.374259	13.766137
				O	0.645573	14.167661	13.814891
85, $\nu^{\neq} = 712.54\ i\text{cm}^{-1}$				S	0.757268	8.476604	14.195996
1-TS1D, B3LYP/6-311++G(d,p)=-4884.994739				C	-1.628580	12.342603	4.993190
C	4.122455	8.633040	8.851187	C	-0.605510	13.468371	6.937709
C	3.410276	10.862057	9.639110	C	-0.362899	14.158037	8.200123
C	2.961439	11.998774	10.435966	C	0.332966	13.002518	6.041412
C	3.624153	10.824996	8.277525	H	1.396151	13.132419	6.202386
H	3.483680	11.696253	7.649644	C	-0.254965	12.356825	4.923930
C	4.034479	9.545045	7.825365	H	0.308055	11.921903	4.106200
H	4.254041	9.306141	6.791192	O	0.868763	14.354429	8.511080
O	3.152708	13.162363	14.193422	O	-1.355396	14.518243	8.885735
O	2.747904	13.089578	9.798281	O	0.427581	15.807697	10.710544
O	2.823054	11.833768	11.680787	S	-2.229098	13.111848	6.415783
O	2.186823	14.586466	11.923122	Cl	-0.213890	12.766875	11.188311
O	1.490506	16.799889	13.738688	H	-2.319838	11.915348	4.278593
O	2.875149	15.793651	9.613662	H	-7.538791	11.304066	10.007732
S	3.707474	9.313706	10.381078	H	4.409133	7.591716	8.784205
V	2.021034	12.996492	13.094200	H	-0.102023	6.230340	14.680208
V	1.825226	14.762434	10.136314	O	0.194275	18.109270	12.329906
V	0.764903	15.672507	12.665491	H	1.140994	17.696235	13.187214
C	-6.748966	11.614628	10.679134	O	0.528704	18.597041	11.001259
C	-4.748951	12.662026	11.686932	H	0.537698	17.741071	10.518447
C	-3.525730	13.429719	11.935814	N	-2.363396	18.374236	12.515857
C	-5.417788	11.840706	12.567170	H	-1.272185	18.316281	12.508223
H	-5.075427	11.689531	13.583687	C	-2.781735	19.741553	12.138922

H	-2.320474	19.985084	11.180684	H	-5.349743	-1.485823	0.501658
H	-3.870855	19.793362	12.058696	C	-6.379289	-1.877581	-1.437200
H	-2.433205	20.443936	12.899692	H	-7.174889	-2.539596	-1.114681
C	-2.888533	17.880933	13.810250	O	-1.492023	3.343790	-1.753575
H	-3.980999	17.848376	13.780694	O	-3.198896	0.109988	0.602636
H	-2.487348	16.881512	13.981812	O	-2.661949	0.897247	-1.454088
H	-2.563769	18.556872	14.605502	O	-1.175811	2.093026	0.697608
H	-2.601408	17.712335	11.754139	O	-2.633055	1.527382	2.973153
N	1.618278	14.631687	16.194848	S	-4.840358	-0.438343	-2.935434
H	2.625963	14.649190	16.011458	V	-0.985187	1.933212	-1.235796
C	1.145946	15.896939	16.816742	V	-1.800879	0.702895	1.906732
H	1.441791	16.718512	16.164104	C	-1.657292	-5.833738	3.611032
H	0.057360	15.847336	16.871560	C	-1.466832	-3.440554	3.018289
H	1.580672	16.000753	17.813668	C	-0.988422	-2.109157	2.635102
C	1.260603	13.393620	16.939648	C	-2.764682	-3.821154	3.276704
H	0.172160	13.325107	16.967825	H	-3.589724	-3.121793	3.217392
H	1.675243	12.543822	16.396847	C	-2.874297	-5.194955	3.618163
H	1.671575	13.441903	17.950476	H	-3.808891	-5.689487	3.857467
H	1.191148	14.541004	15.224568	O	-1.856640	-1.195794	2.511832
				O	0.264757	-1.988547	2.445224
				O	0.076077	0.834451	2.326991
85				S	-0.359623	-4.775356	3.189711
1-3D, B3LYP/6-311++G(d,p)=-4885.007189				C	0.457227	-1.099128	-6.773949
C	3.872962	-5.146628	-1.734960	C	0.892215	0.028869	-4.621283
C	3.411862	-2.829222	-1.019903	C	0.770513	0.727316	-3.345956
C	2.976478	-1.637299	-0.300483	C	2.039629	-0.474774	-5.196808
C	3.962027	-2.894213	-2.282734	H	3.011310	-0.368528	-4.730288
H	4.150079	-2.006862	-2.874339	C	1.789851	-1.121589	-6.433915
C	4.228135	-4.225421	-2.692771	H	2.556393	-1.582849	-7.045908
H	4.658502	-4.493187	-3.650858	O	1.861948	0.886285	-2.682389
O	2.433385	-0.469890	3.267130	O	-0.365459	1.129322	-2.985939
O	3.168812	-0.512773	-0.899958	O	0.896533	2.358037	-0.680790
O	2.465217	-1.775370	0.839360	S	-0.513862	-0.293012	-5.597994
O	2.159709	1.072519	0.973891	Cl	-0.068111	-0.603687	-0.454004
O	1.587814	2.976520	2.805466	H	-0.004335	-1.519059	-7.658054
O	3.575858	2.155871	-1.008058	H	-6.789192	-1.770904	-3.603989
S	3.206263	-4.412851	-0.323257	H	3.965667	-6.223387	-1.790257
V	1.439867	-0.469697	2.014288	H	-1.456833	-6.874219	3.830736
V	2.325696	1.222440	-0.841010	O	0.498659	4.233595	1.233170
V	0.666609	2.324770	1.276684	H	1.563227	3.949869	2.787334
C	-6.197002	-1.489552	-2.743053	O	-0.046489	4.925686	0.083606
C	-4.506353	-0.511290	-1.226366	H	0.170393	4.323851	-0.659825
C	-3.372605	0.216358	-0.647477	N	-2.539640	4.311157	1.075463
C	-5.407877	-1.316434	-0.566647	H	-1.839651	4.858011	0.538417

C	-3.848916	4.252349	0.383026	C	-5.397674	19.942635	17.654701
H	-3.672575	3.916281	-0.639505	H	-4.688920	19.717277	18.442230
H	-4.486543	3.539102	0.909439	C	-6.711549	20.444487	17.848767
H	-4.310970	5.242468	0.385786	H	-7.142857	20.661004	18.819523
C	-2.583712	4.765531	2.487883	O	-2.119461	19.564128	12.381126
H	-3.151344	4.037467	3.068169	O	-2.920757	18.941329	16.578665
H	-1.557306	4.804483	2.853556	O	-3.791256	19.127734	14.495773
H	-3.043781	5.755498	2.537696	O	-1.016464	18.238299	14.532286
H	-2.092182	3.354841	1.033547	O	-0.159434	18.965547	17.043061
N	3.912757	1.810624	3.224281	S	-6.431686	20.177971	15.291973
H	3.018145	2.363938	3.020723	V	-2.515751	18.275655	13.218485
C	4.310945	2.036384	4.632283	V	-1.207373	17.929359	16.461194
H	3.470431	1.759659	5.270410	C	-3.765582	14.203335	21.483073
H	5.179742	1.419468	4.873659	C	-2.720580	15.351484	19.558696
H	4.555735	3.091669	4.774036	C	-2.062518	15.678208	18.290551
C	4.953848	2.117838	2.215545	C	-3.175337	16.229703	20.516928
H	5.818314	1.468125	2.372916	H	-3.071357	17.302276	20.407045
H	4.533441	1.955458	1.223496	C	-3.774161	15.570784	21.622731
H	5.255222	3.162888	2.321171	H	-4.193334	16.082501	22.481647
H	3.574044	0.830786	3.132053	O	-1.902007	16.906497	18.024257
				O	-1.720305	14.691600	17.560641
				O	-0.274174	16.366858	15.825749
85, $\nu^{\neq} = 658.94$ *i*cm^{-1}				S	-3.029794	13.695795	20.005931
1-TS2D, B3LYP/6-311++G(d,p)=-4884.974982				C	-8.062952	16.799308	10.376097
C	-5.425177	10.065411	15.595833	C	-5.763799	16.352220	11.168359
C	-3.923495	11.770640	14.622359	C	-4.427406	16.446336	11.763797
C	-2.896458	12.791772	14.400715	C	-6.335603	15.259266	10.556312
C	-4.856773	11.309623	13.720409	H	-5.807735	14.319244	10.451556
H	-4.905522	11.682942	12.704758	C	-7.655338	15.515969	10.099925
C	-5.718410	10.329254	14.278895	H	-8.276134	14.786453	9.592213
H	-6.521010	9.844002	13.735203	O	-3.711244	15.396441	11.727047
O	0.450029	13.642305	16.093982	O	-4.109650	17.565283	12.273006
O	-2.834558	13.302204	13.239856	O	-1.451011	16.780610	12.578492
O	-2.142925	13.065725	15.387082	S	-6.849570	17.714985	11.194828
O	-0.535030	14.901526	13.854990	Cl	-3.212997	16.023174	14.977108
O	1.607976	16.612107	14.054085	H	-9.016888	17.253363	10.141776
O	-1.133949	14.260343	11.248681	H	-8.393161	20.985559	16.524535
S	-4.100597	11.006917	16.178968	H	-5.925215	9.368886	16.256067
V	-0.845714	14.529581	15.806192	H	-4.156916	13.467231	22.173051
V	-1.937065	14.901930	12.451245	O	0.275939	17.603635	12.276407
V	-0.060402	16.672317	13.980940	H	2.054190	17.392542	13.078646
C	-7.383385	20.621729	16.662614	O	1.919551	18.133878	12.265289
C	-5.094867	19.750223	16.325031	H	2.132110	17.710967	11.414760
C	-3.846652	19.230721	15.760020	N	-0.057122	20.603618	14.043552

H	-0.238139	20.700703	13.039453	C	-2.812523	12.166122	13.283601
C	-0.958932	21.504787	14.811606	C	-3.479723	9.966129	14.386177
H	-1.979488	21.322143	14.474569	H	-2.698355	9.997203	15.135701
H	-0.863283	21.252249	15.868515	C	-4.437904	8.929448	14.240577
H	-0.676113	22.544719	14.632773	H	-4.489045	8.053956	14.877739
C	1.384431	20.732226	14.374982	O	-3.406279	15.632566	11.697703
H	1.511540	20.435963	15.417738	O	-1.866385	12.334143	14.117014
H	1.944263	20.060189	13.723986	O	-3.130831	12.944066	12.329169
H	1.707525	21.765418	14.226350	O	-1.183159	14.820384	13.056615
H	-0.368444	19.601726	14.247098	O	-0.437205	14.264544	15.638540
N	1.361527	13.127367	13.551762	S	-4.952233	10.629503	12.360737
H	0.659356	13.913167	13.478308	V	-2.286182	14.530727	11.462599
C	2.619777	13.510020	12.869695	V	-0.294408	13.553383	14.223166
H	2.967080	14.445900	13.310239	C	3.075549	7.752892	14.714208
H	3.364192	12.721156	12.998824	C	2.081177	9.997770	14.431802
H	2.407097	13.654536	11.808425	C	1.752671	11.354067	13.988114
C	0.702050	11.890601	13.054781	C	1.451285	9.258059	15.408615
H	1.399084	11.052365	13.119517	H	0.610812	9.646752	15.970707
H	-0.172017	11.706107	13.680337	C	2.022924	7.969204	15.571851
H	0.382222	12.059082	12.025500	H	1.672510	7.233940	16.287246
H	1.474752	13.079061	14.579336	O	0.782492	11.932462	14.576949
				O	2.459789	11.842634	13.057042
				O	1.188561	14.485199	13.353079

85, $\nu^{\neq} = 811.06\ i\text{cm}^{-1}$

1-TS1F, B3LYP/6-311++G(d,p)=-4885.000742

C	4.599532	9.812177	7.347550	S	3.386835	9.110163	13.694404
C	3.224986	11.622755	8.320021	C	-4.463921	11.402804	6.344610
C	2.580297	12.587477	9.214724	C	-2.812213	12.720296	7.628200
C	3.022147	11.471881	6.966242	C	-2.099974	13.484982	8.653337
H	2.327759	12.096157	6.417301	C	-2.354641	12.371338	6.376895
C	3.812007	10.432994	6.407475	H	-1.371040	12.657999	6.025350
H	3.799344	10.156171	5.359423	C	-3.303465	11.616057	5.639272
O	3.790605	14.173985	12.545143	H	-3.136938	11.245825	4.634142
O	1.720269	13.362987	8.697103	O	-0.922525	13.860429	8.382958
O	2.933811	12.552620	10.437520	O	-2.728689	13.699142	9.742138
O	1.705906	15.079054	10.927635	O	-0.722674	15.504347	10.733002
O	-0.172731	17.173793	12.793841	S	-4.421798	12.116492	7.916071
O	0.845765	16.031300	8.405903	Cl	-0.087511	12.529884	11.347014
S	4.393652	10.480613	8.926111	H	-5.342517	10.860365	6.020759
V	2.416251	13.566239	12.050911	H	-6.112399	8.527133	12.858967
V	0.533080	14.816079	9.344274	H	5.290557	8.993841	7.193063
V	0.256284	15.725872	12.236847	H	3.682406	6.861204	14.626657
C	-5.296788	9.156111	13.190990	O	2.302517	16.802907	12.297487
C	-3.629829	10.962505	13.446305	O	2.144647	18.207709	11.994302
				H	1.187835	18.309185	12.202538
				H	2.263809	16.012730	11.279443

N	-2.814720	16.392381	14.352475	C	-2.834639	-2.544708	2.316592
H	-2.041210	15.823105	13.898629	C	-2.278624	-1.239755	1.949050
C	-2.225904	17.409282	15.257897	C	-2.370224	-3.415142	3.278059
H	-1.560232	18.039904	14.668320	H	-1.502720	-3.188570	3.885846
H	-3.021573	18.000281	15.717216	C	-3.139776	-4.605448	3.354904
H	-1.653953	16.880848	16.022604	H	-2.937703	-5.417351	4.044232
C	-3.735907	15.423236	15.007357	O	-3.707515	1.931943	0.244729
H	-4.552542	15.963926	15.490546	O	-1.262395	-0.846439	2.603205
H	-4.123034	14.757341	14.235914	O	-2.874515	-0.615788	1.013746
H	-3.160844	14.852906	15.738213	O	-1.227587	1.570206	1.305366
H	-3.280386	16.813900	13.540337	O	-0.026922	1.465918	3.761860
N	2.899273	15.975228	14.758361	S	-4.224904	-3.187220	1.484357
H	3.050269	16.457792	13.840475	V	-2.453614	1.010447	-0.066697
C	2.063312	16.842622	15.625785	V	0.043387	0.655140	2.392325
H	1.202602	17.167030	15.039966	C	4.316324	-4.530459	2.851412
H	1.726676	16.265135	16.488490	C	2.963886	-2.483331	2.555086
H	2.649229	17.707148	15.945328	C	2.368090	-1.239973	2.063189
C	4.161054	15.488673	15.364736	C	2.610063	-3.193756	3.681117
H	3.924610	14.908998	16.259958	H	1.817290	-2.864414	4.341838
H	4.660935	14.860678	14.627507	C	3.387697	-4.368721	3.852359
H	4.785802	16.344416	15.630462	H	3.266415	-5.064500	4.674777
H	2.301981	15.181965	14.426267	O	1.422005	-0.737228	2.742507
				O	2.846165	-0.758702	0.989392
				O	1.169603	1.714136	1.200414
85				S	4.259221	-3.259173	1.685293
1-3F, B3LYP/6-311++G(d,p)=-4885.013417				C	-4.897163	-2.977273	-4.419589
C	4.480377	-3.231832	-4.588397	C	-3.280163	-1.306582	-3.579921
C	2.969049	-1.505495	-3.666418	C	-2.540900	-0.334006	-2.773279
C	2.302885	-0.511318	-2.819917	C	-2.970097	-1.754963	-4.844589
C	2.598992	-1.914994	-4.927980	H	-2.102480	-1.395304	-5.384158
H	1.732226	-1.505823	-5.432472	C	-3.899454	-2.713187	-5.327567
C	3.467301	-2.905415	-5.458062	H	-3.834108	-3.187060	-6.300356
H	3.348737	-3.357354	-6.436295	O	-1.480764	0.148428	-3.273680
O	3.703115	1.673149	0.113225	O	-3.017848	-0.058157	-1.627820
O	1.251698	0.024969	-3.286732	O	-1.164888	2.143730	-1.113768
O	2.841002	-0.283764	-1.687196	S	-4.723070	-2.065634	-2.963799
O	1.337522	2.025247	-1.333502	Cl	0.028221	-0.635584	-0.446218
O	-0.932887	4.004082	0.888453	H	-5.726442	-3.663404	-4.531738
O	-0.030439	2.483636	-3.693184	H	-4.904707	-5.400843	2.293470
S	4.394587	-2.341055	-3.111583	H	5.272778	-3.953202	-4.739386
V	2.372928	0.821975	-0.107528	H	5.029639	-5.336225	2.737522
V	-0.065667	1.358930	-2.599834	O	1.274576	4.081025	-0.137488
V	-0.127414	2.773574	0.224850	O	1.135477	5.404419	0.425499
C	-4.173354	-4.618404	2.448371	H	0.171122	5.382648	0.638914

H	1.838982	2.790010	-1.664796	C	-3.448866	11.259957	14.086927
N	-2.908335	2.866321	2.825981	C	-2.424992	12.254879	13.759077
H	-2.124974	2.421181	2.255102	C	-3.411019	10.318771	15.091875
C	-2.357261	3.940171	3.688772	H	-2.567383	10.232258	15.765771
H	-1.881085	4.676766	3.042588	C	-4.577234	9.510323	15.127931
H	-3.161953	4.392363	4.273578	H	-4.743151	8.713570	15.844052
H	-1.610498	3.487157	4.342313	O	-2.788696	15.793835	11.994337
C	-3.592038	1.768464	3.560999	O	-1.363073	12.240480	14.454865
H	-4.411083	2.179960	4.155124	O	-2.683594	13.036117	12.785564
H	-3.971712	1.057531	2.827362	O	-0.801162	14.777592	13.666477
H	-2.855058	1.284960	4.203738	O	0.499223	13.850953	15.971263
H	-3.529391	3.234504	2.097910	S	-4.925716	11.158905	13.166913
N	3.116360	3.691715	1.838451	V	-1.739329	14.587044	12.020810
H	2.374693	3.772627	1.103205	V	0.251786	13.401428	14.469894
C	2.504566	3.815740	3.185564	C	3.531364	7.542507	13.727565
H	1.741383	3.044799	3.295585	C	2.564373	9.805622	13.956291
H	3.280302	3.695037	3.945292	C	2.268294	11.235363	13.846164
H	2.054455	4.807082	3.262417	C	1.855852	8.853826	14.655737
C	4.176550	4.684512	1.533774	H	0.969663	9.103262	15.226558
H	4.970426	4.610998	2.280168	C	2.412099	7.554244	14.525798
H	4.571324	4.460863	0.542044	H	2.002932	6.667537	14.996424
H	3.730311	5.679459	1.542120	O	1.252750	11.669124	14.466159
H	3.476428	2.741645	1.661615	O	3.064696	11.934562	13.145598
				O	1.683505	14.512259	13.557550
				S	3.924846	9.109287	13.118450
85				C	-3.782559	11.340287	6.861021
1-3G, B3LYP/6-311++G(d,p)=-4885.021061				C	-2.274897	12.839900	8.120908
C	5.031438	10.226728	7.271160	C	-1.634460	13.669937	9.143506
C	3.644606	11.928260	8.409039	C	-1.805622	12.556653	6.857230
C	3.012209	12.814038	9.389781	H	-0.868619	12.957716	6.490406
C	3.381721	11.845622	7.059592	C	-2.672148	11.696450	6.132958
H	2.639635	12.472008	6.579915	H	-2.483211	11.352837	5.122304
C	4.178957	10.870007	6.405671	O	-0.537276	14.227919	8.834995
H	4.125297	10.651937	5.345129	O	-2.232983	13.781226	10.255395
O	4.352909	14.290720	12.898621	O	-0.094874	15.660053	11.389857
O	2.091006	13.579169	8.957973	S	-3.791090	12.041690	8.438626
O	3.426959	12.712846	10.591329	Cl	0.390724	12.715848	11.549510
O	2.591689	15.150857	10.981019	H	-4.595160	10.695953	6.551858
O	1.106022	16.360815	8.999805	H	-6.442206	9.397911	13.951567
S	4.878542	10.796556	8.893577	H	5.741691	9.444338	7.037821
V	3.023016	13.717346	12.252760	H	4.142675	6.690125	13.461456
V	1.015761	15.013749	9.820543	O	1.893946	17.049621	12.714818
V	0.715854	15.987112	12.980834	H	2.693503	16.037078	11.378079
C	-5.479220	9.850791	14.148032	O	-0.087799	17.215375	14.058095

O	-1.273870	16.961985	14.805910	V	0.428689	15.660402	12.394686
H	-1.427420	16.001719	14.577270	C	-5.228681	9.083585	13.039795
N	3.399476	15.173359	15.461211	C	-3.556832	10.874857	13.366780
H	4.204038	15.505952	14.921472	C	-2.732509	12.080749	13.249602
C	2.793469	16.256128	16.284355	C	-3.426489	9.854473	14.282948
H	2.541309	17.089038	15.625612	H	-2.657023	9.863208	15.045259
H	1.881499	15.857750	16.730856	C	-4.387306	8.826332	14.096190
H	3.500780	16.571714	17.054201	H	-4.452343	7.935364	14.710325
C	3.770573	13.939749	16.209833	O	-3.307707	15.606400	11.782438
H	2.859836	13.535720	16.652696	O	-1.801960	12.220888	14.104348
H	4.187550	13.229689	15.494626	O	-3.033160	12.883059	12.309711
H	4.504759	14.188821	16.979039	O	-1.117128	14.726083	13.136024
H	2.698399	14.902505	14.715541	O	-0.437467	14.102214	15.715947
N	-1.516546	17.769049	10.553225	S	-4.863920	10.576410	12.253103
H	-2.274793	17.280669	11.072481	V	-2.178347	14.515014	11.540224
C	-1.162300	19.046527	11.227172	V	-0.243726	13.453386	14.279867
H	-0.933407	18.827069	12.271873	C	3.207268	7.682961	14.761366
H	-0.284451	19.468989	10.734995	C	2.180841	9.915589	14.494134
H	-2.005881	19.735987	11.156444	C	1.844646	11.277769	14.074584
C	-1.845850	17.863271	9.107697	C	1.518000	9.134275	15.414756
H	-0.973856	18.242922	8.574667	H	0.642103	9.489533	15.943888
H	-2.075699	16.859783	8.747369	C	2.108066	7.852592	15.569520
H	-2.704761	18.524232	8.975546	H	1.737421	7.089393	16.244340
H	-0.734787	17.089992	10.680746	O	0.830042	11.816017	14.614659
				O	2.596953	11.809559	13.199740
				O	1.284948	14.428677	13.474404
85, $\nu^{\neq} = 569.79$ *i*cm^{-1}				S	3.541134	9.076872	13.799491
1-TS2F, B3LYP/6-311++G(d,p)=-4884.98836				C	-4.256737	11.710542	6.177898
C	4.831065	9.774461	7.610402	C	-2.610076	12.891998	7.593662
C	3.436616	11.589701	8.544843	C	-1.913173	13.572269	8.687205
C	2.782002	12.565738	9.419881	C	-2.117928	12.597402	6.341558
C	3.224239	11.397983	7.197647	H	-1.112296	12.866772	6.042592
H	2.513014	11.993833	6.638806	C	-3.063721	11.920158	5.527990
C	4.025589	10.356461	6.660657	H	-2.872155	11.600948	4.509861
H	4.007226	10.049442	5.621129	O	-0.713679	13.926632	8.475093
O	3.932630	14.215224	12.806064	O	-2.566933	13.742996	9.764352
O	1.907776	13.315859	8.888255	O	-0.583287	15.500273	10.894564
O	3.148033	12.564430	10.641030	S	-4.249177	12.332605	7.788338
O	1.848519	14.956279	11.146707	Cl	0.053075	12.470844	11.391216
O	0.066725	16.967467	13.345969	H	-5.140707	11.219682	5.792272
O	1.169966	16.033398	8.750328	H	-6.042046	8.467486	12.679330
S	4.627343	10.482129	9.171985	H	5.533012	8.962491	7.472393
V	2.581355	13.550141	12.253913	H	3.836626	6.806478	14.679268
V	0.713853	14.757812	9.569485	O	1.555023	17.245170	12.127092

O	2.815744	17.122380	10.953134	V	0.710217	16.168414	13.250213
H	2.308577	17.441474	10.175941	C	-6.183965	11.161450	15.146068
H	2.600962	16.057797	10.924957	C	-4.008930	12.313202	14.915013
N	-2.751118	16.201375	14.528652	C	-2.896639	13.166877	14.493643
H	-1.973269	15.662274	14.036379	C	-4.013834	11.390174	15.937353
C	-2.166870	17.126184	15.531523	H	-3.141249	11.212456	16.554012
H	-1.473006	17.788959	15.014563	C	-5.263164	10.729844	16.071024
H	-2.964595	17.690214	16.020914	H	-5.472895	9.970463	16.815630
H	-1.620244	16.522046	16.256998	O	-2.846791	16.664496	12.522930
C	-3.695538	15.193342	15.082029	O	-1.796603	13.026733	15.107297
H	-4.514633	15.702052	15.595385	O	-3.130611	13.967945	13.528201
H	-4.076646	14.598971	14.251499	O	-0.889373	15.436770	14.090042
H	-3.140290	14.557537	15.772787	O	0.223136	14.468377	16.452923
H	-3.199835	16.700956	13.753250	S	-5.547675	12.377251	14.098510
N	3.326848	16.546535	14.149036	V	-2.043689	15.284473	12.555360
H	3.572004	15.612020	13.743760	V	-0.033512	13.938430	15.000315
C	4.529083	17.416186	14.099758	C	2.519434	7.690063	14.964752
H	4.859610	17.480730	13.062303	C	1.799511	10.052647	14.840894
H	4.268222	18.409515	14.470438	C	1.628470	11.464181	14.486848
H	5.314747	16.977987	14.718146	C	1.108674	9.337374	15.792959
C	2.729787	16.364789	15.499934	H	0.337704	9.791505	16.403387
H	2.421679	17.339254	15.883699	C	1.522837	7.981034	15.865283
H	1.869750	15.702671	15.403396	H	1.103460	7.253022	16.550376
H	3.478462	15.919457	16.158406	O	0.733341	12.110618	15.106816
H	2.609553	16.929092	13.491237	O	2.390036	11.924049	13.581230
				O	1.500414	14.736546	13.870361
				S	2.970390	9.060289	14.015179

85, $\nu^{\neq} = 251.80\ i\text{cm}^{-1}$

1-TS2G, B3LYP/6-311++G(d,p)=-4884.986848

C	3.414697	9.280136	7.807188	C	-5.086904	11.917096	8.052083
C	2.479703	11.316890	8.851725	C	-3.206369	13.231324	8.971559
C	2.139229	12.411885	9.767313	C	-2.325455	14.041736	9.815784
C	2.043810	11.136594	7.556986	C	-2.918429	12.683910	7.740848
H	1.357723	11.826572	7.080759	H	-1.958217	12.827171	7.260426
C	2.581343	9.967317	6.957019	C	-3.998889	11.930481	7.211639
H	2.359588	9.645251	5.945991	H	-3.973959	11.418371	6.256453
O	4.081835	13.925471	12.766771	O	-1.165706	14.296452	9.375591
O	1.354565	13.306283	9.315533	O	-2.802581	14.437100	10.924958
O	2.689181	12.378589	10.914737	O	-0.316682	15.886665	11.736989
O	2.165515	14.986729	11.234911	S	-4.814369	12.816898	9.499831
O	0.818508	16.156415	9.191360	Cl	-0.234690	12.947522	12.116114
S	3.555596	10.039399	9.351754	H	-6.034622	11.418587	7.895936
V	2.553666	13.592770	12.522818	H	-7.205630	10.825537	15.025998
V	0.563844	14.937996	10.180138	H	3.947594	8.359730	7.607390
				H	3.011798	6.738937	14.809897
				O	1.917977	17.115616	12.438070

H	2.242822	16.330926	11.805873	V	2.454171	13.632919	12.424783
O	0.321964	17.615839	14.238347	V	0.447313	14.938933	9.848680
O	-0.670448	17.666570	15.246666	V	0.261820	15.557569	12.643449
H	-1.106807	16.780929	15.102168	C	-4.984548	8.827044	13.639500
N	4.381720	14.929893	9.995875	C	-3.415985	10.719326	13.896483
H	3.366795	14.923222	10.462296	C	-2.668707	11.968757	13.741285
C	5.081074	16.119783	10.543526	C	-3.194143	9.718208	14.816994
H	5.104775	16.020167	11.629294	H	-2.402805	9.781452	15.553921
H	6.094691	16.182641	10.139520	C	-4.095792	8.632149	14.670422
H	4.512113	17.009434	10.266041	H	-4.087078	7.745403	15.293870
C	4.261304	14.899768	8.518187	O	-3.503154	15.439846	12.323880
H	5.247215	15.000536	8.056849	O	-1.720991	12.174947	14.563828
H	3.799463	13.958311	8.219541	O	-3.041252	12.740834	12.801989
H	3.611127	15.722126	8.213944	O	-1.166129	14.723584	13.556715
H	4.826881	14.080906	10.353526	O	-0.339353	14.102783	16.113173
N	-1.228467	18.267165	10.936203	S	-4.737401	10.330450	12.828584
H	-0.641514	17.411911	11.076383	V	-2.332837	14.414296	11.991448
C	-1.704467	18.286822	9.528328	V	-0.194737	13.447866	14.675681
H	-2.255147	17.362994	9.346218	C	3.437199	7.781391	14.870495
H	-2.352209	19.152827	9.377780	C	2.323799	9.979935	14.679792
H	-0.837501	18.323533	8.868601	C	1.912997	11.328273	14.282776
C	-0.474393	19.467325	11.384992	C	1.773922	9.190983	15.666237
H	-1.112874	20.348191	11.291525	H	0.941875	9.526975	16.273033
H	-0.175890	19.313256	12.422918	C	2.413856	7.928851	15.776676
H	0.414249	19.571551	10.760789	H	2.131277	7.163524	16.490526
H	-2.020313	18.059541	11.573522	O	0.941647	11.845057	14.921665
				O	2.559815	11.867057	13.332918
				O	1.269747	14.421847	13.798974
91				S	3.637828	9.172508	13.868554
2-2, B3LYP/6-311++G(d,p)=-5000.835715				C	-4.506746	11.624237	6.676845
C	4.888240	10.466549	7.420308	C	-2.859515	12.860919	8.043995
C	3.329653	12.017683	8.550051	C	-2.144906	13.549584	9.120568
C	2.610013	12.841351	9.523537	C	-2.423303	12.644432	6.755553
C	3.127346	11.961423	7.188789	H	-1.456752	12.991503	6.411255
H	2.361217	12.549062	6.697785	C	-3.369457	11.935496	5.970162
C	4.021833	11.070028	6.540199	H	-3.217743	11.666738	4.931005
H	4.026222	10.883021	5.472475	O	-0.983855	13.981570	8.856861
O	3.878642	14.200197	12.862394	O	-2.754646	13.640875	10.237517
O	1.682049	13.580237	9.081383	O	-0.870824	15.484213	11.226878
O	2.990120	12.750204	10.736184	S	-4.445705	12.187982	8.307394
O	1.624919	15.172785	11.465938	Cl	-0.017495	12.534698	11.730806
O	0.372534	17.034745	13.216060	H	-5.378531	11.090277	6.321983
O	0.743955	16.207221	8.975886	H	-5.770020	8.159055	13.311020
S	4.629207	10.969806	9.051617	H	5.665146	9.748189	7.193664

H	4.082178	6.922659	14.737779	O	4.487433	15.341713	12.465667
O	4.205428	17.219289	12.461952	O	2.120830	12.732755	9.723561
O	3.141680	17.622486	11.555646	O	3.869682	12.937061	11.159168
H	2.598210	16.803249	11.491859	O	1.964968	15.006729	11.322911
H	4.756567	16.626881	11.871704	O	-0.260709	17.007371	13.145492
N	-2.785390	16.236480	14.921252	O	0.315590	14.819037	9.074810
H	-2.027706	15.654378	14.452273	S	5.670701	11.029065	9.805320
C	-2.158953	17.399829	15.596324	V	3.337697	14.252929	12.541364
H	-1.577238	17.951227	14.855935	V	0.668173	13.927087	10.338388
H	-2.931484	18.034397	16.036414	V	0.603344	15.713102	12.817958
H	-1.493183	17.018640	16.372587	C	-1.934844	8.557034	17.025163
C	-3.563862	15.325658	15.802791	C	-0.989009	10.721953	16.298967
H	-4.356765	15.886018	16.302979	C	-0.694732	11.973392	15.597369
H	-3.990513	14.540670	15.176971	C	-0.312195	10.180317	17.369840
H	-2.877045	14.885627	16.527114	H	0.544549	10.671436	17.814895
H	-3.360752	16.515329	14.115292	C	-0.856122	8.937820	17.787917
N	3.117855	16.233575	14.802167	H	-0.466980	8.349111	18.610789
H	3.559242	16.523638	13.889645	O	-2.769907	14.406067	13.422412
C	2.533145	17.433630	15.454536	O	0.281699	12.659928	16.036053
H	1.843594	17.897294	14.750372	O	-1.452288	12.265592	14.618085
H	2.001082	17.122045	16.356368	O	-0.186734	14.713102	14.240387
H	3.339564	18.123167	15.712200	O	1.221920	15.316316	16.523199
C	4.113392	15.512093	15.637798	S	-2.303493	9.699337	15.784679
H	3.624093	15.165894	16.550846	V	-1.404595	13.634798	13.167335
H	4.483365	14.666071	15.060120	V	1.306047	14.232904	15.359322
H	4.930433	16.193178	15.885381	C	6.526266	10.084855	16.266040
H	2.361065	15.563724	14.537250	C	4.767591	11.739326	15.737470
C	4.868803	15.385819	9.579753	C	3.898404	12.721261	15.084147
H	5.164128	14.471503	9.051150	C	4.656378	11.237408	17.015524
H	3.776951	15.468617	9.580248	H	3.868470	11.551924	17.689133
H	5.284832	16.250050	9.058577	C	5.666951	10.288036	17.319791
O	5.407247	15.402445	10.906928	H	5.754792	9.776261	18.271428
H	4.995765	14.681455	11.424352	O	2.932633	13.182657	15.774559
				O	4.179349	13.035283	13.890123
				O	2.145155	15.176235	13.875203
91, $\nu^{\neq} = 1076.95\ i\text{cm}^{-1}$				S	6.119625	11.041653	14.888014
2-TS1, B3LYP/6-311++G(d,p)=-5000.795919				C	-3.303914	8.487959	9.888612
C	5.792014	9.976536	8.442024	C	-2.002824	10.557704	10.255580
C	4.060747	11.500581	9.332861	C	-1.422838	11.787818	10.797463
C	3.295472	12.464580	10.128075	C	-1.687701	9.937340	9.066961
C	3.662161	10.861447	8.179949	H	-0.942442	10.338227	8.390868
H	2.688036	11.030844	7.737674	C	-2.435719	8.749641	8.855478
C	4.656392	9.986988	7.667734	H	-2.336506	8.116042	7.981510
H	4.538707	9.392402	6.768934	O	-0.521302	12.352986	10.110217

O	-1.869756	12.182393	11.922853	C	5.300932	-3.391639	-3.530753
O	-0.472895	14.692294	11.768574	C	3.573740	-1.876643	-2.616717
S	-3.225521	9.680230	11.134825	C	2.841460	-0.847875	-1.872479
Cl	1.271438	12.379042	12.881237	C	3.067708	-2.758445	-3.545650
H	-3.985390	7.652548	9.982040	H	2.020372	-2.762040	-3.821856
H	-2.528818	7.658033	17.125520	C	4.059437	-3.627783	-4.071328
H	6.694933	9.402086	8.281424	H	3.865212	-4.393346	-4.813909
H	7.376588	9.416623	16.227734	O	4.085445	2.503267	-0.247022
O	2.041146	17.119893	12.091798	O	1.593441	-0.766500	-2.090577
O	1.564411	18.376792	11.585628	O	3.528872	-0.137145	-1.067557
H	0.823778	18.085960	10.980701	O	1.507312	1.720512	-0.900746
H	2.183143	16.184669	11.322616	O	-0.389293	3.964493	1.360396
N	-1.939652	16.135111	15.544619	O	-0.431493	1.028345	-2.756363
H	-1.146767	15.656224	15.019272	S	5.283944	-2.109683	-2.374197
C	-1.495244	17.473184	16.009186	V	3.099633	1.326282	0.196034
H	-1.200723	18.051895	15.133789	V	0.129023	0.405032	-1.409132
H	-2.307025	17.963577	16.551651	V	0.329799	2.698249	0.703156
H	-0.632634	17.324779	16.660682	C	-0.930599	-4.255858	5.799823
C	-2.362600	15.204520	16.626319	C	-0.317096	-2.078570	4.803139
H	-3.180676	15.651321	17.195582	C	-0.261621	-0.857743	3.994135
H	-2.684672	14.273104	16.160358	C	0.589169	-2.502050	5.750104
H	-1.499631	15.022168	17.268413	H	1.470993	-1.924220	5.998671
H	-2.675880	16.196561	14.833801	C	0.236039	-3.751501	6.324001
N	3.590073	17.303524	14.376311	H	0.818499	-4.257753	7.085365
H	3.886976	17.504258	13.415782	O	-2.880207	1.295254	2.044711
C	2.712162	18.386754	14.888062	O	0.724819	-0.082386	4.198112
H	1.940308	18.573061	14.140485	O	-1.216623	-0.686792	3.169457
H	2.262182	18.041074	15.820782	O	-0.201495	1.696226	2.347008
H	3.303519	19.288932	15.061509	O	1.452490	2.673287	4.290180
C	4.745947	16.954576	15.238269	S	-1.615978	-3.222975	4.598145
H	4.362702	16.592127	16.194304	V	-1.535383	0.553396	1.633491
H	5.308013	16.166295	14.736722	V	1.467710	1.497503	3.220479
H	5.373123	17.835752	15.392286	C	7.198884	-2.010353	3.829235
H	2.994018	16.431663	14.237706	C	5.211677	-0.611849	3.377453
C	-1.697981	17.332908	10.275869	C	4.157790	0.191051	2.754321
H	-1.907162	16.441614	10.875226	C	5.326152	-0.956527	4.706272
H	-1.924567	18.224698	10.864486	H	4.603984	-0.634599	5.446781
H	-2.323304	17.330852	9.374617	C	6.468046	-1.758557	4.966199
O	-0.313052	17.405982	9.923846	H	6.737381	-2.134482	5.946679
H	-0.060190	16.559030	9.497006	O	3.236746	0.628966	3.506660
				O	4.247739	0.384699	1.501220
				O	1.986507	2.358287	1.497889
91				S	6.510562	-1.277967	2.425911
2-3, B3LYP/6-311++G(d,p)=-5000.807928				C	-3.537135	-5.159428	-0.407433

C	-2.326408	-3.014165	-0.610069	H	-1.811907	5.121980	-2.227031
C	-1.762947	-1.682046	-0.388192	O	-0.749738	3.700336	-3.241587
C	-2.097653	-3.854318	-1.677190	H	-0.721211	2.718571	-3.277194
H	-1.447789	-3.575696	-2.497722				
C	-2.794399	-5.085614	-1.561871				
H	-2.748237	-5.881619	-2.296280	91, $\nu^{\neq} = 374.36\ i\text{cm}^{-1}$			
O	-0.957372	-1.239749	-1.263462	2-TS2, B3LYP/6-311++G(d,p)=-5000.796221			
O	-2.115934	-1.073977	0.668743	C	5.317557	-3.359361	-3.499198
O	-0.842868	1.473855	-0.006634	C	4.073736	-3.612661	-4.026308
S	-3.401065	-3.734587	0.557726	S	5.300404	-2.057960	-2.364296
Cl	1.264599	-0.629557	1.004989	H	6.244204	-3.873711	-3.717916
H	-4.157240	-5.981052	-0.073578	C	3.080160	-2.740590	-3.508120
H	-1.419651	-5.186871	6.055065	H	3.878876	-4.392590	-4.753683
H	6.225980	-3.907844	-3.751840	C	3.587245	-1.839654	-2.598651
H	8.106593	-2.593339	3.744170	H	2.030532	-2.756256	-3.775108
O	0.751874	4.165187	-0.585622	C	2.854237	-0.803811	-1.864200
O	1.458224	3.982105	-1.862788	O	1.604410	-0.731014	-2.074428
H	0.650721	3.988522	-2.477021	O	3.536993	-0.077050	-1.074235
H	1.657989	2.484247	-1.545794	V	0.163991	0.438938	-1.359950
N	-1.738888	3.132424	3.913106	V	3.069432	1.384013	0.180353
H	-1.008288	2.689788	3.277764	O	-0.431741	1.040651	-2.730238
C	-1.371145	4.535432	4.226366	O	1.461306	1.730820	-0.811114
H	-1.286666	5.079233	3.286206	O	-0.916675	-1.223664	-1.219247
H	-2.133424	4.977779	4.872485	O	4.055893	2.571508	-0.254652
H	-0.402071	4.517713	4.726385	O	4.219374	0.425044	1.489438
C	-1.880224	2.247836	5.100931	C	-1.744335	-1.670835	-0.370569
H	-2.637427	2.657810	5.773051	C	4.137110	0.185651	2.732281
H	-2.176149	1.258871	4.751453	C	-2.290470	-3.008712	-0.607986
H	-0.910247	2.194357	5.596528	O	-2.138628	-1.066070	0.675572
H	-2.587559	3.071193	3.339393	C	5.202342	-0.629553	3.322347
N	3.082519	4.966336	0.545259	O	3.215923	0.584540	3.509230
H	2.097055	4.790383	0.218295	C	-2.016773	-3.850191	-1.663035
C	3.094112	5.267667	2.000508	S	-3.398550	-3.735450	0.524016
H	2.625179	4.435138	2.524856	C	5.329899	-1.020316	4.636730
H	4.127997	5.388296	2.331512	S	6.499124	-1.250539	2.338043
H	2.536434	6.190527	2.173915	V	1.458466	1.469268	3.237833
C	3.692886	6.003543	-0.322934	H	-1.339659	-3.568297	-2.460074
H	4.744278	6.127603	-0.055089	C	-2.706156	-5.087669	-1.568076
H	3.598812	5.671782	-1.357108	C	-3.488487	-5.164754	-0.440479
H	3.157005	6.944852	-0.184200	H	4.610335	-0.731714	5.393301
H	3.556118	4.054540	0.365478	C	6.480643	-1.821456	4.859699
C	-1.897955	4.058627	-2.459639	C	7.204812	-2.026537	3.709361
H	-2.816430	3.888647	-3.034597	O	-0.205123	1.695096	2.342820
H	-1.938186	3.489420	-1.525440	O	1.438932	2.635817	4.318259

O	1.992761	2.363773	1.542008	O	0.737212	4.158997	-0.631892
O	0.689464	-0.097994	4.218378	H	1.659778	2.882486	-1.686168
H	-2.626329	-5.885815	-2.297336	O	1.433278	3.874449	-1.912202
H	-4.112266	-5.991064	-0.125552	H	0.367546	3.772877	-2.607983
H	6.760263	-2.229796	5.824276	O	-0.633732	3.537174	-3.139686
H	8.116568	-2.598497	3.596975	C	-1.788777	3.989794	-2.375317
V	-1.557387	0.556513	1.643004	H	-0.633572	2.513775	-3.126756
H	-0.994390	2.710668	3.260220	H	-2.667000	3.881408	-3.014204
V	0.354500	2.656004	0.712759	H	-1.890105	3.397919	-1.464110
H	2.061549	4.798402	0.214344	H	-1.620249	5.037020	-2.129209
C	-0.303510	-0.862651	4.009909				
O	-2.893916	1.317277	2.051168				
O	-0.873563	1.470506	0.007059	82			
N	-1.719068	3.169660	3.890127	2-5, B3LYP/6-311++G(d,p)=-4808.559438			
O	-0.335364	3.976972	1.321228	C	4.694421	8.784323	7.127958
N	3.033035	4.983898	0.575954	C	3.138701	10.601199	7.753105
C	-0.366627	-2.091955	4.805888	C	2.451342	11.709139	8.420987
O	-1.261067	-0.673382	3.192095	C	2.761759	9.954936	6.596888
C	-1.330903	4.570943	4.184279	H	1.872308	10.236396	6.046513
C	-1.872630	2.301905	5.088959	C	3.655705	8.912639	6.236736
H	-2.568105	3.111977	3.316683	H	3.537223	8.285056	5.360757
C	2.994831	5.285231	2.030592	O	3.767910	14.469109	10.950229
C	3.664116	6.025850	-0.269790	O	1.373442	12.119984	7.893012
H	3.521581	4.074739	0.406166	O	2.992722	12.158445	9.480359
C	0.539732	-2.533722	5.744106	O	1.196681	14.362777	9.660182
S	-1.674711	-3.223982	4.591674	O	0.559538	16.734739	11.318119
Cl	1.235454	-0.667075	1.053992	O	-0.132312	14.378238	7.098308
H	-1.229859	5.097002	3.235563	S	4.602073	9.927797	8.418024
H	-2.089761	5.036037	4.818473	V	2.517576	13.497448	10.853052
H	-0.365700	4.544476	4.691410	V	-0.015224	13.452880	8.376602
H	-2.625626	2.729834	5.754693	V	0.036192	15.083442	10.841627
H	-2.180244	1.312438	4.751076	C	-4.712433	8.966319	14.740350
H	-0.903558	2.242483	5.585449	C	-3.130391	10.740597	14.061224
H	2.522917	4.445255	2.539742	C	-2.426866	11.817587	13.360352
H	4.016605	5.419745	2.392553	C	-2.762601	10.123788	15.236322
H	2.419221	6.200173	2.186872	H	-1.868898	10.408458	15.778091
H	4.701526	6.165706	0.041244	C	-3.671634	9.105978	15.627426
H	3.624068	5.688597	-1.306042	H	-3.562074	8.503222	16.521809
H	3.111088	6.961161	-0.159617	O	-3.703448	14.519109	10.749360
H	1.427018	-1.965642	5.995654	O	-1.342812	12.228062	13.875809
C	0.179123	-3.787369	6.304327	O	-2.961858	12.242713	12.287808
C	-0.993142	-4.276584	5.778493	O	-1.134038	14.414544	12.043345
H	0.760682	-4.307209	7.057221	O	0.196319	14.486467	14.603663
H	-1.488196	-5.207012	6.024138	S	-4.603728	10.069189	13.416642

V	-2.467218	13.532868	10.875750	H	-1.736321	17.619354	8.384251
V	0.065237	13.525548	13.353273	H	-1.454330	16.624058	6.936458
C	4.388838	8.426399	14.264463	H	-2.954588	17.608411	7.061910
C	2.998849	10.416785	13.799339	C	-3.549729	14.915144	7.327132
C	2.410143	11.629244	13.225915	H	-2.786177	14.506638	6.663944
C	2.560351	9.708941	14.896669	H	-3.995265	14.115334	7.919541
H	1.691043	10.014426	15.466110	H	-4.316615	15.443674	6.756377
C	3.359399	8.566695	15.164783	H	-2.145432	15.297576	8.802150
H	3.180556	7.877398	15.982122				
O	1.386162	12.101586	13.808365				
O	2.989707	12.110324	12.199629	98			
O	1.310520	14.372622	12.109398	2-6, B3LYP/6-311++G(d,p)= -5478.464389			
S	4.401137	9.677307	13.074674	C	5.703597	-2.963652	-2.135593
C	-4.413309	8.393691	7.610155	C	4.197709	-1.326215	-1.057217
C	-2.994278	10.375914	8.019168	C	3.318846	-0.605478	-0.132068
C	-2.387788	11.595456	8.558020	C	4.511041	-0.984077	-2.353951
C	-2.566062	9.630701	6.942722	H	4.114723	-0.091529	-2.822578
H	-1.692252	9.906990	6.365312	C	5.377120	-1.923431	-2.972927
C	-3.381696	8.493074	6.706874	H	5.739428	-1.837930	-3.991108
H	-3.212806	7.778154	5.909674	O	2.905296	-0.521609	3.728134
O	-1.357068	12.035879	7.962588	O	2.793135	0.466427	-0.558441
O	-2.960128	12.114160	9.569941	O	3.171129	-1.116443	1.024273
O	-1.247969	14.353701	9.594776	O	1.502761	1.002611	1.949301
S	-4.407443	9.678116	8.763750	O	-0.265104	1.712246	4.234094
Cl	0.011578	11.794210	10.890217	O	2.204442	3.041575	0.240019
H	-5.174508	7.626119	7.660041	S	4.960837	-2.819790	-0.583508
H	-5.537913	8.268835	14.796488	V	1.907036	-0.853136	2.538763
H	5.509535	8.073391	7.093025	V	1.364028	1.708352	0.089701
H	5.138646	7.646605	14.236363	V	-0.220121	1.174899	2.518279
O	-0.464626	16.727074	10.316921	C	-5.052709	-3.606098	-2.752338
N	2.964985	15.895271	13.396056	C	-3.856874	-2.580679	-0.847113
H	3.627673	16.157145	12.660096	C	-3.169683	-1.659834	0.062445
C	2.316993	17.082272	14.013054	C	-4.053630	-3.933882	-0.682797
H	1.845136	17.665493	13.221371	H	-3.700570	-4.462340	0.194340
H	1.550527	16.718218	14.698546	C	-4.741662	-4.522732	-1.776168
H	3.064139	17.677554	14.543041	H	-4.991716	-5.575551	-1.841673
C	3.622618	14.969953	14.358659	O	-3.229524	2.217653	0.506754
H	2.854561	14.592832	15.035085	O	-2.715362	-2.151100	1.141614
H	4.055869	14.146150	13.790505	O	-3.102346	-0.444505	-0.304726
H	4.397804	15.504891	14.911963	O	-1.818372	0.429195	2.060666
H	2.221817	15.326573	12.873810	O	-2.482376	-1.552040	3.821268
N	-2.880398	15.860256	8.262058	S	-4.511003	-2.014316	-2.360189
H	-3.540084	16.153306	8.988897	V	-2.065559	1.172402	0.237116
C	-2.215905	17.019101	7.610130	V	-1.488835	-1.476202	2.572615

C	1.972694	-7.247281	2.272317	N	3.320678	2.399891	3.239463
C	0.910955	-5.020172	2.426604	H	2.565229	1.857621	2.742100
C	0.642862	-3.582452	2.502357	C	2.823762	3.792188	3.434067
C	-0.008817	-6.045001	2.395838	H	1.923082	3.750504	4.047386
H	-1.075398	-5.860138	2.434109	H	3.598941	4.392606	3.914925
C	0.600609	-7.324006	2.308839	H	2.563674	4.190108	2.452401
H	0.051835	-8.258229	2.273223	C	4.559973	2.277319	2.420747
O	-0.577816	-3.227066	2.523954	H	5.374203	2.815759	2.910273
O	1.655410	-2.813854	2.525766	H	4.797017	1.216129	2.332017
O	0.106509	-0.589292	3.184874	H	4.346409	2.697479	1.437420
S	2.545070	-5.620272	2.342973	H	3.438271	1.905425	4.128641
C	-1.284337	1.596351	-6.098153	N	-3.916304	0.830254	3.586314
C	-0.536625	1.543505	-3.742452	H	-3.687445	-0.044247	4.089948
C	-0.468987	1.519197	-2.280138	C	-3.822475	2.018183	4.472784
C	0.502322	1.740917	-4.622618	H	-2.831421	2.021548	4.929773
H	1.521537	1.875970	-4.282726	H	-3.945142	2.913444	3.860835
C	0.073941	1.770453	-5.976258	H	-4.601585	1.968920	5.236327
H	0.737269	1.913836	-6.821726	C	-5.186567	0.680847	2.828729
O	0.675295	1.681524	-1.758377	H	-5.281563	1.527120	2.147431
O	-1.562963	1.320544	-1.661366	H	-5.124797	-0.241975	2.250102
O	-0.415428	1.996145	0.810487	H	-6.025666	0.637693	3.526235
S	-2.060555	1.387784	-4.569097	H	-3.123851	0.865043	2.896897
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H	-1.867351	1.569084	-7.009378				
H	-5.568272	-3.786821	-3.686486	98			
H	6.339391	-3.811652	-2.354106	2-TS3, B3LYP/6-311++G(d,p)= -5478.441874			
H	2.677571	-8.065642	2.205274	C	5.915570	11.158494	7.768376
O	-0.468044	2.779708	3.278497	C	4.404344	12.804489	8.826396
C	-0.393837	5.140055	-0.527058	C	3.554531	13.552716	9.757725
C	0.708744	5.347695	-1.370836	C	4.607589	13.055770	7.487867
C	0.584925	5.165044	-2.744728	H	4.132378	13.887766	6.982631
C	-0.636664	4.777512	-3.302307	C	5.476884	12.111667	6.880311
C	-1.727410	4.560019	-2.462891	H	5.761805	12.132148	5.834466
C	-1.613491	4.735338	-1.082192	O	3.401314	13.868908	13.652130
H	1.664999	5.634454	-0.944425	O	2.937495	14.557850	9.291815
H	1.450862	5.321114	-3.382678	O	3.518792	13.131256	10.956842
H	-0.728531	4.621725	-4.372742	O	1.812446	15.224756	11.878268
H	-2.675075	4.225297	-2.874759	O	0.145835	15.968658	14.178193
H	-2.469015	4.521895	-0.455380	O	2.249633	17.149937	10.016783
S	-0.142637	5.415645	1.211317	S	5.276201	11.391211	9.355400
C	-1.800659	5.137802	1.905326	V	2.343661	13.434244	12.538126
H	-2.520923	5.861092	1.511564	V	1.496629	15.752721	9.990558
H	-2.137359	4.119286	1.706146	V	0.111384	15.410650	12.572224
H	-1.697465	5.276228	2.984093	C	-4.947343	9.870124	8.176116

C	-3.606009	11.132866	9.826095	C	0.408781	19.289339	7.715682
C	-2.865105	12.165480	10.558312	C	-0.748132	18.873977	7.053568
C	-3.750040	9.805894	10.164082	C	-1.857975	18.462128	7.792942
H	-3.302648	9.391121	11.059126	C	-1.817336	18.449967	9.185776
C	-4.521138	9.080714	9.217382	H	1.361575	19.602249	9.619886
H	-4.747279	8.023568	9.299072	H	1.281655	19.602092	7.150362
O	-3.091612	16.016061	10.699881	H	-0.780104	18.851286	5.968762
O	-2.309821	11.812561	11.642335	H	-2.752168	18.112677	7.286746
O	-2.855898	13.329267	10.047574	H	-2.665733	18.069316	9.736861
O	-1.477353	14.507476	12.297626	S	-0.482978	18.908461	11.616119
O	-1.838273	12.602684	14.244598	C	-2.208476	18.898705	12.179974
S	-4.414732	11.505955	8.328056	H	-2.754385	19.735540	11.737400
V	-1.875158	15.023088	10.425705	H	-2.672984	17.946286	11.916312
V	-0.986942	12.658575	12.890400	H	-2.164919	19.008910	13.264733
C	2.730199	7.045179	12.536011	N	3.598494	16.629252	13.157777
C	1.568581	9.221961	12.696983	H	2.823471	16.229315	12.560337
C	1.232075	10.647969	12.738419	C	3.095340	17.836628	13.859868
C	0.705860	8.152678	12.788547	H	2.199556	17.555788	14.415038
H	-0.361649	8.286563	12.913871	H	3.870180	18.222794	14.526178
C	1.372686	6.902486	12.697806	H	2.830642	18.582315	13.108612
H	0.873114	5.941606	12.747677	C	4.782722	16.830445	12.283250
O	0.002185	10.943579	12.853059	H	5.605672	17.247843	12.867728
O	2.202628	11.463578	12.641847	H	5.062834	15.859103	11.872616
O	0.594161	13.647303	13.260132	H	4.496608	17.499012	11.470407
S	3.218722	8.700584	12.491170	H	3.766959	15.843074	13.804996
C	-1.707403	15.720847	4.063561	N	-3.335315	14.903432	14.083135
C	-0.725730	15.548836	6.328010	H	-2.967695	14.070311	14.579739
C	-0.511640	15.426099	7.774771	C	-3.222922	16.130805	14.907635
C	0.205362	15.879805	5.370761	H	-2.172650	16.260196	15.175489
H	1.244906	16.052916	5.620404	H	-3.554373	16.981190	14.308969
C	-0.357245	15.977699	4.069628	H	-3.846564	16.033667	15.799171
H	0.209275	16.224325	3.178682	C	-4.677001	14.611584	13.518432
O	0.669750	15.622423	8.190528	H	-4.940973	15.407153	12.820243
O	-1.530210	15.130112	8.475923	H	-4.613444	13.665510	12.978667
O	-0.249927	15.977708	10.766089	H	-5.409120	14.539373	14.325772
S	-2.312887	15.350567	5.639223	H	-2.645859	14.951238	13.283675
Cl	0.325885	12.966476	10.267698				
H	-2.375663	15.718622	3.212422				
H	-5.542954	9.572316	7.323094	189			
H	6.578181	10.326457	7.568949	3-1, B3LYP/6-311++G(d,p)=-10881.6232896			
H	3.469018	6.260541	12.438202	O	3.719804	14.714444	10.860627
O	-0.108648	17.225741	12.938774	O	1.132388	14.521233	9.629934
C	-0.656884	18.872438	9.844583	O	0.005599	16.768244	10.922210
C	0.457398	19.295627	9.107008	O	-0.343005	14.513304	7.178821

V	2.491968	13.713440	10.774717	O	1.176819	12.208340	7.925861
V	-0.152294	13.599138	8.455639	O	4.552777	6.049915	7.800126
V	-0.014629	15.182309	10.923975	O	3.208889	3.678606	7.824382
O	-3.759631	14.806920	10.988232	O	5.639060	7.372819	9.291133
O	-1.177578	14.553480	12.219783	O	2.902687	12.365093	9.391319
O	0.297075	14.514961	14.670937	O	2.602067	2.178023	9.415317
V	-2.556657	13.776377	11.077021	S	-0.260170	2.415546	9.137753
V	0.083993	13.602469	13.396479	S	4.093249	9.781958	8.906178
O	1.280812	14.517927	12.102886	C	-1.519535	3.306214	8.350210
O	-1.326209	14.547555	9.746731	C	-2.907089	3.138304	8.804438
N	2.941000	16.069665	13.359293	C	-1.030625	4.192457	7.406972
H	3.598630	16.327033	12.616699	H	-1.678400	4.849853	6.840010
C	2.249075	17.254873	13.931742	O	-3.801838	3.832001	8.236032
H	1.764621	17.794713	13.116139	O	-3.080463	2.299651	9.747477
H	1.490016	16.888703	14.624588	C	-4.083399	8.387300	13.798132
H	2.970019	17.893884	14.446447	C	-1.261505	3.271132	13.685192
C	3.618062	15.189174	14.351581	C	-2.860669	10.522335	13.765129
H	2.857647	14.818468	15.039979	C	-2.341043	11.839598	13.370538
H	4.064843	14.355659	13.808008	C	-2.689229	3.079671	13.392387
H	4.384145	15.756970	14.884064	C	-4.980232	7.272179	13.463575
H	2.213660	15.475436	12.855560	C	-2.297000	9.609614	14.638555
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C	-2.232930	17.298567	7.906717	H	-2.729184	7.513834	15.244493
H	-1.735867	17.829865	8.720348	C	-0.683681	4.175695	14.557883
H	-1.482824	16.913399	7.214428	H	-1.274007	4.815682	15.202116
H	-2.939747	17.952099	7.390655	O	-1.279212	12.246362	13.929846
C	-3.648523	15.263111	7.494048	O	-4.806799	6.173572	14.070082
H	-2.897292	14.872894	6.806357	O	-3.523751	3.768504	14.051901
H	-4.114067	14.441785	8.040425	O	-5.859580	7.519447	12.575612
H	-4.401683	15.846733	6.960240	O	-3.000665	12.442261	12.463952
H	-2.236616	15.522191	8.988419	O	-2.954244	2.249780	12.464330
C	3.885026	8.281689	8.066381	S	-0.086754	2.418019	12.741384
C	0.934983	3.237564	8.191916	S	-4.254773	9.890471	12.955188
C	2.715373	10.446308	8.094455	C	1.193914	3.279893	13.526626
C	2.228365	11.776841	8.486095	C	2.576873	3.076999	13.072715
C	2.357606	3.011993	8.485307	C	0.726761	4.180059	14.467688
C	4.753740	7.145367	8.403813	H	1.390333	4.822976	15.032991
C	2.129558	9.545917	7.222805	O	3.488602	3.749479	13.639594
H	1.238984	9.786177	6.655115	O	2.729241	2.232412	12.131338
C	2.802024	8.302939	7.205656	C	4.210976	8.285395	13.397135
H	2.510041	7.438824	6.621465	C	2.973405	10.411916	13.428144
C	0.379300	4.153681	7.316920	C	2.426993	11.729186	13.073225
H	0.984982	4.777537	6.671117	C	5.060945	7.158607	12.986226

C	2.500639	9.517048	14.371489	H	7.752744	-0.414847	14.191827
H	1.660163	9.745250	15.015505	C	5.085015	0.370437	14.288738
C	3.210724	8.295201	14.352680	H	5.197869	1.244181	14.931730
H	3.000382	7.436705	14.978661	H	4.096959	0.374474	13.826573
O	1.438237	12.156452	13.740015	H	5.243175	-0.552073	14.851589
O	4.929378	6.062933	13.609109	H	5.901441	1.377357	12.671629
O	5.838239	7.385297	12.004045	N	8.688322	5.319203	7.876249
O	3.006849	12.324502	12.107733	H	9.307545	5.779521	8.550685
S	4.292336	9.769182	12.507981	C	9.296077	4.087564	7.306230
C	-4.409662	8.386031	8.467840	H	9.574228	3.430105	8.131891
C	-3.119729	10.481063	8.431768	H	8.535760	3.599149	6.694976
C	-2.540868	11.785247	8.783450	H	10.170397	4.347971	6.705600
C	-5.287310	7.281722	8.881509	C	8.204851	6.310194	6.875007
C	-2.669590	9.572651	7.490297	H	7.436299	5.825046	6.272066
H	-1.823926	9.778492	6.845535	H	7.773961	7.151669	7.419124
C	-3.409772	8.368850	7.512027	H	9.039421	6.640506	6.252747
H	-3.221027	7.504007	6.887899	H	7.848264	5.029183	8.464423
O	-1.541831	12.186198	8.115649	O	-8.378324	6.997776	11.499867
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S	-4.453910	9.873347	9.353695	V	-6.910898	6.439560	11.271567
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Cl	-4.118788	5.106084	11.144386	O	-4.742034	0.476827	11.047094
O	4.344096	0.363814	10.837375	O	-5.703886	2.781494	12.462489
O	5.363926	2.640003	9.415953	O	-6.208668	3.967202	15.017240
O	7.966700	2.550748	10.514533	V	-4.438683	2.028338	11.180443
O	5.898377	3.806527	6.858489	V	-5.413974	4.294819	13.689185
V	4.080293	1.922221	10.699805	O	-6.901659	4.930687	12.537053
V	5.112094	4.157348	8.185607	O	-5.820689	2.766930	9.987923
V	6.605483	3.361699	10.584430	N	-8.959287	5.546660	13.997031
O	8.143427	6.790196	10.368686	H	-9.567338	6.020638	13.321896
O	6.739190	4.742138	11.810785	C	-9.596986	4.331680	14.570108
O	6.167575	3.598785	14.370104	H	-9.891573	3.679384	13.746043
V	6.662338	6.269802	10.598212	H	-8.848634	3.826089	15.182160
V	5.383973	4.181028	13.125422	H	-10.464386	4.614875	15.170458
O	5.480406	2.628721	11.890552	C	-8.450735	6.527617	14.995720
O	6.614842	4.758524	9.336397	H	-7.694810	6.024611	15.599983
N	6.097393	0.473486	13.201306	H	-7.998469	7.356352	14.449391
H	5.931891	-0.256421	12.501232	H	-9.276588	6.880794	15.617050
C	7.513283	0.505497	13.654570	H	-8.127036	5.234526	13.409057
H	8.150819	0.619493	12.776013	N	-6.494727	0.624983	8.683598
H	7.630894	1.375501	14.302306	H	-6.350724	-0.108240	9.384892

C	-7.908120	0.694527	8.226691	O	3.002549	12.424673	9.537023
H	-8.544558	0.826731	9.103491	O	1.209760	14.566280	9.663528
H	-8.000581	1.566596	7.577656	O	0.004026	16.814176	10.877625
H	-8.170903	-0.219725	7.689930	O	2.874936	2.370407	9.513136
C	-5.482781	0.493225	7.598807	O	-0.131510	14.533020	7.136181
H	-5.570460	1.368898	6.954505	S	0.049613	2.572146	9.127499
H	-4.496145	0.471241	8.063477	S	4.290342	9.891099	9.085812
H	-5.664429	-0.425378	7.036660	V	2.507151	13.773993	10.887598
H	-6.275534	1.524185	9.212132	V	-0.001952	13.626769	8.425881
				V	-0.013145	15.227881	10.884927
				C	-1.198467	3.415204	8.274041
199				C	-2.598107	3.210404	8.676409
3-2, B3LYP/6-311++G(d,p)=-11149.0490483				C	-0.694907	4.296750	7.333975
O	8.269185	7.009026	11.063903	H	-1.335527	4.925676	6.727907
O	6.223198	3.836795	7.097556	O	-3.491097	3.866523	8.063298
O	8.220936	2.833614	10.945534	O	-2.780055	2.379885	9.624530
O	4.364401	0.564154	10.934353	C	-4.143787	8.412857	13.604464
O	5.686170	2.725698	9.649948	C	-1.187444	3.321799	13.700694
O	6.815371	4.927042	12.144827	C	-2.965834	10.572249	13.613979
V	5.472764	4.300117	8.391272	C	-2.446733	11.893336	13.233160
V	6.789526	6.451072	10.903950	C	-2.593684	3.138841	13.308204
V	4.260125	2.151825	10.900347	C	-4.996305	7.275258	13.233009
V	6.811252	3.558320	10.849333	C	-2.431720	9.680354	14.526808
O	6.342042	3.883714	14.641493	H	-1.572392	9.925125	15.138977
O	5.668479	2.744707	12.139024	C	-3.108530	8.439918	14.521809
O	6.860206	4.938938	9.666563	H	-2.851474	7.581032	15.129631
V	5.444737	4.266524	13.393806	C	-0.659673	4.153758	14.671932
C	4.195829	8.408280	8.196003	H	-1.283703	4.743929	15.331975
C	1.261087	3.407445	8.213004	O	-8.287846	6.907042	11.111116
C	2.956644	10.534645	8.188576	O	-6.210708	3.941170	14.736496
C	2.401593	11.838358	8.579704	O	-3.752157	14.826432	10.750812
C	2.671076	3.204666	8.569908	O	-1.425308	12.321755	13.849278
C	5.054839	7.284482	8.594340	O	-8.095718	2.665757	10.998556
C	2.472427	9.642724	7.248252	O	-4.823446	6.183279	13.851797
H	1.623847	9.871995	6.615355	O	-3.475472	3.811375	13.920144
C	3.184367	8.421510	7.252160	O	-5.838309	7.497810	12.303696
H	2.968560	7.567029	6.622403	O	-4.437421	0.500319	10.845478
C	0.718701	4.292897	7.299269	O	-3.060107	12.475996	12.282515
H	1.332710	4.918837	6.663180	O	-1.240094	14.602905	12.123296
O	3.721309	14.783841	11.038818	O	-2.787048	2.328520	12.346082
O	1.369065	12.250007	7.971125	O	-5.545829	2.767994	12.212663
O	4.914989	6.183222	7.990165	O	-6.817970	4.854413	9.747124
O	3.555197	3.864893	7.954996	O	0.106634	14.598536	14.651498
O	5.851812	7.527180	9.562079	S	0.037322	2.535547	12.764719

S	-4.300941	9.903807	12.737510	V	-5.410974	4.287283	8.492557
V	-2.548869	13.805549	10.912231	Cl	-0.035347	12.004968	10.910215
V	-5.359402	4.289359	13.449662	Cl	3.999447	5.035347	10.922869
V	-6.796891	6.388562	10.954203	Cl	-3.967332	5.132737	10.965503
V	-4.196333	2.061782	10.990893	N	2.763041	16.216026	13.431842
V	-6.734827	3.480187	10.985205	H	3.452213	16.473304	12.718513
V	-0.039949	13.673687	13.376467	C	2.001566	17.393953	13.926229
C	1.273146	3.327960	13.683879	H	1.545602	17.890284	13.067808
C	2.669611	3.154536	13.264539	H	1.217365	17.023454	14.588131
C	0.754660	4.155261	14.664262	H	2.671301	18.072995	14.458609
H	1.384025	4.746680	15.318363	C	3.411290	15.390202	14.487700
O	3.579999	3.763311	13.906643	H	2.625586	15.015824	15.145113
O	2.839578	2.409431	12.249555	H	3.913740	14.555656	13.996680
C	4.061287	8.336969	13.554249	H	4.128160	15.999341	15.042637
C	2.821300	10.461721	13.543298	H	2.084584	15.581014	12.909177
C	2.307843	11.792128	13.179566	N	-2.822519	16.129053	8.271789
C	4.966786	7.237232	13.197659	H	-3.517007	16.406255	8.972530
C	2.285878	9.548011	14.433529	C	-2.085293	17.296964	7.720337
H	1.403055	9.763026	15.023058	H	-1.640441	17.844733	8.553046
C	2.998297	8.326739	14.439985	H	-1.293589	16.911048	7.076501
H	2.747277	7.456925	15.034806	H	-2.768845	17.935682	7.156659
O	1.289627	12.220848	13.797839	C	-3.455377	15.241771	7.256361
O	4.849922	6.138803	13.820015	H	-2.662987	14.850742	6.617077
O	5.800493	7.498925	12.270185	H	-3.943406	14.422756	7.786283
O	2.948353	12.391890	12.257096	H	-4.182523	15.811348	6.673624
O	1.219201	14.578934	12.139517	H	-2.131952	15.534837	8.823894
S	4.196508	9.837262	12.698130	N	-8.959317	5.427056	13.570501
C	-4.208822	8.378963	8.258771	H	-8.087451	5.143020	13.027659
C	-2.940724	10.487192	8.268417	C	-8.536048	6.424701	14.592222
C	-2.392574	11.799312	8.637879	H	-8.082966	7.267403	14.068399
C	-5.088605	7.264152	8.637414	H	-9.404409	6.751069	15.168611
C	-2.436848	9.577630	7.355826	H	-7.796969	5.946907	15.236472
H	-1.563462	9.788051	6.750732	C	-9.585709	4.191967	14.112468
C	-3.164912	8.366493	7.350963	H	-10.491556	4.447053	14.666864
H	-2.938055	7.499522	6.742744	H	-9.815943	3.530089	13.275693
O	-6.138277	3.692779	7.220159	H	-8.853875	3.711366	14.763390
O	-1.362252	12.203196	8.021214	H	-9.547125	5.880452	12.864082
O	-4.940530	6.165683	8.022856	N	-6.096324	0.574097	8.416368
O	-5.905280	7.500114	9.584696	H	-5.927823	1.483670	8.944974
O	-3.014134	12.414983	9.564105	C	-5.041201	0.467747	7.370687
O	-1.253187	14.577423	9.644378	H	-4.072197	0.482126	7.871391
O	-5.549512	2.745520	9.734282	H	-5.171273	-0.460951	6.810882
O	-6.805456	4.882930	12.224080	H	-5.133954	1.334578	6.715235
S	-4.310782	9.871314	9.130927	C	-7.493447	0.591592	7.907144

H	-7.705244	-0.335856	7.370543	O	5.599829	2.708341	9.546489
H	-8.166000	0.710036	8.758574	O	6.777867	4.944774	12.162307
H	-7.591238	1.453972	7.246058	V	5.425779	4.286408	8.399425
H	-5.953763	-0.148247	9.129258	V	6.750386	6.411108	10.889240
O	6.850714	-0.496399	9.585443	V	4.272065	2.147352	10.897517
O	7.413653	0.570975	8.773474	V	7.041742	3.533923	10.902012
H	6.852017	1.340057	9.023394	O	6.326041	3.848017	14.633696
H	5.983757	-0.667859	9.113588	O	5.722705	2.781657	12.118225
N	9.054705	5.522460	13.339482	O	6.845916	4.859248	9.672740
H	8.148927	5.153901	12.923615	V	5.439894	4.265904	13.382382
C	9.944887	4.378402	13.655813	C	4.154439	8.393886	8.201419
H	10.091146	3.798962	12.742692	C	1.232335	3.383929	8.219323
H	10.899423	4.744997	14.039787	C	2.931556	10.529436	8.196640
H	9.445493	3.762293	14.405638	C	2.388892	11.839507	8.583678
C	8.692916	6.394087	14.490132	C	2.640265	3.185164	8.595362
H	9.599604	6.804644	14.939586	C	5.012015	7.266368	8.589617
H	8.057704	7.196308	14.112032	C	2.423296	9.632449	7.274009
H	8.135735	5.791964	15.209025	H	1.564145	9.862271	6.655820
H	9.419992	6.098428	12.569077	C	3.125487	8.405874	7.276677
N	6.907547	0.211718	12.257807	H	2.890429	7.546354	6.660896
H	6.773011	-0.041972	11.242728	C	0.699443	4.256642	7.288033
C	8.362680	0.185631	12.560168	H	1.320307	4.868904	6.645372
H	8.864491	0.851605	11.859895	O	3.721291	14.788898	11.032124
H	8.518090	0.523975	13.587254	O	1.356827	12.254442	7.976432
H	8.725898	-0.837156	12.442973	O	4.852275	6.162337	7.994668
C	6.095542	-0.691631	13.116948	O	3.526194	3.834429	7.962004
H	6.212543	-0.387942	14.159446	O	5.834070	7.499980	9.535558
H	5.055283	-0.603109	12.807485	O	2.997749	12.427690	9.534738
H	6.447323	-1.716680	12.983250	O	1.205683	14.572522	9.664414
H	6.533370	1.180062	12.349095	O	0.005490	16.822574	10.880231
C	4.312641	0.230465	7.308917	O	2.829419	2.389619	9.569525
H	3.263548	0.322138	7.001964	O	-0.141999	14.539099	7.140237
H	4.717413	1.226050	7.514338	S	0.012458	2.569205	9.139272
H	4.884830	-0.222779	6.497516	S	4.276307	9.883833	9.076026
O	4.434472	-0.641012	8.440294	V	2.505861	13.779846	10.885319
H	4.022595	-0.209956	9.214266	V	-0.010490	13.633888	8.430604
				V	-0.013573	15.236282	10.888415
				C	-1.227405	3.404835	8.266203
199, $\nu^{\neq} = 1091.63$ *i*cm^{-1}				C	-2.627192	3.209431	8.667195
3-TS1, B3LYP/6-311++G(d,p)=-11149.0099695				C	-0.714459	4.268829	7.314900
O	8.228637	6.975791	11.009740	H	-1.348089	4.891200	6.694736
O	6.250730	3.890048	7.107748	O	-3.518926	3.871687	8.057971
O	8.604259	3.471257	11.190509	O	-2.814060	2.376596	9.613286
O	4.483227	0.580357	10.979327	C	-4.134584	8.421046	13.610904

C	-1.185868	3.319203	13.681779	C	2.294583	9.561308	14.441491
C	-2.958217	10.581362	13.623063	H	1.418145	9.780703	15.038918
C	-2.441475	11.903672	13.244089	C	3.003395	8.337828	14.444734
C	-2.593241	3.137768	13.292904	H	2.755396	7.470410	15.044306
C	-4.988327	7.283935	13.239572	O	1.296405	12.232822	13.801990
C	-2.420157	9.686972	14.531120	O	4.844468	6.143207	13.816518
H	-1.558601	9.930281	15.140734	O	5.775835	7.492384	12.244118
C	-3.096131	8.446070	14.524640	O	2.949234	12.398994	12.254439
H	-2.836389	7.585510	15.128935	O	1.221836	14.587251	12.140061
C	-0.659717	4.172143	14.635629	S	4.188971	9.838944	12.686615
H	-1.285519	4.779690	15.277934	C	-4.222390	8.389654	8.268503
O	-8.292550	6.923443	11.136533	C	-2.951641	10.496431	8.279965
O	-6.198690	3.951416	14.746746	C	-2.401670	11.807629	8.649506
O	-3.753497	14.836434	10.763882	C	-5.104026	7.275873	8.646669
O	-1.418823	12.332253	13.858252	C	-2.449066	9.586866	7.366582
O	-8.115178	2.687178	11.021929	H	-1.575498	9.796636	6.761525
O	-4.812548	6.190709	13.855019	C	-3.178486	8.376514	7.360797
O	-3.470171	3.814761	13.907650	H	-2.952189	7.509417	6.752558
O	-5.833560	7.508865	12.313887	O	-6.169067	3.709848	7.230375
O	-4.465409	0.503654	10.847383	O	-1.372735	12.211459	8.030252
O	-3.058145	12.488001	12.296478	O	-4.960005	6.178147	8.030206
O	-1.237615	14.613289	12.130328	O	-5.918358	7.512833	9.595776
O	-2.794319	2.325608	12.334109	O	-3.019977	12.423366	9.577936
O	-5.555882	2.777292	12.218944	O	-1.257532	14.586096	9.651529
O	-6.834872	4.869313	9.761799	O	-5.574756	2.754869	9.740202
O	0.114694	14.610567	14.654958	O	-6.807388	4.896039	12.238317
S	0.041182	2.508126	12.769334	S	-4.322279	9.881306	9.142202
S	-4.295872	9.914438	12.749106	V	-5.433820	4.299704	8.500444
V	-2.550132	13.815217	10.923477	Cl	-0.038076	12.013964	10.917058
V	-5.355470	4.297866	13.453850	Cl	3.984565	5.034351	10.908970
V	-6.803525	6.402087	10.970027	Cl	-3.978011	5.138459	10.962519
V	-4.217202	2.064494	10.990019	N	2.768713	16.224167	13.427312
V	-6.749571	3.493220	10.997463	H	3.456460	16.481446	12.712652
V	-0.034816	13.684074	13.381381	C	2.008032	17.402044	13.923074
C	1.275078	3.317940	13.676095	H	1.550477	17.898267	13.065442
C	2.675500	3.132752	13.274115	H	1.225035	17.031343	14.586287
C	0.754220	4.170238	14.633579	H	2.678637	18.081137	14.454309
H	1.382888	4.776297	15.274749	C	3.418821	15.398374	14.481965
O	3.576989	3.765434	13.907129	H	2.634297	15.024138	15.140870
O	2.866571	2.353298	12.291597	H	3.920100	14.563629	13.990085
C	4.057367	8.341769	13.548458	H	4.136878	16.007350	15.035592
C	2.824086	10.470747	13.543457	H	2.089038	15.588948	12.905989
C	2.311496	11.801270	13.180360	N	-2.834376	16.130302	8.279387
C	4.955043	7.236869	13.185531	H	-3.527232	16.406819	8.982053

C	-2.102880	17.299081	7.722392	H	7.892580	6.130495	15.073518
H	-1.656981	17.850540	8.552110	H	9.501455	5.989289	12.605354
H	-1.312132	16.914032	7.076861	N	6.627312	0.423787	12.869009
H	-2.790402	17.934154	7.159413	H	6.553455	0.007058	11.933544
C	-3.468060	15.238446	7.268491	C	8.050212	0.504679	13.285830
H	-2.676741	14.847995	6.627534	H	8.611295	0.970767	12.475169
H	-3.951858	14.419440	7.802267	H	8.105417	1.114622	14.189790
H	-4.198880	15.804356	6.686768	H	8.431331	-0.499651	13.484386
H	-2.140032	15.539724	8.830708	C	5.713332	-0.244197	13.828561
N	-8.957321	5.430748	13.591620	H	5.710714	0.328218	14.758289
H	-8.086056	5.151882	13.044345	H	4.715849	-0.250562	13.388506
C	-8.533598	6.426972	14.614356	H	6.056184	-1.264537	14.014537
H	-8.086635	7.273258	14.091011	H	6.271559	1.407399	12.681423
H	-9.400485	6.747875	15.196057	C	9.571140	4.070870	8.103439
H	-7.789328	5.950295	15.253469	H	9.040614	4.848304	8.660984
C	-9.575805	4.191190	14.132433	H	10.459051	3.767543	8.662564
H	-10.480585	4.440377	14.691287	H	9.879674	4.458170	7.124908
H	-9.805950	3.530710	13.294544	O	8.759443	2.902057	7.946081
H	-8.839009	3.712151	14.778910	H	7.910300	3.169214	7.535111
H	-9.550108	5.883547	12.889079				
N	-6.088750	0.587331	8.401831				
H	-5.937368	1.497010	8.935215	199			
C	-5.026983	0.500727	7.360924	3-3, B3LYP/6-311++G(d,p)=-11149.0225828			
H	-4.060773	0.527516	7.866363	O	8.270631	6.963848	11.070400
H	-5.140834	-0.427698	6.797146	O	6.173784	3.909101	7.138558
H	-5.129071	1.368640	6.708342	O	8.514634	3.347379	11.660175
C	-7.483205	0.584147	7.885905	O	4.531411	0.517827	10.963512
H	-7.677438	-0.344514	7.344756	O	5.543947	2.684187	9.541797
H	-8.162057	0.687724	8.734320	O	6.716909	4.984968	12.149724
H	-7.591961	1.447388	7.227670	V	5.406239	4.330538	8.458670
H	-5.937498	-0.134510	9.113677	V	6.798265	6.396772	10.887126
O	7.277624	1.470179	10.391331	V	4.272012	2.091590	10.921688
O	8.552666	1.047750	9.883039	V	7.085458	3.429888	10.950235
H	8.715831	1.722662	9.164326	O	6.277303	3.890090	14.615659
H	6.419667	1.837046	9.603700	O	5.753878	2.740679	12.060933
N	8.999864	5.553905	13.386903	O	6.920473	4.786834	9.715962
H	8.121143	5.179113	12.919014	V	5.418880	4.267678	13.335335
C	9.763852	4.430812	13.985008	C	4.212995	8.429156	8.210600
H	10.011852	3.731274	13.186624	C	1.227224	3.345975	8.247223
H	10.666586	4.813353	14.466961	C	2.989609	10.564393	8.219546
H	9.116237	3.944987	14.716711	C	2.439029	11.870406	8.609598
C	8.561163	6.600225	14.350607	C	2.635949	3.157315	8.624419
H	9.433290	7.028278	14.849520	C	5.064276	7.293758	8.586721
H	8.023775	7.366826	13.791877	C	2.461435	9.661482	7.314125

H	1.587135	9.887348	6.716191	O	-3.482097	3.776362	13.890739
C	3.162345	8.435119	7.310245	O	-5.808438	7.498309	12.298413
H	2.911618	7.570004	6.708810	O	-4.519456	0.474726	10.833265
C	0.697424	4.234090	7.328556	O	-3.043628	12.473442	12.288189
H	1.321223	4.861765	6.703985	O	-1.240600	14.612485	12.130002
O	3.723636	14.835719	11.060767	O	-2.823136	2.271315	12.324965
O	1.404263	12.275207	7.999684	O	-5.577540	2.764853	12.203483
O	4.852540	6.184440	8.011174	O	-6.827367	4.871192	9.743676
O	3.508332	3.836074	8.005187	O	0.094716	14.625193	14.663587
O	5.927302	7.504384	9.494682	S	0.020857	2.435529	12.761734
O	3.039392	12.463404	9.562624	S	-4.273065	9.898828	12.737859
O	1.217985	14.590498	9.678713	V	-2.539389	13.803214	10.916524
O	-0.011353	16.831412	10.882907	V	-5.358655	4.285672	13.436074
O	2.834203	2.339170	9.582654	V	-6.785619	6.402961	10.951791
O	-0.117876	14.536065	7.147958	V	-4.247015	2.031185	10.977602
S	0.003994	2.509831	9.143308	V	-6.760307	3.494614	10.980277
S	4.355528	9.925336	9.071715	V	-0.037496	13.696231	13.389965
V	2.519890	13.813716	10.908102	C	1.257025	3.262249	13.649575
V	0.017150	13.636050	8.441796	C	2.658507	3.087679	13.249069
V	-0.013950	15.245092	10.895149	C	0.738736	4.131334	14.593479
C	-1.232644	3.357601	8.276803	H	1.370040	4.749448	15.220271
C	-2.635722	3.161931	8.665635	O	3.548613	3.753668	13.852996
C	-0.716074	4.240569	7.345221	O	2.862304	2.284232	12.283088
H	-1.348145	4.873168	6.733976	C	4.018975	8.342433	13.489885
O	-3.518663	3.832314	8.052453	C	2.815350	10.487782	13.531392
O	-2.834323	2.324276	9.604826	C	2.317727	11.828802	13.193041
C	-4.111082	8.405184	13.599358	C	4.907142	7.232517	13.111181
C	-1.203653	3.263805	13.662578	C	2.271740	9.565820	14.407768
C	-2.940104	10.568834	13.616477	H	1.396601	9.783431	15.007768
C	-2.428103	11.893974	13.239608	C	2.964456	8.333334	14.385175
C	-2.612478	3.087908	13.278062	H	2.704990	7.456398	14.965683
C	-4.964857	7.268958	13.224837	O	1.302843	12.257955	13.817449
C	-2.402812	9.675275	14.525821	O	4.782083	6.137804	13.738131
H	-1.544289	9.920429	15.139000	O	5.725115	7.491906	12.169351
C	-3.075647	8.432431	14.516444	O	2.965250	12.440577	12.282474
H	-2.815857	7.572724	15.121981	O	1.218997	14.609286	12.154667
C	-0.674558	4.132638	14.600342	S	4.173340	9.856090	12.662567
H	-1.298860	4.752250	15.232400	C	-4.179836	8.371632	8.260467
O	-8.269777	6.939261	11.114922	C	-2.907003	10.477807	8.276111
O	-6.207065	3.952798	14.729173	C	-2.361357	11.790990	8.647127
O	-3.749877	14.814666	10.748272	C	-5.067496	7.261184	8.635162
O	-1.411551	12.329550	13.858589	C	-2.400376	9.566498	7.366761
O	-8.133654	2.701423	10.998862	H	-1.523828	9.774670	6.765443
O	-4.792732	6.173655	13.837380	C	-3.130971	8.356615	7.358497

H	-2.902354	7.489034	6.751771	H	-9.821781	3.579729	13.289935
O	-6.167182	3.710369	7.213906	H	-8.849300	3.750535	14.772042
O	-1.328643	12.196584	8.035683	H	-9.530298	5.927039	12.876916
O	-4.926115	6.161630	8.021303	N	-6.158789	0.586544	8.394991
O	-5.885403	7.503604	9.579947	H	-5.982603	1.492255	8.928184
O	-2.988830	12.406077	9.569874	C	-5.102438	0.474840	7.351138
O	-1.245082	14.581000	9.652036	H	-4.134435	0.478495	7.853917
O	-5.590574	2.743807	9.725103	H	-5.239988	-0.450256	6.787124
O	-6.805794	4.897689	12.220396	H	-5.185600	1.345353	6.699298
S	-4.282862	9.864723	9.131509	C	-7.554448	0.619691	7.883103
V	-5.427763	4.287838	8.487304	H	-7.774080	-0.303136	7.341658
Cl	-0.008925	12.021939	10.924875	H	-8.227721	0.740313	8.733685
Cl	3.971540	4.972457	10.834328	H	-7.642705	1.486122	7.225969
Cl	-3.969276	5.106418	10.951817	H	-6.024293	-0.139788	9.105469
N	2.754200	16.243608	13.460369	N	8.825503	5.636071	13.569712
H	3.446528	16.501999	12.750422	H	7.997097	5.216319	13.048768
C	1.991465	17.420563	13.954799	C	9.572635	4.574863	14.290000
H	1.539717	17.919895	13.095859	H	9.903622	3.840218	13.556843
H	1.204110	17.048644	14.612141	H	10.421442	5.018190	14.816328
H	2.659275	18.097655	14.492064	H	8.882878	4.106231	14.992933
C	3.397271	15.414136	14.516536	C	8.293728	6.719239	14.440561
H	2.608645	15.038900	15.169911	H	9.117596	7.189370	14.982112
H	3.900140	14.579977	14.025324	H	7.789681	7.446926	13.804824
H	4.112914	16.020864	15.075729	H	7.580472	6.271695	15.133729
H	2.077657	15.610793	12.932648	H	9.376308	6.047768	12.808394
N	-2.820181	16.118172	8.271253	O	7.906431	1.824158	10.101390
H	-3.518454	16.391569	8.969731	O	7.296387	1.044300	9.015671
C	-2.089673	17.290166	7.719710	H	7.810459	1.446404	8.237914
H	-1.651009	17.842515	8.552679	H	6.021650	1.910347	9.098096
H	-1.293429	16.908550	7.078911	N	7.083529	-0.015150	11.912886
H	-2.776047	17.923047	7.152859	H	7.561010	0.708116	11.313991
C	-3.443876	15.224388	7.255947	C	7.298163	0.289859	13.352279
H	-2.646933	14.837846	6.619592	H	6.922063	1.294867	13.544476
H	-3.927329	14.402888	7.786229	H	6.754515	-0.439776	13.956321
H	-4.173639	15.787473	6.670149	H	8.366990	0.233840	13.568886
H	-2.126835	15.529880	8.826496	C	7.525537	-1.362346	11.474550
N	-8.943451	5.467344	13.580032	H	6.967385	-2.123772	12.023314
H	-8.077761	5.173616	13.032016	H	7.334114	-1.446648	10.404403
C	-8.503383	6.460168	14.599248	H	8.594708	-1.467405	11.670109
H	-8.044683	7.298187	14.072782	H	6.076178	0.108674	11.673120
H	-9.364606	6.795610	15.181144	C	9.475099	3.287210	7.640690
H	-7.765372	5.974337	15.238708	H	9.925941	3.873134	6.830687
C	-9.579826	4.238968	14.125490	H	9.059217	3.961692	8.395804
H	-10.479725	4.503540	14.685136	H	10.242421	2.661666	8.101114

O	8.469864	2.407117	7.115331	V	2.526291	13.818526	10.890812
H	7.691576	2.960511	6.887036	V	0.016749	13.630997	8.431853
				V	-0.011613	15.243068	10.883749
				C	-1.242357	3.357270	8.278316
199, $\nu^{\neq} = 362.30\ i\text{cm}^{-1}$				C	-2.645980	3.157004	8.660811
3-TS2, B3LYP/6-311++G(d,p)=-11149.0108582				C	-0.723469	4.256746	7.363943
O	8.292820	6.936386	11.065865	H	-1.354190	4.900124	6.762638
O	6.151856	3.910559	7.152704	O	-3.528204	3.830539	8.049604
O	8.461897	3.245151	11.612825	O	-2.847494	2.312019	9.593078
O	4.543674	0.506322	10.942931	C	-4.100134	8.398541	13.594190
O	5.542684	2.742953	9.604944	C	-1.203301	3.260580	13.649044
O	6.715740	4.962612	12.133653	C	-2.926727	10.561095	13.609096
V	5.388470	4.306809	8.510191	C	-2.415908	11.886771	13.232400
V	6.808376	6.395890	10.888679	C	-2.611670	3.081901	13.267548
V	4.290519	2.087587	10.896210	C	-4.957426	7.263921	13.222549
V	7.011102	3.422362	10.937222	C	-2.385557	9.665206	14.513811
O	6.280305	3.897519	14.617882	H	-1.523343	9.908067	15.122704
O	5.728007	2.735337	12.089822	C	-3.059742	8.423039	14.505705
O	6.922098	4.803113	9.706349	H	-2.797295	7.561829	15.107944
V	5.411908	4.272084	13.342730	C	-0.676668	4.128836	14.588742
C	4.209776	8.423181	8.230142	H	-1.302901	4.744203	15.223073
C	1.217578	3.348719	8.257282	O	-8.268914	6.940135	11.121565
C	2.987781	10.559577	8.220168	O	-6.203331	3.950228	14.730071
C	2.440412	11.869477	8.598804	O	-3.746944	14.808035	10.745538
C	2.625852	3.155923	8.635193	O	-1.397269	12.321758	13.848327
C	5.063700	7.290794	8.613501	O	-8.140128	2.702489	11.004651
C	2.450667	9.644157	7.332725	O	-4.785702	6.168351	13.834557
H	1.570257	9.861757	6.740677	O	-3.481571	3.767667	13.883795
C	3.150777	8.417268	7.339904	O	-5.803749	7.495110	12.298951
H	2.893457	7.543100	6.754583	O	-4.530494	0.468975	10.831251
C	0.690026	4.252237	7.352515	O	-3.035006	12.467666	12.284058
H	1.315668	4.892315	6.742582	O	-1.234642	14.608562	12.121363
O	3.727151	14.844360	11.042507	O	-2.824789	2.266318	12.313697
O	1.403065	12.270106	7.989887	O	-5.580826	2.761183	12.202609
O	4.846578	6.176407	8.055308	O	-6.833403	4.870233	9.745972
O	3.498686	3.844179	8.027162	O	0.105665	14.620060	14.651521
O	5.935587	7.516644	9.511909	S	0.024614	2.440137	12.744625
O	3.045781	12.472207	9.542881	S	-4.264858	9.893870	12.736041
O	1.218493	14.590588	9.664570	V	-2.534986	13.797682	10.911191
O	-0.012262	16.829412	10.871051	V	-5.356505	4.280926	13.435176
O	2.828694	2.327698	9.580308	V	-6.785887	6.401541	10.954440
O	-0.121921	14.529322	7.137048	V	-4.254201	2.025150	10.973589
S	-0.007485	2.496459	9.134863	V	-6.765250	3.492956	10.982242
S	4.360888	9.930709	9.069101	V	-0.027016	13.691976	13.377088

C	1.257695	3.269175	13.633922	H	1.550958	17.915620	13.094645
C	2.661284	3.100098	13.233063	H	1.217177	17.039855	14.608712
C	0.736636	4.132925	14.580815	H	2.673870	18.086861	14.488874
H	1.366211	4.751707	15.208615	C	3.407439	15.401897	14.502625
O	3.544924	3.765877	13.851207	H	2.619748	15.025614	15.156510
O	2.869981	2.308073	12.262715	H	3.907752	14.568644	14.007301
C	4.051114	8.354864	13.496564	H	4.125408	16.005543	15.062189
C	2.838317	10.495379	13.519915	H	2.084327	15.606214	12.922215
C	2.334826	11.832175	13.175507	N	-2.824939	16.107778	8.264850
C	4.943372	7.244096	13.129686	H	-3.522085	16.380008	8.964917
C	2.292406	9.574826	14.396467	C	-2.098327	17.280754	7.710613
H	1.412040	9.791589	14.989071	H	-1.659021	17.834870	8.542078
C	2.989788	8.345109	14.383643	H	-1.302590	16.900249	7.068506
H	2.729473	7.468947	14.964860	H	-2.787243	17.911650	7.144585
O	1.318342	12.258825	13.799601	C	-3.448854	15.211534	7.251965
O	4.807842	6.150766	13.756253	H	-2.652419	14.825893	6.614417
O	5.775930	7.500280	12.199940	H	-3.929330	14.389588	7.784259
O	2.978048	12.444374	12.261998	H	-4.181128	15.772303	6.667040
O	1.225170	14.609372	12.140454	H	-2.128692	15.521425	8.819262
S	4.205294	9.865240	12.663483	N	-8.936825	5.469450	13.588250
C	-4.184414	8.367986	8.257514	H	-8.073091	5.173806	13.037643
C	-2.908748	10.472523	8.271357	C	-8.491720	6.461129	14.606304
C	-2.361320	11.785270	8.641444	H	-8.032408	7.298058	14.078637
C	-5.072959	7.258655	8.633641	H	-9.350585	6.798609	15.190541
C	-2.404989	9.560777	7.360871	H	-7.753099	5.973520	15.243703
H	-1.529242	9.767958	6.758032	C	-9.574314	4.242411	14.135162
C	-3.137230	8.351850	7.353634	H	-10.472142	4.508712	14.697351
H	-2.910892	7.484109	6.746269	H	-9.819887	3.583853	13.300118
O	-6.178047	3.708316	7.214855	H	-8.842993	3.752293	14.779537
O	-1.329644	12.190462	8.028179	H	-9.524338	5.930564	12.886621
O	-4.934865	6.159314	8.018772	N	-6.157670	0.584895	8.389476
O	-5.888252	7.501887	9.580478	H	-5.987375	1.492055	8.922500
O	-2.986947	12.400590	9.565373	C	-5.100732	0.479337	7.345662
O	-1.244512	14.576485	9.643369	H	-4.132792	0.490520	7.848422
O	-5.599770	2.740832	9.724390	H	-5.231934	-0.447405	6.782800
O	-6.805272	4.896129	12.222556	H	-5.189844	1.348584	6.692931
S	-4.283718	9.860915	9.129256	C	-7.553481	0.608125	7.878120
V	-5.436317	4.285684	8.487175	H	-7.767128	-0.316486	7.337276
Cl	-0.003302	12.020775	10.913488	H	-8.227376	0.724505	8.728822
Cl	3.956540	5.052391	10.860976	H	-7.648033	1.473542	7.220515
Cl	-3.973120	5.101598	10.945975	H	-6.017625	-0.139378	9.101131
N	2.763243	16.236086	13.450861	O	7.867742	1.806739	10.013164
H	3.454241	16.495312	12.739888	O	7.176332	1.110529	8.900298
C	2.003751	17.412585	13.950900	H	7.774819	1.733561	7.966195

H	6.277118	1.623973	8.998888	O	5.785133	2.851958	12.010742
N	7.073578	0.002315	11.894341	O	6.874059	4.814668	9.789691
H	7.540546	0.705549	11.265006	V	5.493974	4.330046	13.375153
C	7.337714	0.329635	13.320455	C	4.224993	8.368760	8.294842
H	6.977275	1.341054	13.507185	C	1.199441	3.577809	8.291253
H	6.805265	-0.384155	13.952824	C	2.954731	10.474571	8.234188
H	8.412222	0.265615	13.504303	C	2.395309	11.787174	8.590660
C	7.480216	-1.359958	11.471475	C	2.596884	3.379937	8.698434
H	6.935047	-2.100110	12.060834	C	5.116726	7.283512	8.716627
H	7.240545	-1.471566	10.413320	C	2.463048	9.540705	7.339291
H	8.555084	-1.477265	11.625029	H	1.597482	9.733383	6.717335
H	6.058705	0.134391	11.678432	C	3.193330	8.330443	7.373570
C	9.322478	3.253600	7.703348	H	2.977958	7.449578	6.780914
H	9.794559	3.762409	6.861215	C	0.670855	4.475236	7.380638
H	8.932179	3.969918	8.428219	H	1.291117	5.133293	6.784444
H	10.023721	2.571849	8.181869	O	3.720459	14.776562	11.006876
O	8.234817	2.441625	7.169101	O	1.356089	12.178373	7.980632
H	7.448400	3.060488	6.978526	O	5.014286	6.155736	8.147833
N	8.854355	5.547132	13.532774	O	3.492411	4.066597	8.102268
H	8.012496	5.148037	13.018894	O	5.927963	7.559364	9.651788
C	9.595290	4.461977	14.222384	O	3.004276	12.402471	9.524468
H	9.893244	3.730497	13.471932	O	1.205999	14.531490	9.638716
H	10.464086	4.880732	14.736207	O	0.001455	16.790497	10.833594
H	8.911172	3.998407	14.934165	O	2.768866	2.549978	9.643399
C	8.353515	6.624401	14.429274	O	-0.131149	14.462719	7.115101
H	9.193945	7.075211	14.961831	S	-0.024041	2.686684	9.132139
H	7.847679	7.367709	13.813268	S	4.315280	9.884632	9.126895
H	7.646672	6.175789	15.128128	V	2.510387	13.760162	10.867085
H	9.398116	5.963186	12.768734	V	-0.007413	13.572505	8.416431
				V	-0.014356	15.204149	10.856148
				C	-1.258444	3.520949	8.252875
199				C	-2.660651	3.261506	8.608711
3-4, B3LYP/6-311++G(d,p)=-11149.0310224				C	-0.743098	4.443255	7.359471
O	8.320953	7.023386	11.056624	H	-1.375060	5.074522	6.746768
O	6.145699	3.905201	7.223968	O	-3.562839	3.908808	8.000391
O	8.647682	3.612094	11.901454	O	-2.836245	2.390747	9.522386
O	4.503770	0.613460	10.928570	C	-4.129302	8.399048	13.589062
O	5.358520	2.777660	9.411419	C	-1.149577	3.336634	13.605451
O	6.927918	5.060414	12.324157	C	-2.954819	10.560662	13.605521
V	5.421582	4.256713	8.562830	C	-2.440170	11.884584	13.229007
V	6.850588	6.437638	10.990052	C	-2.553921	3.140050	13.214389
V	4.294626	2.179829	10.870385	C	-4.983050	7.261438	13.219158
V	7.195616	3.457936	10.970012	C	-2.409748	9.661727	14.504760
O	6.258591	3.763278	14.645199	H	-1.543750	9.902117	15.109178

C	-3.084550	8.420284	14.495796	O	2.958466	12.391091	12.244978
H	-2.819891	7.556724	15.093615	O	1.221399	14.568624	12.114519
C	-0.644694	4.223382	14.539819	S	4.253831	9.872179	12.735394
H	-1.286369	4.842371	15.154826	C	-4.283761	8.377081	8.240922
O	-8.311090	6.889529	11.161661	C	-2.983188	10.464665	8.261248
O	-6.150629	3.910532	14.726998	C	-2.412680	11.764867	8.638610
O	-3.751766	14.810095	10.732630	C	-5.170355	7.268537	8.621090
O	-1.414951	12.311704	13.839932	C	-2.505019	9.559612	7.330516
O	-8.106190	2.648617	11.025715	H	-1.636859	9.765074	6.716214
O	-4.796684	6.166023	13.827895	C	-3.251977	8.360150	7.319394
O	-3.434989	3.801561	13.840772	H	-3.046987	7.497455	6.697460
O	-5.838214	7.486733	12.302796	O	-6.229110	3.691415	7.208718
O	-4.437700	0.499169	10.792594	O	-1.377194	12.155571	8.022378
O	-3.061273	12.471756	12.285977	O	-5.045520	6.176572	7.990194
O	-1.237322	14.589808	12.102711	O	-5.967290	7.501178	9.585711
O	-2.752124	2.336414	12.247588	O	-3.022421	12.383588	9.570441
O	-5.529510	2.756752	12.183943	O	-1.256150	14.541606	9.623374
O	-6.865948	4.847720	9.754996	O	-5.586602	2.745260	9.707499
O	0.110423	14.598726	14.627530	O	-6.800042	4.865172	12.231226
S	0.099638	2.512544	12.733950	S	-4.351982	9.859249	9.132839
S	-4.297961	9.897177	12.736919	V	-5.484446	4.293346	8.467411
V	-2.551555	13.786926	10.901970	Cl	-0.035620	11.982587	10.911075
V	-5.328510	4.271405	13.424465	Cl	4.061197	5.192095	11.050135
V	-6.822138	6.377552	10.969490	Cl	-3.993550	5.141943	10.911939
V	-4.203199	2.062147	10.933001	N	2.754048	16.227043	13.391743
V	-6.749166	3.468148	10.984576	H	3.440576	16.487129	12.676979
V	-0.033784	13.665591	13.358255	C	1.981084	17.400442	13.879365
C	1.312218	3.365082	13.630883	H	1.520288	17.887145	13.018029
C	2.723996	3.190633	13.262811	H	1.200561	17.026012	14.543404
C	0.768535	4.240016	14.554114	H	2.644208	18.089034	14.407736
H	1.382375	4.874241	15.182023	C	3.410140	15.413846	14.452472
O	3.596814	3.869660	13.878095	H	2.627867	15.035279	15.111604
O	2.955390	2.365692	12.323731	H	3.921379	14.581724	13.966423
C	4.155976	8.391338	13.629532	H	4.120477	16.033253	15.004465
C	2.873668	10.491189	13.577364	H	2.081216	15.582249	12.873401
C	2.331493	11.801391	13.183433	N	-2.817290	16.088934	8.238166
C	5.072375	7.297488	13.279416	H	-3.510110	16.380869	8.934450
C	2.365267	9.589936	14.495641	C	-2.069803	17.243756	7.672890
H	1.484031	9.802165	15.088675	H	-1.620962	17.797906	8.499201
C	3.101692	8.382931	14.525344	H	-1.280859	16.843138	7.034656
H	2.872287	7.522657	15.142427	H	-2.747503	17.881124	7.100685
O	1.305478	12.224487	13.792572	C	-3.456140	15.194142	7.233159
O	4.979016	6.206773	13.921415	H	-2.665999	14.787891	6.600570
O	5.890628	7.558944	12.337502	H	-3.952544	14.386501	7.772685

H	-4.177084	15.762355	6.641456	H	4.670194	-0.397450	13.197131
H	-2.131541	15.495758	8.797758	H	5.930841	-1.228979	14.172597
N	-8.930916	5.386089	13.621996	H	6.166452	1.399684	12.816428
H	-8.068252	5.113316	13.058858	C	6.915609	-1.070797	9.739199
C	-8.494301	6.380354	14.641366	H	6.079442	-0.416351	9.484878
H	-8.060983	7.231128	14.113867	H	7.523149	-1.279981	8.851316
H	-9.352548	6.694287	15.239418	H	6.524288	-2.010606	10.137346
H	-7.736597	5.904870	15.265388	O	7.722035	-0.486028	10.774432
C	-9.534396	4.141660	14.168783	H	7.957850	0.428542	10.495072
H	-10.430530	4.384768	14.743971	O	8.114684	-2.095370	12.984826
H	-9.776127	3.483197	13.332568	H	8.252813	-1.645691	12.126789
H	-8.784410	3.663684	14.800698	H	7.996683	-3.029879	12.762734
H	-9.538048	5.838832	12.931796				
N	-6.105521	0.572856	8.378086				
H	-5.953788	1.485775	8.905415	190			
C	-5.066565	0.496663	7.313689	3-5, B3LYP/6-311++G(d,p)=-10956.774145			
H	-4.089735	0.542993	7.796874	O	8.292225	6.999913	10.783318
H	-5.178025	-0.437148	6.758391	O	6.271987	3.947466	7.181901
H	-5.197593	1.358667	6.658482	O	8.550102	3.128915	10.434901
C	-7.511274	0.549161	7.894548	O	4.587583	0.504479	11.097201
H	-7.705448	-0.383934	7.361072	O	5.676635	2.828764	9.767747
H	-8.171727	0.646811	8.758044	O	6.844268	4.880710	12.111983
H	-7.646922	1.408317	7.235964	V	5.441804	4.324447	8.472930
H	-5.928301	-0.144209	9.088924	V	6.813692	6.443766	10.907564
N	8.897022	5.989324	13.750428	V	4.313809	2.060071	10.970283
H	8.080133	5.539709	13.211301	V	6.868925	3.507528	10.940674
C	9.553030	4.953319	14.588079	O	6.180360	3.803446	14.697211
H	9.911218	4.163708	13.928318	O	5.619878	2.772114	12.222052
H	10.377758	5.398327	15.149892	O	6.868432	4.955755	9.657656
H	8.799061	4.546753	15.263943	V	5.434553	4.323033	13.404253
C	8.366489	7.153476	14.507590	C	4.138015	8.413561	8.244606
H	9.175072	7.626005	15.069919	C	1.283990	3.317943	8.292642
H	7.931795	7.852968	13.794094	C	2.925335	10.553712	8.202561
H	7.592209	6.790841	15.185708	C	2.392699	11.875178	8.565688
H	9.512599	6.316712	12.999309	C	2.695099	3.121178	8.654162
O	7.830910	2.165691	10.226491	C	5.008574	7.296514	8.633647
N	6.559834	0.505428	13.179538	C	2.402801	9.638494	7.306482
H	6.863296	-0.011457	12.329174	H	1.537499	9.858373	6.693291
C	7.751616	0.823419	14.013241	C	3.100003	8.409348	7.329628
H	8.442382	1.409146	13.404135	H	2.855076	7.537171	6.735848
H	7.424915	1.426725	14.860980	C	0.753790	4.221793	7.389645
H	8.211623	-0.113562	14.326188	H	1.377987	4.857697	6.773951
C	5.505492	-0.267070	13.885615	O	3.711677	14.839193	11.009424
H	5.185136	0.299399	14.762356	O	1.360670	12.283790	7.954756

O	4.861388	6.193170	8.028010	O	-6.796841	4.837189	9.729179
O	3.563716	3.802835	8.033662	O	0.112815	14.581835	14.647263
O	5.841760	7.544422	9.565426	S	0.024567	2.474871	12.785478
O	3.011227	12.478052	9.500481	S	-4.271222	9.875890	12.731381
O	1.191208	14.597527	9.652654	V	-2.549778	13.786805	10.920449
O	-0.038251	16.824369	10.884624	V	-5.372263	4.266509	13.440741
O	2.914108	2.291855	9.593948	V	-6.775256	6.372383	10.934685
O	-0.163323	14.560117	7.133137	V	-4.221900	2.007129	11.000792
S	0.060371	2.471732	9.178973	V	-6.739388	3.463966	10.969440
S	4.273087	9.921106	9.086363	V	-0.021554	13.663933	13.365973
V	2.508167	13.815888	10.863633	C	1.251223	3.361730	13.627114
V	-0.018426	13.650472	8.419074	C	2.656526	3.181191	13.240443
V	-0.029028	15.238253	10.888294	C	0.724201	4.259003	14.539117
C	-1.176420	3.335358	8.327818	H	1.348704	4.916110	15.131959
C	-2.582052	3.139494	8.709441	O	3.530691	3.868299	13.848286
C	-0.659322	4.230994	7.408806	O	2.868235	2.338429	12.308340
H	-1.291616	4.874195	6.809064	C	4.183049	8.414064	13.578893
O	-3.459757	3.808518	8.087337	C	2.913885	10.521897	13.540471
O	-2.787623	2.304692	9.649437	C	2.365805	11.830370	13.156757
C	-4.118672	8.381169	13.592767	C	5.071252	7.299438	13.219205
C	-1.208147	3.313392	13.665762	C	2.407266	9.622102	14.461271
C	-2.929163	10.535094	13.604890	H	1.532043	9.839365	15.061259
C	-2.411376	11.858180	13.227643	C	3.135484	8.411113	14.482299
C	-2.615928	3.096716	13.301102	H	2.906921	7.551166	15.099821
C	-4.979187	7.249378	13.220984	O	1.340399	12.243499	13.775600
C	-2.395778	9.637285	14.512164	O	4.924819	6.204983	13.839662
H	-1.532537	9.874801	15.121687	O	5.898629	7.532367	12.281052
C	-3.079636	8.400453	14.506121	O	2.981343	12.433093	12.218336
H	-2.824924	7.538932	15.111205	O	1.219602	14.598985	12.130002
C	-0.688703	4.231937	14.560240	S	4.287344	9.896727	12.690310
H	-1.320093	4.865822	15.170675	C	-4.166862	8.354173	8.252634
O	-8.263177	6.903363	11.079859	C	-2.920013	10.475441	8.264419
O	-6.231887	3.930713	14.725496	C	-2.385450	11.792956	8.635891
O	-3.764773	14.796147	10.772484	C	-5.041496	7.234419	8.629792
O	-1.384334	12.284372	13.835429	C	-2.406353	9.571185	7.351938
O	-8.108812	2.663898	10.971891	H	-1.534978	9.790876	6.747230
O	-4.818284	6.157132	13.842259	C	-3.121829	8.352368	7.346178
O	-3.494734	3.776393	13.910138	H	-2.885698	7.488260	6.737343
O	-5.816601	7.476800	12.288306	O	-6.095484	3.673021	7.211608
O	-4.487782	0.449803	10.855002	O	-1.363784	12.211789	8.014813
O	-3.035320	12.445387	12.286346	O	-4.882456	6.132778	8.024081
O	-1.241697	14.589207	12.127193	O	-5.867105	7.472711	9.568822
O	-2.817675	2.256037	12.367088	O	-3.008631	12.397210	9.568320
O	-5.568411	2.741846	12.208276	O	-1.270225	14.578558	9.649925

O	-5.550471	2.714463	9.730928	H	-5.169089	-0.485764	6.802888
O	-6.805909	4.869380	12.206330	H	-5.110586	1.309639	6.712935
S	-4.284475	9.845351	9.125081	C	-7.494510	0.590590	7.869599
V	-5.376603	4.257622	8.493653	H	-7.709583	-0.332615	7.326972
Cl	-0.009884	12.014680	10.894265	H	-8.177489	0.714006	8.711996
Cl	3.999785	5.144678	10.937490	H	-7.573006	1.456251	7.210239
Cl	-3.956031	5.090267	10.966793	H	-5.980823	-0.170594	9.110856
N	2.785354	16.186186	13.462014	N	8.973886	5.570908	8.268537
H	3.473219	16.456387	12.752116	H	8.126925	5.236142	8.829930
C	2.040734	17.357433	13.996030	C	8.484947	6.610387	7.321016
H	1.585734	17.885015	13.155822	H	8.028443	7.410199	7.905086
H	1.256352	16.976377	14.651649	H	9.321163	6.992723	6.731546
H	2.721589	18.012781	14.543713	H	7.736667	6.147096	6.676720
C	3.431315	15.322661	14.489313	C	9.620161	4.394500	7.628753
H	2.645842	14.936320	15.139938	H	10.494948	4.717604	7.059928
H	3.923301	14.498424	13.971202	H	9.903920	3.691100	8.412614
H	4.156977	15.908341	15.057819	H	8.881062	3.928755	6.975568
H	2.096560	15.575680	12.924878	H	9.577676	6.002435	8.974719
N	-2.855674	16.140275	8.311729	N	6.152773	0.648667	13.617805
H	-3.546413	16.404356	9.021172	H	6.088281	-0.090491	12.911399
C	-2.126905	17.318845	7.772142	C	7.493966	0.689395	14.258576
H	-1.678344	17.856058	8.609705	H	8.244582	0.801945	13.475210
H	-1.337993	16.945360	7.117590	H	7.519498	1.562762	14.911575
H	-2.816622	17.962825	7.222064	H	7.659444	-0.228204	14.827642
C	-3.491102	15.263947	7.288719	C	5.008402	0.541380	14.564412
H	-2.701259	14.885637	6.638659	H	5.027614	1.419924	15.210538
H	-3.971111	14.435163	7.810792	H	4.087962	0.530276	13.979672
H	-4.225342	15.837414	6.718774	H	5.102493	-0.374371	15.152169
H	-2.158568	15.540997	8.850910	H	6.011860	1.548074	13.055783
N	-8.957402	5.443501	13.543731	O	8.048524	2.252895	11.450400
H	-8.087087	5.146784	13.005206				
C	-8.526058	6.439616	14.563594				
H	-8.059874	7.274422	14.038635	206			
H	-9.392820	6.779218	15.134732	3-6, B3LYP/6-311++G(d,p)=-11626.6796464			
H	-7.795986	5.955020	15.213001	O	8.288404	6.953988	10.763793
C	-9.600919	4.218155	14.087500	O	6.264295	3.934614	7.179481
H	-10.505710	4.486165	14.637518	O	8.504198	3.134549	11.402491
H	-9.836139	3.556218	13.252143	O	4.468636	0.530432	11.096788
H	-8.877497	3.730919	14.742889	O	5.562989	2.779182	9.665596
H	-9.536560	5.901553	12.833149	O	6.840885	4.940362	12.160637
N	-6.105026	0.555293	8.398124	V	5.381811	4.281550	8.451243
H	-5.933453	1.461501	8.931988	V	6.796685	6.425635	10.945024
C	-5.036591	0.439990	7.367019	V	4.249448	2.096605	10.893620
H	-4.074539	0.442603	7.881140	V	6.816115	3.501108	10.914523

O	6.183237	3.748552	14.662210	H	-1.537271	9.859750	15.113860
O	5.637491	2.815598	12.117837	C	-3.086534	8.391717	14.488806
O	6.814455	4.873916	9.706618	H	-2.832101	7.525332	15.086995
V	5.457884	4.349379	13.396303	C	-0.710584	4.257718	14.536573
C	4.141467	8.395578	8.253215	H	-1.350794	4.869429	15.160379
C	1.224864	3.311766	8.203088	O	-8.283761	6.914890	11.079554
C	2.930163	10.536729	8.222892	O	-6.241171	3.931009	14.708749
C	2.398002	11.857664	8.586922	O	-3.764170	14.791119	10.766905
C	2.630386	3.145721	8.595720	O	-1.389379	12.280952	13.842637
C	5.011379	7.273732	8.631466	O	-8.132977	2.669311	10.967743
C	2.403905	9.624836	7.325611	O	-4.829062	6.157685	13.817264
H	1.536605	9.847796	6.716385	O	-3.508053	3.782208	13.875853
C	3.100170	8.395278	7.342162	O	-5.824202	7.482810	12.265677
H	2.852557	7.524618	6.747339	O	-4.503996	0.465380	10.832440
C	0.692091	4.185957	7.273427	O	-3.040798	12.448488	12.294720
H	1.313315	4.812008	6.644639	O	-1.243899	14.585035	12.129972
O	3.711273	14.832685	11.018996	O	-2.817734	2.291756	12.309880
O	1.366938	12.266142	7.973741	O	-5.583193	2.750517	12.184223
O	4.858562	6.176644	8.017346	O	-6.833557	4.845170	9.716253
O	3.501946	3.837970	7.988850	O	0.104498	14.581573	14.652225
O	5.850786	7.509731	9.559804	S	0.028447	2.548464	12.726842
O	3.014403	12.461245	9.522724	S	-4.277570	9.880917	12.725136
O	1.193580	14.584257	9.660257	V	-2.550785	13.780897	10.923019
O	-0.038076	16.815697	10.881915	V	-5.386688	4.269081	13.421003
O	2.832931	2.349581	9.565299	V	-6.798384	6.380264	10.921088
O	-0.157037	14.536385	7.138421	V	-4.240535	2.024294	10.965511
S	0.006158	2.477590	9.105014	V	-6.764741	3.471892	10.955458
S	4.280497	9.899625	9.100338	V	-0.026202	13.660339	13.372948
V	2.508682	13.807729	10.876455	C	1.242358	3.430109	13.592727
V	-0.013800	13.632202	8.428577	C	2.650025	3.258533	13.204305
V	-0.028559	15.229545	10.891723	C	0.702488	4.300799	14.521881
C	-1.234652	3.313011	8.231353	H	1.317111	4.949482	15.134104
C	-2.635553	3.131078	8.635586	O	3.529796	3.931931	13.815591
C	-0.721763	4.186395	7.288916	O	2.851907	2.432173	12.257452
H	-1.356301	4.811649	6.672653	C	4.210920	8.433172	13.612333
O	-3.519197	3.803098	8.025076	C	2.925829	10.531197	13.571685
O	-2.830179	2.305971	9.586280	C	2.367264	11.833242	13.180718
C	-4.126000	8.380190	13.575728	C	5.097815	7.320402	13.244334
C	-1.217195	3.353027	13.620426	C	2.436430	9.635303	14.505554
C	-2.934765	10.532557	13.603315	H	1.566628	9.850680	15.114095
C	-2.416446	11.857134	13.233256	C	3.173964	8.429810	14.528110
C	-2.621823	3.122612	13.254449	H	2.958495	7.572929	15.154615
C	-4.988094	7.251621	13.198442	O	1.337489	12.242843	13.794315
C	-2.401505	9.627793	14.503619	O	4.966834	6.227413	13.869805

O	5.905096	7.556591	12.286379	H	-3.964725	14.423224	7.808267
O	2.980929	12.434549	12.240060	H	-4.213164	15.822998	6.711850
O	1.217454	14.594667	12.138016	H	-2.151331	15.527306	8.848954
S	4.293980	9.909452	12.710862	N	-8.964640	5.455867	13.544631
C	-4.191027	8.352957	8.239182	H	-8.098519	5.157106	13.000474
C	-2.926663	10.464341	8.268261	C	-8.524335	6.449873	14.562693
C	-2.384730	11.777573	8.645547	H	-8.059856	7.284259	14.035562
C	-5.076566	7.238549	8.607184	H	-9.386590	6.790836	15.139825
C	-2.415078	9.559744	7.354898	H	-7.791168	5.962934	15.206832
H	-1.538331	9.774882	6.756347	C	-9.608384	4.231947	14.091296
C	-3.140368	8.346750	7.339336	H	-10.509117	4.502134	14.646896
H	-2.906780	7.483078	6.728928	H	-9.850522	3.571377	13.256827
O	-6.165634	3.683260	7.193003	H	-8.882381	3.742105	14.741858
O	-1.358658	12.191476	8.028440	H	-9.546597	5.916265	12.837852
O	-4.927739	6.139100	7.994648	N	-6.172532	0.559009	8.400885
O	-5.901475	7.478737	9.546421	H	-5.985684	1.466245	8.929614
O	-3.006852	12.383406	9.577687	C	-5.119938	0.433739	7.355088
O	-1.267483	14.565620	9.652873	H	-4.150795	0.430162	7.855734
O	-5.586546	2.722536	9.706709	H	-5.267351	-0.491690	6.794051
O	-6.823296	4.876889	12.192957	H	-5.196605	1.302992	6.700682
S	-4.301174	9.841174	9.118169	C	-7.569099	0.605212	7.892024
V	-5.426641	4.264285	8.465143	H	-7.799742	-0.316846	7.353804
Cl	-0.008958	12.006740	10.911596	H	-8.238788	0.736141	8.743863
Cl	3.997651	5.179563	10.910803	H	-7.649544	1.470670	7.232564
Cl	-3.981109	5.094592	10.920634	H	-6.044519	-0.166531	9.113101
N	2.781471	16.181477	13.471302	N	9.020032	5.532074	8.439599
H	3.471049	16.450366	12.762567	H	8.128540	5.131210	8.829158
C	2.036481	17.353756	14.002375	C	8.667368	6.355256	7.250842
H	1.583849	17.880872	13.160591	H	7.990501	7.143767	7.582804
H	1.250252	16.973913	14.656490	H	9.574643	6.786110	6.822538
H	2.716468	18.009201	14.551040	H	8.156499	5.713451	6.532073
C	3.424524	15.318680	14.501026	C	9.972337	4.418271	8.199258
H	2.637289	14.933403	15.150161	H	10.922769	4.817221	7.838904
H	3.917312	14.493649	13.984965	H	10.110182	3.880553	9.138866
H	4.149093	15.904580	15.070713	H	9.533045	3.749741	7.457053
H	2.093234	15.570863	12.933205	H	9.321434	6.141727	9.215533
N	-2.846021	16.126843	8.306771	N	6.366192	0.440108	13.090700
H	-3.537462	16.394217	9.014303	H	5.739451	0.073317	12.346970
C	-2.113468	17.302329	7.765671	C	7.761637	-0.029595	12.889022
H	-1.665245	17.840498	8.602802	H	8.054644	0.225799	11.869932
H	-1.324156	16.925356	7.113608	H	8.410110	0.482410	13.602001
H	-2.800614	17.946562	7.212660	H	7.802473	-1.109582	13.043980
C	-3.481490	15.249321	7.284895	C	5.777314	0.188543	14.432104
H	-2.691232	14.867245	6.637546	H	6.354955	0.737635	15.176827

H	4.751182	0.558950	14.423724	C	2.428451	9.657998	7.342898
H	5.792671	-0.883221	14.639593	H	1.558895	9.879609	6.736375
H	6.306423	1.464011	12.897350	C	3.126077	8.429443	7.358363
O	7.978571	2.227565	10.404206	H	2.877757	7.557889	6.765244
C	4.972801	-0.021874	7.836240	C	0.763817	4.179405	7.317970
C	3.879301	-0.746335	8.338408	H	1.387161	4.821469	6.707685
C	2.604474	-0.542755	7.820758	O	3.696933	14.871673	11.041240
C	2.396346	0.378740	6.789999	O	1.385360	12.292269	7.986341
C	3.481277	1.097668	6.292354	O	4.868059	6.205821	8.041738
C	4.764837	0.906018	6.809626	O	3.567105	3.815160	8.009886
H	4.028138	-1.447155	9.153702	O	5.888574	7.539494	9.561189
H	1.766519	-1.097005	8.234410	O	3.024648	12.494892	9.542787
H	1.398823	0.544064	6.394348	O	1.187016	14.606146	9.670882
H	3.335954	1.836650	5.509373	O	-0.067550	16.828861	10.884972
H	5.578691	1.507549	6.426824	O	2.908439	2.305824	9.577651
S	6.561526	-0.352341	8.566717	O	-0.152986	14.549084	7.143047
C	7.667772	0.773230	7.662872	S	0.073168	2.435707	9.114212
H	7.716252	0.517084	6.600353	S	4.309734	9.935306	9.112182
H	7.350283	1.809063	7.789771	V	2.502230	13.838011	10.892834
H	8.654803	0.642009	8.113081	V	-0.007226	13.645411	8.433569
				V	-0.045072	15.242810	10.896792
				C	-1.165677	3.289486	8.254797
206, $\nu^{\neq} = 386.15$ *i*cm^{-1}				C	-2.568887	3.103765	8.648691
3-TS3, B3LYP/6-311++G(d,p)=-11626.656705				C	-0.649837	4.181500	7.331732
O	8.305914	7.008470	10.834221	H	-1.282939	4.821680	6.729474
O	6.311938	3.999919	7.198696	O	-3.448123	3.778659	8.034702
O	8.525065	3.222204	11.403632	O	-2.770936	2.273369	9.593302
O	4.616928	0.548902	11.135875	C	-4.102607	8.362684	13.566046
O	5.586477	2.837015	9.682687	C	-1.177263	3.333373	13.619066
O	6.834175	4.978381	12.158088	C	-2.927999	10.524301	13.596607
V	5.438133	4.330420	8.487927	C	-2.419263	11.853389	13.228485
V	6.815136	6.447016	10.959180	C	-2.580387	3.097450	13.253919
V	4.335345	2.097435	10.934623	C	-4.956354	7.228522	13.186985
V	6.923241	3.483557	10.906820	C	-2.389592	9.623364	14.497660
O	6.220827	3.786944	14.655923	H	-1.528147	9.861704	15.109375
O	5.701665	2.844096	12.145639	C	-3.065049	8.381988	14.481146
O	6.905284	4.895831	9.712777	H	-2.804995	7.517480	15.079648
V	5.484352	4.390583	13.383303	C	-0.674943	4.252823	14.522729
C	4.169887	8.431035	8.266203	H	-1.318282	4.872351	15.135515
C	1.295243	3.284367	8.228542	O	-8.242125	6.879642	11.052651
C	2.955387	10.570968	8.238812	O	-6.203898	3.907955	14.694401
C	2.416506	11.888011	8.603434	O	-3.776983	14.775636	10.754443
C	2.703208	3.116931	8.621656	O	-1.399511	12.286411	13.843348
C	5.038643	7.306610	8.644005	O	-8.079732	2.635149	10.943613

O	-4.793018	6.135406	13.806037	C	-3.085368	8.331503	7.339219
O	-3.468651	3.759928	13.869983	H	-2.841349	7.468201	6.732356
O	-5.791772	7.454954	12.252116	O	-6.087737	3.653131	7.180772
O	-4.456568	0.433417	10.828549	O	-1.339614	12.193528	8.027307
O	-3.043913	12.438739	12.286400	O	-4.862256	6.112169	7.989130
O	-1.262326	14.590094	12.129288	O	-5.853156	7.449096	9.532238
O	-2.775317	2.259280	12.315199	O	-2.996748	12.374160	9.568450
O	-5.537583	2.722162	12.174754	O	-1.273723	14.569016	9.652461
O	-6.777808	4.813378	9.698487	O	-5.527021	2.693706	9.697986
O	0.074574	14.598890	14.657997	O	-6.780851	4.847087	12.175723
S	0.073209	2.520180	12.738942	S	-4.268164	9.821531	9.107163
S	-4.263615	9.862476	12.715208	V	-5.359333	4.236258	8.458403
V	-2.556519	13.774700	10.916520	Cl	-0.005119	12.021008	10.917527
V	-5.345170	4.244388	13.408872	Cl	4.014464	5.214376	10.918158
V	-6.754199	6.349254	10.902358	Cl	-3.934338	5.069340	10.919050
V	-4.190167	1.991852	10.963771	N	2.758253	16.197502	13.494747
V	-6.713612	3.441723	10.940056	H	3.450290	16.464443	12.787528
V	-0.043576	13.675506	13.378873	C	2.015666	17.371205	14.025377
C	1.282381	3.417843	13.594430	H	1.567156	17.901207	13.183170
C	2.693175	3.249026	13.212847	H	1.226324	16.993026	14.676713
C	0.737920	4.300371	14.509398	H	2.696110	18.023800	14.576906
H	1.349870	4.961317	15.111039	C	3.396144	15.331274	14.524758
O	3.564318	3.934838	13.823064	H	2.606142	14.946566	15.170845
O	2.906690	2.414298	12.277262	H	3.888328	14.505968	14.008610
C	4.203432	8.461894	13.614648	H	4.120501	15.914464	15.097520
C	2.918383	10.560141	13.582169	H	2.069727	15.589895	12.953460
C	2.359518	11.862166	13.195419	N	-2.853799	16.121340	8.301026
C	5.092648	7.350759	13.242431	H	-3.550281	16.384293	9.005205
C	2.429238	9.660690	14.512846	C	-2.124476	17.301017	7.764946
H	1.559323	9.873535	15.122183	H	-1.683506	17.840632	8.604993
C	3.167244	8.455354	14.531001	H	-1.329627	16.928550	7.117021
H	2.952320	7.596090	15.154390	H	-2.811836	17.942239	7.208649
O	1.326566	12.268307	13.806969	C	-3.478913	15.241250	7.275107
O	4.966831	6.258261	13.871094	H	-2.683015	14.864179	6.631736
O	5.892754	7.587860	12.281407	H	-3.960127	14.411929	7.795252
O	2.975351	12.469972	12.259961	H	-4.210819	15.811227	6.698623
O	1.199174	14.617336	12.148737	H	-2.158437	15.524742	8.846443
S	4.286263	9.940828	12.718520	N	-8.920548	5.435687	13.525061
C	-4.141408	8.331784	8.232783	H	-8.054701	5.131590	12.983234
C	-2.893814	10.453254	8.263469	C	-8.478421	6.431771	14.540301
C	-2.364781	11.772105	8.640504	H	-8.009847	7.262444	14.010968
C	-5.021295	7.212196	8.598148	H	-9.340524	6.778022	15.114516
C	-2.369646	9.550216	7.355779	H	-7.748177	5.944548	15.187528
H	-1.490823	9.770474	6.762161	C	-9.569938	4.216363	14.074907

H	-10.470424	4.491944	14.628277	H	5.273395	-1.423812	9.420160
H	-9.813724	3.553911	13.242389	H	3.002214	-1.793608	8.517846
H	-8.846834	3.725799	14.728157	H	2.137581	-0.347024	6.686464
H	-9.499039	5.895858	12.815216	H	3.578030	1.460434	5.759672
N	-6.121762	0.534703	8.393216	H	5.816585	1.855849	6.675746
H	-5.930456	1.441894	8.921502	S	7.298459	0.433676	8.862078
C	-5.067076	0.402384	7.350666	C	8.247591	1.295381	7.576505
H	-4.099357	0.395115	7.854096	H	8.234092	0.716348	6.649827
H	-5.217467	-0.523225	6.790615	H	7.833428	2.292775	7.416849
H	-5.137602	1.271083	6.694816	H	9.266956	1.366868	7.959695
C	-7.516621	0.588923	7.880735				
H	-7.751682	-0.332258	7.342847				
H	-8.187530	0.725174	8.730764	207			
H	-7.589929	1.454208	7.220208	3-7, B3LYP/6-311++G(d,p)=-11701.89745			
H	-5.999942	-0.190452	9.106879	O	8.252677	6.985433	10.737386
N	9.223705	5.547273	8.686105	O	6.262898	3.912580	7.141147
H	8.300347	5.104469	8.938815	O	8.546908	3.230765	11.327836
C	9.034845	6.320419	7.431848	O	4.422616	0.560142	10.980971
H	8.254517	7.061394	7.612384	O	5.582530	2.774998	9.632790
H	9.970527	6.813053	7.159018	O	6.825644	4.950613	12.121447
H	8.710233	5.636295	6.646459	V	5.387543	4.272612	8.414836
C	10.284965	4.511466	8.668181	V	6.765787	6.433384	10.908401
H	11.258572	4.985952	8.527282	V	4.245741	2.126293	10.868571
H	10.245550	3.974418	9.617770	V	6.823468	3.510309	10.888281
H	10.082093	3.821457	7.847301	O	6.246441	3.805207	14.658372
H	9.335341	6.196105	9.487717	O	5.688600	2.777700	12.095287
N	6.642885	1.052856	13.782032	O	6.795424	4.888499	9.672430
H	6.274586	1.749183	13.069707	V	5.483786	4.322794	13.384518
C	7.547912	0.108271	13.075329	C	4.097754	8.376452	8.214010
H	8.332916	0.687694	12.587891	C	1.220163	3.320533	8.157242
H	7.965283	-0.606568	13.788167	C	2.883439	10.516275	8.190780
H	6.958306	-0.402501	12.313089	C	2.354507	11.837268	8.559462
C	5.461366	0.432976	14.441473	C	2.625971	3.143419	8.549349
H	5.794285	-0.302118	15.177613	C	4.973557	7.258640	8.592992
H	4.893712	1.229549	14.924300	C	2.358572	9.606638	7.290240
H	4.855646	-0.036236	13.665027	H	1.491440	9.830314	6.680964
H	7.146180	1.646418	14.449433	C	3.056805	8.377789	7.302686
O	7.871336	2.003053	10.279910	H	2.810539	7.509182	6.704250
C	5.706387	0.221566	8.092273	C	0.683837	4.192753	7.227507
C	4.905227	-0.806676	8.608443	H	1.302267	4.813434	6.590413
C	3.625474	-1.008536	8.100477	O	3.699018	14.801042	10.986914
C	3.141655	-0.196733	7.072071	O	1.323032	12.251372	7.950612
C	3.949648	0.813406	6.548590	O	4.833879	6.160557	7.977458
C	5.229063	1.032411	7.056867	O	3.511827	3.795968	7.916906

O	5.803948	7.502662	9.526920	S	0.047914	2.560535	12.721327
O	2.975498	12.436097	9.495368	S	-4.295632	9.890977	12.731003
O	1.173665	14.573126	9.638324	V	-2.569632	13.792660	10.916390
O	-0.040257	16.814374	10.860180	V	-5.366763	4.272430	13.433095
O	2.815475	2.363785	9.531556	V	-6.808626	6.376075	10.941667
O	-0.184395	14.536071	7.121537	V	-4.220731	2.039625	10.968621
S	0.003208	2.502037	9.077965	V	-6.755914	3.469141	10.976387
S	4.233923	9.877672	9.066443	V	-0.037723	13.665254	13.358678
V	2.486576	13.786596	10.850312	C	1.267346	3.408383	13.612407
V	-0.044258	13.630004	8.410848	C	2.672248	3.233752	13.209806
V	-0.039415	15.228258	10.873901	C	0.733146	4.258126	14.563367
C	-1.239857	3.338100	8.209204	H	1.351871	4.883417	15.195562
C	-2.638445	3.157765	8.626015	O	3.565122	3.887186	13.823042
C	-0.730262	4.202828	7.257010	O	2.854093	2.431900	12.240553
H	-1.366272	4.828866	6.642971	C	4.161396	8.404377	13.578015
O	-3.527905	3.828633	8.023199	C	2.885497	10.508457	13.544118
O	-2.822521	2.333598	9.579146	C	2.336092	11.814993	13.157154
C	-4.131731	8.390343	13.579759	C	5.052416	7.294479	13.207093
C	-1.193623	3.352541	13.632319	C	2.393597	9.612185	14.476514
C	-2.950071	10.547705	13.600976	H	1.526019	9.829630	15.087548
C	-2.436506	11.873354	13.228818	C	3.126123	8.403132	14.495292
C	-2.597441	3.137404	13.257524	H	2.908350	7.546082	15.120805
C	-4.990496	7.257783	13.208195	O	1.312660	12.234497	13.775137
C	-2.406655	9.644564	14.496861	O	4.932072	6.200482	13.828517
H	-1.538901	9.879877	15.100750	O	5.854965	7.543171	12.246904
C	-3.086050	8.405486	14.485622	O	2.951305	12.412577	12.214643
H	-2.823133	7.539335	15.080452	O	1.207219	14.586938	12.115890
C	-0.680825	4.227562	14.573695	S	4.249191	9.882094	12.679547
H	-1.316205	4.827010	15.214276	C	-4.230586	8.363683	8.242610
O	-8.296301	6.901572	11.109871	C	-2.969486	10.476662	8.263953
O	-6.212963	3.928936	14.724947	C	-2.424760	11.789541	8.638084
O	-3.778110	14.809292	10.763727	C	-5.109644	7.246428	8.616286
O	-1.409262	12.298813	13.836696	C	-2.462483	9.573240	7.346908
O	-8.116496	2.653231	10.993048	H	-1.589669	9.790049	6.743256
O	-4.821551	6.164771	13.825983	C	-3.185998	8.359310	7.335705
O	-3.484370	3.796339	13.879570	H	-2.955064	7.495848	6.724008
O	-5.834788	7.484599	12.281508	O	-6.180718	3.680658	7.209520
O	-4.475273	0.478954	10.834738	O	-1.401780	12.201326	8.014391
O	-3.063219	12.463742	12.291255	O	-4.961265	6.148351	8.000967
O	-1.254538	14.593526	12.117290	O	-5.928305	7.482025	9.562047
O	-2.794403	2.317234	12.303065	O	-3.040293	12.396531	9.573582
O	-5.561898	2.753758	12.196064	O	-1.287377	14.570491	9.640342
O	-6.842140	4.841042	9.736207	O	-5.579427	2.729196	9.719368
O	0.107070	14.588569	14.634976	O	-6.816724	4.872145	12.213891

S	-4.337165	9.851328	9.122978	C	-7.601243	0.615399	7.952464
V	-5.438895	4.270327	8.476313	H	-7.846725	-0.308124	7.423308
Cl	-0.044487	12.005684	10.895509	H	-8.256437	0.756712	8.813808
Cl	3.972128	5.129098	10.865278	H	-7.685731	1.477542	7.289143
Cl	-3.986485	5.111493	10.922779	H	-6.063293	-0.159328	9.154931
N	2.802568	16.145564	13.446327	N	9.069228	5.519271	8.508892
H	3.491967	16.401167	12.732376	H	8.173191	5.077339	8.834697
C	2.083878	17.331305	13.983201	C	8.771039	6.285726	7.269591
H	1.635700	17.867882	13.144991	H	8.016843	7.034582	7.515826
H	1.295072	16.966181	14.642570	H	9.682362	6.767564	6.909581
H	2.779997	17.973332	14.527491	H	8.368802	5.596065	6.526531
C	3.436968	15.270291	14.470958	C	10.117503	4.474834	8.395700
H	2.647677	14.899530	15.125986	H	11.065675	4.937168	8.113219
H	3.910154	14.436373	13.950902	H	10.201829	3.975924	9.362286
H	4.176784	15.842304	15.035137	H	9.805094	3.754579	7.637728
H	2.099621	15.548535	12.912307	H	9.255952	6.170568	9.291287
N	-2.858698	16.144919	8.303817	N	6.836970	0.234991	12.520186
H	-3.545501	16.417663	9.013741	H	6.895019	-0.095852	11.516385
C	-2.117819	17.314407	7.761147	C	8.201368	0.419927	13.079456
H	-1.662105	17.847925	8.597203	H	8.735684	1.137263	12.458605
H	-1.333895	16.930990	7.106333	H	8.117709	0.808159	14.096647
H	-2.801111	17.964995	7.210763	H	8.714965	-0.543641	13.081232
C	-3.504543	15.273321	7.283485	C	5.985956	-0.706722	13.293806
H	-2.719356	14.884792	6.633789	H	5.874364	-0.329872	14.312840
H	-3.993185	14.451097	7.807945	H	5.017481	-0.760345	12.798724
H	-4.232978	15.853339	6.712664	H	6.467078	-1.686896	13.305761
H	-2.166972	15.538856	8.843257	H	6.365149	1.157153	12.477523
N	-8.940650	5.456511	13.591237	O	8.043648	2.312132	10.324948
H	-8.081576	5.154267	13.038040	C	5.310254	-0.094715	8.039943
C	-8.487272	6.452544	14.601636	C	4.429060	-1.060705	8.516538
H	-8.027476	7.284760	14.067081	C	3.132639	-1.094870	8.004934
H	-9.342549	6.796327	15.187412	C	2.737581	-0.174246	7.030340
H	-7.747634	5.966206	15.238759	C	3.637139	0.785346	6.561832
C	-9.580964	4.235728	14.148590	C	4.933246	0.838974	7.075985
H	-10.474646	4.509575	14.713708	H	4.749496	-1.733249	9.304211
H	-9.834611	3.573494	13.318845	H	2.423967	-1.826589	8.381633
H	-8.848669	3.745864	14.792029	H	1.720223	-0.192728	6.650341
H	-9.529132	5.916285	12.889396	H	3.323497	1.520515	5.827192
N	-6.197367	0.562348	8.439990	H	5.615323	1.624217	6.764889
H	-5.995494	1.472310	8.959855	S	6.973117	0.033110	8.733195
C	-5.161713	0.424111	7.379484	C	7.802862	-1.020477	7.490437
H	-4.185268	0.417356	7.865826	H	7.343733	-2.011907	7.511026
H	-5.323204	-0.503535	6.825903	H	7.688442	-0.560772	6.505071
H	-5.242705	1.290181	6.721312	H	8.859376	-1.081702	7.763544

O	7.026272	-0.823499	10.012788	V	0.023309	13.575842	8.394616
				V	-0.014161	15.191985	10.845557
				C	-1.135176	3.264881	8.288229
207, $\nu^{\neq} = 427.16\ i\text{cm}^{-1}$				C	-2.540212	3.075105	8.675969
3-TS4, B3LYP/6-311++G(d,p)=-11701.867125				C	-0.615004	4.144235	7.355390
O	8.320132	6.971638	10.882735	H	-1.244845	4.774976	6.739903
O	6.358499	3.854963	7.265934	O	-3.420464	3.740130	8.053363
O	8.560621	3.235495	11.465895	O	-2.740569	2.249848	9.625183
O	4.635220	0.522251	11.155094	C	-4.101236	8.348850	13.555694
O	5.623344	2.789226	9.749693	C	-1.158175	3.318443	13.657897
O	6.845342	4.951199	12.220618	C	-2.927034	10.510585	13.573291
V	5.480471	4.261335	8.530260	C	-2.414589	11.835520	13.196196
V	6.829273	6.415523	11.004874	C	-2.559827	3.085675	13.283385
V	4.351011	2.072674	10.998583	C	-4.952042	7.210697	13.182317
V	6.936900	3.473966	10.985887	C	-2.392348	9.617207	14.484077
O	6.250827	3.743245	14.722539	H	-1.533429	9.860802	15.097255
O	5.722229	2.810949	12.212329	C	-3.067528	8.375729	14.474932
O	6.924666	4.856990	9.764834	H	-2.809962	7.516097	15.081467
V	5.503614	4.347169	13.457619	C	-0.658696	4.240346	14.560685
C	4.206564	8.355652	8.265890	H	-1.303830	4.865605	15.165697
C	1.325241	3.258811	8.274046	O	-8.231525	6.836009	11.044274
C	2.981115	10.488913	8.223942	O	-6.188181	3.893757	14.708189
C	2.437127	11.806252	8.582819	O	-3.747836	14.744273	10.693944
C	2.729808	3.084118	8.672730	O	-1.396421	12.270887	13.812223
C	5.078260	7.240048	8.659696	O	-8.052570	2.590233	10.962428
C	2.472152	9.574728	7.318873	O	-4.787301	6.122263	13.809240
H	1.611213	9.792722	6.698868	O	-3.450499	3.753334	13.890044
C	3.176415	8.349754	7.342428	O	-5.785897	7.428742	12.244157
H	2.941804	7.478557	6.743124	O	-4.419023	0.404358	10.865886
C	0.798858	4.141197	7.347957	O	-3.033312	12.414897	12.246602
H	1.424804	4.772725	6.729318	O	-1.239230	14.556597	12.079066
O	3.725242	14.796533	11.006589	O	-2.749827	2.244589	12.346462
O	1.409027	12.208740	7.960292	O	-5.513037	2.696087	12.197255
O	4.935588	6.135613	8.054421	O	-6.758454	4.766177	9.705498
O	3.608509	3.751140	8.044505	O	0.090190	14.579839	14.612563
O	5.904856	7.485452	9.595100	S	0.095074	2.494510	12.792169
O	3.040959	12.414059	9.524168	S	-4.259127	9.841597	12.692027
O	1.218797	14.537963	9.629381	V	-2.533663	13.737947	10.868177
O	-0.026704	16.777971	10.821040	V	-5.329001	4.226673	13.422182
O	2.922642	2.291665	9.646188	V	-6.741525	6.310203	10.899807
O	-0.110681	14.471088	7.097115	V	-4.160708	1.964715	10.993247
S	0.098303	2.423878	9.166237	V	-6.690282	3.403256	10.956385
S	4.325240	9.859509	9.116302	V	-0.030414	13.646266	13.341207
V	2.523411	13.770611	10.862536	C	1.301879	3.391954	13.651520

C	2.713492	3.216598	13.278541	H	1.250572	16.970160	14.609837
C	0.754373	4.281872	14.557649	H	2.724521	17.994460	14.505232
H	1.364404	4.943300	15.160701	C	3.414833	15.299060	14.483127
O	3.583573	3.909516	13.883751	H	2.620979	14.924025	15.130190
O	2.931226	2.372508	12.352418	H	3.905919	14.466698	13.977349
C	4.204630	8.420279	13.644367	H	4.139229	15.885363	15.052632
C	2.917115	10.516422	13.585403	H	2.095457	15.546561	12.904225
C	2.361595	11.815687	13.182716	N	-2.808214	16.068574	8.234157
C	5.099961	7.310532	13.284665	H	-3.505734	16.341560	8.933462
C	2.427728	9.627422	14.525987	C	-2.069113	17.239452	7.692006
H	1.557304	9.846470	15.132401	H	-1.627778	17.782488	8.529645
C	3.167235	8.423052	14.559412	H	-1.274327	16.856975	7.049864
H	2.952682	7.571526	15.193529	H	-2.750202	17.880903	7.128337
O	1.328156	12.231542	13.786306	C	-3.435130	15.184923	7.212354
O	4.982670	6.222017	13.921903	H	-2.639193	14.797584	6.575160
O	5.899603	7.547972	12.322109	H	-3.924200	14.362908	7.736747
O	2.982379	12.410478	12.242312	H	-4.160696	15.755473	6.628494
O	1.222120	14.569378	12.107106	H	-2.118945	15.471594	8.786566
S	4.286417	9.888869	12.730785	N	-8.909624	5.404975	13.525593
C	-4.130394	8.280631	8.219106	H	-8.042128	5.101033	12.986586
C	-2.878374	10.399207	8.237684	C	-8.472538	6.409097	14.535138
C	-2.345342	11.718242	8.607431	H	-8.006548	7.238269	14.001197
C	-5.010628	7.163721	8.591244	H	-9.336668	6.755544	15.106160
C	-2.355938	9.489896	7.335270	H	-7.741234	5.928747	15.186289
H	-1.476443	9.704935	6.740747	C	-9.554676	4.186455	14.082471
C	-3.074313	8.272808	7.325603	H	-10.456761	4.461924	14.633262
H	-2.832256	7.405311	6.723977	H	-9.795085	3.517856	13.253898
O	-6.060151	3.588837	7.196231	H	-8.830257	3.702881	14.739461
O	-1.316686	12.130968	7.993925	H	-9.489491	5.858375	12.812537
O	-4.850961	6.060505	7.988141	N	-6.094293	0.480258	8.437097
O	-5.842387	7.405357	9.524075	H	-5.901983	1.392112	8.956518
O	-2.976820	12.329209	9.529731	C	-5.041131	0.337989	7.394324
O	-1.242043	14.515692	9.602130	H	-4.072693	0.334802	7.896439
O	-5.498392	2.652322	9.720986	H	-5.192638	-0.592650	6.842994
O	-6.765264	4.815856	12.182851	H	-5.112343	1.200613	6.730571
S	-4.254362	9.775602	9.084674	C	-7.489950	0.530047	7.926078
V	-5.337272	4.186084	8.470363	H	-7.725817	-0.395994	7.396986
Cl	0.006919	11.970083	10.891591	H	-8.159564	0.674287	8.775789
Cl	4.034482	5.164990	10.950731	H	-7.564044	1.389223	7.257713
Cl	-3.918500	5.044151	10.930033	H	-5.971736	-0.238475	9.157087
N	2.784102	16.157058	13.441850	N	9.281154	5.446389	8.779089
H	3.479930	16.414566	12.734891	H	8.344491	5.038833	9.041479
C	2.043753	17.338844	13.957727	C	9.100104	6.222751	7.524719
H	1.600395	17.861845	13.108456	H	8.352616	6.994234	7.716009

H	10.049235	6.677033	7.232827
H	8.735762	5.547476	6.749018
C	10.299383	4.367626	8.742174
H	11.286109	4.799907	8.562463
H	10.268517	3.844585	9.699548
H	10.040440	3.676787	7.937591
H	9.430772	6.092173	9.573973
N	6.796274	0.989218	13.778933
H	6.392409	1.645821	13.058780
C	7.934028	0.239708	13.173724
H	8.676674	0.964893	12.840619
H	8.353519	-0.439080	13.919740
H	7.570579	-0.313444	12.305882
C	5.677662	0.147649	14.285679
H	6.054747	-0.544399	15.041557
H	4.924822	0.810361	14.715188
H	5.250273	-0.387628	13.437361
H	7.112985	1.634233	14.512472
O	7.891872	1.990852	10.422094
C	5.660927	-0.035936	8.335308
C	5.014049	-1.203941	8.736079
C	3.787193	-1.524716	8.158236
C	3.215741	-0.677072	7.206347
C	3.878587	0.488501	6.817446
C	5.108260	0.822307	7.383897
H	5.467389	-1.833048	9.492589
H	3.271030	-2.430058	8.463560
H	2.250584	-0.921966	6.772543
H	3.433671	1.157195	6.086648
H	5.597999	1.744718	7.100167
S	7.192185	0.378619	9.206305
C	8.239903	0.848565	7.799469
H	8.249313	0.044580	7.060637
H	7.839439	1.776303	7.381960
H	9.235747	1.017181	8.213539
O	7.715883	-0.882224	9.839417

4

H_2O_2, B3LYP/6-311++G(d,p)=-151.6197

O	-0.084196	0.213180	0.354700
H	-0.327447	1.129298	0.132302
O	1.335028	0.251550	0.031507
H	1.708152	0.055865	0.909223

6

CH_3OH, B3LYP/6-311++G(d,p)=-115.77696

C	-1.654178	-0.803575	0.032180
H	-1.280250	-1.830782	0.050280
H	-1.295816	-0.325908	-0.893062
H	-2.754293	-0.841080	0.000353
O	-1.161556	-0.169901	1.201787
H	-1.485036	0.743155	1.199261

3

H_2O, B3LYP/6-311++G(d,p)=-76.472682

O	-0.368409	0.356883	-0.004989
H	0.598980	0.406205	-0.004989
H	-0.644837	1.285248	-0.004989

9

$CH_3OH + H_2O$, B3LYP/6-311++G(d,p)=-192.25204

O	2.007765	4.234619	-1.385705
H	2.133668	4.722839	-2.215845
H	2.385901	4.821687	-0.712317
C	4.012503	2.171522	-3.644987
H	4.242256	1.248294	-3.089633
H	2.990285	2.081675	-4.046587
H	4.703545	2.236819	-4.490986
O	4.192658	3.336855	-2.862121
H	3.538484	3.313923	-2.139064

16

S1, B3LYP/6-311++G(d,p)=-669.889369

C	-0.395336	-0.094024	0.279020
C	0.968860	-0.003314	-0.020057
C	1.554857	1.246100	-0.235427
C	0.796052	2.411610	-0.156409
C	-0.566023	2.320620	0.142189
C	-1.159497	1.081325	0.358469
H	1.582784	-0.893868	-0.087838
H	2.615260	1.300583	-0.466749
H	1.257419	3.380012	-0.324878
H	-1.171404	3.220517	0.207393

H	-2.219371	1.018833	0.590236	H	2.100179	0.326972	1.671050
S	-1.258380	-1.624883	0.573865	H	1.492629	-1.174920	2.442398
C	0.047941	-2.878428	0.385688	H	2.769314	-1.272522	1.185263
H	-0.436705	-3.842104	0.559218	O	-0.547731	-0.057737	0.704581
H	0.468956	-2.870201	-0.623275	O	0.406613	-2.334931	0.011157
H	0.842438	-2.743282	1.124500				

17

S2, B3LYP/6-311++G(d,p)=-745.10085

C	-0.393039	-0.055127	0.121818
C	0.967088	0.024617	-0.177417
C	1.560702	1.280623	-0.299861
C	0.798600	2.436265	-0.108650
C	-0.557730	2.339140	0.207791
C	-1.161303	1.086553	0.328277
H	1.558032	-0.878665	-0.310267
H	2.618003	1.357967	-0.536687
H	1.266249	3.412510	-0.198312
H	-1.145260	3.239460	0.363996
H	-2.210238	0.969694	0.584353
S	-1.203971	-1.673548	0.320051
C	-1.303474	-2.042976	-1.477419
H	-1.892695	-1.259517	-1.960510
H	-0.295938	-2.087091	-1.899643
H	-1.801699	-3.009947	-1.582831
O	-2.616200	-1.409533	0.794244

18

PhSOOCH3, B3LYP/6-311++G(d,p)=-820.338352

S	0.581371	-0.899185	0.279267
C	1.315586	-0.148058	-1.176795
C	1.140972	1.218253	-1.396519
C	2.050427	-0.945570	-2.054010
C	1.731200	1.799749	-2.517952
H	0.537012	1.800201	-0.708509
C	2.635913	-0.352482	-3.171882
H	2.138511	-2.010442	-1.866724
C	2.479113	1.016551	-3.400071
H	1.601013	2.860981	-2.707526
H	3.207002	-0.959267	-3.868133
H	2.935289	1.473674	-4.273376
C	1.883064	-0.732342	1.522894

21

H_2O_2+PhSOCH3, B3LYP/6-311++G(d,p)=-896.730848

C	-0.039532	0.807328	0.301820
C	1.006812	0.670319	1.214370
C	1.486914	1.804653	1.868038
C	0.910872	3.052668	1.617315
C	-0.147314	3.169618	0.714197
C	-0.631741	2.041493	0.050728
H	1.440947	-0.306115	1.415768
H	2.304030	1.713641	2.577722
H	1.283110	3.932815	2.133434
H	-0.598164	4.140045	0.527447
H	-1.459528	2.092574	-0.649428
S	-0.691150	-0.658406	-0.548380
C	0.642872	-0.784434	-1.794113
H	0.662462	0.144591	-2.368976
H	1.595436	-0.943207	-1.281733
H	0.396884	-1.635904	-2.430036
O	-1.934803	-0.170537	-1.296122
O	-2.371622	-2.090760	-3.176886
H	-2.347149	-1.298096	-2.580483
O	-1.568365	-3.002244	-2.376903
H	-2.264093	-3.546248	-1.968462

21, $\nu^{\neq} = 856.96\ i\text{cm}^{-1}$

TS_{OX}, B3LYP/6-311++G(d,p)=-896.681446

C	-0.538273	-0.280349	1.326523
C	0.399683	-0.497680	2.339287
C	0.831425	0.599016	3.084375
C	0.328156	1.875522	2.823220
C	-0.622079	2.067024	1.818255
C	-1.066870	0.983476	1.062621
H	0.751860	-1.500010	2.552798
H	1.556010	0.451523	3.879450
H	0.669151	2.721520	3.412714

H	-1.022305	3.057950	1.626039
H	-1.821359	1.100168	0.291428
S	-1.149833	-1.640333	0.317889
C	0.149123	-1.737868	-0.954200
H	0.146106	-0.799298	-1.512860
H	1.106230	-1.905002	-0.459243
H	-0.099207	-2.573867	-1.612126
O	-2.419726	-1.213055	-0.353331
O	0.286467	-4.614103	2.363153
H	1.164234	-4.443742	1.977505
O	-0.529944	-3.043778	1.515790
H	-0.698917	-3.990708	1.250908

7

I, B3LYP/6-311++G(d,p)=-846.251992

B	-0.856348	-0.359041	0.175531
O	-1.908883	0.538024	0.609208
O	0.375850	-0.516058	0.915285
O	-0.535989	-0.094911	-1.419935
O	-1.504870	-1.833662	-0.174977
V	-1.229028	-1.703196	-1.991755
O	-0.340672	-2.744304	-2.754477

11

II, B3LYP/6-311++G(d,p)=-997.891795

S	-1.131907	-0.463986	-0.124345
O	-2.526999	0.014888	-0.241868
O	-0.297418	0.032209	0.943228
O	-0.475962	-0.336486	-1.584012
O	-1.171178	-2.083095	-0.194229
V	-0.814084	-2.147728	-2.033329
O	0.383178	-2.961657	-2.635312
O	-3.299165	-0.536184	-2.800620
H	-3.102838	-0.342085	-1.830458
O	-2.604154	-1.817875	-2.977433
H	-2.829317	-2.018458	-3.903959

11, $\nu^{\neq}$ = 762.71 *i*cm^{-1}

TSIA, B3LYP/6-311++G(d,p)=-997.870728

S	-0.045639	0.876278	1.400949
O	-1.331078	1.543953	1.463804
O	0.976954	1.082974	2.401925
O	0.573718	1.045207	-0.107042
O	-0.265087	-0.741161	1.160325
V	0.312186	-0.751151	-0.578307
O	1.583339	-1.578585	-0.958934
O	-0.789922	1.213951	-2.694779
H	-0.528875	1.624092	-1.837699
O	-0.778009	-0.415531	-2.047278
H	-0.606514	-0.825233	-2.916488

11, $\nu^{\neq}$ = 1539.79 *i*cm^{-1}

TSIB, B3LYP/6-311++G(d,p)=-997.845633

S	-1.819534	-0.693549	-0.520571
O	-3.231603	-0.369044	-0.576752
O	-0.982318	-0.275607	0.583035
O	-1.115280	-0.310377	-1.960816
O	-1.600689	-2.282252	-0.848668
V	-0.765203	-2.036167	-2.481910
O	0.787906	-2.541887	-2.738135
H	0.346284	-2.578506	-3.926441
O	-0.731667	-2.289253	-4.562930
O	-1.634191	-3.267831	-3.903186
H	-2.493869	-3.062138	-4.325642

11, $\nu^{\neq}$ = 1182.95 *i*cm^{-1}

TSIC, B3LYP/6-311++G(d,p)=-997.865958

S	-2.421983	-0.618185	-0.903988
O	-3.660245	-0.151636	-1.499659
O	-2.033798	-0.252800	0.439536
O	-1.162473	-0.186197	-1.946699
O	-2.198998	-2.172394	-1.189229
V	-0.793814	-2.059811	-2.470469
O	0.513374	-2.863671	-2.173694
H	-1.374001	-0.232456	-3.235174
O	-1.067917	-0.939973	-4.159138
O	-2.133778	-1.959849	-4.156717
H	-1.970207	-2.395437	-5.017623

11

IIIA, B3LYP/6-311++G(d,p)=-997.910557

S	0.184963	-0.424062	1.579693

O	-1.046724	-0.329234	2.337816
O	1.413766	-0.895473	2.179473
O	0.417919	0.912585	0.712872
O	-0.085947	-1.270677	0.180050
V	0.013592	0.118013	-0.982614
O	1.193499	-0.127974	-1.968094
O	-0.469498	1.969909	-1.421365
H	-1.012077	2.331239	-0.685186
O	-1.607799	0.125850	-1.869974
H	-1.570072	0.242011	-2.839553

11

IIIB, B3LYP/6-311++G(d,p)=-997.904801

S	-1.327514	-0.736770	-0.252028
O	-2.618069	-0.111475	-0.051354
O	-0.298832	-0.709963	0.768579
O	-0.696773	-0.300442	-1.700098
O	-1.525754	-2.271310	-0.811366
V	-0.813825	-1.962864	-2.480122
O	0.792924	-2.533129	-2.824029
H	1.547299	-2.513756	-2.208950
O	-2.035758	-1.762199	-3.802886
O	-2.139175	-3.198363	-3.494738
H	-2.988367	-3.253574	-3.004790

11

IIIC, B3LYP/6-311++G(d,p)=-997.899345

S	-0.914344	0.780277	1.304520
O	-1.972784	1.652140	0.831310
O	-0.469139	0.796574	2.677712
O	0.518703	1.262119	0.312479
O	-0.902516	-0.617673	0.654429
V	0.553851	-0.524538	-0.688639
O	1.877539	-1.311285	-0.391267
H	0.324252	2.094721	-0.160350
O	0.321393	0.054807	-2.442043
O	-0.358502	-1.254838	-2.359940
H	0.242561	-1.838676	-2.867296

11, $\nu^{\neq} = 1735.62\ i\text{cm}^{-1}$

TSII, B3LYP/6-311++G(d,p)=-997.869675

S	-1.275266	-0.209233	-0.357643
O	-2.680416	-0.042780	-0.056582
O	-0.246959	0.564451	0.301072
O	-1.032029	-0.276169	-1.953220
O	-0.862312	-1.827268	-0.236081
V	-0.701071	-2.123289	-2.002241
O	0.751230	-2.586457	-2.343169
O	-1.409178	-1.994211	-4.039020
H	-0.802821	-2.498110	-4.621798
O	-1.956233	-3.356661	-2.542496
H	-2.210402	-2.772313	-3.541030

11

IV, B3LYP/6-311++G(d,p)=-997.917206

S	-1.181437	-0.169617	-0.539139
O	-2.449058	0.218425	0.043958
O	0.021228	0.607325	-0.318340
O	-1.347364	-0.540851	-2.093661
O	-0.876845	-1.751497	-0.192829
V	-1.018724	-2.446139	-1.881474
O	0.352155	-3.203248	-2.220017
O	-1.460762	-2.155173	-3.924600
H	-1.482043	-1.188470	-4.065831
O	-2.076383	-3.759450	-1.734401
H	-0.794085	-2.539927	-4.520245

25

V, B3LYP/6-311++G(d,p)=-1666.570551

S	0.702871	-0.440046	-0.326927
O	1.089281	-0.024320	-1.682933
O	1.407736	0.121794	0.805942
O	0.662218	-2.049674	-0.264046
O	-0.892659	-0.276968	-0.171023
V	-1.228610	-2.141674	-0.200454
O	-1.914394	-2.800313	1.059512
O	-1.905301	-2.692640	-1.588022
C	-2.036857	-0.842310	-4.260608
C	-1.653583	0.232330	-3.450271
C	-2.237728	1.472914	-3.696466
C	-3.191778	1.619123	-4.706640
C	-3.571147	0.524402	-5.490299
C	-3.002605	-0.725960	-5.266744

H	-0.915576	0.130170	-2.665025	S	0.660773	-0.520840	-0.321236
H	-1.944747	2.322467	-3.088551	O	1.057746	0.071627	-1.609854
H	-3.645256	2.589639	-4.882785	O	1.336377	-0.086142	0.883632
H	-4.310332	0.643696	-6.275872	O	0.646094	-2.122393	-0.479704
H	-3.281467	-1.589752	-5.859583	O	-0.941864	-0.434653	-0.192025
S	-1.387272	-2.468026	-3.953436	V	-1.245081	-2.288043	-0.449233
C	0.405794	-2.302292	-3.775578	O	-1.840350	-3.085642	0.765406
H	0.805958	-2.094792	-4.770913	O	-1.765409	-2.661722	-2.292102
H	0.633466	-1.498556	-3.068724	C	-2.036573	-0.779984	-4.151354
H	0.765308	-3.259196	-3.392843	C	-1.615225	0.360062	-3.459283
O	-1.710401	-3.387125	-5.093191	C	-2.201907	1.578154	-3.797422
				C	-3.179774	1.640792	-4.793655
				C	-3.580414	0.486987	-5.471697
25, $\nu^{\neq} = 570.53$ *i*cm^{-1}				C	-3.006564	-0.742912	-5.155747
TSIII, B3LYP/6-311++G(d,p)=-1666.564246				H	-0.850328	0.319771	-2.691242
S	-0.295129	-0.671375	-2.310571	H	-1.889955	2.477454	-3.276653
O	0.125614	-0.124809	-3.608085	H	-3.630230	2.596066	-5.045408
O	0.111822	0.002555	-1.095923	H	-4.337678	0.542227	-6.247030
O	0.055914	-2.245808	-2.271228	H	-3.295275	-1.654160	-5.667216
O	-1.889147	-0.922746	-2.348643	S	-1.363143	-2.372544	-3.749014
V	-1.740228	-2.801908	-2.445472	C	0.420322	-2.219921	-3.761467
O	-2.357307	-3.654679	-1.276774	H	0.707967	-2.046062	-4.800534
O	-2.068824	-3.464099	-3.967685	H	0.737178	-1.401040	-3.107669
C	-2.478055	-1.703983	-6.418230	H	0.814528	-3.173286	-3.401731
C	-2.375773	-0.502991	-5.706969	O	-1.814712	-3.383838	-4.700573
C	-3.201928	0.551577	-6.090072				
C	-4.110728	0.395486	-7.139921				
C	-4.203130	-0.819542	-7.824902	18			
C	-3.390005	-1.890080	-7.462730	VI, B3LYP/6-311++G(d,p)= -1844.257194			
H	-1.674394	-0.372063	-4.891420	S	-4.369031	0.626256	-1.568581
H	-3.132398	1.495328	-5.559180	O	-4.463233	-0.644201	-2.254863
H	-4.752269	1.223849	-7.424277	O	-5.524674	1.457373	-1.320389
H	-4.909251	-0.935637	-8.640829	O	-3.123373	1.481979	-2.116914
H	-3.443149	-2.843547	-7.976148	O	-3.548507	0.418264	-0.128096
S	-1.523428	-3.120006	-5.935666	V	-2.005140	1.219538	-0.578984
C	0.177732	-2.561468	-5.713197	O	-1.827918	2.471721	0.326655
H	0.571717	-2.339286	-6.707868	S	1.000028	-1.816004	-3.124239
H	0.198452	-1.684553	-5.059529	O	2.252878	-1.784767	-3.840890
H	0.715732	-3.391669	-5.251243	O	0.077176	-2.922356	-3.202641
O	-1.603617	-4.195746	-6.958577	O	0.237776	-0.401384	-3.185137
				O	1.300353	-1.474278	-1.499476
				V	0.529168	0.116242	-1.360335
25				O	-0.631328	-0.004772	-0.144664
VI, B3LYP/6-311++G(d,p)=-1666.630085				O	-0.635486	1.525393	-1.995931

H	-0.978690	1.447715	-2.908280	H	-2.396267	3.583094	-2.450069
O	1.830475	1.153804	-0.908166	O	1.731358	1.299230	-2.160061
H	1.692098	2.014557	-0.467709	H	1.559427	2.250868	-2.289723

18, $\nu^{\neq} = 64.32\ i\text{cm}^{-1}$

TSIV, B3LYP/6-311++G(d,p)= -1844.236525

S	-4.534224	0.930957	-1.468109
O	-4.676533	0.889983	-2.911045
O	-5.667209	0.796422	-0.581509
O	-3.677484	2.292074	-1.052579
O	-3.293352	0.022307	-0.991662
V	-2.105885	1.465349	-0.681020
O	-1.677512	1.885909	0.758362
S	1.502534	-2.269088	-2.788966
O	2.759374	-2.113648	-3.480282
O	0.761157	-3.504440	-2.741899
O	0.491358	-1.015329	-3.159157
O	1.651594	-1.660247	-1.225799
V	0.639907	-0.220088	-1.530570
O	-0.741460	-0.154841	-0.708739
O	-0.990427	2.243926	-1.883723
H	-1.379317	2.411247	-2.762648
O	1.473445	1.279565	-1.531811
H	0.866605	2.065021	-1.547483

18

IX, B3LYP/6-311++G(d,p)= -1844.243062

S	-4.308201	0.628690	-0.974243
O	-5.378547	1.401215	-1.568779
O	-4.551143	-0.483157	-0.086842
O	-3.219080	1.672083	-0.276857
O	-3.173822	0.275281	-2.073519
V	-1.868829	1.482884	-1.461024
O	-0.526270	1.031374	-0.624280
S	1.074163	-2.424931	-1.793100
O	2.415367	-2.746969	-1.362274
O	0.113527	-3.435059	-2.170589
O	1.161610	-1.276161	-3.016682
O	0.405763	-1.290113	-0.865260
V	0.471813	0.112252	-2.133754
O	-0.871162	0.612047	-2.956953
O	-1.647138	3.112449	-2.034633

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3G, B3LYP/6-311++G(d,p)= -4613.577864

C	2.132670	13.051828	4.688841
C	1.693096	13.850667	6.994960
C	1.753815	14.118556	8.453215
C	0.740986	14.268809	6.098096
H	-0.100786	14.875551	6.408725
C	0.992419	13.812639	4.773197
H	0.354567	14.035248	3.923588
O	4.806806	14.122627	11.015404
O	0.803568	14.808407	8.921042
O	2.741990	13.607368	9.058309
O	2.352953	15.364804	10.973496
O	1.839838	14.997437	15.534469
O	0.156903	16.992687	10.691800
S	2.914931	12.877684	6.223172
V	3.305838	13.643020	11.011580
V	0.393372	15.439089	10.815044
V	1.784282	14.733217	13.730489
C	-3.482561	7.596241	13.440276
C	-1.656550	9.270966	13.550153
C	-0.862880	10.524973	13.581629
C	-1.194332	7.978504	13.589786
H	-0.135681	7.758980	13.656140
C	-2.241155	7.015538	13.528326
H	-2.079964	5.942191	13.545204
O	-1.821844	14.216589	14.605276
O	0.389741	10.377847	13.642289
O	-1.532489	11.596990	13.531836
O	0.681121	13.031312	14.289699
O	2.780939	11.292878	14.870020
S	-3.393679	9.325102	13.428871
V	-0.955777	13.542416	13.468801
V	1.904393	11.734518	13.631336
C	4.183972	7.774951	8.589124
C	3.533664	9.376410	10.366579
C	3.277556	10.596125	11.169378
C	3.209222	8.078964	10.677639
H	2.712474	7.828037	11.606948

C	3.583545	7.157561	9.659054	V	3.281849	13.650720	10.996410
H	3.410280	6.087481	9.715337	V	0.352754	15.406604	10.794170
O	2.695665	10.428987	12.271425	V	1.748608	14.729626	13.703259
O	3.672470	11.684093	10.663186	C	-3.478717	7.585689	13.435394
O	2.760184	13.415796	12.913152	C	-1.662509	9.269712	13.548006
S	4.298206	9.488534	8.805561	C	-0.875997	10.526700	13.579830
C	-5.598887	12.804986	9.039656	C	-1.192989	7.979720	13.588624
C	-3.507232	13.762280	9.964436	H	-0.133396	7.765395	13.656902
C	-2.353439	14.113057	10.826931	C	-2.234433	7.011374	13.525605
C	-3.743855	14.156477	8.670556	H	-2.067762	5.938986	13.543099
H	-3.058032	14.809249	8.144396	O	-1.851536	14.215451	14.597368
C	-4.945366	13.609097	8.138173	O	0.377959	10.387656	13.641379
H	-5.305046	13.799007	7.131763	O	-1.550085	11.596210	13.529107
O	-1.493445	14.881442	10.317558	O	0.658325	13.049631	14.271510
O	-2.347867	13.610432	11.982032	O	2.756567	11.315765	14.877515
O	0.254790	14.985931	12.751652	S	-3.399619	9.314667	13.423904
S	-4.757643	12.699991	10.548880	V	-0.991203	13.542205	13.458487
Cl	0.526223	12.457877	11.059506	V	1.886666	11.744077	13.631311
H	-6.525098	12.263981	8.892822	C	4.203531	7.775971	8.619549
H	-4.442112	7.098951	13.376253	C	3.537398	9.385058	10.383183
H	2.549018	12.580120	3.807793	C	3.270431	10.607399	11.176164
H	4.556815	7.313487	7.683495	C	3.220702	8.087567	10.702864
O	2.637695	16.075190	13.498518	H	2.723426	7.839289	11.632601
O	1.232524	14.111892	16.478120	C	3.604249	7.161789	9.692037
H	0.844953	13.436197	15.849568	H	3.438516	6.091015	9.755343
H	2.651188	15.928727	11.718514	O	2.684615	10.444660	12.277503
				O	3.659714	11.695470	10.665011
				O	2.740573	13.427295	12.905702
67				S	4.306023	9.491434	8.823861
H-1, B3LYP/6-311++G(d,p)= -4765.213938				C	-5.638978	12.776063	9.041033
C	2.128190	13.069678	4.670158	C	-3.543988	13.731627	9.957669
C	1.675220	13.847085	6.980073	C	-2.389638	14.084962	10.815382
C	1.729510	14.106008	8.438462	C	-3.778421	14.116192	8.660286
C	0.720019	14.261198	6.084318	H	-3.090349	14.762095	8.128636
H	-0.128601	14.857389	6.396699	C	-4.982069	13.569641	8.132648
C	0.979353	13.817226	4.757093	H	-5.341257	13.752982	7.124994
H	0.341501	14.039344	3.907526	O	-1.525060	14.844746	10.298605
O	4.775169	14.146989	11.000662	O	-2.382094	13.593781	11.975456
O	0.768140	14.780288	8.909645	O	0.215956	14.986095	12.727373
O	2.721085	13.604284	9.045637	S	-4.799142	12.680121	10.551241
O	2.305015	15.361880	10.958889	Cl	0.510904	12.466797	11.048898
O	1.807633	15.004122	15.504966	H	-6.567856	12.238447	8.899098
O	0.102145	16.966675	10.655721	H	-4.435532	7.083416	13.370148
S	2.909785	12.893747	6.204213	H	2.552251	12.609599	3.786713

H	4.582599	7.310811	7.718466	V	1.905899	11.735903	13.612374
O	2.584272	16.097175	13.488245	C	4.368362	7.497646	8.909722
O	1.215103	14.123106	16.458420	C	3.620732	9.223231	10.523994
H	0.819323	13.445026	15.839201	C	3.302923	10.495191	11.212690
H	2.624719	15.963775	11.663318	C	3.358403	7.945657	10.954669
O	1.590564	18.676521	13.215596	H	2.868838	7.757737	11.902500
H	1.996839	17.822287	13.487300	C	3.788268	6.953277	10.029440
O	1.973241	18.706371	11.811350	H	3.669147	5.885801	10.185421
H	1.228756	18.207975	11.406793	O	2.725810	10.396706	12.328176
				O	3.641628	11.555009	10.615886
				O	2.844028	13.322068	12.894270
67, $\nu^{\neq} = 1675.30$ *i*cm^{-1}				S	4.396515	9.227101	8.964754
TSH1, B3LYP/6-311++G(d,p)= -4765.162387				C	-5.819957	12.726332	9.501912
C	2.349296	13.417460	4.592400	C	-3.652371	13.719664	10.174215
C	1.756242	13.968511	6.935702	C	-2.432784	14.119868	10.909374
C	1.725891	14.088460	8.412258	C	-3.976221	13.991145	8.867189
C	0.880329	14.507949	6.026356	H	-3.320184	14.571126	8.229568
H	0.035160	15.107230	6.342143	C	-5.222160	13.423120	8.480002
C	1.219186	14.192991	4.680135	H	-5.651961	13.521717	7.488326
H	0.651343	14.526981	3.817370	O	-1.584226	14.798968	10.271738
O	4.700990	14.104340	10.817623	O	-2.359810	13.743501	12.113500
O	0.761296	14.751710	8.888165	O	0.149539	15.034812	12.742265
O	2.653021	13.487087	9.028443	S	-4.872560	12.748202	10.949393
O	2.159001	15.075393	11.231449	Cl	0.459300	12.405836	11.055893
O	1.938503	15.048989	15.243390	H	-6.762948	12.195195	9.476266
O	0.215291	16.897960	10.563269	H	-4.548847	7.258241	13.009096
S	3.016961	13.061182	6.148943	H	2.822902	13.038097	3.695804
V	3.239419	13.506668	10.960906	H	4.774248	6.973240	8.054013
V	0.309779	15.331052	10.775250	O	2.759137	16.202126	13.379925
V	1.915144	14.871265	13.414390	O	1.382537	14.220762	16.249049
C	-3.579180	7.726101	13.122757	H	0.953280	13.517238	15.692863
C	-1.716199	9.343496	13.368726	H	2.737420	16.052695	10.942798
C	-0.892646	10.571539	13.485066	O	3.929917	16.383295	8.960108
C	-1.286181	8.039552	13.340295	H	4.388898	15.687674	9.475180
H	-0.234814	7.789132	13.411793	O	3.268189	17.101650	10.510335
C	-2.354522	7.109318	13.200720	H	2.494478	17.493547	10.062884
H	-2.220017	6.033223	13.155530				
O	-1.692605	14.197936	14.707708				
O	0.353312	10.391937	13.567304	67			
O	-1.543781	11.661004	13.477567	H-2, B3LYP/6-311++G(d,p)= -4765.198702			
O	0.644016	12.981764	14.194431	C	2.447819	13.670565	4.694600
O	2.689587	11.296899	14.909716	C	1.790256	14.121861	7.041077
S	-3.448404	9.449572	13.214722	C	1.722199	14.184297	8.518348
V	-0.895710	13.587679	13.493733	C	0.940882	14.702643	6.132051

H	0.090968	15.294192	6.449548	C	-5.220141	13.317390	8.568565
C	1.316598	14.444508	4.783781	H	-5.650340	13.393382	7.575189
H	0.774700	14.818123	3.920614	O	-1.607267	14.778909	10.343388
O	4.635553	14.217677	10.959678	O	-2.371297	13.746329	12.201169
O	0.741645	14.820855	8.997820	O	0.053886	15.004550	12.870473
O	2.633464	13.561309	9.137204	S	-4.861988	12.684663	11.048014
O	2.012373	14.977490	11.409401	Cl	0.395103	12.339553	11.161432
O	1.849908	15.041038	15.220314	H	-6.740013	12.077231	9.581788
O	0.167675	16.931425	10.724669	H	-4.691560	7.294862	12.981171
S	3.072370	13.248011	6.252002	H	2.946578	13.329807	3.796148
V	3.194360	13.562559	11.067891	H	4.983360	7.155464	8.047160
V	0.272167	15.354575	10.878774	O	2.947826	16.136215	13.392394
V	1.970795	14.891670	13.391028	O	1.147190	14.369153	16.238700
C	-3.715045	7.746688	13.100686	H	0.781878	13.593456	15.741021
C	-1.827568	9.333456	13.355769	H	3.220782	17.091527	11.658565
C	-0.983216	10.546140	13.477675	O	3.944268	16.352570	8.882966
C	-1.418833	8.022506	13.333142	H	4.153447	15.845483	9.698034
H	-0.372459	7.754438	13.412950	O	3.137004	17.702961	10.901984
C	-2.501374	7.109854	13.188049	H	2.237659	17.503021	10.585283
H	-2.384354	6.031667	13.145810				
O	-1.720008	14.123565	14.763318				
O	0.257852	10.344893	13.577607	67, $\nu^{\neq} = 807.20\ i\text{cm}^{-1}$			
O	-1.619468	11.647269	13.459579	TSH2, B3LYP/6-311++G(d,p)= -4765.191538			
O	0.502467	12.877226	14.289155	C	2.353274	12.584707	4.968076
O	2.579417	11.199526	14.961414	C	1.885814	13.499105	7.224587
S	-3.556598	9.467779	13.189754	C	1.881067	13.789955	8.678151
V	-0.888527	13.562846	13.550274	C	1.103226	14.067322	6.249580
V	1.837187	11.663816	13.649730	H	0.371670	14.830575	6.485116
C	4.536569	7.640263	8.905827	C	1.370846	13.544308	4.953110
C	3.688048	9.290731	10.547633	H	0.857764	13.864560	4.051828
C	3.312364	10.531933	11.262233	O	4.690210	13.464747	11.303252
C	3.456193	7.992864	10.933170	O	1.034569	14.644401	9.062594
H	2.947726	7.759974	11.860826	O	2.714404	13.138083	9.371249
C	3.944001	7.043439	9.991894	O	2.230760	14.805753	11.536688
H	3.856229	5.968424	10.112926	O	1.792681	15.370872	15.274145
O	2.704731	10.379906	12.358555	O	0.728004	16.967846	10.587670
O	3.635125	11.617248	10.707691	S	2.967073	12.305124	6.561958
O	2.808141	13.283365	13.026562	V	3.146419	13.145373	11.342257
S	4.506483	9.366994	9.012403	V	0.579591	15.412495	10.875941
C	-5.806712	12.625446	9.600487	V	2.093939	14.805535	13.483146
C	-3.658544	13.665753	10.259631	C	-4.672101	8.751538	13.530555
C	-2.446397	14.097810	10.985759	C	-2.557162	10.026696	13.737126
C	-3.985165	13.912803	8.948235	C	-1.528723	11.092251	13.785898
H	-3.338341	14.494430	8.302748	C	-2.375113	8.672455	13.875883

H	-1.394131	8.247445	14.049463	O	3.692401	17.054136	10.325110
C	-3.588891	7.938573	13.758946	H	2.735703	17.237032	10.338054
H	-3.654510	6.858053	13.837013				
O	-1.753417	14.823866	14.692697				
O	-0.341522	10.703245	13.975120	67			
O	-1.963360	12.271692	13.620520	H-3, B3LYP/6-311++G(d,p)= -4765.303791			
O	0.324771	13.254082	14.410191	C	4.521607	9.529134	7.338686
O	1.982894	11.346491	15.454374	C	3.349441	11.490923	8.297994
S	-4.229390	10.422477	13.452079	C	2.850285	12.562182	9.191081
V	-0.947873	14.054156	13.584398	C	2.979972	11.235364	7.000142
V	1.402211	11.750593	14.031992	H	2.245915	11.846934	6.489870
C	3.477943	6.878639	9.811853	C	3.653144	10.109965	6.447064
C	2.907933	8.816807	11.246955	H	3.497705	9.746291	5.436331
C	2.735504	10.173448	11.814530	O	4.387456	14.241985	12.331750
C	2.474665	7.623533	11.771522	O	1.978305	13.329892	8.699815
H	1.938890	7.579834	12.711920	O	3.350897	12.586485	10.352640
C	2.802266	6.509147	10.949188	O	2.040474	15.046512	10.997098
H	2.545493	5.482117	11.188337	O	1.046030	17.058050	12.773084
O	2.123155	10.237368	12.918327	O	1.164335	15.977858	8.462267
O	3.213808	11.126646	11.142050	S	4.530193	10.343225	8.865705
O	2.664439	13.081398	13.308472	V	2.948272	13.649324	12.018643
S	3.722753	8.589422	9.724582	V	0.831451	14.810567	9.471265
C	-5.778737	13.567529	9.416149	V	0.776145	15.570095	12.293815
C	-3.525271	14.301745	10.133253	C	-5.065803	9.332667	13.280608
C	-2.295715	14.587199	10.902378	C	-3.290598	11.043850	13.533129
C	-3.748385	14.511549	8.794050	C	-2.418724	12.232566	13.382485
H	-2.989260	14.943764	8.153581	C	-3.131094	9.984044	14.391992
C	-5.043484	14.091952	8.380759	H	-2.298253	9.935966	15.082862
H	-5.410547	14.169949	7.362473	C	-4.150656	9.001206	14.249769
O	-1.329892	15.086826	10.267812	H	-4.199761	8.088614	14.835254
O	-2.334158	14.307102	12.135529	O	-3.038542	15.792361	11.844782
O	0.214874	15.269769	12.827659	O	-1.411391	12.276811	14.141859
S	-4.903913	13.573063	10.908197	O	-2.780238	13.070284	12.507203
Cl	0.238135	12.418211	11.352729	O	-0.686870	14.863253	13.185722
H	-6.785382	13.171207	9.376996	O	0.200479	13.926745	15.735675
H	-5.704923	8.454957	13.398992	S	-4.696805	10.844947	12.524551
H	2.746185	12.027461	4.127163	V	-1.915963	14.695909	11.676685
H	3.839052	6.235801	9.019194	V	0.217119	13.474685	14.223555
O	3.370057	15.722088	13.547784	C	3.614421	7.600348	14.081986
O	0.711399	15.273196	16.132335	C	2.590299	9.857091	14.047618
H	0.455311	14.270391	16.263102	C	2.256072	11.271348	13.759314
H	3.732252	16.251611	10.874092	C	1.933589	8.989788	14.886067
O	0.579792	13.187566	17.254401	H	1.060357	9.297952	15.448009
H	1.162870	12.593580	16.726633	C	2.521226	7.693744	14.908335

H	2.147807	6.868249	15.505929	O	0.049382	17.250755	13.619945
O	1.243111	11.731834	14.353307	O	0.677506	13.910962	9.386730
O	3.023515	11.861462	12.944359	S	6.332157	10.631488	10.739741
O	1.724302	14.358755	13.347307	V	3.967676	14.467300	12.564806
S	3.942107	9.088832	13.262566	V	1.219639	13.432835	10.786547
C	-4.274264	11.238076	6.802186	V	1.015130	15.908438	12.968936
C	-2.588549	12.672966	7.916905	C	-1.228186	9.552630	18.769917
C	-1.847195	13.529225	8.872150	C	-0.218795	11.373182	17.423109
C	-2.167234	12.213415	6.693161	C	0.093274	12.372833	16.373467
H	-1.190796	12.467136	6.298876	C	0.466686	11.133116	18.588685
C	-3.134777	11.390763	6.050624	H	1.350781	11.700825	18.852061
H	-2.990074	10.929850	5.078708	C	-0.112175	10.089039	19.363940
O	-0.689109	13.881228	8.514270	H	0.282155	9.751006	20.316991
O	-2.456668	13.811578	9.943300	O	-2.191676	14.139830	13.713784
O	-0.370351	15.536142	10.828088	O	1.129506	13.068843	16.571776
S	-4.183972	12.091404	8.305003	O	-0.702398	12.406523	15.390897
Cl	0.245128	12.443418	11.304275	O	0.316713	14.851430	14.684182
H	-5.157516	10.663339	6.554050	O	2.240958	15.675735	16.547316
H	-5.931817	8.763639	12.967146	S	-1.590025	10.311564	17.256973
H	5.151630	8.663318	7.179208	V	-0.722214	13.565876	13.726567
H	4.239004	6.733464	13.907617	V	2.001060	14.524171	15.467703
O	0.456469	18.654761	10.175949	C	7.555027	10.689829	16.289129
O	1.655776	18.482832	10.095142	C	5.656354	12.218582	15.841030
H	3.489173	16.301728	10.387997	C	4.695784	13.161263	15.223219
O	3.639845	18.418611	12.619675	C	5.578232	11.625232	17.077046
H	2.764962	18.037501	12.806343	H	4.752022	11.823794	17.748828
O	4.412536	16.556632	10.578972	C	6.668943	10.748427	17.336964
H	4.665378	15.851312	11.206383	H	6.787636	10.183658	18.256170
H	3.965687	17.855099	11.886227	O	3.683216	13.460323	15.907879
				O	4.987121	13.574188	14.065867
				O	2.592514	15.326022	13.727304
67, $\nu^{\neq} = 1824.44\ i\text{cm}^{-1}$				S	7.071678	11.698989	14.968885
TSH3, B3LYP/6-311++G(d,p)= -4765.157053				C	-2.055549	7.567802	11.728542
C	6.446041	9.206673	9.763794	C	-1.072138	9.835672	11.543344
C	4.679386	10.877696	10.246860	C	-0.662996	11.240638	11.776585
C	3.900717	12.025650	10.771492	C	-0.711610	9.015045	10.502874
C	4.259449	9.896752	9.382281	H	-0.058271	9.360104	9.710787
H	3.252550	9.887112	8.983216	C	-1.276503	7.712632	10.606713
C	5.272984	8.937316	9.102264	H	-1.109016	6.919129	9.885317
H	5.136536	8.085043	8.444175	O	0.095492	11.749967	10.907916
O	5.044027	15.565651	12.225900	O	-1.113009	11.788620	12.818453
O	2.700779	12.097097	10.379446	O	0.221974	14.461743	12.178897
O	4.525627	12.787743	11.567404	S	-2.109438	9.014950	12.676417
O	2.751513	14.639903	11.030106	Cl	1.990194	12.346326	13.486794

H	-2.594104	6.685414	12.050055
H	-1.853595	8.750433	19.140547
H	7.367484	8.639190	9.733275
H	8.461128	10.101204	16.221866
O	1.505416	16.825401	11.736541
O	-0.850304	17.016297	15.153193
H	-0.547602	16.049623	15.180051
H	2.457974	15.572893	10.945565
O	-0.211102	17.586963	17.378256
H	-0.532539	17.420836	16.148932
O	1.098263	18.031305	17.186746
H	1.593099	17.179264	17.046855

67

H-4, B3LYP/6-311++G(d,p)= -4765.249363

C	5.317535	10.689664	7.533212
C	3.679934	12.262382	8.517572
C	2.901037	13.121752	9.439234
C	3.483617	12.069163	7.171374
H	2.684695	12.568621	6.636851
C	4.424422	11.165411	6.603521
H	4.437500	10.880962	5.556012
O	4.055145	14.720295	12.818910
O	1.944437	13.768587	8.916946
O	3.277735	13.097589	10.647902
O	2.038379	15.421774	11.028424
O	-0.444716	17.110048	13.758425
O	0.806706	16.357005	8.785654
S	5.028509	11.333913	9.112448
V	2.671509	14.106769	12.304573
V	0.625971	15.094903	9.731453
V	0.526123	16.453152	12.682298
C	-4.873449	9.017462	12.737482
C	-3.252970	10.840928	13.177499
C	-2.464343	12.095758	13.139714
C	-3.081176	9.765627	14.014410
H	-2.302602	9.753300	14.767279
C	-4.011891	8.718259	13.764334
H	-4.037538	7.784737	14.317355
O	-3.277332	15.744198	11.958992
O	-1.531602	12.185961	13.982673
O	-2.822142	12.926800	12.243268
O	-1.440669	14.718936	13.447630
O	-0.184437	14.015796	15.804439
S	-4.561326	10.578062	12.057379
V	-2.036195	14.775619	11.880591
V	-0.104073	13.654408	14.272922
C	4.005791	8.238185	14.563600
C	2.679650	10.314421	14.347319
C	2.182154	11.658983	13.986977
C	2.066222	9.377254	15.143722
H	1.104472	9.566721	15.604955
C	2.827523	8.182436	15.269131
H	2.516339	7.322127	15.853213
O	1.081413	12.013773	14.482297
O	2.915136	12.331818	13.206300
O	1.251701	14.834652	13.428530
S	4.207068	9.743398	13.736789
C	-4.301433	11.406849	6.918398
C	-2.629269	12.867119	8.016623
C	-1.902807	13.745662	8.959382
C	-2.183351	12.358320	6.821056
H	-1.195048	12.586645	6.441026
C	-3.143476	11.520425	6.187877
H	-2.980810	11.020851	5.238242
O	-0.731582	14.083492	8.628477
O	-2.519014	14.083283	10.004425
O	-0.555721	15.755258	11.204123
S	-4.237632	12.314164	8.389705
Cl	0.265395	12.797608	11.374612
H	-5.184200	10.830763	6.671786
H	-5.669216	8.399664	12.341103
H	6.131186	9.994129	7.370482
H	4.766509	7.471498	14.488509
O	1.553702	17.662857	12.313335
O	3.071537	17.681898	10.073886
H	2.599620	17.916710	10.913470
H	2.690057	16.099674	10.702838
O	6.397770	12.282765	12.546813
O	6.088456	13.123730	13.530890
H	5.299015	13.656683	13.202896
H	2.337180	17.553941	9.442574

67, $v^{\neq} = 443.05\ i\text{cm}^{-1}$

TSH4, B3LYP/6-311++G(d,p)= -4765.197008

C	6.027575	9.481135	10.839063

C	4.622757	11.524397	10.878319	C	0.838797	14.613808	7.783588
C	3.667213	12.597599	11.248716	C	1.915410	13.441988	5.768403
C	5.361398	11.410539	9.726362	H	2.899719	13.388455	6.217334
H	5.302167	12.154362	8.941209	C	1.559158	12.941173	4.484471
C	6.169623	10.238744	9.702414	H	2.254036	12.450502	3.810187
H	6.823291	9.969287	8.878703	O	1.935826	14.607021	8.410529
O	2.274038	13.739866	14.786162	O	-0.263380	15.076659	8.176445
O	3.513730	13.511173	10.386784	O	0.563284	16.018480	10.690579
O	3.113433	12.474212	12.377744	S	-0.604656	13.938020	5.483187
O	2.352834	15.116695	12.333889	Cl	0.458098	12.966827	10.650578
O	-0.661250	17.295763	13.183320	H	-0.299117	12.854384	3.295481
O	3.344868	16.255469	10.051617	H	-5.153320	10.582190	6.455057
S	4.905269	10.183768	11.954191	H	6.519167	8.546107	11.076166
V	1.655771	13.544569	13.346093	H	0.188980	6.391306	13.941204
V	2.269613	15.121543	10.336588	O	1.860623	17.903918	12.274017
V	0.543065	16.417730	12.647700	O	4.512886	16.690094	12.659126
C	-4.775728	10.931695	7.407638	H	3.911380	17.299953	13.133625
C	-3.642621	12.194986	9.215022	H	3.228515	15.478137	12.634498
C	-2.842702	13.167407	9.999165	O	2.242122	18.191334	13.540218
C	-4.313163	11.090478	9.680068	O	1.641683	16.792979	14.386723
H	-4.312419	10.830024	10.731413	H	0.952871	17.256092	14.899281
C	-4.965920	10.364728	8.644060	H	4.265187	16.822969	11.720719
H	-5.544770	9.461266	8.808124				
O	-1.771877	16.918886	9.423904				
O	-2.780801	12.960013	11.238960	67			
O	-2.303095	14.094282	9.312838	H-5, B3LYP/6-311++G(d,p)= -4765.266411			
O	-1.829730	15.387603	11.501505	C	4.081533	9.992839	7.381549
O	-2.743736	14.265821	13.866485	C	3.127004	12.006958	8.466292
S	-3.794582	12.355450	7.487044	C	2.746625	13.067899	9.429935
V	-1.116664	15.599398	9.994547	C	2.696802	11.848064	7.171655
V	-1.702552	13.925756	12.726371	H	2.000628	12.542843	6.718080
C	-0.220775	7.384576	13.808381	C	3.244816	10.692463	6.546734
C	-0.534150	9.833750	13.579744	H	3.022942	10.390679	5.528004
C	-0.335402	11.299937	13.482736	O	4.207252	14.400588	12.747634
C	-1.707588	9.133923	13.442854	O	1.987034	13.973733	8.972989
H	-2.645875	9.638660	13.247272	O	3.227104	12.965395	10.591666
C	-1.530076	7.727631	13.575344	O	2.077779	15.462056	11.337623
H	-2.335491	7.004164	13.496359	O	-1.479156	17.635034	13.108909
O	-1.365252	11.987409	13.261596	O	1.045493	16.618595	9.051353
O	0.848858	11.712194	13.633829	S	4.206856	10.726386	8.944420
O	0.040124	14.577224	13.219534	V	2.727735	13.873786	12.415185
S	0.815281	8.770334	13.865837	V	0.761602	15.319630	9.899019
C	0.231425	13.141228	4.194579	V	-0.479038	16.424838	12.900296
C	0.855864	14.014511	6.428350	C	-4.791631	8.866316	13.377774

C	-3.188366	10.746549	13.592435	O	4.760282	15.915530	10.496916
C	-2.413771	11.999176	13.411019	H	4.795258	15.420218	11.348678
C	-2.992117	9.771105	14.538848	O	1.016456	16.875167	13.666628
H	-2.204126	9.852722	15.277626	H	1.485567	15.964906	13.729637
C	-3.912031	8.691379	14.417794	H	4.534093	15.219142	9.860866
H	-3.918390	7.823769	15.070061				
O	-3.378201	15.319391	11.822086				
O	-1.485989	12.199113	14.233624				
O	-2.769111	12.729071	12.437957				
O	-1.159043	14.905465	13.532146				
O	-0.068672	13.903343	15.983540				
S	-4.509218	10.348481	12.528692				
V	-2.047556	14.480758	11.766218				
V	0.066362	13.529737	14.451928				
C	3.561794	7.706908	14.182223				
C	2.483448	9.940904	14.202465				
C	2.116519	11.357173	13.950272				
C	1.849664	9.037895	15.020050				
H	0.970619	9.312487	15.590293				
C	2.467872	7.755367	15.010985				
H	2.114564	6.907471	15.589443				
O	1.099809	11.777850	14.567266				
O	2.855433	11.980151	13.135478				
O	1.565734	14.377830	13.744662				
S	3.852560	9.223261	13.398701				
C	-3.497268	11.609564	6.144338				
C	-2.192003	13.049448	7.684314				
C	-1.679556	13.799253	8.856626				
C	-1.627793	12.959917	6.435301				
H	-0.706781	13.476373	6.193541				
C	-2.376318	12.134584	5.549401				
H	-2.094205	11.936709	4.520116				
O	-0.614523	14.446892	8.673414				
O	-2.358757	13.706982	9.917499				
O	-0.641892	15.814362	11.191525				
S	-3.655015	12.111033	7.793665				
Cl	0.217305	12.835574	11.420072				
H	-4.233712	10.950700	5.702105				
H	-5.585577	8.200606	13.063783				
H	4.621341	9.080225	7.162897				
H	4.206765	6.859475	13.987302				
O	1.061328	18.796452	11.220347				
O	2.261554	18.617358	11.212070				
H	2.874526	15.924835	10.999124				