

Supporting Information
**Insights into Chiral Sulfide/Selenide Electrophilic
Carbothiolation of Alkynes: Mechanism and Origin of
Axial Chirality**

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Table of Contents

Part 1: Computational methods	2
Part 2: Additionally computational results	4
2.1 Other unfavorable pathway for the formation of Int1	4
2.2 The role of chiral sulfide catalyst.....	4
2.3 Local electrophilic (P_k^+) and nucleophilic (P_k^-) Parr function analyses on R1 , Int1 , and Int02	5
2.4 The formation of thiiranium ion intermediate catalyzed by chiral selenide catalyst.....	6
2.5 NCI and AIM analyses of TS2R-Se and TS2S-Se	6
2.6 Different configurations of TS2R&TS2S	8
2.7 NCI and AIM analyses of TS2R and TS2S	11
2.8 The FMO overlap mode and ELF analyses for the formation of thiiranium ion intermediate	12
2.9 The volume of R groups of R2 involved in the axially chiral products	12
Part 3: Energy values and Cartesian coordinates of all the optimized structures	15
3.1 Absolute SPE and GFE of the optimized structures by using B3LYP-D3 method.....	15
3.2 Absolute SPE and GFE of the optimized structures by other DFT methods.....	16
3.3 The Cartesian coordinates and representative vibrational frequencies of all the stationary points	18

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Part 1: Computational methods

All theoretical calculations were performed in Gaussian 09¹. All structures were completely optimized by using the B3LYP-D3² method and the 6-31G(d, p) basis set in dichloromethane solvent with the integral equation formalism polarizable continuum model (IEF-PCM)³. Frequency calculations were carried out at the same level to confirm all the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency), and provided the thermal relative Gibbs free energy correction.

All the energies discussed in the main text are the relative Gibbs free energies (GFE), which are obtained by the addition of the thermal Gibbs free energy corrections (GFEC) at the B3LYP-D3/6-31G(d, p)/IEF-PCM_{dichloromethane} level and the single-point energies (SPE) at a higher computational level of B3LYP-D3/6-311++G(2df, 2pd)/IEF-PCM_{dichloromethane}. To check whether the selected method is reliable, the additional calculations by employing different DFT methods (including M06-2X⁴/6-31G(d, p)/IEF-PCM_{dichloromethane} and ω B97X-D⁵/6-31G(d, p)/IEF-PCM_{dichloromethane} have been performed for the key transition states involved in the stereoselectivity-determining step, and the computed and test results can be found in the **Table S1**. As summarized in **Table S1**, there are tiny differences between the energies calculated by different methods. Thus, the selected DFT method is suitable in this work.

Table S1. The relative Gibbs free energies (kcal/mol) of transition states **TS2R&TS2S** calculated by the three calculation methods below.

Method	B3LYP-D3	M06-2X	ω B97XD
TS2R	2.2	2.0	2.1
TS2S	0	0	0

We further computed the single-point energies for the key transition states **TS2R&TS2S** optimized at the B3LYP-D3/6-31G(d, p)/IEF-PCM_{dichloromethane} level by

using the higher basis set 6-311++G(2df, 2pd). As summarized in **Table S2**, the single-point energies of transition states **TS2R&TS2S** calculated by 6-311++G(2df, 2pd) basis set are close to those obtained by the selected basis set 6-31G(d, p). Thus, the calculated results should be reliable and the selected basis set is suitable for the study in this work.

Table S2. The relative energies (kcal/mol) of transition states **TS2R&TS2S** calculated by two different basis sets including 6-31G(d, p) and 6-311++G(2df, 2pd).

Basis Set	6-31G(d, p)	6-311++G(2df,2pd)
TS2R	1.6	2.2
TS2S	0.0	0.0

Noncovalent interactions (NCIs) and atom-in-molecule (AIM)⁶ analyses were plotted using NCIPLOT (version 1.0)⁷ and Multiwfn (version 3.3.8)⁸. Most of the significant three-dimensional structures were illustrated with CYLview⁹. In addition, the extent of enantioselectivity, in terms of enantiomeric excess (*ee*), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

$$eq. 1: \frac{[S]}{[R]} = \frac{\exp\left(-\Delta G_{[S]}^{\ddagger}/RT\right)}{\exp\left(-\Delta G_{[R]}^{\ddagger}/RT\right)} = \exp\left(\Delta\Delta G_{[R]-[S]}^{\ddagger}/RT\right)$$

$$eq. 2: ee = \frac{[S] - [R]}{[S] + [R]} \times 100\% = \frac{\frac{[S]}{[R]} - 1}{\frac{[S]}{[R]} + 1} \times 100\%$$

where ΔG^{\ddagger} is the Gibbs free energy barrier of the competing diastereomeric transition state and $\Delta\Delta G^{\ddagger}$ is the difference between the Gibbs free energy barriers of two diastereomeric transition states.

Part 2: Additionally computational results

2.1 Other unfavorable pathway for the formation of Int1

In addition, we considered and discussed other possible pathways to activate the electrophilic sulfur reagent. As shown in **Fig. S1**, the reactant **R1** and Lewis acid **TMSOTf** were proposed to be transformed to 1-(trimethylsilyl)pyrrolidine-2,5-dione (donated as **P1**) and *P*-methylphenylthiotrifluoromethanesulfonic acid (donated as **P2**). Then, the **Cat** nucleophilically attacks on the S atom of **P2** to form **Int1** via a S_N2 type transition state **TS1'** with an energy barrier of 31.0 kcal/mol, showing that this pathway is difficult to happen under the experimental conditions.

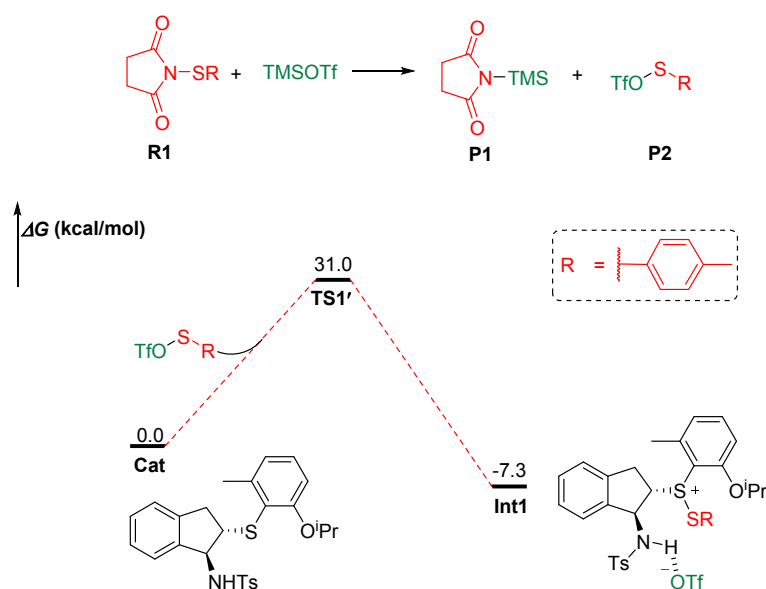


Fig. S1. The relative Gibbs free energy profiles of transformation from **Cat** and **P2** to **Int1**.

2.2 The role of chiral sulfide catalyst

In order to understand the actual role of chiral sulfide, we analyzed global reaction index (GRI)¹⁰. The global electrophilicity index ω is calculated from the electronic chemical potential μ and the chemical hardness η with the equation $\omega = (\mu^2/2\eta)$, which can be computed by using the energies of the frontier molecular orbitals (HOMO and LUMO), *i.e.* E_H and E_L , respectively, and the equations are $\mu \approx (E_H + E_L)/2$ and $\eta \approx (E_L - E_H)$. According to the HOMO energies obtained within the Kohn–Sham¹¹ scheme,

Domingo¹² and co-workers defined a global nucleophilicity index N ($N = E_{\text{HOMO(S)}} - E_{\text{HOMO(TCE)}}$) to handle the nucleophilicity scale. As shown in **Table S3**, the electrophilicity index (ω) of the reactant **R1** (1.33 eV) is enhanced to 2.93 eV in intermediate **Int1** after the complexation with the catalyst. The computed results show that the catalyst can strengthen the electrophilicity of **R1** to promote the subsequent reaction with the nucleophile acetylide.

Table S3. GRI analysis of **R1**, **Int1**, and **Int02**

SP	E_{HOMO} (a.u.)	E_{LUMO} (a.u.)	η (a.u.)	μ (a.u.)	ω (eV)	N (eV)
R1	-0.250	-0.038	-0.144	0.212	1.33	2.01
Int1	-0.242	-0.103	-0.173	0.139	2.93	2.21
Int02	-0.225	-0.102	-0.163	0.123	2.96	2.69

2.3 Local electrophilic (P_k^+) and nucleophilic (P_k^-) Parr function analyses on **R1**, **Int1**, and **Int02**.

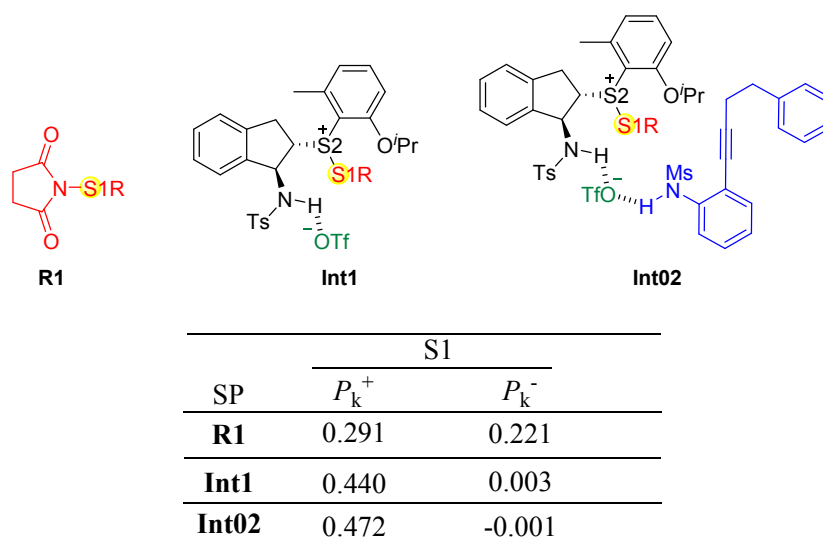


Fig. S2. Local electrophilic (P_k^+) and nucleophilic (P_k^-) Parr function analyses on **R1**, **Int1**, and **Int02**.

2.4 The formation of thiiranium ion intermediate catalyzed by chiral selenide catalyst

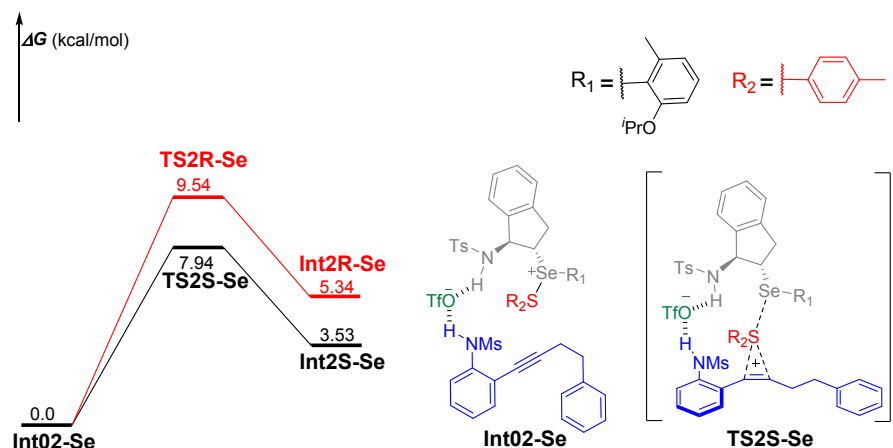
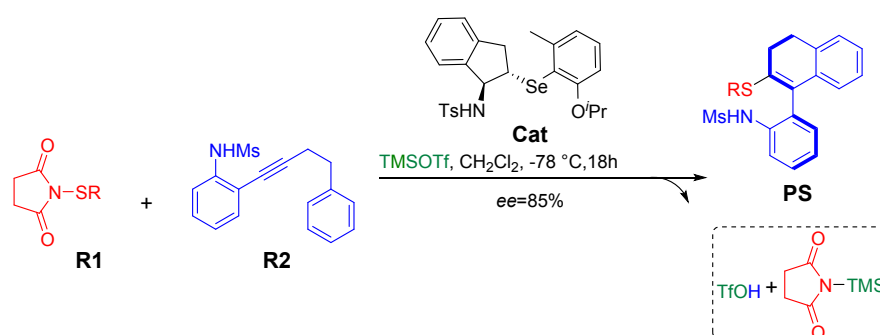


Fig. S3. The relative Gibbs free energy profiles of the chiral selenide-catalyzed electrophilic carbothiolation reaction of alkyne.

2.5 NCI and AIM analyses of TS2R-Se and TS2S-Se

As shown in **Scheme S1**, the relatively low stereoselectivity (85% *ee*) was obtained by using selenide catalyst in experiment¹³. Herein, we also computed the formation process of thiiranium ion intermediate with the presence of selenide catalyst. As summarized in **Fig. 2** and **S3**, the energy difference between **TS2R-Se** and **TS2S-Se** is only 1.6 kcal/mol, which is smaller than the energy difference between **TS2R** and **TS2S** (2.2 kcal/mol). Attracted by this puzzle, the topology analyses on the key transition states **TS2R-Se** and **TS2S-Se** was performed to characterize the stereoselectivity-determining factors by using noncovalent interaction (NCI) and Bader's atoms-in-molecules (AIM) methods. As shown in **Fig. S4**, the NCI analyses of the transition states **TS2R-Se** and **TS2S-Se** indicate that the hydrogen bond N-H...O interactions would be the key for determining the stereoselectivity. Correspondingly, Laplacian values at the bond critical points (BCPs) along the bond paths were summarized in **Fig. S4c**. The quantitatively analysis results indicate that there are more and stronger hydrogen bond C-H...O interactions in **TS2S-Se** compared with those in the other transition state.

Hence, the C-H...O hydrogen bond interactions would lead to the energetical favorability of *SR* configurational transition state **TS2S-Se**, which is the key to control the stereoselectivity. By comparing **Fig. 2** and **Fig. S4**, the energy difference between **TS2R-Se** and **TS2S-Se** is relatively smaller and the lower *ee* value is obtained by using selenide catalyst, which is mainly because that the strength of the ¹N-H...O interaction in **TS2R-Se** becomes stronger than that in **TS2R**.



Scheme. S1 Representative strategies for the organocatalytic preparation of axially chiral compounds using alkynes.

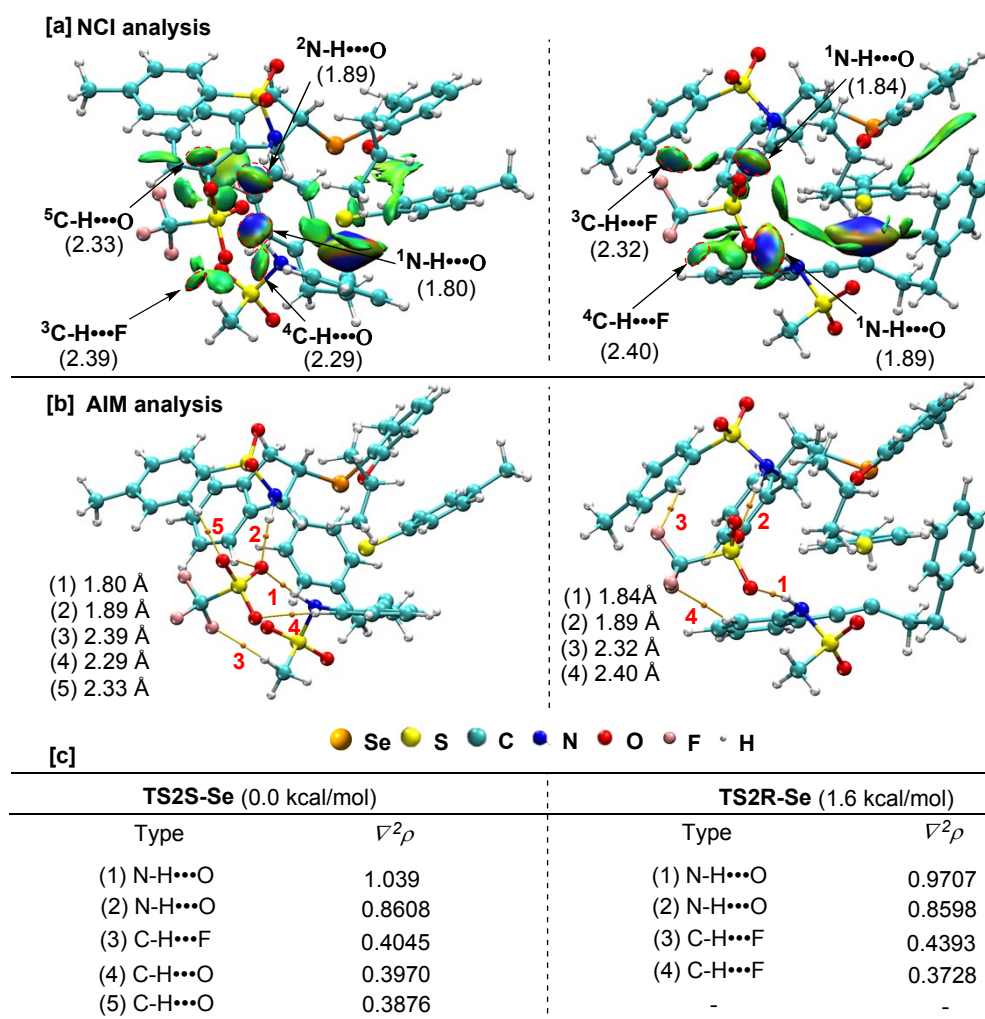
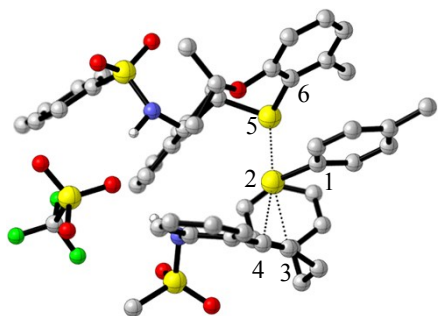


Fig. S4 (a) NCI and (b) AIM analyses of the transition states **TS2S-Se** and **TS2R-Se** (Distance in Å) and (c) summary of Laplacian values ($\nabla^2\rho$, eÅ⁻³).

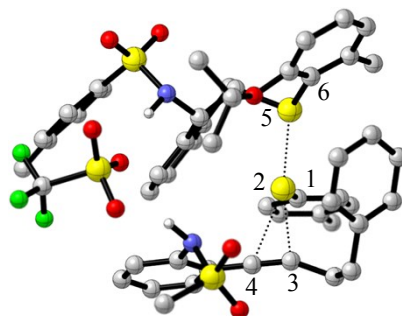
2.6 Different configurations of **TS2R**&**TS2S**

To ensure the selected configuration of the stereochemical transition state **TS2R**&**TS2S** with the lowest energy, we have searched multiple possible conformations in the second step. By rotating the dihedral angle $\Phi_1(\text{C1-S2-C3-C4})$ and dihedral angle $\Phi_2(\text{C1-S2-S5-C6})$ in stereo-controlling transition states **TS2S** and **TS2R**, we have totally constructed $2 \times 9 = 18$ conformations as the initial structures, which have subsequently been optimized at the B3LYP-D3/6-31G(d, p)//IEFPCM_{dichloromethane} level. Actually, we have only obtained ten conformations after optimization. As depicted in **Fig. S5**, we have located ten diastereoselective transition states, and selected the two lowest energy

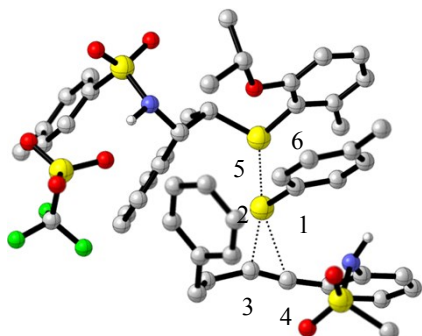
conformations (denoted as **TS2S** and **TS2R**) with the dihedral angles $\Phi_1(\text{C1-S2-C3-C4})$ of $101^\circ/-96^\circ$ and the dihedral angles $\Phi_2(\text{C1-S2-S5-C6})$ of $-31^\circ/-143^\circ$, separately.



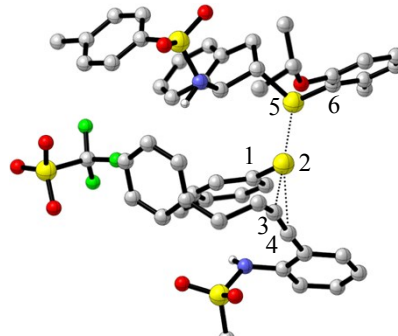
TS2S $\Phi_1 = 101^\circ/\Phi_2 = -31^\circ$ 0.0



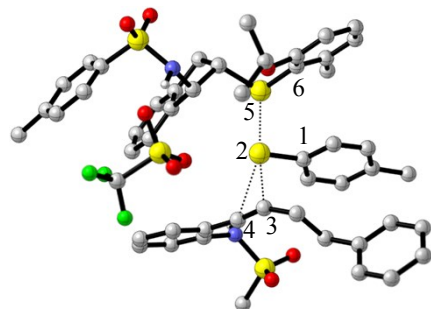
TS2R $\Phi_1 = -96^\circ/\Phi_2 = -143^\circ$ 1.6



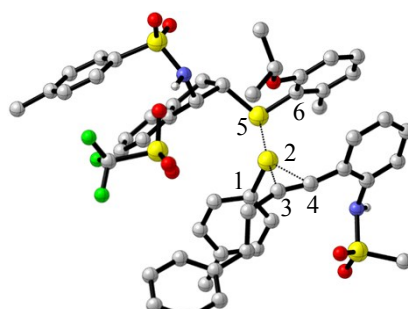
TS2S $\Phi_1 = -60^\circ/\Phi_2 = 9^\circ$ 15.4



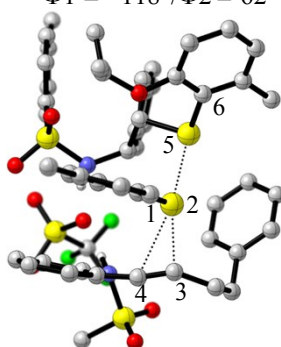
TS2R $\Phi_1 = 66^\circ/\Phi_2 = -165^\circ$ 17.4



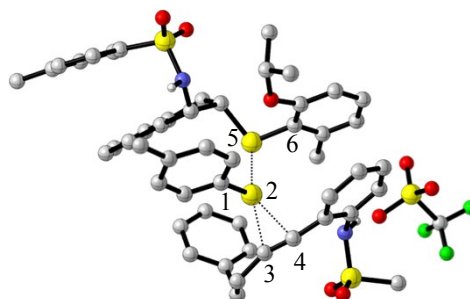
TS2S $\Phi_1 = -118^\circ/\Phi_2 = -62^\circ$ 11.1



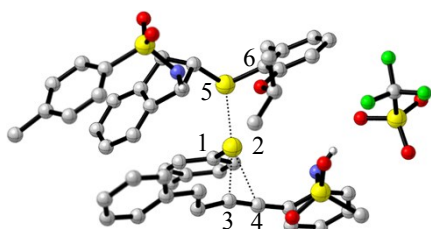
TS2R $\Phi_1 = 120^\circ/\Phi_2 = -146^\circ$ 12.3



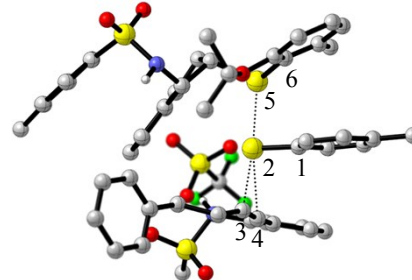
TS2S $\Phi_1 = 57^\circ/\Phi_2 = 48^\circ$ 13.2



TS2R $\Phi_1 = -84^\circ/\Phi_2 = -35^\circ$ 35.56



TS2S $\Phi_1 = 92^\circ/\Phi_2 = -134^\circ$ 3.5



TS2R $\Phi_1 = -102^\circ/\Phi_2 = 106^\circ$ 16.0

Fig. S5. Different configurations of the transition states **TS2Rs** and **TS2Ss** with different dihedral Φ_1 and Φ_2 angles optimized at the B3LYP-D3/6-31G(d, p)/IEF-PCM_{dichloromethane} level of theory (energy in kcal/mol)

2.7 NCI and AIM analyses of **TS2R** and **TS2S**

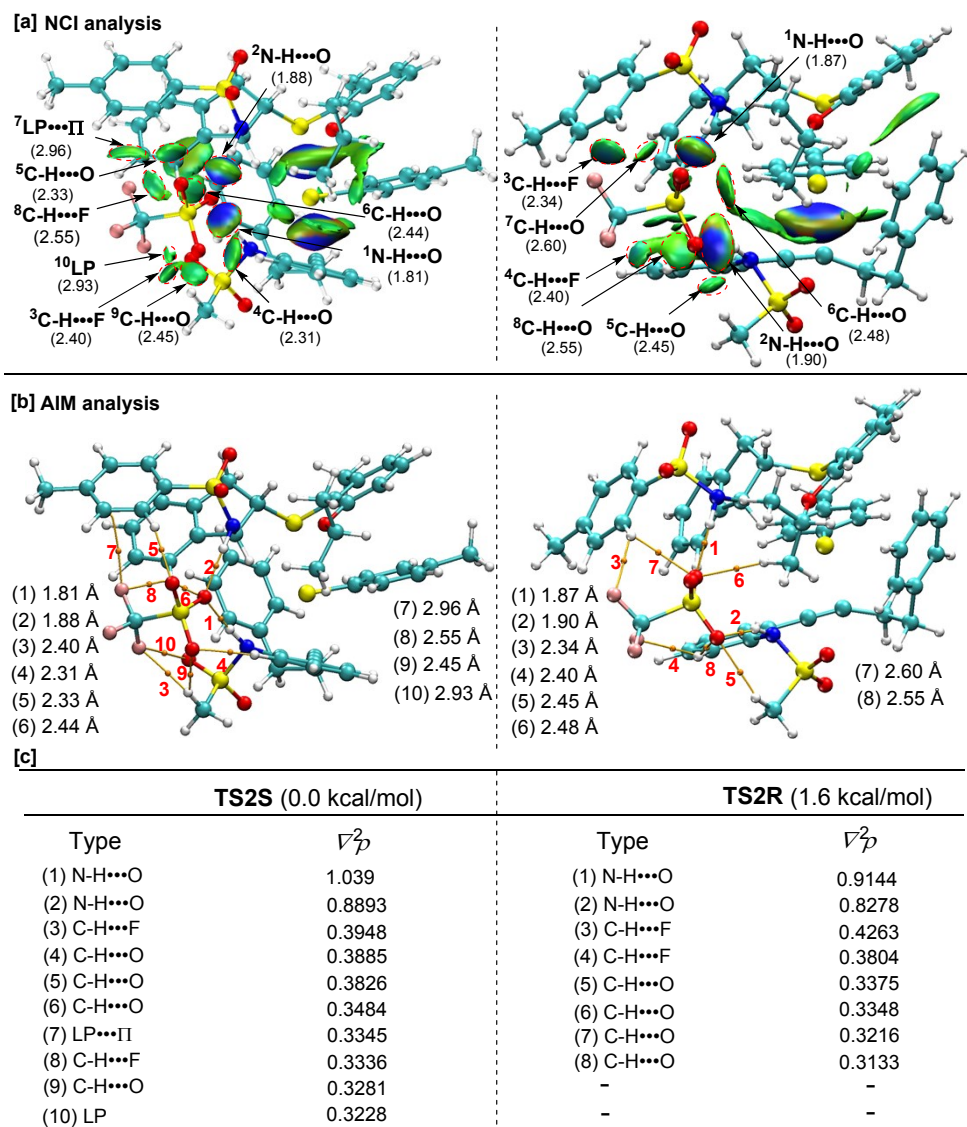


Fig. S6 (a) NCI and (b) AIM analyses of the transition states **TS2S** and **TS2R** (Distance in Å), and (c) complete summary of Laplacian values ($\nabla^2\rho$, eÅ⁻³).

2.8 The FMO overlap mode and ELF analyses for the formation of thiiranium ion intermediate

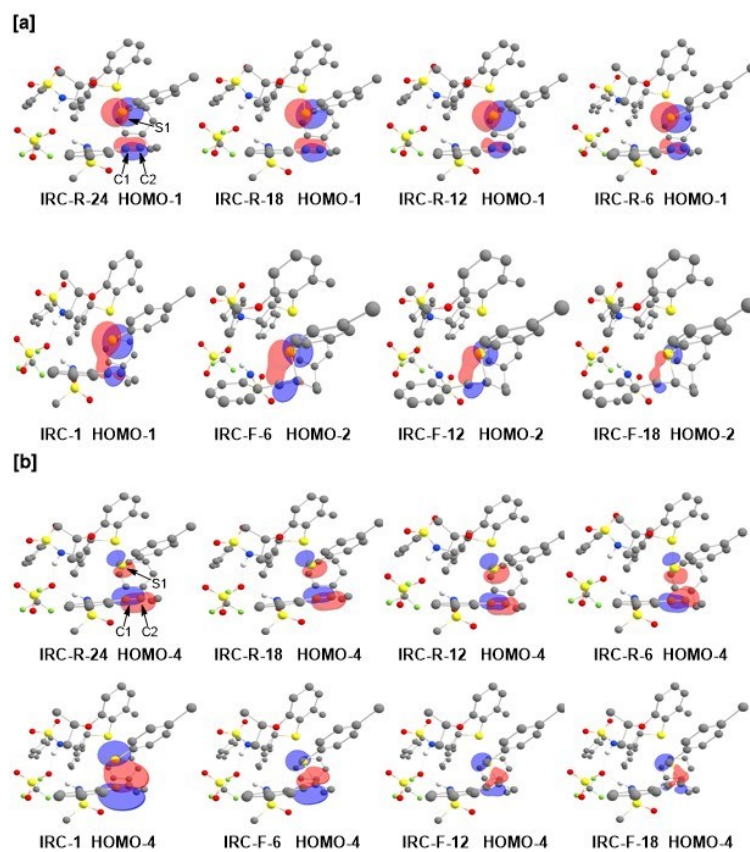


Fig. S7 The orbital pictures for (a) S1-C1 and (b) S1-C2 σ bonds of several representative IRC points of **TS2S** (IRC-1 is the structure of transition state, F represents forward direction, R represents reverse direction, and only the orbital pictures of the key atoms (S1, C1, and C2 atoms) are shown).

2.9 The volume of R groups of R2 involved in the axially chiral products

To obtain the relationship of substituent groups and the energy barriers of corresponding racemization between the enantioselective products, the typical functional groups, *i.e.* H, CH₃, *t*Pr, and *p*-methylphenylthio (PMP) group, were employed for molecular simulations. The molecular volume of organic compounds has good additivity, that is, the molecular volume of organic compounds is equal to the sum of the topological volumes of the functional groups of its components, and the

molecular volume of organic compounds can be calculated by the following equation (eq. 3)¹⁴, in which V_m is the molecular volume, d is molecular radius.

$$\text{eq. 3: } V_M = \frac{M(\text{molecular weight})}{d \times 6.023 \times 10^{23}} = \frac{1.6603M}{d}$$

Table S4. Summary of the volumes of each groups.

Groups	Volume (cm ³ /mol)
H	9.8
CH ₃	22.8
ⁱ Pr	50.5
PMP	102.1

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Part 3: Energy values and Cartesian coordinates of all the optimized structures

3.1 Absolute SPE and GFE of the optimized structures by using B3LYP-D3 method

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
cat	-2085.117451	0.437191	-2084.680259
TMSOTf	-1370.768509	0.097153	-1370.671356
Int01	-3455.910905	0.55935	-3455.351556
R1	-1029.254348	0.156823	-1029.097525
P1	-769.417227	0.152415	-769.264812
TS1	-4485.153821	0.744016	-4484.409805
Int1	-3715.743902	0.563577	-3715.180325
TS1'	-3715.691662	0.561379	-3715.130283
R2	-1261.400584	0.251548	-1261.149036
Int02	-4977.192798	0.847912	-4976.344885
TS2S	-4977.186903	0.848351	-4976.338551
Ts2R	-4977.183576	0.847495	-4976.336081
TS2'S	-4977.181614	0.847605	-4976.334009
TS2'R	-4977.176463	0.841788	-4976.334675
Int2S	-4977.198984	0.849864	-4976.34912
Int2R	-4977.197088	0.847777	-4976.349311
TS3S	-4977.195027	0.851929	-4976.343098
TS3R	-4977.192049	0.848746	-4976.343303
Int3S	-4977.196456	0.848594	-4976.347862
Int3R	-4977.195385	0.844518	-4976.350866
TS4S	-4977.194445	0.84865	-4976.345796
TS4R	-4977.193964	0.849067	-4976.344897

PS	-1930.045922	0.358692	-1929.68723
TfOH	-962.018555	0.004259	-962.014296
Int02-se	-6978.4284	0.847553	-6977.580848
TS2S-Se	-6978.41537	0.849457	-6977.565914
TS2R-Se	-6978.405254	0.847574	-6977.55768
Int2S-se	-6978.419211	0.850159	-6977.569052
Int2R-se	-6978.411859	0.846501	-6977.565359
TS5	-1261.429415	0.261453	-1261.167962
TS6	-1300.780013	0.285126	-1300.494887
TS7	-1379.363968	0.342668	-1379.0213
TS8	-1929.977347	0.359503	-1929.617844

3.2 Absolute SPE and GFE of the optimized structures by other DFT methods

Table S10. Absolute SPE and GFE of the optimized structures obtained at the M06-2X/6-31G(d, p)/IEF-PCM_{dichloromethane} level.

	SPE(a.u.)	GFEC(a.u.)	CFE(a.u.)	$\Delta\Delta G^\ddagger$
TS2R	-4975.630848	0.860363	-4974.770485	2.0
TS2S	-4975.633867	0.860157	-4974.77371	0.0

Table S11. Absolute SPE and GFE of the Optimized Structures obtained at the ω B97X-D /6-31G(d, p)/IEF-PCM_{dichloromethane} level..

	SPE(a.u.)	GFEC(a.u.)	CFE(a.u.)	$\Delta\Delta G^\ddagger$
TS2R	-4976.022087	0.86361	-4975.158477	2.1
TS2S	-4976.02706	0.865268	-4975.161792	0.0

Table 12 Absolute SPE and GFE of the different conformers of TS2R/S

	SPE(a.u.)	GFEC(a.u.)	CFE(a.u.)
TS2R($\Phi_1=-96^\circ/\Phi_2=-143^\circ$)	-4977.183576	0.847495	-4976.336081

TS2R($\Phi_1=66^\circ/\Phi_2=-165^\circ$)	-4977.158625	0.847843	-4976.310782
TS2R($\Phi_1=120^\circ/\Phi_2=-146^\circ$)	-4977.159441	0.840488	-4976.318953
TS2R($\Phi_1=-84^\circ/\Phi_2=-35^\circ$)	-4977.122475	0.840592	-4976.281883
TS2R($\Phi_1=-102^\circ/\Phi_2=106^\circ$)	-4977.156219	0.843183	-4976.313036
TS2S($\Phi_1=101^\circ/\Phi_2=-31^\circ$)	-4977.186903	0.848351	-4976.338551
TS2S($\Phi_1=-60^\circ/\Phi_2=9^\circ$)	-4977.162922	0.848999	-4976.313924
TS2S($\Phi_1=-118^\circ/\Phi_2=48^\circ$)	-4977.161364	0.840484	-4976.320881
TS2S($\Phi_1=92^\circ/\Phi_2=-134^\circ$)	-4977.163089	0.845703	-4976.317386
TS2S($\Phi_1=57^\circ/\Phi_2=48^\circ$)	-4977.178459	0.845546	-4976.332913

3.3 The Cartesian coordinates and representative vibrational frequencies of all the stationary points

Cat

Cartesian coordinates

C	0.606689	-1.623985	0.303637
C	1.182754	-1.239256	-0.909193
C	2.358121	-1.831033	-1.368763
C	2.958742	-2.824474	-0.593625
C	2.379110	-3.220940	0.618356
C	1.200399	-2.624756	1.073421
C	-0.615118	-0.796474	0.615263
C	-0.906680	-0.033682	-0.698199
C	0.375823	-0.141786	-1.574864
H	2.806915	-1.515907	-2.306653
H	3.878402	-3.292825	-0.931041
H	2.853066	-3.998203	1.210771
H	0.758016	-2.930308	2.017548
H	-1.467347	-1.394350	0.949998
H	-1.161629	1.003697	-0.517584
H	-0.394922	-0.077538	1.412716
S	1.747385	2.046208	-0.506089
O	0.754914	2.122049	0.576453
O	2.242617	3.268450	-1.155695
C	3.166340	1.151920	0.113829
C	3.064645	0.429829	1.302821
C	4.341436	1.143023	-0.640589
C	4.153259	-0.325559	1.727098
H	2.145487	0.454743	1.874813
C	5.419819	0.380467	-0.199843

H	4.413730	1.727081	-1.551983
C	5.338629	-0.373770	0.979882
H	4.076214	-0.897967	2.646662
H	6.337015	0.368325	-0.781460
C	6.483265	-1.250591	1.420927
H	7.428899	-0.938479	0.970206
H	6.598043	-1.241219	2.508794
H	6.300277	-2.290191	1.122695
N	1.048877	1.170078	-1.755009
H	1.657054	1.206898	-2.568354
S	-2.301638	-0.774357	-1.674049
C	-3.620474	-0.827532	-0.462878
C	-4.275518	-2.047535	-0.193367
C	-4.019535	0.353910	0.208828
C	-5.315992	-2.063919	0.745460
C	-5.045511	0.305081	1.160535
C	-5.689426	-0.903272	1.418081
H	-5.822702	-3.000451	0.958029
H	-5.346234	1.201633	1.688314
H	-6.488786	-0.934435	2.152553
C	-3.870548	-3.329753	-0.881421
H	-4.040132	-3.279775	-1.962309
H	-2.803703	-3.531172	-0.741034
H	-4.440532	-4.175761	-0.489460
O	-3.371049	1.498134	-0.143382
C	-3.351875	2.651541	0.734015
C	-2.721685	3.762762	-0.094137
C	-2.556686	2.348824	2.001867
H	-4.384664	2.927436	0.982940
H	-3.283198	3.920099	-1.018763

H	-2.716010	4.696080	0.476095
H	-1.688452	3.505026	-0.346292
H	-1.515742	2.134021	1.744361
H	-2.578063	3.215774	2.669160
H	-2.973610	1.493705	2.539908
H	0.126800	-0.419382	-2.605238

Vibrational frequencies

17.7335	21.8435	27.7049
39.5180	52.3877	57.5079
61.4505	62.9074	76.1294
77.2802	86.2123	106.6104
127.0794	133.5766	140.5329
162.0468	176.7592	182.1948
194.2187	231.3712	238.4467
241.7713	245.4405	257.6924
268.0465	279.4818	293.2740
304.6298	311.6807	329.2584

TMSOTf

Si	-2.022035	-0.197998	0.012443
C	-1.668141	-1.378252	-1.391303
H	-1.184249	-2.291373	-1.034250
H	-2.605953	-1.656438	-1.884205
H	-1.016956	-0.908719	-2.133526
C	-2.893074	-0.986482	1.461874
H	-2.342149	-1.859950	1.823417
H	-3.002669	-0.278350	2.288601
H	-3.893426	-1.316148	1.160826
C	-2.779471	1.411264	-0.555042
H	-2.870599	2.118140	0.275387

H	-2.161837	1.867833	-1.333497
H	-3.779810	1.236706	-0.965742
O	-0.461366	0.221847	0.751394
S	0.796732	0.888070	0.071020
O	1.400034	1.839422	0.995224
O	0.520619	1.264587	-1.315005
C	1.925717	-0.600437	0.013628
F	1.362710	-1.557966	-0.727181
F	3.083519	-0.234317	-0.534966
F	2.135320	-1.055745	1.247104

Vibrational frequencies

32.2977	44.3101	64.5507
115.2338	135.3656	137.4954
149.3335	158.8933	174.5119
187.0846	198.1919	208.9054
235.1604	247.3644	298.2855
309.8910	328.2869	394.4772
491.5861	534.8717	556.7906
589.0807	599.9792	663.5628
706.8802	709.9580	712.7540
762.5653	786.2463	787.2033

Int01

Cartesian coordinates

C	0.804792	2.986841	-1.070083
C	-0.149552	1.975569	-1.197948
C	-1.420506	2.233822	-1.710474
C	-1.730886	3.537103	-2.099773
C	-0.775499	4.555946	-1.983848
C	0.495669	4.288366	-1.469139

C	2.075924	2.465947	-0.440697
C	1.891802	0.927423	-0.412524
C	0.392975	0.648278	-0.718612
H	-2.155226	1.436983	-1.784309
H	-2.717033	3.764746	-2.493152
H	-1.028369	5.565821	-2.293847
H	1.229419	5.084315	-1.375611
H	2.976319	2.765970	-0.984602
H	2.155423	0.500023	0.548296
H	2.175002	2.843582	0.583993
S	-0.599451	0.783523	1.880579
O	0.667125	1.398642	2.306247
O	-1.250400	-0.246836	2.705951
C	-1.783428	2.101045	1.626117
C	-1.338943	3.421379	1.555256
C	-3.126499	1.777186	1.425238
C	-2.255972	4.424899	1.259484
H	-0.292261	3.650066	1.712712
C	-4.027788	2.794980	1.125133
H	-3.461505	0.750987	1.502703
C	-3.606462	4.128783	1.025356
H	-1.913874	5.453155	1.191086
H	-5.072809	2.548178	0.961268
C	-4.570378	5.220342	0.634528
H	-5.607371	4.930449	0.822592
H	-4.365761	6.148018	1.177055
H	-4.476603	5.442743	-0.435525
N	-0.308807	0.012412	0.423159
H	-1.141522	-0.488067	0.124071
S	2.912398	0.026472	-1.670081

C	4.521067	0.036852	-0.879767
C	5.623535	0.647879	-1.510402
C	4.692337	-0.625942	0.362281
C	6.877483	0.591739	-0.885493
C	5.952362	-0.655687	0.972018
C	7.036145	-0.048181	0.340604
H	7.730349	1.062734	-1.364974
H	6.090948	-1.153491	1.923480
H	8.012318	-0.076681	0.815774
C	5.484147	1.356179	-2.837622
H	5.200278	0.662279	-3.635971
H	4.704281	2.122920	-2.799194
H	6.425933	1.831853	-3.122399
O	3.583771	-1.220394	0.881087
C	3.528785	-1.653845	2.262047
C	2.247513	-2.471480	2.356349
C	3.521660	-0.454867	3.207660
H	4.391174	-2.302168	2.465452
H	2.276444	-3.312197	1.658322
H	2.121920	-2.861267	3.370418
H	1.383821	-1.846199	2.112869
H	4.413256	0.163668	3.078963
H	2.636937	0.160547	3.023220
H	3.495743	-0.803417	4.244708
H	0.284805	-0.106182	-1.502174
Si	-0.924538	-4.133241	-0.127397
C	-1.154121	-3.641340	1.656634
H	-1.115006	-2.559267	1.806053
H	-2.106288	-4.014178	2.046208
H	-0.348452	-4.087010	2.251078

C	-1.008397	-5.976712	-0.408077
H	-1.936401	-6.394770	-0.006648
H	-0.953957	-6.213091	-1.474982
H	-0.168090	-6.468813	0.093682
C	0.531397	-3.314363	-0.958485
H	0.656786	-2.280816	-0.630974
H	1.444369	-3.858468	-0.692057
H	0.437011	-3.329648	-2.047829
O	-3.733385	-2.575675	-2.784547
S	-2.902388	-2.289727	-1.625532
O	-1.822174	-1.302125	-1.715691
O	-2.416084	-3.626994	-0.976237
C	-4.022122	-1.658617	-0.270779
F	-5.025212	-2.499657	-0.057472
F	-3.296536	-1.528418	0.852434
F	-4.491456	-0.461834	-0.625197

Vibrational frequencies

21.2951	22.6146	24.2916
29.2816	31.9317	35.3309
42.5491	46.6675	51.7258
51.7596	61.8995	64.4910
65.7672	66.9024	69.7363
78.3420	80.9070	86.7800
94.1151	106.2654	108.8491
121.1140	135.2688	142.0087
142.7198	145.4658	149.8493
165.1334	169.9725	179.6261

R1

Cartesian coordinates

C	-2.244306	1.126730	-0.400798
C	-2.162339	-1.207554	-0.093826
C	-3.135907	-0.979044	-1.238915
C	-3.175179	0.541390	-1.451222
H	-2.781145	-1.532988	-2.111510
H	-4.104208	-1.401100	-0.956530
H	-2.817368	0.850140	-2.436835
H	-4.169244	0.974808	-1.314568
N	-1.735262	0.055419	0.361596
O	-1.795513	-2.270201	0.359361
O	-1.966753	2.293419	-0.230956
S	-0.628733	0.265433	1.684563
C	0.937225	0.132761	0.825242
C	1.477629	-1.129394	0.542938
C	1.627590	1.290249	0.445167
C	2.699661	-1.223691	-0.118865
H	0.927963	-2.021197	0.824017
C	2.853887	1.180035	-0.208778
H	1.199262	2.265472	0.651238
C	3.409427	-0.074354	-0.499041
H	3.111286	-2.204162	-0.342760
H	3.384347	2.081208	-0.504077
C	4.751030	-0.187226	-1.180251
H	5.557801	-0.234399	-0.438661
H	4.815338	-1.093452	-1.789187
H	4.948350	0.675657	-1.822452

Vibrational frequencies

29.9130	35.8768	43.1811
47.7101	69.0891	98.9067
125.6987	187.4835	240.2166

279.1407	304.4854	368.8172
385.7577	407.5906	421.4249
499.7424	529.2294	560.8180
564.9866	581.6380	638.6731
647.1302	648.0938	657.3403
723.1039	813.0384	831.1253
838.0134	856.2275	939.0596

P1

Cartesian coordinates

C	-1.134149	-1.150210	-0.000035
C	-1.264435	1.158462	-0.000140
C	-2.713251	0.678570	-0.000197
C	-2.626461	-0.848730	0.000257
H	-3.214539	1.090466	0.879743
H	-3.214224	1.089883	-0.880597
H	-3.076169	-1.315195	0.880895
H	-3.076770	-1.315838	-0.879724
N	-0.411256	0.046746	-0.000266
O	-0.905612	2.321221	-0.000034
O	-0.627545	-2.260109	-0.000004
Si	1.422893	0.026715	-0.000052
C	2.049595	1.792192	-0.000502
H	1.712160	2.340396	0.882091
H	3.145898	1.771356	-0.001100
H	1.711171	2.340456	-0.882670
C	1.929406	-0.880711	1.562474
H	1.484990	-1.878807	1.583969
H	3.019106	-0.982376	1.610310
H	1.601873	-0.334717	2.453385

C	1.929763	-0.882034	-1.561667
H	1.485420	-1.880196	-1.582090
H	1.602341	-0.337092	-2.453252
H	3.019480	-0.983709	-1.609207

Vibrational frequencies

27.1351	49.8445	72.3022
139.6009	156.1962	157.1730
159.2419	173.7559	175.6845
203.5150	215.9442	239.9359
296.3351	337.3216	471.8127
563.1506	565.5223	575.7509
615.3425	659.2711	671.6328
705.0496	705.2891	705.7461
783.5940	787.7659	841.2473
873.7725	879.1360	882.7261

TS1

Cartesian coordinates

C	1.386281	-3.373384	-1.678868
C	1.770136	-2.035205	-1.594737
C	2.873839	-1.546787	-2.293148
C	3.603949	-2.433947	-3.084093
C	3.228925	-3.781502	-3.169155
C	2.119115	-4.260847	-2.468460
C	0.175017	-3.662362	-0.823532
C	-0.253590	-2.272431	-0.284864
C	0.862534	-1.253556	-0.672386
H	3.169104	-0.506445	-2.196540
H	4.472496	-2.080422	-3.631065
H	3.807819	-4.461532	-3.787123

H	1.832870	-5.306387	-2.538335
H	-0.619199	-4.170069	-1.381067
H	-0.410952	-2.263820	0.785814
H	0.432523	-4.301659	0.026095
S	2.391318	-1.541641	1.615604
O	1.736561	-2.853670	1.760158
O	2.549941	-0.653867	2.775660
C	4.011656	-1.796159	0.909102
C	4.352232	-3.032821	0.364397
C	4.889300	-0.710423	0.857237
C	5.594422	-3.175648	-0.249746
H	3.651093	-3.857536	0.406265
C	6.118707	-0.869157	0.227943
H	4.614406	0.236469	1.302605
C	6.487855	-2.099343	-0.339803
H	5.866225	-4.135031	-0.679693
H	6.799530	-0.024611	0.175896
C	7.804031	-2.245713	-1.061628
H	8.583347	-1.631784	-0.601191
H	8.143006	-3.285077	-1.072921
H	7.706273	-1.919471	-2.104238
N	1.473701	-0.654297	0.528888
H	1.937639	0.235121	0.332799
S	-1.884800	-1.778229	-1.026384
C	-3.089284	-2.593831	-0.001858
C	-4.119367	-3.306370	-0.655609
C	-3.077444	-2.440442	1.409849
C	-5.096626	-3.915781	0.135000
C	-4.064925	-3.081452	2.168954
C	-5.060089	-3.809928	1.525097

H	-5.891370	-4.476722	-0.345164
H	-4.067041	-2.999501	3.247499
H	-5.826482	-4.295701	2.121060
C	-4.200885	-3.407938	-2.160704
H	-4.341040	-2.421023	-2.614287
H	-3.292242	-3.838951	-2.591782
H	-5.045906	-4.034319	-2.452732
O	-2.122494	-1.635761	1.916358
C	-1.912291	-1.486959	3.353723
C	-1.103955	-0.208429	3.510356
C	-1.196323	-2.720087	3.893479
H	-2.892406	-1.358856	3.827703
H	-1.624530	0.644282	3.068977
H	-0.945350	-0.012410	4.575146
H	-0.125958	-0.308627	3.032514
H	-1.774980	-3.631727	3.721471
H	-0.221824	-2.825683	3.407490
H	-1.040372	-2.613388	4.971002
H	0.457856	-0.384344	-1.199058
C	-2.961348	3.137090	0.977339
C	-2.978685	3.494789	-1.259292
C	-4.288083	4.123206	-0.775694
C	-4.263793	3.906506	0.733220
H	-4.316605	5.173259	-1.079853
H	-5.114686	3.612315	-1.278336
H	-4.244080	4.832436	1.315547
H	-5.093821	3.300231	1.106098
N	-2.243739	2.960470	-0.203448
O	-2.653289	3.455806	-2.441501
O	-2.635868	2.720030	2.083747

S	-2.075096	0.499015	-0.584090
C	-3.847582	0.454175	-0.706851
C	-4.618429	0.303539	0.455731
C	-4.478161	0.576087	-1.953424
C	-6.006802	0.269522	0.364419
H	-4.123654	0.229360	1.416449
C	-5.868418	0.533760	-2.029409
H	-3.879553	0.722942	-2.845368
C	-6.653208	0.372753	-0.876819
H	-6.597966	0.155136	1.268525
H	-6.352760	0.630768	-2.996871
C	-8.155360	0.285384	-0.971690
H	-8.636699	0.690742	-0.077328
H	-8.534452	0.823854	-1.844461
H	-8.472302	-0.760328	-1.067563
Si	0.286004	3.380371	-0.274984
C	0.350934	2.397605	1.316407
H	0.034117	1.365901	1.168891
H	1.360748	2.393730	1.730847
H	-0.340622	2.828521	2.040378
C	-0.246747	5.179688	-0.189111
H	-0.831334	5.360209	0.717079
H	0.620204	5.845159	-0.188139
H	-0.872814	5.421680	-1.052493
C	0.327089	2.582154	-1.971887
H	0.832541	1.614675	-1.937785
H	-0.671810	2.475311	-2.388322
H	0.915563	3.230194	-2.630965
O	4.182586	3.458327	-1.737366
S	3.378530	2.929092	-0.636799

O	3.026426	1.495265	-0.666911
O	2.185650	3.830725	-0.292968
C	4.418521	3.119229	0.899662
F	4.644484	4.404751	1.160940
F	3.794834	2.555164	1.943539
F	5.587067	2.490995	0.711368

Vibrational frequencies

-141.4257	17.1491	18.2812
20.7515	28.4456	31.0756
32.4247	35.3018	36.0993
39.9563	44.4312	46.4004
47.0180	49.3119	53.3544
54.3046	60.0467	62.9953
66.8305	71.7406	75.0190
76.9208	81.4690	82.8083
84.9914	87.2735	94.4433
99.2026	104.7661	108.8173

Int1

Cartesian coordinates

C	-0.566482	-2.053640	-1.952554
C	0.360890	-1.089511	-1.555727
C	1.554077	-0.901671	-2.252697
C	1.810809	-1.711838	-3.359288
C	0.883739	-2.682425	-3.761715
C	-0.312426	-2.859433	-3.062409
C	-1.762002	-2.087546	-1.030841
C	-1.561533	-0.857081	-0.116449
C	-0.111394	-0.333333	-0.328680
H	2.265414	-0.152747	-1.921651
H	2.737475	-1.590771	-3.911906

H	1.097528	-3.304015	-4.626216
H	-1.029300	-3.613018	-3.375814
H	-2.717846	-2.086715	-1.564824
H	-1.769635	-1.053181	0.927877
H	-1.753963	-2.980328	-0.398142
S	1.106616	-1.921868	1.562806
O	-0.107599	-2.759589	1.541131
O	1.764018	-1.600714	2.836035
C	2.318935	-2.682512	0.491277
C	1.961425	-3.772803	-0.300234
C	3.589495	-2.109034	0.407523
C	2.892946	-4.283942	-1.199949
H	0.967641	-4.196341	-0.222006
C	4.503346	-2.629497	-0.503147
H	3.861073	-1.272996	1.038072
C	4.167263	-3.714060	-1.327414
H	2.618980	-5.127650	-1.826444
H	5.488698	-2.178886	-0.579592
C	5.138339	-4.228701	-2.359956
H	6.174903	-4.041279	-2.067048
H	5.013867	-5.302135	-2.528567
H	4.972098	-3.725447	-3.320465
N	0.683923	-0.442580	0.908327
H	1.489884	0.195008	0.868610
S	-2.737007	0.500849	-0.609533
C	-4.352308	-0.202795	-0.373431
C	-5.245735	-0.178297	-1.465044
C	-4.693323	-0.780595	0.872423
C	-6.487005	-0.794225	-1.285985
C	-5.941171	-1.397276	1.009028

C	-6.819791	-1.396784	-0.071656
H	-7.195788	-0.802958	-2.106963
H	-6.226729	-1.859174	1.944930
H	-7.789336	-1.871687	0.040297
C	-4.889343	0.465874	-2.783259
H	-4.612848	1.517297	-2.654970
H	-4.041264	-0.036502	-3.260333
H	-5.736257	0.420140	-3.469824
O	-3.773640	-0.650410	1.849973
C	-3.823076	-1.447207	3.075370
C	-2.809445	-0.790815	3.998796
C	-3.490654	-2.901541	2.761571
H	-4.828566	-1.353192	3.500709
H	-3.062215	0.258906	4.167282
H	-2.798325	-1.308821	4.961395
H	-1.807037	-0.846860	3.563871
H	-4.181471	-3.323637	2.026990
H	-2.469570	-2.980717	2.377093
H	-3.563214	-3.496788	3.676306
H	-0.084692	0.743014	-0.524573
S	-2.492298	1.994581	0.918999
C	-1.666334	3.254275	-0.029636
C	-2.384959	4.078176	-0.910976
C	-0.290510	3.451381	0.160259
C	-1.717458	5.079007	-1.607852
H	-3.451905	3.931617	-1.045417
C	0.356554	4.472821	-0.530590
H	0.278106	2.829397	0.841511
C	-0.339327	5.292230	-1.430115
H	-2.272621	5.713004	-2.293324

H	1.417537	4.624273	-0.361944
C	0.379244	6.363573	-2.209615
H	-0.278320	7.209428	-2.428968
H	1.254137	6.731904	-1.667732
H	0.732108	5.965313	-3.168743
O	4.118034	3.271133	-0.437746
S	3.312776	2.480019	0.513593
O	2.487455	1.407517	-0.123528
O	2.605797	3.247418	1.561377
C	4.558836	1.484364	1.472586
F	5.394547	2.276799	2.155902
F	3.923753	0.679384	2.348902
F	5.287291	0.705330	0.651063

Vibrational frequencies

11.8494	19.3620	22.6997
25.1254	28.6702	30.2102
33.5112	43.1405	45.9621
48.6856	54.0034	55.7862
58.3551	66.1072	67.1819
70.5645	72.3891	76.5250
79.1777	82.7687	87.3431
87.9083	102.1805	111.1312
119.2515	136.0764	143.5801
148.3770	166.1612	170.1841

TS1'

Cartesian coordinates

C	-1.007425	4.082526	-0.857991
C	-1.344286	3.154896	-1.847013
C	-1.934539	3.558245	-3.043546
C	-2.177659	4.917416	-3.248488

C	-1.835041	5.852791	-2.262995
C	-1.250745	5.441350	-1.062394
C	-0.424032	3.405798	0.357987
C	-0.160683	1.956976	-0.112500
C	-0.988670	1.746463	-1.426043
H	-2.204640	2.824434	-3.797061
H	-2.633187	5.252618	-4.175496
H	-2.026490	6.908192	-2.434527
H	-0.990769	6.169210	-0.298761
H	0.475200	3.902708	0.731886
H	-0.413249	1.210513	0.629304
H	-1.153991	3.388360	1.172101
S	-3.457510	1.277956	-0.310247
O	-4.432551	2.046221	-1.102424
O	-2.999927	1.876144	0.962950
C	-4.094520	-0.353383	0.020876
C	-4.831883	-1.013213	-0.961270
C	-3.740115	-0.983262	1.214064
C	-5.194391	-2.341225	-0.747661
H	-5.103280	-0.500578	-1.877598
C	-4.115773	-2.306721	1.410560
H	-3.168457	-0.445454	1.960408
C	-4.823971	-3.011226	0.426456
H	-5.756807	-2.870203	-1.511456
H	-3.824298	-2.812763	2.325622
C	-5.130946	-4.473911	0.624187
H	-4.204680	-5.056916	0.560744
H	-5.564383	-4.661461	1.611828
H	-5.821308	-4.851816	-0.133833
N	-2.160659	0.856490	-1.309072

H	-1.904624	-0.121505	-1.145779
S	1.620005	1.684741	-0.571287
C	2.585267	2.323445	0.768050
C	3.748908	3.070279	0.472493
C	2.268456	2.002987	2.117809
C	4.551448	3.507062	1.530189
C	3.087229	2.463594	3.156852
C	4.219604	3.213155	2.853668
H	5.440200	4.091340	1.313423
H	2.851657	2.231651	4.187226
H	4.853250	3.567503	3.660889
C	4.131331	3.405221	-0.949254
H	4.359471	2.503521	-1.529015
H	3.316643	3.918047	-1.470266
H	5.014910	4.047088	-0.969421
O	1.160387	1.250955	2.292871
C	0.669785	0.878039	3.607117
C	1.435624	-0.336729	4.121834
C	-0.811219	0.591945	3.405123
H	0.792836	1.733948	4.281049
H	2.511516	-0.148234	4.162237
H	1.093382	-0.592664	5.129010
H	1.256501	-1.192800	3.464563
H	-1.334219	1.463874	3.006359
H	-0.930050	-0.233055	2.699069
H	-1.269618	0.306497	4.356462
H	-0.383388	1.249180	-2.192285
S	2.618542	-1.095111	0.688803
C	3.362532	-1.971012	-0.551950
C	4.180304	-1.308732	-1.522683

C	3.224632	-3.391538	-0.632785
C	4.847982	-2.034438	-2.481322
H	4.264575	-0.228096	-1.481245
C	3.912112	-4.104849	-1.595610
H	2.573710	-3.890659	0.072586
C	4.728212	-3.446162	-2.535349
H	5.473816	-1.529252	-3.210489
H	3.813871	-5.184522	-1.641445
C	5.446803	-4.211198	-3.605215
H	6.489290	-3.885826	-3.684220
H	5.420621	-5.287953	-3.428151
H	4.980374	-4.013532	-4.578780
O	0.254956	-1.117177	-0.249178
S	-0.411467	-2.400310	-0.659018
O	0.430180	-3.324735	-1.440715
O	-1.777555	-2.159736	-1.172677
C	-0.660093	-3.297757	0.962371
F	-1.097211	-2.462766	1.919369
F	-1.557695	-4.282612	0.816107
F	0.497993	-3.835469	1.383028

Vibrational frequencies

-93.6174	11.5075	17.3691
20.5739	25.2877	33.0311
39.4049	39.8544	44.7261
46.3582	52.1863	54.7669
56.5003	60.6271	62.4504
65.6012	70.7335	76.4328
83.7675	84.4668	86.7043
90.7619	98.9722	102.5885
117.6305	123.0875	126.2378

136.0358

145.1162

153.9565

R2

Cartesian coordinates

C	5.764518	0.441318	-1.127309
C	4.373292	0.387223	-1.025383
C	3.758020	-0.142088	0.117196
C	4.568480	-0.619171	1.156209
C	5.960119	-0.566767	1.058588
C	6.562396	-0.036241	-0.084739
H	6.224753	0.859337	-2.017957
H	3.756270	0.763404	-1.837757
H	4.104006	-1.030315	2.049272
H	6.573140	-0.936454	1.875537
H	7.644786	0.007896	-0.161225
C	2.252797	-0.245086	0.203985
C	1.739572	-1.592958	-0.373364
H	1.780655	0.576961	-0.345230
H	1.927342	-0.165890	1.246913
C	0.282736	-1.682900	-0.334001
H	2.091798	-1.698401	-1.407201
H	2.183021	-2.422325	0.190893
C	-0.930063	-1.700779	-0.270130
C	-2.350114	-1.569372	-0.212609
C	-3.191364	-2.632945	0.156761
C	-2.931666	-0.312701	-0.517520
C	-4.567598	-2.443744	0.255672
H	-2.749740	-3.598637	0.378507
C	-4.312008	-0.131642	-0.420237
C	-5.125527	-1.192594	-0.022742
H	-5.204652	-3.271258	0.550701

H	-4.729411	0.840394	-0.654745
H	-6.197885	-1.044653	0.054376
S	-1.858806	2.079176	0.110203
O	-0.729301	2.818793	-0.467375
O	-3.157026	2.732163	0.307259
C	-1.348605	1.365271	1.683573
H	-0.432424	0.796985	1.522722
H	-1.182589	2.193189	2.373998
H	-2.149008	0.718559	2.043819
N	-2.094646	0.763395	-0.937632
H	-1.175929	0.444040	-1.245202

Vibrational frequencies

14.3321	20.8619	29.5222
38.7980	57.8579	69.0577
78.8361	95.6790	108.5316
136.0944	180.0852	212.5068
243.8856	264.9072	275.5612
291.4484	340.8441	362.6679
366.3517	391.3374	416.2066
416.6705	460.7037	474.3007
490.5777	504.8267	526.8402
558.2038	561.8401	601.7402

Int02

Cartesian coordinates

C	-1.396733	-2.371428	2.150907
C	-1.630363	-1.271700	1.324448
C	-2.555125	-0.288351	1.670384
C	-3.252968	-0.426351	2.871070
C	-3.015281	-1.522742	3.710661
C	-2.083577	-2.502735	3.357609

C	-0.395664	-3.317274	1.533610
C	0.179683	-2.520043	0.335403
C	-0.794172	-1.337583	0.063749
H	-2.717436	0.565827	1.027935
H	-3.978659	0.328301	3.157843
H	-3.559708	-1.611695	4.646015
H	-1.903831	-3.353561	4.008528
H	0.369605	-3.655976	2.238853
H	0.320254	-3.119033	-0.557770
H	-0.888210	-4.210256	1.137911
S	-2.560734	-2.799591	-1.513583
O	-1.848671	-4.022959	-1.102356
O	-2.957893	-2.611451	-2.915971
C	-4.033900	-2.666339	-0.509141
C	-4.175716	-3.475548	0.619122
C	-5.008125	-1.729902	-0.859139
C	-5.307758	-3.329784	1.414907
H	-3.412316	-4.202502	0.866049
C	-6.134654	-1.603183	-0.050410
H	-4.882642	-1.100783	-1.733670
C	-6.298079	-2.388263	1.099272
H	-5.420831	-3.951410	2.298297
H	-6.889929	-0.867221	-0.308703
C	-7.491552	-2.197937	2.001562
H	-8.351048	-1.802111	1.453805
H	-7.787260	-3.136476	2.479164
H	-7.254416	-1.485287	2.801078
N	-1.537654	-1.511589	-1.202036
H	-1.976688	-0.628262	-1.487108
S	1.935728	-2.024480	0.818255

C	2.933872	-2.794522	-0.426587
C	4.018926	-3.587399	0.007677
C	2.685185	-2.548162	-1.800878
C	4.823818	-4.171642	-0.971879
C	3.504192	-3.169234	-2.753220
C	4.561110	-3.967363	-2.327431
H	5.658397	-4.794981	-0.669529
H	3.326576	-3.028230	-3.810554
H	5.195131	-4.438837	-3.071848
C	4.318750	-3.813236	1.470321
H	4.547086	-2.871366	1.978840
H	3.470772	-4.267950	1.991674
H	5.180579	-4.473355	1.583229
O	1.673499	-1.705249	-2.073719
C	1.410391	-1.261206	-3.442146
C	0.790957	0.120668	-3.320583
C	0.510449	-2.269703	-4.143548
H	2.375855	-1.175591	-3.953880
H	1.460121	0.814066	-2.808329
H	0.588411	0.519706	-4.318129
H	-0.150413	0.078369	-2.770444
H	-0.466563	-2.303816	-3.657015
H	0.370643	-1.972534	-5.187273
H	0.947393	-3.272000	-4.129290
H	-0.253165	-0.403280	-0.107887
O	-2.333246	1.223394	-1.256296
S	-3.513431	1.845360	-1.948451
O	-4.253061	0.904737	-2.810468
O	-3.230596	3.183943	-2.509772
C	-4.684554	2.216449	-0.543807

F	-4.148685	3.124123	0.286405
F	-5.836256	2.701529	-1.025456
F	-4.950340	1.109793	0.167311
S	2.245434	0.178964	0.590663
C	3.938696	0.061888	0.077572
C	4.279876	0.203152	-1.275784
C	4.941340	-0.181913	1.028352
C	5.610233	0.095995	-1.666001
H	3.505548	0.396708	-2.007492
C	6.266997	-0.300387	0.621030
H	4.671017	-0.278381	2.074388
C	6.622097	-0.170981	-0.730332
H	5.868558	0.209317	-2.715051
H	7.037491	-0.496907	1.360999
C	8.051318	-0.344260	-1.176687
H	8.303909	0.348621	-1.984522
H	8.210536	-1.359993	-1.558620
H	8.752553	-0.187578	-0.353076
C	2.552330	-0.697038	4.290460
C	3.180608	0.545724	4.211714
C	2.459830	1.697484	3.859950
C	1.089726	1.579156	3.605434
C	0.452088	0.339283	3.699006
C	1.181856	-0.802294	4.034971
H	3.126912	-1.579006	4.560146
H	4.243956	0.626875	4.427574
H	0.518408	2.456581	3.320996
H	-0.611538	0.265142	3.504128
H	0.680518	-1.762206	4.105096
C	3.169239	3.026211	3.730074

C	4.093053	3.104223	2.485662
H	2.440451	3.839595	3.677844
H	3.796571	3.199212	4.612339
C	3.370611	3.137227	1.219509
H	4.788056	2.254270	2.488352
H	4.713558	4.007037	2.556017
C	2.738271	3.211297	0.185776
C	2.093846	3.364616	-1.075880
C	2.871896	3.711365	-2.199122
C	0.702825	3.175944	-1.249683
C	2.292895	3.871842	-3.454392
H	3.940330	3.843511	-2.065261
C	0.127511	3.359287	-2.512227
C	0.916035	3.699443	-3.610320
H	2.914186	4.132539	-4.305452
H	-0.941096	3.216882	-2.628609
H	0.452575	3.827218	-4.583441
S	-0.710249	3.825172	0.968527
O	0.412187	4.536770	1.590985
O	-1.628834	3.042884	1.808313
C	-1.648337	5.038178	0.018960
H	-0.951983	5.549730	-0.646111
H	-2.079597	5.738637	0.735555
H	-2.423470	4.528629	-0.552023
N	-0.114235	2.719707	-0.165787
H	-0.913176	2.159084	-0.493316

Vibrational frequencies

12.8544	18.5585	21.3581
23.5384	28.7136	32.6603
37.7187	38.9240	39.8785

42.2024	43.0770	47.0192
48.9549	51.2586	54.1642
56.5810	58.8119	60.3124
63.1108	64.9220	66.4927
73.1565	75.2764	79.5580
80.8720	86.9228	89.0377
94.0817	95.9783	97.7300

TS2S

Cartesian coordinates

C	-1.209364	-2.632341	1.933611
C	-1.489494	-1.458737	1.232585
C	-2.500425	-0.592088	1.643558
C	-3.241774	-0.924613	2.778455
C	-2.961012	-2.097998	3.491668
C	-1.940498	-2.957941	3.076050
C	-0.107214	-3.418099	1.267530
C	0.455367	-2.449529	0.191505
C	-0.600656	-1.315804	0.016664
H	-2.700568	0.320549	1.097474
H	-4.037240	-0.264706	3.110620
H	-3.540933	-2.340468	4.377336
H	-1.727195	-3.867711	3.630224
H	0.656066	-3.758682	1.972831
H	0.642164	-2.939810	-0.757225
H	-0.504632	-4.306033	0.764948
S	-2.197777	-2.696695	-1.807184
O	-1.385073	-3.902715	-1.570571
O	-2.599306	-2.333175	-3.174703
C	-3.694547	-2.857509	-0.837837
C	-3.772236	-3.833765	0.156587

C	-4.756070	-1.985484	-1.082812
C	-4.929570	-3.924499	0.923579
H	-2.940788	-4.507454	0.321032
C	-5.906266	-2.095304	-0.304996
H	-4.685758	-1.227763	-1.855470
C	-6.008855	-3.053997	0.712064
H	-4.993431	-4.678772	1.702619
H	-6.729632	-1.410146	-0.482013
C	-7.233759	-3.125547	1.589251
H	-8.107523	-2.690612	1.096730
H	-7.469600	-4.157624	1.865058
H	-7.068774	-2.569535	2.520331
N	-1.302945	-1.383070	-1.287469
H	-1.831314	-0.521133	-1.467840
S	2.133532	-1.844187	0.758473
C	3.218676	-2.486715	-0.495681
C	4.328946	-3.261431	-0.101657
C	3.009883	-2.143278	-1.854356
C	5.200157	-3.719087	-1.095543
C	3.886749	-2.638731	-2.828031
C	4.973370	-3.416370	-2.437398
H	6.055335	-4.324445	-0.812738
H	3.735503	-2.412528	-3.874849
H	5.653883	-3.790671	-3.196178
C	4.595101	-3.595166	1.346382
H	4.784099	-2.690185	1.932858
H	3.741567	-4.103010	1.805965
H	5.469703	-4.243081	1.435578
O	1.964406	-1.322744	-2.097547
C	1.703305	-0.820788	-3.438317

C	0.951739	0.487028	-3.250497
C	0.913422	-1.850789	-4.237851
H	2.669255	-0.613805	-3.915598
H	1.540481	1.199396	-2.669804
H	0.734667	0.934268	-4.224236
H	0.008001	0.310157	-2.732505
H	-0.076471	-1.987742	-3.797612
H	0.790361	-1.502427	-5.267990
H	1.424921	-2.816614	-4.262114
H	-0.124853	-0.332353	-0.019089
O	-2.567916	1.182808	-1.182632
S	-3.821174	1.805544	-1.732317
O	-4.547128	0.948033	-2.685488
O	-3.648114	3.225715	-2.109644
C	-4.926269	1.896966	-0.231971
F	-4.378752	2.697814	0.697216
F	-6.124035	2.389370	-0.571905
F	-5.099354	0.685264	0.316000
S	2.402924	0.719665	0.638323
C	4.084028	0.478372	0.128920
C	4.462171	0.632915	-1.212396
C	5.036202	0.074223	1.078813
C	5.772131	0.367351	-1.595621
H	3.729331	0.952931	-1.943595
C	6.340164	-0.201432	0.678172
H	4.738857	-0.044839	2.116186
C	6.725308	-0.073743	-0.664625
H	6.056574	0.480429	-2.637792
H	7.067107	-0.532234	1.414535
C	8.117193	-0.445208	-1.107445

H	8.440389	0.153962	-1.963261
H	8.144729	-1.497673	-1.415571
H	8.844068	-0.320129	-0.300336
C	2.585714	-0.815992	4.522760
C	2.985355	0.513031	4.382514
C	2.073042	1.500468	3.981301
C	0.744796	1.132688	3.743196
C	0.337378	-0.194910	3.897146
C	1.256289	-1.173642	4.278383
H	3.307024	-1.569521	4.826673
H	4.018529	0.788488	4.583506
H	0.024176	1.879105	3.421919
H	-0.696274	-0.462371	3.716641
H	0.935409	-2.205397	4.387058
C	2.537164	2.924636	3.772354
C	3.497321	3.086973	2.567032
H	1.681300	3.588375	3.624868
H	3.081201	3.273945	4.657608
C	2.850081	2.909661	1.262239
H	4.339412	2.390481	2.649571
H	3.920145	4.098818	2.571004
C	2.304863	3.188779	0.191043
C	1.672095	3.511996	-1.030936
C	2.439305	3.972418	-2.120071
C	0.273363	3.338712	-1.183432
C	1.830943	4.250528	-3.338995
H	3.509297	4.094770	-1.992161
C	-0.323803	3.622884	-2.413264
C	0.452165	4.070907	-3.483846
H	2.428369	4.600395	-4.174098

H	-1.393680	3.481409	-2.524534
H	-0.026295	4.283243	-4.434525
S	-1.018998	3.781167	1.151579
O	0.132062	4.527305	1.675771
O	-1.781611	2.890833	2.036127
C	-2.136687	4.975648	0.397332
H	-1.560036	5.564112	-0.317191
H	-2.514913	5.609702	1.200577
H	-2.943235	4.441894	-0.103291
N	-0.491681	2.789775	-0.115770
H	-1.283529	2.213813	-0.442439

Vibrational frequencies

-196.7066	14.6968	20.2533
24.5417	28.5190	28.7166
33.2427	35.8511	38.0783
38.8501	41.7585	46.6848
49.3590	50.1763	52.7159
55.9207	58.8043	60.2317
62.8357	65.5090	67.6853
71.0456	72.6351	75.0356
78.3441	81.9990	91.2141
91.8757	92.4020	95.5801

TS2R

Cartesian coordinates

C	0.379600	-3.404689	-0.360335
C	0.876032	-2.101727	-0.282311
C	1.734749	-1.594457	-1.255987
C	2.090992	-2.421192	-2.323400
C	1.590000	-3.726670	-2.411314
C	0.732384	-4.228312	-1.429025

C	-0.504906	-3.722139	0.820281
C	-0.746789	-2.340516	1.485914
C	0.368306	-1.391349	0.954742
H	2.124307	-0.585486	-1.173389
H	2.759129	-2.046708	-3.091391
H	1.872960	-4.355171	-3.250729
H	0.342344	-5.239493	-1.500994
H	-1.431675	-4.228380	0.536240
H	-0.744902	-2.380338	2.573182
H	0.019174	-4.365881	1.532346
S	2.448543	-2.167120	2.622926
O	1.689914	-3.388030	2.942672
O	3.149089	-1.428986	3.684563
C	3.652060	-2.560787	1.360406
C	3.619912	-3.792661	0.710020
C	4.554884	-1.564973	0.984862
C	4.499922	-4.016420	-0.346064
H	2.905524	-4.547915	1.014244
C	5.417916	-1.801649	-0.079571
H	4.568662	-0.616090	1.502078
C	5.396557	-3.024195	-0.767504
H	4.475238	-4.970098	-0.865080
H	6.106130	-1.017946	-0.383204
C	6.285112	-3.252397	-1.964687
H	6.578011	-4.302488	-2.053527
H	5.756686	-2.982274	-2.887533
H	7.191794	-2.643184	-1.915718
N	1.376338	-1.059254	1.982784
H	1.895323	-0.208169	1.735236
S	-2.479805	-1.791407	1.029678

C	-3.154648	-1.162971	2.551693
C	-4.370355	-1.719049	3.005533
C	-2.502995	-0.138681	3.278204
C	-4.875028	-1.288425	4.236603
C	-3.019176	0.248026	4.523460
C	-4.194401	-0.333315	4.990793
H	-5.801448	-1.714495	4.607618
H	-2.520585	1.001289	5.118004
H	-4.589191	-0.024974	5.954004
C	-5.130737	-2.747309	2.201841
H	-5.413466	-2.352817	1.219985
H	-4.532789	-3.646954	2.025948
H	-6.044062	-3.039847	2.724239
O	-1.415692	0.406864	2.696079
C	-0.790047	1.598724	3.259652
C	-0.189791	2.327288	2.071835
C	0.229717	1.211959	4.324509
H	-1.580266	2.218190	3.698751
H	-0.958668	2.613705	1.352997
H	0.333508	3.228005	2.401695
H	0.531213	1.685729	1.565777
H	1.025203	0.604646	3.890660
H	0.671066	2.116936	4.752453
H	-0.234940	0.640677	5.132788
H	-0.047619	-0.415826	0.704340
S	-2.291423	-0.092989	-0.891369
C	-2.726555	-1.422758	-1.996494
C	-1.732730	-2.125406	-2.692355
C	-4.076599	-1.762941	-2.172722
C	-2.095430	-3.148018	-3.564027

H	-0.688560	-1.875338	-2.549405
C	-4.422575	-2.793336	-3.042867
H	-4.841314	-1.229216	-1.616817
C	-3.440676	-3.498055	-3.756464
H	-1.317360	-3.692053	-4.091910
H	-5.468874	-3.057160	-3.169042
C	-3.821280	-4.590993	-4.723266
H	-3.059653	-5.375173	-4.758669
H	-4.777553	-5.048660	-4.455944
H	-3.922159	-4.189183	-5.738954
O	2.737899	3.536098	0.441436
S	3.315972	2.360833	1.154945
O	2.757563	1.064146	0.672845
O	3.443404	2.496302	2.614450
C	5.071054	2.310334	0.520905
F	5.676332	3.486757	0.718717
F	5.776585	1.356297	1.153984
F	5.088638	2.034268	-0.795564
C	-5.893666	1.177353	0.973662
C	-5.706507	1.634334	-0.329911
C	-4.673386	2.532852	-0.633843
C	-3.835641	2.975726	0.395317
C	-4.032219	2.529071	1.704257
C	-5.056707	1.628685	1.997366
H	-6.693128	0.475903	1.195367
H	-6.366267	1.289771	-1.123418
H	-3.024964	3.664357	0.172209
H	-3.381476	2.884610	2.496607
H	-5.197449	1.273098	3.011247
C	-4.451144	2.970248	-2.062220

C	-3.930393	1.825837	-2.961485
H	-3.741284	3.800703	-2.107946
H	-5.394283	3.317008	-2.500099
C	-2.555844	1.403376	-2.651290
H	-4.596406	0.958011	-2.902489
H	-3.924314	2.154738	-4.007325
C	-1.334790	1.345899	-2.830050
C	0.055431	1.288693	-3.050141
C	0.560741	0.472354	-4.084692
C	0.953186	2.046590	-2.256358
C	1.927704	0.401494	-4.319848
H	-0.136549	-0.103577	-4.682795
C	2.324835	1.958052	-2.500175
C	2.807959	1.136663	-3.519177
H	2.308241	-0.230672	-5.114725
H	3.006056	2.527826	-1.882524
H	3.878266	1.076641	-3.688471
S	-0.217863	4.352427	-1.476836
O	-1.028875	4.268643	-2.697652
O	-0.832461	4.774293	-0.212126
C	1.204392	5.409733	-1.800087
H	1.706973	5.033938	-2.692425
H	0.831078	6.421655	-1.963005
H	1.862394	5.359849	-0.932179
N	0.456331	2.822095	-1.176406
H	1.155152	2.932557	-0.429916

Vibrational frequencies

-220.6519	11.0810	19.8079
22.4681	26.0517	27.8365
32.9345	34.9775	37.2791

40.1044	41.0421	43.1690
46.4957	47.8868	48.5232
50.7270	52.9820	54.5051
56.3508	58.9344	63.4570
67.7035	68.1403	72.5587
73.1524	74.4120	81.0989
89.0178	93.7604	95.2443

TS2'S

Cartesian coordinates

C	-2.900627	2.886337	-1.594294
C	-2.559432	1.658587	-1.016567
C	-3.183442	0.476924	-1.415915
C	-4.148213	0.533689	-2.422689
C	-4.488229	1.759835	-3.008242
C	-3.872049	2.944790	-2.594038
C	-2.110573	4.013334	-0.968603
C	-0.955408	3.275593	-0.249947
C	-1.474638	1.835594	0.030113
H	-2.944056	-0.462174	-0.934348
H	-4.634737	-0.381715	-2.745340
H	-5.240301	1.791834	-3.791607
H	-4.141798	3.894103	-3.048574
H	-1.765685	4.760934	-1.688017
H	-0.585565	3.759440	0.648768
H	-2.715168	4.526376	-0.213969
S	-3.247540	2.123821	2.164677
O	-3.447136	3.534500	1.796904
O	-3.096992	1.738518	3.576756
C	-4.593704	1.161625	1.485101
C	-5.545638	1.773547	0.672311

C	-4.619985	-0.214634	1.727347
C	-6.531263	0.987738	0.079723
H	-5.493585	2.840165	0.489671
C	-5.612897	-0.981097	1.126352
H	-3.869532	-0.687169	2.350842
C	-6.572069	-0.397898	0.283807
H	-7.267934	1.455939	-0.566527
H	-5.640447	-2.050869	1.311609
C	-7.589289	-1.251401	-0.430653
H	-7.827833	-2.155675	0.136370
H	-8.517285	-0.703377	-0.615717
H	-7.195253	-1.568869	-1.403997
N	-1.839573	1.605998	1.441508
H	-1.680634	0.626198	1.682226
S	0.478345	3.195481	-1.463702
C	1.894756	3.956362	-0.714540
C	2.707968	4.741117	-1.568267
C	2.293593	3.688656	0.621129
C	3.898916	5.265955	-1.061982
C	3.493306	4.238907	1.093298
C	4.284435	5.014261	0.252526
H	4.527121	5.872346	-1.706457
H	3.821612	4.052185	2.106002
H	5.214688	5.425086	0.632862
C	2.336729	5.002377	-3.009088
H	2.343357	4.078151	-3.598328
H	1.334027	5.430914	-3.098816
H	3.048611	5.693123	-3.465993
O	1.485943	2.885439	1.355597
C	1.767590	2.669610	2.770911

C	0.973422	1.447999	3.200595
C	1.379525	3.911612	3.569227
H	2.837558	2.452858	2.870555
H	1.164294	0.591164	2.553175
H	1.259140	1.177255	4.221418
H	-0.096092	1.658620	3.182644
H	0.306321	4.095054	3.459400
H	1.595686	3.753155	4.629800
H	1.918642	4.802254	3.238599
H	-0.675119	1.108873	-0.109102
S	1.188497	0.632704	-1.760780
C	2.820694	0.860137	-1.128943
C	3.819028	1.414505	-1.944288
C	3.122348	0.509271	0.197165
C	5.091314	1.639532	-1.427177
H	3.590756	1.675752	-2.972189
C	4.403036	0.716651	0.691956
H	2.353536	0.071074	0.818496
C	5.402834	1.299697	-0.103485
H	5.854018	2.084416	-2.059586
H	4.630592	0.428802	1.714376
C	6.766261	1.588102	0.468474
H	7.535133	1.603753	-0.308722
H	6.769456	2.571632	0.954530
H	7.048705	0.849000	1.223421
O	-0.691516	-3.508464	0.913719
S	-0.569021	-2.105492	1.365832
O	-1.621611	-1.190355	0.849490
O	0.805365	-1.542301	1.302281
C	-0.967392	-2.137590	3.184931

F	-0.121628	-2.911963	3.865158
F	-0.911229	-0.886963	3.677950
F	-2.218478	-2.597744	3.362549
C	-4.581753	-3.207225	-1.674994
C	-3.194298	-3.218276	-1.526478
C	-2.358040	-3.249835	-2.652797
C	-2.941887	-3.261315	-3.926232
C	-4.330475	-3.248749	-4.076792
C	-5.155361	-3.222964	-2.949681
H	-5.215828	-3.184423	-0.794968
H	-2.748009	-3.191421	-0.537402
H	-2.303563	-3.280229	-4.806327
H	-4.766510	-3.262091	-5.071570
H	-6.235643	-3.221418	-3.063300
C	-0.855304	-3.183496	-2.484665
C	-0.429427	-1.710722	-2.316000
H	-0.345453	-3.618341	-3.350379
H	-0.547895	-3.735649	-1.592439
C	1.018047	-1.512108	-2.071491
H	-0.721475	-1.128227	-3.197959
H	-0.966593	-1.277516	-1.468727
C	2.162061	-1.997882	-1.954054
C	3.514622	-2.285400	-1.795220
C	4.386204	-2.104016	-2.904449
C	4.050339	-2.719381	-0.538819
C	5.738645	-2.356349	-2.788607
H	3.959518	-1.753565	-3.837618
C	5.426357	-2.964833	-0.448374
C	6.250422	-2.792970	-1.556131
H	6.398998	-2.209342	-3.635969

H	5.840399	-3.273038	0.501382
H	7.314465	-2.980852	-1.452403
S	3.128239	-4.265354	1.517110
O	4.458727	-4.884359	1.548566
O	2.467332	-3.876849	2.763950
C	2.021014	-5.318767	0.572033
H	2.453076	-5.463441	-0.419130
H	1.949444	-6.270226	1.102081
H	1.050173	-4.821380	0.526885
N	3.227528	-2.845796	0.587532
H	2.319321	-2.361021	0.596884

Vibrational frequencies

-164.6682	17.3651	20.3998
21.0605	27.0532	27.5071
30.5479	31.8322	34.3706
36.4176	40.4045	41.6620
41.8820	46.1620	52.2909
55.1856	57.1395	57.9614
62.8167	65.2920	67.3302
69.8692	71.5803	72.1409
76.2885	76.8806	82.5755
85.5246	86.3991	91.9862

TS2'R

Cartesian coordinates

C	-2.929371	-2.562640	1.668090
C	-2.623041	-1.434658	0.901183
C	-3.408111	-0.284462	0.972756
C	-4.501553	-0.272229	1.839756
C	-4.799446	-1.393085	2.625124
C	-4.016588	-2.547028	2.542115

C	-1.985852	-3.699571	1.359306
C	-0.819468	-3.005436	0.611810
C	-1.396878	-1.675225	0.038007
H	-3.172740	0.576486	0.360122
H	-5.125382	0.614352	1.906042
H	-5.649744	-1.366566	3.300633
H	-4.254157	-3.419573	3.144365
H	-1.661025	-4.250879	2.245853
H	-0.362065	-3.610385	-0.166686
H	-2.460972	-4.412213	0.678894
S	-2.755672	-2.682080	-2.178132
O	-2.634450	-4.038772	-1.619010
O	-2.541935	-2.459480	-3.615431
C	-4.378848	-2.053853	-1.758084
C	-5.214380	-2.799580	-0.927919
C	-4.750671	-0.787570	-2.215225
C	-6.440218	-2.261000	-0.546678
H	-4.898551	-3.775150	-0.578675
C	-5.978035	-0.265101	-1.817876
H	-4.082417	-0.210752	-2.844715
C	-6.835288	-0.985797	-0.973915
H	-7.092732	-2.833026	0.106740
H	-6.263370	0.727604	-2.152839
C	-8.131865	-0.385079	-0.491223
H	-8.912059	-1.144906	-0.387436
H	-7.993243	0.075373	0.494909
H	-8.494091	0.392082	-1.169581
N	-1.616480	-1.722885	-1.425389
H	-1.631262	-0.798094	-1.860304
S	0.515045	-2.675467	1.883573

C	2.004607	-3.379185	1.198047
C	2.776116	-4.234369	2.012137
C	2.468853	-2.973361	-0.078911
C	4.009694	-4.681876	1.525443
C	3.706014	-3.446831	-0.539687
C	4.465160	-4.287424	0.269336
H	4.613517	-5.341385	2.140634
H	4.091982	-3.149855	-1.505436
H	5.429578	-4.630399	-0.092127
C	2.313824	-4.657863	3.386553
H	2.249289	-3.803687	4.069513
H	1.319216	-5.113104	3.351781
H	3.008910	-5.381179	3.818823
O	1.672173	-2.117333	-0.760321
C	2.113279	-1.550038	-2.029440
C	1.458183	-0.185631	-2.147672
C	1.734852	-2.500168	-3.158818
H	3.197735	-1.412832	-1.982728
H	1.634101	0.413265	-1.253383
H	1.881661	0.353315	-2.998387
H	0.384697	-0.284821	-2.300105
H	0.647930	-2.619903	-3.188214
H	2.068615	-2.091947	-4.117712
H	2.194605	-3.483389	-3.024617
H	-0.669644	-0.868202	0.135131
S	1.547723	-0.233210	1.813547
C	0.467624	0.599180	2.936915
C	-0.689355	1.221363	2.441984
C	0.746775	0.640702	4.314227
C	-1.557011	1.864878	3.318457

H	-0.898058	1.209328	1.380624
C	-0.120248	1.305333	5.174321
H	1.637615	0.153562	4.697214
C	-1.284849	1.927235	4.691469
H	-2.455861	2.331440	2.926466
H	0.101146	1.338352	6.237478
C	-2.201694	2.676763	5.623844
H	-2.156307	2.278660	6.641173
H	-1.913802	3.734405	5.671921
H	-3.239316	2.637449	5.280723
O	-1.225425	1.486405	-0.741942
S	-1.576728	1.962000	-2.099229
O	-1.973788	0.889610	-3.041914
O	-0.627040	2.970198	-2.653357
C	-3.130274	2.953907	-1.832239
F	-2.892103	3.961002	-0.975095
F	-3.575548	3.465283	-2.984827
F	-4.093057	2.174946	-1.307681
C	7.342446	-2.161008	-1.082685
C	6.903136	-1.134187	-0.244903
C	6.014324	-0.158240	-0.714646
C	5.585052	-0.221445	-2.048240
C	6.023568	-1.247726	-2.888637
C	6.898756	-2.224535	-2.406404
H	8.028809	-2.912186	-0.702382
H	7.243492	-1.095546	0.787030
H	4.896046	0.533430	-2.419006
H	5.679019	-1.285253	-3.918168
H	7.237424	-3.024724	-3.057811
C	5.419470	0.872088	0.218990

C	4.307637	0.197588	1.063931
H	4.990823	1.695402	-0.354038
H	6.176994	1.298601	0.884345
C	3.202350	1.094849	1.471364
H	3.855761	-0.602942	0.467537
H	4.722535	-0.298811	1.947946
C	2.703987	2.236877	1.555179
C	1.805706	3.304977	1.598806
C	1.433964	3.905741	2.824042
C	1.114595	3.655482	0.401076
C	0.356667	4.776024	2.869889
H	1.970441	3.632764	3.725106
C	0.011172	4.506218	0.473110
C	-0.365755	5.052528	1.700129
H	0.056276	5.220213	3.812440
H	-0.547548	4.726267	-0.429192
H	-1.225358	5.713909	1.742255
S	2.949789	3.563789	-1.570467
O	3.907875	3.937691	-0.521974
O	3.296192	2.520539	-2.541406
C	2.472088	5.044681	-2.477183
H	2.126137	5.787049	-1.756684
H	3.351686	5.402641	-3.014069
H	1.675525	4.770235	-3.170161
N	1.515647	3.076444	-0.816989
H	0.762405	2.966869	-1.514049

Vibrational frequencies

-150.1060	11.4747	15.7926
18.9576	20.7086	25.2815
27.9494	29.7893	33.9599

34.4135	35.8784	38.7909
39.5048	42.4591	45.9083
48.9131	53.0564	54.0473
55.2375	59.1242	60.5184
60.9095	64.7132	66.8100
68.2748	70.2371	71.8722
74.6757	76.2236	78.4254

Int2S

Cartesian coordinates

C	-1.286974	-2.629363	2.087079
C	-1.478200	-1.492749	1.297847
C	-2.388027	-0.502057	1.662470
C	-3.123631	-0.671015	2.837469
C	-2.933481	-1.806036	3.636929
C	-2.010271	-2.790011	3.269466
C	-0.285711	-3.566033	1.455315
C	0.363225	-2.725034	0.322596
C	-0.609772	-1.533973	0.058729
H	-2.518133	0.380747	1.050535
H	-3.840890	0.088061	3.134837
H	-3.505551	-1.920691	4.553227
H	-1.865804	-3.668868	3.891960
H	0.451350	-3.946888	2.167161
H	0.516413	-3.304478	-0.583037
H	-0.793871	-4.430987	1.015259
S	-2.344668	-2.903869	-1.652718
O	-1.643331	-4.156454	-1.323345
O	-2.720847	-2.613448	-3.045478
C	-3.847345	-2.855376	-0.679237
C	-3.985063	-3.696018	0.426363

C	-4.847790	-1.946451	-1.026481
C	-5.138483	-3.610809	1.200012
H	-3.201977	-4.401862	0.672666
C	-5.996456	-1.880131	-0.241327
H	-4.726418	-1.293755	-1.884062
C	-6.156275	-2.698656	0.884779
H	-5.247332	-4.257269	2.066087
H	-6.771780	-1.164854	-0.499280
C	-7.375763	-2.576241	1.764341
H	-8.228278	-2.166533	1.215861
H	-7.666725	-3.544050	2.183261
H	-7.172827	-1.904455	2.607502
N	-1.350132	-1.636515	-1.224165
H	-1.807578	-0.750125	-1.461671
S	2.051469	-2.134310	0.845409
C	3.086216	-2.721464	-0.491164
C	4.155428	-3.595606	-0.213612
C	2.872569	-2.253585	-1.809663
C	4.974705	-4.020085	-1.268092
C	3.693598	-2.709967	-2.850024
C	4.737166	-3.589303	-2.569988
H	5.795792	-4.700066	-1.061939
H	3.532670	-2.381402	-3.867962
H	5.369943	-3.937029	-3.381296
C	4.444858	-4.069616	1.190180
H	4.719358	-3.232142	1.840588
H	3.568287	-4.544769	1.640936
H	5.270714	-4.785481	1.193754
O	1.864824	-1.354295	-1.968646
C	1.583754	-0.792996	-3.274872

C	0.875248	0.527048	-3.016754
C	0.745012	-1.759899	-4.105288
H	2.539833	-0.583556	-3.772135
H	1.489322	1.174742	-2.388922
H	0.689135	1.045751	-3.961168
H	-0.082853	0.369311	-2.518706
H	-0.228514	-1.908557	-3.633624
H	0.592150	-1.350562	-5.108945
H	1.236930	-2.731002	-4.203548
H	-0.046305	-0.606828	-0.067999
O	-2.323055	1.110562	-1.272277
S	-3.530206	1.733057	-1.918652
O	-4.226674	0.842269	-2.862301
O	-3.296873	3.127148	-2.359919
C	-4.725810	1.932075	-0.496007
F	-4.318684	2.906736	0.332888
F	-5.939604	2.250603	-0.964813
F	-4.823970	0.798944	0.211926
S	2.481273	1.212870	0.763643
C	4.038197	0.568756	0.149193
C	4.370593	0.666200	-1.203129
C	4.863052	-0.115312	1.047841
C	5.539772	0.061761	-1.656478
H	3.726747	1.196637	-1.895448
C	6.027493	-0.713189	0.573017
H	4.586332	-0.196848	2.094573
C	6.377844	-0.645629	-0.782914
H	5.795050	0.124246	-2.709929
H	6.667264	-1.253306	1.264698
C	7.599219	-1.360499	-1.299709

H	8.028931	-0.849682	-2.165869
H	7.324425	-2.373810	-1.614245
H	8.370625	-1.448561	-0.529752
C	2.743778	-0.495957	4.512958
C	3.069848	0.856236	4.399395
C	2.100815	1.797784	4.020646
C	0.794491	1.358589	3.773737
C	0.462573	0.006395	3.897119
C	1.436968	-0.924129	4.258723
H	3.506654	-1.213808	4.800655
H	4.087586	1.183532	4.599921
H	0.035066	2.068834	3.460704
H	-0.551694	-0.318221	3.699371
H	1.179556	-1.975761	4.337705
C	2.480343	3.248108	3.805801
C	3.460604	3.444420	2.619247
H	1.587974	3.847397	3.614512
H	2.977392	3.654460	4.693579
C	2.928698	2.928070	1.344053
H	4.412844	2.941686	2.820823
H	3.669790	4.508894	2.470611
C	2.418023	3.034227	0.176798
C	1.876220	3.593210	-1.031090
C	2.710626	4.174016	-1.998229
C	0.493276	3.445484	-1.275339
C	2.166510	4.598340	-3.208246
H	3.772453	4.270234	-1.800142
C	-0.038030	3.865415	-2.495601
C	0.801179	4.431877	-3.457625
H	2.808387	5.045908	-3.959310

H	-1.099294	3.732646	-2.682119
H	0.382472	4.750567	-4.406708
S	-0.913621	3.747684	0.993491
O	0.217419	4.455816	1.610320
O	-1.728075	2.827210	1.795292
C	-1.975216	4.984627	0.228966
H	-1.344969	5.632734	-0.380526
H	-2.439345	5.549926	1.038404
H	-2.720805	4.477654	-0.382137
N	-0.309696	2.812747	-0.284181
H	-1.064033	2.212013	-0.659427

Vibrational frequencies

17.2786	19.6616	20.9490
27.4828	30.2783	34.0956
36.4156	39.7365	42.2465
42.7847	46.1468	49.0663
52.3311	53.4700	56.8382
58.6129	61.9180	62.9182
67.1401	67.3341	73.8254
75.4664	80.1441	81.9470
84.0143	86.9389	90.4344
91.6672	92.5726	97.0761

Int2R

Cartesian coordinates

C	0.213975	-3.182548	-1.249825
C	0.706713	-1.969271	-0.763638
C	1.584217	-1.189642	-1.517998
C	1.965365	-1.647957	-2.781350
C	1.469283	-2.861379	-3.276523
C	0.592774	-3.636636	-2.513341

C	-0.689095	-3.849850	-0.242060
C	-0.928960	-2.758463	0.838652
C	0.194740	-1.694703	0.635395
H	1.981199	-0.263245	-1.116497
H	2.653291	-1.061136	-3.379847
H	1.773894	-3.204495	-4.261137
H	0.210301	-4.576987	-2.900381
H	-1.621380	-4.209232	-0.687226
H	-0.905564	-3.158720	1.850289
H	-0.185105	-4.707945	0.212171
S	2.283300	-2.971487	1.956504
O	1.515813	-4.224787	1.875788
O	2.993905	-2.616486	3.194865
C	3.489914	-2.966425	0.634669
C	3.441918	-3.927213	-0.373810
C	4.424049	-1.930467	0.603483
C	4.334697	-3.828128	-1.438103
H	2.707514	-4.722142	-0.331605
C	5.298523	-1.838408	-0.474172
H	4.453584	-1.199820	1.398634
C	5.260714	-2.777928	-1.514904
H	4.297587	-4.567313	-2.233040
H	6.008951	-1.017454	-0.507711
C	6.163419	-2.639300	-2.715428
H	6.465001	-3.615516	-3.106348
H	5.642760	-2.111977	-3.524592
H	7.065175	-2.068308	-2.478077
N	1.222099	-1.706338	1.705114
H	1.755698	-0.829951	1.720724
S	-2.628074	-2.033037	0.587658

C	-3.287027	-1.853002	2.240659
C	-4.463507	-2.550274	2.585018
C	-2.705121	-0.942605	3.155835
C	-5.034606	-2.334720	3.846895
C	-3.281074	-0.766763	4.421821
C	-4.443809	-1.458978	4.753519
H	-5.940326	-2.868174	4.118682
H	-2.838454	-0.092434	5.142773
H	-4.886896	-1.311456	5.733988
C	-5.131273	-3.505746	1.624052
H	-5.508477	-2.984100	0.737759
H	-4.429399	-4.264537	1.265604
H	-5.974097	-4.008988	2.104522
O	-1.616846	-0.262529	2.716473
C	-0.948095	0.708173	3.563917
C	-0.248735	1.661496	2.609653
C	0.001839	0.000991	4.525843
H	-1.706883	1.267637	4.124807
H	-0.964593	2.161866	1.955890
H	0.301913	2.422880	3.168049
H	0.465583	1.121511	1.987795
H	0.739841	-0.578081	3.966952
H	0.524690	0.737942	5.142592
H	-0.539313	-0.681157	5.187171
H	-0.226617	-0.693274	0.724298
S	-2.103447	0.807402	-1.299390
C	-2.657228	-0.456991	-2.446043
C	-1.733456	-1.178901	-3.202787
C	-4.024007	-0.753334	-2.494747
C	-2.195007	-2.199328	-4.032632

H	-0.671680	-0.970500	-3.136829
C	-4.462183	-1.777776	-3.328618
H	-4.726600	-0.206208	-1.874361
C	-3.558175	-2.514270	-4.110780
H	-1.474816	-2.770737	-4.609770
H	-5.521234	-2.016354	-3.366240
C	-4.049765	-3.608989	-5.024148
H	-3.260506	-4.333068	-5.242651
H	-4.897383	-4.142742	-4.584900
H	-4.388204	-3.190949	-5.979889
O	2.836638	3.136482	1.401506
S	3.318644	1.795569	1.846733
O	2.713017	0.682839	1.061862
O	3.387840	1.592402	3.301955
C	5.097693	1.793106	1.278599
F	5.736171	2.878502	1.729725
F	5.739776	0.702158	1.731019
F	5.162484	1.784276	-0.065990
C	-5.847901	1.120939	0.501961
C	-5.486809	2.095145	-0.431108
C	-4.422135	2.972127	-0.176084
C	-3.745488	2.872510	1.045740
C	-4.114949	1.906105	1.983892
C	-5.157857	1.019468	1.713811
H	-6.668260	0.442799	0.284371
H	-6.032228	2.168734	-1.369283
H	-2.913732	3.540528	1.250085
H	-3.580923	1.835953	2.924726
H	-5.422670	0.254819	2.436831
C	-3.965765	3.965907	-1.223821

C	-3.436311	3.292054	-2.514178
H	-3.174597	4.602577	-0.821637
H	-4.793392	4.616713	-1.527229
C	-2.300826	2.380254	-2.275285
H	-4.232598	2.723403	-3.006910
H	-3.079538	4.051656	-3.216626
C	-1.074268	2.039082	-2.383467
C	0.326845	2.083734	-2.688800
C	0.817364	1.625237	-3.920135
C	1.214662	2.536920	-1.688398
C	2.190535	1.606720	-4.149054
H	0.122341	1.276861	-4.675973
C	2.589403	2.496138	-1.924015
C	3.070903	2.023256	-3.146061
H	2.573649	1.251511	-5.099489
H	3.268762	2.823976	-1.147420
H	4.142051	1.988784	-3.316342
S	0.043032	4.550097	-0.343236
O	-0.630410	4.848350	-1.615329
O	-0.712967	4.602379	0.913299
C	1.488097	5.612736	-0.192500
H	2.084936	5.497805	-1.098280
H	1.128575	6.637742	-0.091972
H	2.048160	5.294399	0.686771
N	0.676807	2.971781	-0.447186
H	1.335325	2.845897	0.335254

Vibrational frequencies

18.7706	23.2446	24.4254
24.6252	26.0144	28.6609
32.9149	34.6733	36.6783

37.4504	39.2750	40.7384
45.0454	45.9633	51.4574
54.7719	55.6437	56.4884
60.0917	64.2960	65.9905
67.1533	69.6993	72.1766
73.7762	78.8581	83.1669
88.3554	91.1543	94.7733

TS3S

Cartesian coordinates

C	-0.912970	-2.611325	2.357601
C	-1.193858	-1.522864	1.529263
C	-2.090639	-0.527898	1.915216
C	-2.743948	-0.659977	3.146225
C	-2.489165	-1.761875	3.970219
C	-1.565788	-2.743745	3.581990
C	0.111854	-3.523747	1.731388
C	0.634975	-2.725103	0.505991
C	-0.423061	-1.607108	0.229301
H	-2.276097	0.323685	1.278434
H	-3.447576	0.101374	3.458552
H	-3.000540	-1.849185	4.921393
H	-1.361501	-3.587182	4.237759
H	0.914039	-3.790383	2.423064
H	0.766510	-3.347753	-0.375220
H	-0.357644	-4.452580	1.388131
S	-2.216309	-3.147389	-1.277409
O	-1.589245	-4.310392	-0.613169
O	-2.413876	-3.164499	-2.733995
C	-3.825698	-2.877610	-0.544559
C	-4.043034	-3.173560	0.805972

C	-4.836165	-2.328587	-1.335939
C	-5.284253	-2.886501	1.365710
H	-3.253161	-3.610957	1.404013
C	-6.070870	-2.050310	-0.753624
H	-4.649358	-2.094158	-2.372936
C	-6.308830	-2.305856	0.602338
H	-5.455418	-3.097578	2.416462
H	-6.846514	-1.591511	-1.357488
C	-7.612967	-1.891091	1.231416
H	-8.471210	-2.215009	0.631532
H	-7.730790	-2.290756	2.244398
H	-7.663890	-0.790167	1.288103
N	-1.240318	-1.819567	-0.985343
H	-1.742876	-0.967588	-1.256581
S	2.308983	-1.998330	0.897161
C	3.329493	-2.577057	-0.453349
C	4.509504	-3.283907	-0.177982
C	2.994737	-2.238527	-1.791228
C	5.319519	-3.699228	-1.238442
C	3.810724	-2.695107	-2.841816
C	4.963911	-3.413223	-2.556113
H	6.230514	-4.253369	-1.029172
H	3.549454	-2.482317	-3.866187
H	5.586611	-3.760156	-3.376956
C	4.933727	-3.593844	1.241143
H	5.145617	-2.674704	1.798001
H	4.140134	-4.123957	1.789654
H	5.834268	-4.212787	1.249033
O	1.900328	-1.455838	-1.959000
C	1.519647	-0.997198	-3.280159

C	0.725627	0.278043	-3.078798
C	0.730999	-2.077029	-4.006003
H	2.441393	-0.754865	-3.831935
H	1.317714	1.014408	-2.525131
H	0.460366	0.716149	-4.049530
H	-0.192886	0.087920	-2.526423
H	-0.198496	-2.284259	-3.474469
H	0.487443	-1.742960	-5.022776
H	1.298843	-3.008558	-4.087334
H	0.089149	-0.664400	0.004850
O	-2.471110	0.844435	-1.161826
S	-3.803921	1.322191	-1.680973
O	-4.462917	0.398040	-2.617935
O	-3.784696	2.753053	-2.064633
C	-4.866105	1.310618	-0.136620
F	-4.588031	2.389668	0.639279
F	-6.179027	1.349497	-0.475569
F	-4.638096	0.199443	0.590560
S	2.409571	1.296435	0.453751
C	4.057489	0.793147	-0.033031
C	4.380247	0.623674	-1.382860
C	4.974017	0.454451	0.968293
C	5.623501	0.109638	-1.727608
H	3.659609	0.869135	-2.158656
C	6.210220	-0.065673	0.603162
H	4.706864	0.569868	2.014764
C	6.548684	-0.262995	-0.744561
H	5.865546	-0.044693	-2.775479
H	6.916255	-0.343284	1.378171
C	7.850599	-0.915583	-1.124821

H	8.250713	-0.495269	-2.058841
H	7.695398	-1.986721	-1.286352
H	8.605593	-0.803179	-0.341292
C	3.216750	0.056104	4.570640
C	3.298041	1.409137	4.238434
C	2.180250	2.099143	3.760722
C	0.958848	1.412927	3.647145
C	0.870790	0.062403	3.994454
C	2.000213	-0.621663	4.452272
H	4.098075	-0.466354	4.938541
H	4.244148	1.934422	4.348663
H	0.081273	1.929253	3.267905
H	-0.077216	-0.453065	3.910510
H	1.932275	-1.675293	4.705851
C	2.294016	3.544772	3.326932
C	3.188297	3.737760	2.082270
H	1.307146	3.957111	3.105447
H	2.734083	4.143610	4.127336
C	2.651944	3.083128	0.857576
H	4.190684	3.331572	2.265903
H	3.296414	4.802132	1.851412
C	2.113831	3.263599	-0.279781
C	1.442360	3.574632	-1.486172
C	2.160125	4.009102	-2.617379
C	0.050870	3.320311	-1.570265
C	1.494461	4.194575	-3.823427
H	3.227914	4.186099	-2.537539
C	-0.597429	3.499749	-2.792387
C	0.120543	3.934685	-3.905063
H	2.042252	4.534502	-4.693427

H	-1.662688	3.296619	-2.859372
H	-0.395869	4.066576	-4.850377
S	-1.126381	3.829139	0.797514
O	-0.004298	4.723264	1.111550
O	-1.685630	2.945524	1.832988
C	-2.443475	4.839663	0.108590
H	-2.016576	5.416476	-0.710780
H	-2.789568	5.500584	0.905545
H	-3.233243	4.186343	-0.246476
N	-0.632296	2.798391	-0.448954
H	-1.373374	2.108063	-0.677230

Vibrational frequencies

-67.6782	20.1324	23.3579
23.9678	25.8828	31.8482
32.9034	35.0073	40.7273
43.9702	48.0045	50.9637
52.4074	56.0594	59.4257
61.5538	63.1883	64.3096
66.9271	70.3171	72.5996
76.3641	81.0538	83.2724
86.2518	88.6665	89.6248
96.5489	99.3653	106.0947

TS3R

Cartesian coordinates

C	-0.277549	-3.435146	0.436198
C	-0.727787	-2.124120	0.267960
C	-1.617792	-1.542041	1.171345
C	-2.053975	-2.300438	2.260025
C	-1.599573	-3.614215	2.438219
C	-0.710379	-4.189842	1.527220

C	0.641299	-3.845875	-0.688599
C	0.932443	-2.522913	-1.453528
C	-0.162154	-1.508802	-0.994248
H	-1.982197	-0.532943	1.010419
H	-2.752269	-1.870079	2.969889
H	-1.947008	-4.191670	3.290170
H	-0.361206	-5.208858	1.668331
H	1.552570	-4.333446	-0.330666
H	0.908240	-2.653640	-2.533398
H	0.132981	-4.546163	-1.358488
S	-2.231053	-2.314079	-2.670081
O	-1.489552	-3.562112	-2.914759
O	-2.889673	-1.613069	-3.783448
C	-3.483682	-2.637385	-1.433311
C	-3.473952	-3.827858	-0.708899
C	-4.406768	-1.628673	-1.156341
C	-4.396589	-3.994164	0.320946
H	-2.744830	-4.595483	-0.937368
C	-5.311919	-1.805687	-0.115210
H	-4.403976	-0.715273	-1.733202
C	-5.313803	-2.984280	0.645195
H	-4.389513	-4.915010	0.896745
H	-6.014037	-1.009278	0.113258
C	-6.250315	-3.146933	1.816536
H	-6.562028	-4.188135	1.940440
H	-5.753477	-2.843339	2.746556
H	-7.145427	-2.528888	1.705640
N	-1.157100	-1.196595	-2.048697
H	-1.674669	-0.336149	-1.838389
S	2.658021	-1.957328	-1.028698

C	3.325979	-1.330733	-2.566943
C	4.518067	-1.899084	-3.064049
C	2.731385	-0.230241	-3.231053
C	5.084298	-1.374044	-4.233349
C	3.296569	0.246047	-4.423151
C	4.470228	-0.323127	-4.909487
H	6.001212	-1.808213	-4.620088
H	2.839752	1.065254	-4.961775
H	4.905722	0.061046	-5.827206
C	5.203872	-3.050891	-2.365988
H	5.546042	-2.770787	-1.363856
H	4.525498	-3.900182	-2.239082
H	6.073706	-3.382858	-2.938284
O	1.637545	0.312163	-2.643487
C	1.022489	1.512404	-3.185311
C	0.355015	2.196443	-2.005293
C	0.053750	1.152179	-4.307960
H	1.817029	2.165690	-3.561135
H	1.087196	2.460937	-1.242041
H	-0.145647	3.111399	-2.333098
H	-0.397064	1.546374	-1.559144
H	-0.745539	0.512902	-3.929372
H	-0.389313	2.063512	-4.721028
H	0.562133	0.619939	-5.116553
H	0.292318	-0.537662	-0.800791
S	2.214276	0.154436	1.470701
C	2.618824	-1.284429	2.458492
C	1.587497	-2.073189	2.976595
C	3.957675	-1.644180	2.659215
C	1.903971	-3.213882	3.711407

H	0.551110	-1.808659	2.805716
C	4.254541	-2.787760	3.394668
H	4.757923	-1.047265	2.235672
C	3.235438	-3.590422	3.932015
H	1.097156	-3.824379	4.105211
H	5.293194	-3.065013	3.550572
C	3.568610	-4.847892	4.694887
H	2.769935	-5.117431	5.391053
H	3.703046	-5.690525	4.005931
H	4.498802	-4.738366	5.259630
O	-2.758283	3.448557	-0.531837
S	-3.250863	2.280665	-1.323290
O	-2.670716	0.988558	-0.861504
O	-3.309703	2.477135	-2.779615
C	-5.033735	2.153954	-0.784080
F	-5.656378	3.327806	-0.937057
F	-5.684664	1.228333	-1.509458
F	-5.108701	1.793708	0.511214
C	4.977425	1.745071	-1.675333
C	5.167043	1.542404	-0.309444
C	4.568381	2.386938	0.637309
C	3.749053	3.427715	0.182725
C	3.557134	3.635030	-1.185304
C	4.179472	2.803077	-2.116754
H	5.428155	1.067041	-2.393336
H	5.781867	0.712340	0.029523
H	3.239315	4.078085	0.885545
H	2.901884	4.436357	-1.510691
H	4.031233	2.960570	-3.180193
C	4.831805	2.165500	2.114675

C	3.620068	2.351774	3.041327
H	5.606052	2.859989	2.462650
H	5.244525	1.162648	2.262402
C	2.423170	1.542703	2.669782
H	3.899723	2.085264	4.066526
H	3.277488	3.390848	3.063246
C	1.166388	1.446321	2.858564
C	-0.210174	1.413158	3.121365
C	-0.711049	0.639497	4.192724
C	-1.103575	2.089560	2.247216
C	-2.080169	0.524980	4.379071
H	-0.012321	0.129883	4.846414
C	-2.478332	1.947102	2.441966
C	-2.957344	1.165685	3.493721
H	-2.468514	-0.070302	5.197711
H	-3.162073	2.444609	1.766995
H	-4.029408	1.063651	3.627828
S	0.101981	4.366688	1.449215
O	0.920985	4.277065	2.667135
O	0.707904	4.780975	0.182422
C	-1.319249	5.420275	1.782715
H	-1.808003	5.057367	2.687815
H	-0.947701	6.436241	1.922836
H	-1.986638	5.353881	0.922545
N	-0.583926	2.831132	1.163818
H	-1.266089	2.936101	0.396284

Vibrational frequencies

-64.5170	20.1149	22.9396
23.9946	25.6589	27.8600
28.8837	31.7643	32.6097

38.2502	39.9807	41.8894
44.2268	44.6860	48.3797
53.4276	56.0941	57.2953
60.0510	62.8693	64.2534
66.0290	71.8417	72.8181
74.4089	83.1824	83.6644
87.2508	89.6784	93.8608

Int3S

Cartesian coordinates

C	-1.198320	-2.793193	1.895045
C	-1.396397	-1.589358	1.214720
C	-2.317110	-0.644825	1.665124
C	-3.056171	-0.927305	2.815706
C	-2.863254	-2.133462	3.502971
C	-1.930562	-3.071822	3.049545
C	-0.172496	-3.650222	1.193644
C	0.471139	-2.697424	0.150231
C	-0.527773	-1.511472	-0.021787
H	-2.454824	0.288762	1.133267
H	-3.782389	-0.205819	3.177455
H	-3.440706	-2.339349	4.399183
H	-1.783431	-4.004567	3.587226
H	0.563657	-4.079852	1.878291
H	0.654209	-3.188021	-0.800530
H	-0.653590	-4.483820	0.670244
S	-2.208993	-2.797237	-1.855092
O	-1.415736	-4.029302	-1.709555
O	-2.653525	-2.358427	-3.187531
C	-3.676054	-2.982891	-0.842913
C	-3.742477	-4.009849	0.100093

C	-4.725427	-2.076672	-1.000481
C	-4.873093	-4.117148	0.904387
H	-2.924430	-4.712588	0.193935
C	-5.848315	-2.201843	-0.185470
H	-4.666957	-1.282815	-1.737089
C	-5.937162	-3.211683	0.782137
H	-4.927623	-4.911974	1.642944
H	-6.660940	-1.490251	-0.294557
C	-7.130468	-3.304326	1.700053
H	-8.005912	-2.807304	1.273804
H	-7.392613	-4.345019	1.912082
H	-6.911454	-2.822531	2.661017
N	-1.278401	-1.528587	-1.302831
H	-1.778868	-0.646606	-1.452971
S	2.131431	-2.105318	0.760495
C	3.226488	-2.587059	-0.568142
C	4.375078	-3.349738	-0.278548
C	2.989376	-2.131200	-1.887397
C	5.246347	-3.683679	-1.324360
C	3.855733	-2.510648	-2.920967
C	4.979298	-3.281329	-2.629486
H	6.130454	-4.275848	-1.108722
H	3.670458	-2.201063	-3.941275
H	5.651121	-3.565649	-3.433393
C	4.696228	-3.791504	1.128841
H	4.887770	-2.929049	1.776577
H	3.864540	-4.345644	1.574582
H	5.585276	-4.426677	1.140754
O	1.912944	-1.316369	-2.050714
C	1.661524	-0.681483	-3.328554

C	0.916461	0.608431	-3.021084
C	0.873262	-1.617136	-4.240070
H	2.628756	-0.427157	-3.781488
H	1.487323	1.222784	-2.322384
H	0.761852	1.180713	-3.939680
H	-0.058247	0.397149	-2.579099
H	-0.118108	-1.800430	-3.819555
H	0.755796	-1.162380	-5.229210
H	1.384236	-2.575654	-4.362292
H	0.015061	-0.565922	-0.079170
O	-2.478123	1.148937	-1.162834
S	-3.765628	1.750881	-1.656778
O	-4.508032	0.899224	-2.601325
O	-3.631083	3.183075	-2.007968
C	-4.817959	1.792316	-0.117057
F	-4.233983	2.566740	0.815164
F	-6.026159	2.295651	-0.396518
F	-4.970687	0.566159	0.400547
S	2.413164	1.143115	0.618437
C	4.082070	0.655764	0.210406
C	4.504561	0.619480	-1.122642
C	4.921762	0.194476	1.232892
C	5.762546	0.110467	-1.428628
H	3.848676	0.967588	-1.912388
C	6.175085	-0.316924	0.907358
H	4.580328	0.204556	2.262848
C	6.608513	-0.381703	-0.425026
H	6.079720	0.064056	-2.465834
H	6.818840	-0.691139	1.698800
C	7.926391	-1.021674	-0.777687

H	8.369061	-0.568183	-1.669073
H	7.772391	-2.085884	-0.993123
H	8.644754	-0.948775	0.043649
C	2.847546	-0.514959	4.618401
C	2.998013	0.856462	4.407831
C	1.931807	1.631239	3.926601
C	0.701722	1.007328	3.686529
C	0.543812	-0.362594	3.911824
C	1.617147	-1.128859	4.367024
H	3.686669	-1.101290	4.982384
H	3.955288	1.330470	4.614605
H	-0.131583	1.590266	3.303564
H	-0.415093	-0.829192	3.724159
H	1.494438	-2.196486	4.525615
C	2.126123	3.105230	3.639120
C	3.108588	3.393587	2.477531
H	1.170148	3.580707	3.408276
H	2.536007	3.607688	4.523017
C	2.635177	2.895530	1.153978
H	4.081080	2.930304	2.679182
H	3.264650	4.471733	2.384559
C	2.173558	3.336796	0.047456
C	1.577756	3.739505	-1.143307
C	2.358413	4.216432	-2.225199
C	0.172021	3.543995	-1.306217
C	1.755622	4.480456	-3.444285
H	3.423879	4.357629	-2.082062
C	-0.410407	3.798931	-2.546980
C	0.378876	4.260716	-3.602773
H	2.347148	4.846191	-4.275633

H	-1.475034	3.632217	-2.672038
H	-0.088368	4.460242	-4.561983
S	-1.021323	3.990309	1.069716
O	0.142701	4.811892	1.430737
O	-1.622029	3.083103	2.052277
C	-2.286050	5.089680	0.415160
H	-1.822520	5.701352	-0.359978
H	-2.630174	5.710415	1.243854
H	-3.092910	4.486149	0.002974
N	-0.573670	3.007413	-0.237756
H	-1.342527	2.375120	-0.520394

Vibrational frequencies

12.6960	23.5952	25.4300
27.8853	30.6787	32.8486
36.8922	39.5141	43.3473
46.9651	47.2555	50.9291
52.0008	54.4609	57.3814
59.8643	61.1969	62.5630
64.5303	65.1105	68.6967
70.2544	75.5017	77.8926
80.0056	83.8222	85.4280
85.8669	91.6114	92.9517

Int3R

Cartesian coordinates

C	0.052292	-3.441724	-0.743966
C	0.588473	-2.175649	-0.500194
C	1.447077	-1.565081	-1.414378
C	1.763182	-2.247707	-2.591052
C	1.216742	-3.512456	-2.847285
C	0.359667	-4.117825	-1.925424

C	-0.801088	-3.904928	0.410561
C	-0.984558	-2.631115	1.282326
C	0.143742	-1.644524	0.846293
H	1.882355	-0.595263	-1.194581
H	2.440678	-1.799157	-3.308846
H	1.469845	-4.029823	-3.768448
H	-0.058748	-5.100334	-2.125098
H	-1.754141	-4.332751	0.087285
H	-0.926941	-2.839006	2.349290
H	-0.271603	-4.667305	0.989468
S	2.307770	-2.693979	2.244249
O	1.550985	-3.945756	2.405474
O	3.082802	-2.143788	3.367523
C	3.443292	-2.900517	0.873932
C	3.368945	-4.026057	0.056452
C	4.347633	-1.871241	0.608071
C	4.206413	-4.105413	-1.054288
H	2.654942	-4.810008	0.277354
C	5.164292	-1.959207	-0.513959
H	4.398701	-1.011335	1.259541
C	5.099551	-3.071308	-1.367060
H	4.148860	-4.975838	-1.701382
H	5.851492	-1.146163	-0.730725
C	5.937415	-3.132255	-2.620221
H	5.383178	-2.712390	-3.469107
H	6.861504	-2.557155	-2.514857
H	6.198263	-4.162238	-2.879463
N	1.219005	-1.488892	1.855038
H	1.734752	-0.610415	1.738975
S	-2.687968	-1.940843	0.959150

C	-3.283283	-1.433252	2.567543
C	-4.463542	-2.016134	3.072408
C	-2.642413	-0.391808	3.281945
C	-4.976674	-1.560373	4.294969
C	-3.157461	0.022047	4.518402
C	-4.323764	-0.560496	5.010059
H	-5.884856	-2.006607	4.688264
H	-2.666153	0.797967	5.090458
H	-4.720442	-0.227380	5.964609
C	-5.199124	-3.103551	2.323976
H	-5.589802	-2.738620	1.368000
H	-4.539669	-3.945606	2.092905
H	-6.041540	-3.472684	2.914243
O	-1.558860	0.162946	2.688090
C	-0.863688	1.285309	3.291089
C	-0.227710	2.034655	2.132462
C	0.139195	0.784501	4.325728
H	-1.602533	1.941174	3.767190
H	-0.986256	2.385134	1.432239
H	0.330412	2.899545	2.500265
H	0.468602	1.393629	1.592400
H	0.853697	0.104343	3.858693
H	0.690555	1.627365	4.751474
H	-0.363517	0.249313	5.136185
H	-0.259329	-0.636102	0.765119
S	-2.107061	0.492258	-1.276828
C	-2.779275	-0.782930	-2.338365
C	-1.918647	-1.667137	-2.998779
C	-4.167397	-0.926644	-2.454489
C	-2.454193	-2.685628	-3.781864

H	-0.845511	-1.569572	-2.889169
C	-4.685877	-1.952351	-3.243270
H	-4.828178	-0.259258	-1.911960
C	-3.841628	-2.843832	-3.920998
H	-1.781081	-3.377204	-4.280476
H	-5.763160	-2.067505	-3.324959
C	-4.404198	-3.939410	-4.791551
H	-3.820493	-4.860191	-4.697789
H	-5.443589	-4.162276	-4.537049
H	-4.378224	-3.645928	-5.848112
O	2.993212	3.308765	0.958621
S	3.347446	2.024607	1.643326
O	2.744393	0.837844	0.976112
O	3.281372	2.055159	3.111306
C	5.162145	1.845636	1.241497
F	5.832377	2.958978	1.553036
F	5.692416	0.818487	1.923330
F	5.325689	1.598974	-0.074412
C	-5.868206	1.294640	0.472398
C	-5.439351	2.060285	-0.613554
C	-4.336164	2.918172	-0.496822
C	-3.704781	3.031834	0.747036
C	-4.141870	2.278054	1.837901
C	-5.211569	1.392271	1.702592
H	-6.713293	0.621641	0.357223
H	-5.958802	1.981542	-1.566088
H	-2.855146	3.699140	0.850196
H	-3.638462	2.368072	2.794091
H	-5.522662	0.783455	2.545693
C	-3.811003	3.672099	-1.699416

C	-3.272157	2.760266	-2.828018
H	-3.016947	4.359372	-1.397518
H	-4.610511	4.274649	-2.146784
C	-2.093928	1.920604	-2.441849
H	-4.056842	2.073506	-3.166679
H	-2.974183	3.374358	-3.682007
C	-0.846848	1.897546	-2.738165
C	0.506454	1.783491	-2.969073
C	0.985574	1.037368	-4.084003
C	1.432296	2.319606	-2.015055
C	2.335838	0.793447	-4.220446
H	0.267154	0.657401	-4.801245
C	2.791893	2.018371	-2.155108
C	3.229295	1.264479	-3.238861
H	2.707540	0.226070	-5.065936
H	3.493538	2.384829	-1.417584
H	4.289091	1.050575	-3.333600
S	0.156123	4.535447	-1.064415
O	-0.376280	4.630054	-2.429706
O	-0.750377	4.646032	0.080215
C	1.492412	5.723012	-0.852159
H	2.179753	5.617566	-1.691903
H	1.039109	6.715205	-0.838853
H	1.989990	5.502395	0.093451
N	0.974414	3.041231	-0.917393
H	1.650855	3.082823	-0.132095

Vibrational frequencies

5.7690	15.9131	22.8130
23.0598	25.8318	26.2476
30.8757	32.3945	35.1374

35.7898	38.0265	39.2103
40.5904	47.9360	48.2593
49.5427	55.6556	58.9121
59.1751	59.6634	64.4989
67.8551	69.5937	70.3645
73.3217	76.7660	81.5048
83.9659	85.8684	88.6717

TS4S

Cartesian coordinates

C	-4.151499	0.643735	-2.163266
C	-3.137781	-0.148816	-1.617908
C	-2.881991	-1.432224	-2.100820
C	-3.658778	-1.916300	-3.154714
C	-4.670600	-1.123433	-3.712452
C	-4.924487	0.159517	-3.219840
C	-4.260921	1.961493	-1.431701
C	-2.954707	2.033640	-0.598997
C	-2.438667	0.566814	-0.480981
H	-2.105554	-2.039265	-1.647160
H	-3.480854	-2.914795	-3.543578
H	-5.265787	-1.511960	-4.534128
H	-5.714220	0.768390	-3.651801
H	-4.377754	2.817884	-2.100813
H	-3.094508	2.477421	0.381389
H	-5.122792	1.943312	-0.756051
S	-4.060211	-0.400190	1.562963
O	-4.947613	0.758920	1.370958
O	-3.727641	-0.855419	2.922051
C	-4.758752	-1.801903	0.695620
C	-5.851803	-1.625088	-0.150237

C	-4.140434	-3.047339	0.833662
C	-6.326477	-2.714962	-0.875547
H	-6.307988	-0.647148	-0.245348
C	-4.628029	-4.123255	0.097522
H	-3.286331	-3.170714	1.490266
C	-5.718588	-3.973395	-0.772463
H	-7.172864	-2.581987	-1.543155
H	-4.150557	-5.094230	0.194684
C	-6.201401	-5.128526	-1.614006
H	-5.940315	-6.091119	-1.165942
H	-7.285656	-5.095598	-1.755472
H	-5.742352	-5.092759	-2.609777
N	-2.596782	-0.037866	0.861515
H	-1.961489	-0.833315	0.975096
S	-1.656268	3.031214	-1.492770
C	-1.365298	4.461361	-0.461842
C	-1.322737	5.730619	-1.077504
C	-1.064715	4.338556	0.919228
C	-1.020911	6.859139	-0.302447
C	-0.799374	5.488595	1.675574
C	-0.777045	6.739370	1.061796
H	-0.991592	7.835281	-0.777349
H	-0.598268	5.413880	2.736009
H	-0.563004	7.621379	1.658149
C	-1.577024	5.899229	-2.557116
H	-0.810565	5.393329	-3.155214
H	-2.538460	5.464870	-2.848311
H	-1.573203	6.957189	-2.831726
O	-1.032296	3.076679	1.427644
C	-0.935754	2.862031	2.859531

C	-0.456860	1.432016	3.049058
C	-2.297208	3.115356	3.502407
H	-0.180766	3.544115	3.269135
H	0.507912	1.269323	2.566035
H	-0.340666	1.226006	4.117796
H	-1.187043	0.737471	2.637635
H	-3.033594	2.417930	3.091155
H	-2.239149	2.962387	4.584363
H	-2.642417	4.136225	3.317215
H	-1.355750	0.543994	-0.608971
S	0.706502	-0.571870	-2.423599
C	1.330320	0.997267	-1.833275
C	1.713856	1.967242	-2.763672
C	1.323208	1.297317	-0.466399
C	2.074373	3.239562	-2.320832
H	1.724769	1.732770	-3.823157
C	1.718657	2.559340	-0.039362
H	1.013332	0.550299	0.254453
C	2.080723	3.555421	-0.955940
H	2.361497	3.995032	-3.047424
H	1.727191	2.773823	1.022329
C	2.421427	4.943682	-0.477472
H	3.022792	5.487554	-1.211629
H	1.504525	5.518278	-0.302192
H	2.972706	4.913509	0.467321
O	1.014110	-3.875079	1.050984
S	0.328916	-2.591324	1.317329
O	-0.891545	-2.350359	0.506771
O	1.232816	-1.410951	1.424412
C	-0.329827	-2.763944	3.048887

F	0.677055	-3.008338	3.904823
F	-0.949478	-1.640847	3.423826
F	-1.203587	-3.779965	3.111013
C	6.262129	-3.023933	-1.863082
C	5.157449	-3.434770	-2.587262
C	3.910368	-3.587110	-1.948026
C	3.820486	-3.332426	-0.542361
C	4.992361	-3.035107	0.197701
C	6.185745	-2.834726	-0.461364
H	7.209402	-2.867662	-2.369038
H	5.232181	-3.609568	-3.655514
H	2.909241	-3.579334	-0.006440
H	4.925224	-2.930745	1.272859
H	7.077950	-2.557615	0.089916
C	2.681414	-4.042582	-2.689392
C	1.460247	-3.214917	-2.250343
H	2.503345	-5.106027	-2.490712
H	2.844580	-3.933051	-3.764856
C	1.916802	-1.794957	-1.989043
H	0.681794	-3.236009	-3.017082
H	1.009049	-3.605877	-1.333138
C	3.110396	-1.521955	-1.472678
C	4.074653	-0.492519	-1.379951
C	4.690737	-0.054040	-2.580032
C	4.441886	0.117156	-0.138331
C	5.609694	0.976747	-2.579509
H	4.401219	-0.545099	-3.502264
C	5.388966	1.154612	-0.155927
C	5.949374	1.573042	-1.356893
H	6.059486	1.317230	-3.505336

H	5.681119	1.638521	0.764364
H	6.668393	2.386293	-1.336791
S	3.984514	0.334718	2.571407
O	5.403544	0.646009	2.789667
O	2.995498	1.407477	2.746430
C	3.520183	-1.063162	3.590835
H	4.257455	-1.852988	3.449931
H	3.541461	-0.694029	4.617594
H	2.519592	-1.390890	3.314149
N	3.841720	-0.363950	1.021858
H	2.943861	-0.854662	0.918304

Vibrational frequencies

-178.7149	15.0861	19.6551
20.7910	25.9773	27.1318
29.8378	32.1883	36.0214
37.5660	42.5481	44.9609
46.7429	49.3802	52.3340
54.7241	56.0977	59.9198
60.6353	63.5853	65.4758
66.5220	69.7076	70.4421
74.5459	75.8453	80.1210
85.2627	86.3933	88.7913

TS4R

Cartesian coordinates

C	4.230198	1.430732	-1.539241
C	2.871221	1.538811	-1.238098
C	2.123509	2.643727	-1.637827
C	2.760379	3.664083	-2.343877
C	4.124922	3.566521	-2.647329
C	4.866582	2.450242	-2.249692

C	4.814961	0.153276	-0.983298
C	3.585526	-0.646415	-0.483535
C	2.382213	0.337169	-0.461561
H	1.072343	2.712711	-1.389512
H	2.195317	4.538245	-2.653640
H	4.611450	4.366860	-3.197754
H	5.924039	2.379646	-2.490184
H	5.401983	-0.403498	-1.720106
H	3.740053	-1.055296	0.507521
H	5.475904	0.373515	-0.137657
S	2.741115	1.409046	2.068760
O	4.131102	0.922133	2.032236
O	1.939117	1.262686	3.296009
C	2.744245	3.140203	1.622371
C	3.910783	3.740353	1.151394
C	1.532970	3.833150	1.659656
C	3.853140	5.057836	0.703568
H	4.835033	3.176373	1.118160
C	1.492750	5.143195	1.193792
H	0.628573	3.360241	2.021355
C	2.646321	5.771755	0.702158
H	4.755372	5.531292	0.327237
H	0.543343	5.669353	1.195428
C	2.581939	7.168207	0.135669
H	2.415987	7.131239	-0.948168
H	1.761169	7.742816	0.573490
H	3.515086	7.713941	0.303151
N	1.879242	0.578711	0.910093
H	0.909360	0.902220	0.919859
S	3.128271	-2.078306	-1.568524

C	4.434664	-3.241038	-1.177439
C	5.275230	-3.736199	-2.195316
C	4.585595	-3.706887	0.152967
C	6.257739	-4.679920	-1.863976
C	5.584403	-4.638380	0.460589
C	6.411991	-5.119757	-0.552096
H	6.910241	-5.061495	-2.643597
H	5.709598	-4.993248	1.476003
H	7.182993	-5.845131	-0.309398
C	5.139176	-3.272912	-3.626798
H	4.175562	-3.568924	-4.055237
H	5.189118	-2.182015	-3.696968
H	5.930400	-3.699389	-4.248448
O	3.702480	-3.216335	1.065923
C	3.960055	-3.294625	2.488580
C	2.668468	-2.816871	3.139200
C	5.154673	-2.425848	2.876560
H	4.138763	-4.343316	2.760278
H	1.820788	-3.416476	2.796011
H	2.741235	-2.897575	4.227370
H	2.487984	-1.769696	2.879099
H	4.945964	-1.377573	2.643304
H	5.339594	-2.512803	3.951693
H	6.062098	-2.730594	2.349744
H	1.509398	-0.103247	-0.951802
O	-3.243751	2.030254	0.591468
S	-1.886458	2.644853	0.630298
O	-0.796968	1.633262	0.664680
O	-1.748667	3.767119	1.576910
C	-1.690021	3.435630	-1.051014

F	-2.800387	4.092974	-1.395344
F	-0.666555	4.309481	-1.022550
F	-1.415599	2.511633	-1.985032
S	-0.155933	-2.065077	0.371929
C	-1.041101	-1.980778	-1.183679
C	-1.552369	-3.136647	-1.780382
C	-1.222671	-0.733933	-1.795647
C	-2.278552	-3.034503	-2.966989
H	-1.412293	-4.101323	-1.304801
C	-1.945908	-0.649134	-2.980747
H	-0.845752	0.167119	-1.325564
C	-2.504370	-1.791552	-3.572990
H	-2.697814	-3.932248	-3.412557
H	-2.117717	0.325856	-3.422310
C	-3.378464	-1.662497	-4.794946
H	-4.362514	-1.274495	-4.505298
H	-3.525826	-2.625036	-5.292152
H	-2.952762	-0.960328	-5.518553
C	-5.355367	-2.064883	3.546176
C	-4.043893	-2.175488	3.979241
C	-3.092074	-1.213774	3.594842
C	-3.513455	-0.131596	2.763444
C	-4.883644	0.032508	2.439888
C	-5.785001	-0.949731	2.786134
H	-6.073991	-2.833282	3.812886
H	-3.734275	-3.019406	4.586966
H	-2.841054	0.691545	2.565163
H	-5.182058	0.914474	1.889226
H	-6.828880	-0.865914	2.502824
C	-1.647672	-1.283247	4.011914

C	-0.737787	-0.908559	2.829081
H	-1.469908	-0.598405	4.849760
H	-1.415674	-2.293044	4.361621
C	-1.341726	-1.453375	1.555904
H	0.274026	-1.287248	2.975553
H	-0.630888	0.174675	2.707930
C	-2.651113	-1.476405	1.334519
C	-3.637153	-2.192759	0.619847
C	-3.765067	-3.575762	0.917141
C	-4.482780	-1.607832	-0.379506
C	-4.667984	-4.377558	0.249130
H	-3.115726	-3.984483	1.683226
C	-5.413246	-2.438800	-1.030737
C	-5.493870	-3.789161	-0.719542
H	-4.743162	-5.435182	0.475507
H	-6.056458	-2.025313	-1.791069
H	-6.220049	-4.398637	-1.248971
S	-5.099751	0.729860	-1.807169
O	-5.925064	-0.106730	-2.686994
O	-4.071288	1.589995	-2.389545
C	-6.161386	1.743982	-0.776168
H	-6.840774	1.091460	-0.227397
H	-6.713249	2.408051	-1.443670
H	-5.508820	2.310699	-0.111628
N	-4.326301	-0.259858	-0.659730
H	-3.614331	0.281103	-0.158349

Vibrational frequencies

-191.2309	10.2221	15.4433
17.2556	23.2242	24.9091
28.4372	32.7790	34.6289

38.6908	40.9130	44.8681
50.2256	50.8084	53.8440
55.7905	61.1281	63.2239
65.9886	68.2631	69.3970
72.8114	76.1686	78.0069
82.5058	85.1869	87.5658
89.7284	95.4614	97.3193

P

Cartesian coordinates

S	-0.154025	-3.183119	0.128096
C	1.318285	-2.283130	-0.380316
C	2.321079	-1.995107	0.550612
C	1.467979	-1.861476	-1.708517
C	3.444129	-1.268622	0.158997
H	2.204229	-2.305039	1.583647
C	2.585335	-1.116719	-2.081366
H	0.704639	-2.102348	-2.442012
C	3.586672	-0.798970	-1.153284
H	4.207268	-1.032567	0.895734
H	2.676975	-0.769923	-3.106632
C	4.756399	0.071704	-1.536262
H	4.558026	1.105162	-1.230201
H	5.676724	-0.250931	-1.039588
H	4.926841	0.066389	-2.616457
C	-4.536930	2.022736	-0.880957
C	-4.620509	0.675889	-1.242586
C	-3.671153	-0.247312	-0.803718
C	-2.597974	0.185166	0.008008
C	-2.544777	1.534833	0.394345
C	-3.500014	2.448456	-0.049632

H	-5.282076	2.728624	-1.235156
H	-5.440139	0.332653	-1.868575
H	-1.752696	1.870608	1.052732
H	-3.434265	3.488027	0.257562
C	-3.800292	-1.722077	-1.095064
C	-2.433577	-2.382373	-1.287106
H	-4.436610	-1.893930	-1.968508
H	-4.300373	-2.199228	-0.239330
C	-1.460260	-1.985060	-0.199537
H	-2.541225	-3.470806	-1.314751
H	-1.996681	-2.094873	-2.256083
C	-1.553728	-0.786234	0.428740
C	-0.620282	-0.369673	1.521087
C	-0.837406	-0.814973	2.828583
C	0.462765	0.500866	1.272867
C	-0.024307	-0.396262	3.881305
H	-1.666474	-1.491437	3.011635
C	1.284019	0.923670	2.325979
C	1.028621	0.482697	3.623419
H	-0.213717	-0.749475	4.889748
H	2.130266	1.567019	2.121514
H	1.671939	0.816990	4.431688
S	1.451889	2.256575	-0.634863
O	2.759504	2.424469	0.015432
O	1.372060	2.138582	-2.095459
C	0.402263	3.606994	-0.078484
H	0.332926	3.556647	1.009515
H	0.877007	4.539446	-0.386548
H	-0.578799	3.488981	-0.538427
N	0.693232	0.889792	-0.063484

H	0.267225	0.341621	-0.801317
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Vibrational frequencies

16.1217	39.1837	43.1043
51.3399	68.4712	70.8210
74.6617	81.8028	87.1137
95.7216	122.6496	143.1534
160.6300	164.6520	170.0014
198.1607	210.0406	230.7580
242.6304	256.7147	276.8519
300.9574	304.4448	318.2098
330.2888	359.1387	363.3317
366.8427	379.0717	388.9001

TfOH

Cartesian coordinates

O	1.224994	-1.280291	-0.760105
S	0.853369	-0.142783	0.061838
O	1.263734	1.187956	-0.763225
O	1.253585	-0.012595	1.456679
C	-1.011842	0.009511	-0.001722
F	-1.537773	-1.015372	0.663619
F	-1.374362	1.156317	0.570529
F	-1.415269	-0.013971	-1.267743
H	1.425275	1.924129	-0.143505

Vibrational frequencies

18.9089	171.8533	178.2974
275.3438	286.8940	318.4838
335.8720	432.3407	468.9520
548.0644	549.2649	578.0456
752.5267	812.0464	1109.3402
1136.3616	1214.3806	1246.7216

1253.2391

1374.4801

3729.6282

Int02-se

Cartesian coordinates

C	-1.424973	-2.493223	1.989502
C	-1.701579	-1.347680	1.241393
C	-2.655776	-0.421107	1.657114
C	-3.342711	-0.665070	2.847409
C	-3.065302	-1.809524	3.607107
C	-2.103216	-2.730774	3.184638
C	-0.400137	-3.363176	1.301925
C	0.138919	-2.458836	0.171571
C	-0.865052	-1.295717	-0.019847
H	-2.843568	0.472279	1.077079
H	-4.091175	0.043212	3.188741
H	-3.602237	-1.981769	4.535098
H	-1.892805	-3.617686	3.775478
H	0.382791	-3.725115	1.978042
H	0.361549	-2.969560	-0.757693
H	-0.863766	-4.245240	0.849776
S	-2.558967	-2.700467	-1.719860
O	-1.795966	-3.919808	-1.399374
O	-2.957291	-2.423074	-3.106667
C	-4.038181	-2.704505	-0.714275
C	-4.149833	-3.605417	0.345715
C	-5.041302	-1.772432	-0.985289
C	-5.282329	-3.558586	1.153074
H	-3.363287	-4.326126	0.531186
C	-6.166705	-1.744449	-0.165766
H	-4.938277	-1.070969	-1.806204
C	-6.301196	-2.624297	0.917355

H	-5.372207	-4.252297	1.983929
H	-6.944113	-1.012361	-0.361937
C	-7.494705	-2.541241	1.835715
H	-8.370606	-2.136831	1.321221
H	-7.755172	-3.521351	2.245354
H	-7.277407	-1.879985	2.683579
N	-1.599041	-1.398419	-1.298304
H	-2.068884	-0.513015	-1.520781
C	3.032151	-2.627095	-0.547338
C	4.096510	-3.454173	-0.149919
C	2.771753	-2.321105	-1.900153
C	4.897317	-4.000429	-1.156573
C	3.590401	-2.889600	-2.884696
C	4.641254	-3.718226	-2.499380
H	5.722007	-4.651071	-0.885457
H	3.415472	-2.690615	-3.933405
H	5.273377	-4.153982	-3.266852
C	4.385850	-3.737863	1.305344
H	4.717728	-2.830652	1.821474
H	3.498760	-4.105932	1.829704
H	5.173765	-4.486715	1.402119
O	1.745745	-1.475000	-2.121494
C	1.460243	-0.967329	-3.460269
C	0.782056	0.378742	-3.260634
C	0.593481	-1.966503	-4.216674
H	2.419839	-0.816062	-3.968932
H	1.414194	1.067384	-2.697768
H	0.567567	0.828750	-4.233674
H	-0.160135	0.259755	-2.722844
H	-0.380616	-2.059527	-3.731586

H	0.439201	-1.616920	-5.241960
H	1.062609	-2.953123	-4.258624
H	-0.360792	-0.330596	-0.120538
O	-2.447981	1.307240	-1.169591
S	-3.651685	1.933357	-1.815605
O	-4.366037	1.028701	-2.735457
O	-3.415655	3.314463	-2.288945
C	-4.826633	2.170969	-0.386292
F	-4.293734	2.996689	0.527303
F	-5.977771	2.697960	-0.823161
F	-5.093171	1.001445	0.216380
S	2.162574	0.404143	0.474427
C	3.878387	0.288169	0.001376
C	4.258637	0.545799	-1.320139
C	4.838904	-0.114114	0.939784
C	5.592152	0.401775	-1.693936
H	3.517902	0.858370	-2.045931
C	6.165318	-0.269526	0.547323
H	4.542252	-0.292965	1.967616
C	6.562012	-0.027568	-0.776291
H	5.881147	0.606812	-2.720870
H	6.903054	-0.588626	1.278247
C	7.988273	-0.254731	-1.209334
H	8.268217	0.407881	-2.032861
H	8.120381	-1.285899	-1.559316
H	8.688408	-0.097301	-0.384266
C	2.504439	-0.822333	4.112488
C	3.099841	0.438360	4.104766
C	2.347222	1.592948	3.834170
C	0.978826	1.454910	3.583570

C	0.372120	0.195429	3.604928
C	1.132968	-0.945874	3.863100
H	3.104029	-1.704754	4.317694
H	4.162898	0.532792	4.315507
H	0.381227	2.333268	3.365114
H	-0.691554	0.108108	3.417647
H	0.652379	-1.918371	3.890837
C	3.023144	2.945283	3.789991
C	3.947601	3.136635	2.556516
H	2.274286	3.741817	3.794426
H	3.646086	3.072349	4.683136
C	3.228940	3.280481	1.295401
H	4.644559	2.291192	2.484458
H	4.565169	4.030739	2.710906
C	2.594178	3.424510	0.270820
C	1.925122	3.634582	-0.970185
C	2.667552	4.089328	-2.078729
C	0.543286	3.382238	-1.140696
C	2.064855	4.285304	-3.317807
H	3.728629	4.274073	-1.948384
C	-0.056512	3.598974	-2.386320
C	0.698643	4.040597	-3.471638
H	2.659693	4.628285	-4.158498
H	-1.117806	3.406153	-2.498471
H	0.217358	4.193777	-4.432355
S	-0.861216	3.833864	1.133794
O	0.239057	4.563495	1.774520
O	-1.720085	2.957510	1.943453
C	-1.880822	5.049376	0.277827
H	-1.227269	5.629861	-0.373977

H	-2.325368	5.687432	1.042931
H	-2.644968	4.533723	-0.302174
N	-0.236227	2.827985	-0.075517
H	-1.015178	2.250621	-0.421402
Se	1.949755	-1.839678	0.827218

Vibrational frequencies

13.4790	20.7221	25.5936
27.6880	31.2152	32.2354
34.4853	36.7016	41.1266
43.2689	45.6083	47.9549
50.5961	50.9022	51.2698
56.7487	58.6498	59.4985
64.2738	66.8386	70.6918
71.2281	78.8824	81.7970
83.2287	88.0293	89.2232
92.3640	94.9692	98.8220

TS2S-Se

Cartesian coordinates

C	-1.198189	-2.760159	1.758602
C	-1.513477	-1.550876	1.134754
C	-2.523968	-0.724471	1.620942
C	-3.231159	-1.133768	2.752909
C	-2.917747	-2.343602	3.387214
C	-1.897474	-3.163557	2.895742
C	-0.108073	-3.490004	1.012119
C	0.424689	-2.432994	0.016589
C	-0.652566	-1.321374	-0.088367
H	-2.747938	0.217060	1.136062
H	-4.025484	-0.505748	3.144458
H	-3.471430	-2.646283	4.271155

H	-1.658880	-4.101386	3.389415
H	0.673573	-3.884180	1.668530
H	0.689010	-2.832639	-0.955490
H	-0.517772	-4.336160	0.450132
S	-2.239205	-2.631489	-1.973823
O	-1.393873	-3.827483	-1.815319
O	-2.664053	-2.199782	-3.314051
C	-3.719117	-2.880404	-0.998396
C	-3.755228	-3.895148	-0.041020
C	-4.806827	-2.027773	-1.192546
C	-4.896383	-4.044594	0.741244
H	-2.904595	-4.552877	0.084632
C	-5.939988	-2.196181	-0.400796
H	-4.767247	-1.239469	-1.935933
C	-6.000247	-3.194474	0.581091
H	-4.927855	-4.828658	1.492231
H	-6.783937	-1.526969	-0.537855
C	-7.206979	-3.327231	1.476192
H	-8.108758	-2.937401	0.996283
H	-7.386341	-4.369329	1.756275
H	-7.057038	-2.761303	2.403897
N	-1.374814	-1.328601	-1.383425
H	-1.924467	-0.470059	-1.506741
C	3.309636	-2.294319	-0.646390
C	4.420197	-3.095948	-0.335923
C	3.060581	-1.857334	-1.964452
C	5.272721	-3.475406	-1.379136
C	3.918836	-2.266364	-2.993285
C	5.016536	-3.068336	-2.687539
H	6.134138	-4.099332	-1.162555

H	3.746060	-1.960321	-4.016437
H	5.681575	-3.378806	-3.487828
C	4.706436	-3.527326	1.082240
H	4.962434	-2.664807	1.707093
H	3.832418	-4.003101	1.537672
H	5.542519	-4.229161	1.114730
O	1.994033	-1.034356	-2.118440
C	1.682030	-0.458616	-3.415499
C	0.880969	0.800696	-3.126469
C	0.913629	-1.461919	-4.269482
H	2.627834	-0.179906	-3.897081
H	1.439563	1.479133	-2.480197
H	0.651783	1.320171	-4.060736
H	-0.058902	0.547039	-2.632750
H	-0.062000	-1.662032	-3.821411
H	0.758216	-1.051197	-5.271955
H	1.456431	-2.405586	-4.366931
H	-0.203594	-0.324982	-0.078042
O	-2.675237	1.219064	-1.111051
S	-3.961235	1.821364	-1.605337
O	-4.670006	0.992689	-2.596082
O	-3.848747	3.266985	-1.902347
C	-5.047447	1.786779	-0.088622
F	-4.528433	2.570304	0.871232
F	-6.272609	2.234067	-0.391600
F	-5.152993	0.543809	0.402939
S	2.297057	0.958803	0.614587
C	3.990835	0.711234	0.108491
C	4.393238	0.951816	-1.209243
C	4.902963	0.181773	1.032716

C	5.692936	0.643772	-1.599794
H	3.688524	1.359300	-1.924784
C	6.196856	-0.130165	0.624948
H	4.584085	-0.005434	2.052797
C	6.606483	0.075469	-0.699931
H	5.995473	0.818337	-2.628385
H	6.892819	-0.559549	1.340288
C	7.975865	-0.353416	-1.161106
H	8.347025	0.282511	-1.969722
H	7.935062	-1.380835	-1.543508
H	8.701753	-0.335086	-0.343508
C	2.711587	-0.939820	4.245909
C	3.013655	0.421278	4.219267
C	2.024877	1.374119	3.928582
C	0.717107	0.935222	3.700806
C	0.404280	-0.426120	3.751394
C	1.400482	-1.366743	4.014154
H	3.493217	-1.665025	4.453783
H	4.032641	0.749657	4.412440
H	-0.061642	1.654195	3.462759
H	-0.616863	-0.746207	3.590143
H	1.154222	-2.423804	4.041149
C	2.386682	2.837901	3.805749
C	3.304308	3.148356	2.596624
H	1.484058	3.448336	3.720788
H	2.927235	3.166343	4.701256
C	2.655941	2.970242	1.281941
H	4.202679	2.521532	2.629524
H	3.634769	4.191348	2.649131
C	2.116565	3.407452	0.249993

C	1.446127	3.800874	-0.922972
C	2.164980	4.377924	-1.991540
C	0.053343	3.556672	-1.063877
C	1.517410	4.701011	-3.177359
H	3.228659	4.552540	-1.872372
C	-0.581204	3.884215	-2.263072
C	0.148269	4.448101	-3.311777
H	2.075464	5.141456	-3.996546
H	-1.642583	3.685053	-2.368616
H	-0.359743	4.694338	-4.238661
S	-1.198762	3.738320	1.328099
O	-0.073996	4.498124	1.888786
O	-1.892578	2.737468	2.148757
C	-2.393601	4.929350	0.696901
H	-1.859360	5.617318	0.040665
H	-2.802423	5.459520	1.558261
H	-3.170312	4.396726	0.149764
N	-0.654158	2.886176	-0.029412
H	-1.417715	2.284932	-0.378523
Se	2.145131	-1.717188	0.767013

Vibrational frequencies

-202.9359	21.3115	24.6341
28.6444	31.1737	32.2632
36.4140	38.5127	41.4031
42.4054	44.7069	47.4089
48.9193	54.2869	57.1163
58.8853	60.2196	62.4849
66.4923	68.1539	70.3831
75.6999	76.5068	79.8833
81.8986	88.5191	90.8993

93.8785 100.1239 101.1834

TS2R-Se

Cartesian coordinates

C	-0.306844	-3.344669	0.681142
C	-0.858116	-2.082692	0.451374
C	-1.780486	-1.522210	1.334277
C	-2.146840	-2.255401	2.464495
C	-1.592850	-3.519964	2.703727
C	-0.671006	-4.074066	1.812553
C	0.631892	-3.744570	-0.430094
C	0.816057	-2.438580	-1.241738
C	-0.336499	-1.480419	-0.835962
H	-2.212989	-0.547873	1.132122
H	-2.867093	-1.842056	3.161851
H	-1.886630	-4.075780	3.589465
H	-0.241713	-5.053733	2.001908
H	1.579291	-4.146750	-0.058262
H	0.874428	-2.582975	-2.317886
H	0.174606	-4.506116	-1.068592
S	-2.343261	-2.489804	-2.461411
O	-1.535907	-3.712204	-2.607258
O	-3.021986	-1.904448	-3.627226
C	-3.584664	-2.776279	-1.205499
C	-3.552506	-3.931401	-0.426705
C	-4.518124	-1.766838	-0.968236
C	-4.467214	-4.062379	0.615349
H	-2.811734	-4.697096	-0.622689
C	-5.414091	-1.907731	0.086233
H	-4.530834	-0.878341	-1.583209
C	-5.396340	-3.050819	0.899017

H	-4.444280	-4.955496	1.232976
H	-6.124515	-1.110001	0.282945
C	-6.323628	-3.173662	2.082430
H	-6.641797	-4.208805	2.237221
H	-5.815992	-2.849342	2.999467
H	-7.214942	-2.552111	1.962241
N	-1.330717	-1.280548	-1.911368
H	-1.883695	-0.429735	-1.754088
C	3.273817	-1.131693	-2.440291
C	4.468840	-1.704085	-2.912587
C	2.583320	-0.153596	-3.182818
C	4.942145	-1.308621	-4.168501
C	3.068995	0.210376	-4.447161
C	4.240515	-0.371363	-4.925620
H	5.858075	-1.744975	-4.553789
H	2.550629	0.941978	-5.051894
H	4.611529	-0.081832	-5.904076
C	5.241354	-2.709838	-2.092103
H	5.570605	-2.271121	-1.143399
H	4.621679	-3.576483	-1.840507
H	6.124034	-3.056687	-2.633345
O	1.491384	0.381473	-2.593279
C	0.789015	1.498580	-3.212447
C	0.138713	2.240265	-2.060296
C	-0.200340	0.996587	-4.258733
H	1.535963	2.150063	-3.680459
H	0.886282	2.612916	-1.359657
H	-0.442532	3.087500	-2.432523
H	-0.539936	1.579780	-1.520557
H	-0.953280	0.355167	-3.799427

H	-0.703427	1.848878	-4.724380
H	0.303749	0.424143	-5.041990
H	0.039992	-0.471619	-0.669815
S	2.157777	0.233994	1.026777
C	2.605644	-1.033895	2.216700
C	1.618054	-1.725340	2.925204
C	3.959446	-1.331199	2.432214
C	1.988712	-2.694122	3.855936
H	0.570802	-1.513790	2.747590
C	4.313743	-2.304453	3.362503
H	4.721219	-0.807328	1.862820
C	3.336277	-2.998090	4.093251
H	1.212502	-3.231712	4.392943
H	5.363984	-2.533240	3.521586
C	3.729685	-4.027653	5.123188
H	2.938219	-4.767097	5.273279
H	4.644047	-4.553757	4.834141
H	3.921236	-3.551293	6.092535
O	-2.958137	3.415105	-0.783976
S	-3.420435	2.162604	-1.452975
O	-2.829613	0.934268	-0.849177
O	-3.456126	2.201686	-2.923087
C	-5.210715	2.059209	-0.932752
F	-5.852933	3.195916	-1.222946
F	-5.828992	1.046433	-1.565490
F	-5.303907	1.838983	0.391620
C	5.775429	1.251664	-0.729642
C	5.475547	1.840114	0.497960
C	4.440046	2.779716	0.609855
C	3.723727	3.135323	-0.537726

C	4.037612	2.561036	-1.772083
C	5.058155	1.615846	-1.872179
H	6.571954	0.515987	-0.799548
H	6.044596	1.560877	1.382033
H	2.909774	3.851244	-0.460688
H	3.477905	2.846382	-2.657101
H	5.285980	1.157877	-2.827898
C	4.079840	3.357092	1.959445
C	3.541914	2.299733	2.948782
H	3.332792	4.148608	1.852199
H	4.965892	3.805325	2.424740
C	2.222888	1.736265	2.575457
H	4.255637	1.475346	3.050696
H	3.424664	2.752556	3.938842
C	0.995470	1.730642	2.790760
C	-0.385496	1.620163	2.990941
C	-0.882182	0.841600	4.061883
C	-1.295226	2.269324	2.112352
C	-2.249062	0.694289	4.243216
H	-0.175410	0.354988	4.724606
C	-2.667550	2.092071	2.297300
C	-3.137339	1.307463	3.350294
H	-2.626174	0.094608	5.064244
H	-3.357726	2.565327	1.611501
H	-4.207681	1.180353	3.477461
S	-0.116110	4.544986	1.239420
O	0.530478	4.574359	2.557264
O	0.665961	4.832293	0.031631
C	-1.542495	5.645153	1.262440
H	-2.152506	5.389827	2.129864

H	-1.167527	6.666830	1.338263
H	-2.099214	5.493280	0.336845
N	-0.800328	3.005806	1.014217
H	-1.473659	3.056317	0.234921
Se	2.617459	-1.708173	-0.733084

Vibrational frequencies

-203.8739	16.8345	19.8766
21.0476	24.1625	27.3421
30.9315	31.8418	34.9854
38.0475	40.7351	42.5387
45.6552	46.2278	49.5808
54.2214	57.1171	59.7534
62.4743	65.8621	68.5867
69.4023	71.4973	72.2089
77.8292	81.9679	84.5498
91.9079	93.3873	95.1602

Int2S-se

Cartesian coordinates

C	-1.351859	-2.791810	1.761869
C	-1.560738	-1.566459	1.121783
C	-2.466871	-0.632939	1.620684
C	-3.183522	-0.950824	2.776848
C	-2.984288	-2.179745	3.419916
C	-2.065213	-3.106814	2.918047
C	-0.340349	-3.627959	1.015064
C	0.300763	-2.625569	0.027695
C	-0.700056	-1.447574	-0.118762
H	-2.604763	0.321089	1.127020
H	-3.895768	-0.237270	3.180058
H	-3.544454	-2.411831	4.321175

H	-1.910685	-4.056539	3.422775
H	0.399314	-4.094766	1.670867
H	0.563748	-3.058986	-0.931722
H	-0.836605	-4.429260	0.456753
S	-2.370814	-2.693060	-1.987606
O	-1.587592	-3.931846	-1.845452
O	-2.794721	-2.240615	-3.321714
C	-3.846848	-2.868219	-0.988716
C	-3.940467	-3.910447	-0.065586
C	-4.869784	-1.928867	-1.126100
C	-5.072291	-4.000843	0.739350
H	-3.140581	-4.635721	0.014072
C	-5.993661	-2.036969	-0.310781
H	-4.787932	-1.121404	-1.845963
C	-6.109165	-3.062057	0.638002
H	-5.147973	-4.807379	1.463129
H	-6.785144	-1.299514	-0.402646
C	-7.301416	-3.134757	1.559205
H	-8.169621	-2.623082	1.135294
H	-7.580318	-4.170842	1.772788
H	-7.071699	-2.655321	2.518717
N	-1.442768	-1.437785	-1.404748
H	-1.932315	-0.547568	-1.545657
C	3.182380	-2.476047	-0.630575
C	4.243242	-3.363162	-0.387987
C	2.985620	-1.919904	-1.910842
C	5.091353	-3.705153	-1.449573
C	3.835751	-2.286721	-2.962714
C	4.880600	-3.177100	-2.720899
H	5.912640	-4.394060	-1.276052

H	3.698803	-1.882594	-3.956996
H	5.537069	-3.457321	-3.539507
C	4.489245	-3.922475	0.992043
H	4.784355	-3.128366	1.687608
H	3.578807	-4.370031	1.401872
H	5.282444	-4.673888	0.976706
O	1.965208	-1.023616	-2.018492
C	1.651329	-0.420682	-3.298235
C	0.870720	0.843889	-2.977203
C	0.861334	-1.391611	-4.171271
H	2.593642	-0.139061	-3.785802
H	1.455943	1.506669	-2.338339
H	0.630224	1.382907	-3.897509
H	-0.063885	0.604257	-2.466251
H	-0.108075	-1.597946	-3.712798
H	0.695507	-0.951080	-5.159407
H	1.395369	-2.335915	-4.303326
H	-0.170628	-0.493008	-0.150562
O	-2.470453	1.259730	-1.148409
S	-3.718681	1.902665	-1.687691
O	-4.430878	1.086167	-2.685571
O	-3.541345	3.338977	-1.999546
C	-4.852449	1.928885	-0.205811
F	-4.333425	2.697826	0.766276
F	-6.046944	2.425269	-0.552337
F	-5.027002	0.696392	0.290791
S	2.319421	1.265587	0.678319
C	3.942161	0.751391	0.106756
C	4.348739	1.001350	-1.204091
C	4.745803	0.011932	0.980915

C	5.568050	0.492164	-1.643670
H	3.722466	1.573722	-1.879200
C	5.959964	-0.489534	0.521431
H	4.415201	-0.184115	1.995986
C	6.382673	-0.273346	-0.797670
H	5.880529	0.673054	-2.667750
H	6.580582	-1.075367	1.193132
C	7.655402	-0.895596	-1.310597
H	8.102204	-0.299167	-2.110770
H	7.438480	-1.890024	-1.718106
H	8.394256	-1.017846	-0.513702
C	2.837328	-0.824819	4.345472
C	3.020404	0.558335	4.308241
C	1.954868	1.416086	3.994311
C	0.699250	0.857615	3.726891
C	0.508769	-0.525789	3.779576
C	1.577500	-1.369893	4.082643
H	3.674283	-1.474696	4.584750
H	4.000736	0.976531	4.525313
H	-0.132017	1.504888	3.460037
H	-0.471325	-0.939270	3.579005
H	1.430734	-2.444786	4.112336
C	2.166796	2.913549	3.904480
C	3.141818	3.337158	2.776670
H	1.214064	3.420993	3.739099
H	2.589518	3.294793	4.840814
C	2.681810	2.941134	1.432495
H	4.133306	2.901131	2.942451
H	3.252988	4.426132	2.764329
C	2.236074	3.164520	0.258946

C	1.670682	3.793432	-0.899307
C	2.473158	4.411840	-1.869260
C	0.277746	3.662484	-1.100362
C	1.887624	4.892800	-3.038378
H	3.542113	4.494265	-1.706039
C	-0.295347	4.139852	-2.279070
C	0.513070	4.744894	-3.244815
H	2.504245	5.370643	-3.791972
H	-1.363301	4.019234	-2.432473
H	0.062757	5.108093	-4.162929
S	-1.030069	3.834775	1.242600
O	0.109693	4.584134	1.791620
O	-1.726615	2.844387	2.072683
C	-2.213359	5.038046	0.616480
H	-1.670717	5.725667	-0.033015
H	-2.620911	5.565291	1.480200
H	-2.990568	4.513372	0.063158
N	-0.485776	2.979703	-0.112025
H	-1.239720	2.377428	-0.483447
Se	2.017314	-1.948676	0.808389

Vibrational frequencies

16.7639	22.2308	24.8427
27.9011	34.2040	37.2893
40.2428	42.1394	43.8575
45.8969	48.5594	52.0817
56.4608	57.4378	60.0356
60.7269	63.2103	68.0616
73.2535	75.5073	77.5703
81.4074	83.9105	85.0532
87.9547	89.2897	93.9232

94.3282 96.2185 99.6422

Int2R-se

Cartesian coordinates

C	0.014350	-2.559415	1.950535
C	-0.598373	-1.607460	1.133123
C	-1.613494	-0.781509	1.619067
C	-2.024674	-0.938059	2.944111
C	-1.429608	-1.908150	3.761651
C	-0.407428	-2.723194	3.270458
C	1.085453	-3.319459	1.208701
C	1.158095	-2.629712	-0.179088
C	-0.076842	-1.689795	-0.286803
H	-2.098607	-0.065218	0.964985
H	-2.820802	-0.314637	3.335524
H	-1.767996	-2.027606	4.787002
H	0.058777	-3.466494	3.910917
H	2.046767	-3.289564	1.732474
H	1.192888	-3.336628	-1.003819
H	0.806272	-4.371296	1.091576
S	-1.972031	-3.530194	-1.129637
O	-1.074863	-4.585495	-0.631161
O	-2.660114	-3.689135	-2.420739
C	-3.236052	-3.241194	0.104677
C	-3.173397	-3.881144	1.340082
C	-4.241993	-2.317527	-0.183667
C	-4.132936	-3.576815	2.303082
H	-2.375019	-4.584049	1.543814
C	-5.180630	-2.012279	0.795861
H	-4.277798	-1.828998	-1.147448
C	-5.137081	-2.630924	2.054363

H	-4.086920	-4.065889	3.271822
H	-5.947098	-1.274427	0.579100
C	-6.119691	-2.252023	3.134593
H	-6.350643	-3.101419	3.784004
H	-5.702739	-1.460497	3.769878
H	-7.055585	-1.874743	2.713345
N	-1.067890	-2.136488	-1.296800
H	-1.686218	-1.368079	-1.577436
C	3.328479	-1.946797	-2.132581
C	4.443923	-2.760221	-2.400232
C	2.594315	-1.362626	-3.186090
C	4.822910	-2.968855	-3.733450
C	2.991616	-1.584038	-4.512537
C	4.103109	-2.383896	-4.771963
H	5.682156	-3.595442	-3.952456
H	2.446940	-1.143857	-5.337130
H	4.403631	-2.553211	-5.801813
C	5.241210	-3.390146	-1.282271
H	5.745162	-2.627820	-0.677572
H	4.587107	-3.938817	-0.598298
H	5.999418	-4.070193	-1.678109
O	1.545073	-0.582990	-2.820796
C	0.773400	0.146561	-3.809913
C	0.122023	1.278618	-3.033527
C	-0.239305	-0.769450	-4.491344
H	1.467353	0.567551	-4.549601
H	0.869545	1.928160	-2.577868
H	-0.509844	1.881784	-3.690416
H	-0.507938	0.871573	-2.240990
H	-0.928185	-1.185081	-3.754500

H	-0.818465	-0.200614	-5.224240
H	0.249458	-1.600671	-5.005272
H	0.226168	-0.716404	-0.673281
S	1.777541	1.269010	1.215404
C	2.378619	0.292307	2.603852
C	1.514413	-0.088876	3.629482
C	3.722439	-0.101959	2.607476
C	2.010052	-0.855984	4.681352
H	0.463011	0.173338	3.597575
C	4.194389	-0.875419	3.663955
H	4.381914	0.182320	1.794975
C	3.351088	-1.260502	4.717707
H	1.332657	-1.165918	5.470989
H	5.234500	-1.188412	3.667814
C	3.883191	-2.078195	5.867683
H	3.083967	-2.627696	6.372021
H	4.637030	-2.795541	5.530791
H	4.360343	-1.430869	6.613337
O	-3.076793	2.583475	-2.041757
S	-3.440454	1.157019	-2.292054
O	-2.732425	0.216158	-1.380465
O	-3.509446	0.757949	-3.706369
C	-5.203041	1.069059	-1.684636
F	-5.958885	1.995079	-2.285204
F	-5.728618	-0.141834	-1.938818
F	-5.252535	1.271846	-0.354323
C	5.809084	1.309827	-0.206134
C	5.308239	2.472816	0.383286
C	4.197310	3.130265	-0.163167
C	3.608357	2.609225	-1.322241

C	4.104421	1.444884	-1.910369
C	5.200461	0.785687	-1.349705
H	6.670127	0.810911	0.229588
H	5.782879	2.869003	1.277842
H	2.742862	3.110665	-1.746769
H	3.625484	1.044444	-2.795578
H	5.578507	-0.123662	-1.805176
C	3.597476	4.338213	0.525477
C	2.989893	4.003641	1.910497
H	2.817088	4.782475	-0.096710
H	4.361802	5.104327	0.695526
C	1.898771	3.012762	1.852060
H	3.763686	3.616884	2.583105
H	2.563305	4.903462	2.364681
C	0.687122	2.637019	2.015014
C	-0.728883	2.697789	2.250000
C	-1.271014	2.537194	3.532481
C	-1.574943	2.846904	1.129212
C	-2.653688	2.505156	3.696057
H	-0.607718	2.423647	4.382815
C	-2.958470	2.793966	1.303600
C	-3.490645	2.612244	2.581494
H	-3.076321	2.378200	4.686774
H	-3.602954	2.881721	0.437789
H	-4.567643	2.564434	2.705645
S	-0.386654	4.526617	-0.604349
O	0.161315	5.166269	0.600126
O	0.479930	4.307902	-1.768468
C	-1.844100	5.440341	-1.133814
H	-2.511382	5.534051	-0.276004

H	-1.506175	6.420890	-1.471937
H	-2.319545	4.879276	-1.938523
N	-0.982895	2.991963	-0.155219
H	-1.595375	2.652997	-0.911623
Se	2.848607	-1.566704	-0.307395

Vibrational frequencies

14.6316	20.8013	24.4009
28.1108	30.8736	32.1140
33.9159	34.9507	35.7731
37.9793	39.8408	42.9451
45.4128	46.7879	48.0811
51.3875	53.5977	56.7672
59.0809	62.9699	64.4962
68.1181	71.3639	74.8269
79.0133	81.7122	85.8589
89.1539	92.1694	95.4046

TS5

Cartesian coordinates

C	0.472169	-1.412732	0.292631
C	0.904154	-0.136165	0.111682
C	2.404889	0.007217	0.110996
C	3.169531	-1.025768	-0.484800
C	2.439003	-2.267271	-0.932372
C	1.400856	-2.591566	0.153310
H	2.561594	1.723240	1.418734
C	3.101686	1.007657	0.811951
C	4.562709	-0.944787	-0.508989
H	1.914353	-2.102665	-1.884190
H	1.913271	-2.815502	1.101490
C	5.233430	0.116444	0.101052

C	4.496327	1.072750	0.796502
H	5.127528	-1.742856	-0.983923
H	6.317795	0.166904	0.073495
H	4.999642	1.865700	1.341577
C	-0.005829	1.043489	-0.083114
C	-1.396473	0.954783	-0.394320
C	0.511927	2.358964	-0.077959
C	-2.185756	2.103009	-0.529145
C	-0.276163	3.497999	-0.206327
H	1.574782	2.506681	0.017748
C	-1.650331	3.377327	-0.397260
H	-3.234417	1.975497	-0.774978
H	0.193407	4.475977	-0.167557
H	-2.284754	4.252317	-0.494489
H	3.139441	-3.094536	-1.079429
H	0.818379	-3.480899	-0.107893
S	-3.240535	-0.937354	0.323138
O	-2.887581	-2.354744	0.513458
O	-3.428000	-0.054423	1.479964
C	-4.720671	-0.874327	-0.690587
H	-4.535777	-1.444205	-1.601262
H	-5.529829	-1.321591	-0.110815
H	-4.940540	0.168199	-0.920119
N	-2.058511	-0.274545	-0.691401
H	-1.463247	-1.011840	-1.055489
H	-0.557608	-1.649756	0.509816

Vibrational frequencies

-32.0016	28.2857	56.4173
64.5768	97.8496	104.6656
153.8236	172.9365	200.8746

223.8105	228.2130	259.4361
277.3887	286.6101	324.3361
334.7534	359.1455	381.0338
417.6591	435.4252	460.9692
473.5358	482.3302	504.5889
511.6471	529.7166	548.3484
560.0836	601.0445	638.2218

TS6

Cartesian coordinates

C	0.812490	-1.683590	-0.110581
C	1.015093	-0.325696	-0.096549
C	2.468408	0.034430	0.139799
C	3.491686	-0.696521	-0.492738
C	3.039620	-1.874436	-1.307202
C	1.988361	-2.589269	-0.455479
H	2.070960	1.500991	1.674444
C	2.839956	0.973208	1.119914
C	4.833640	-0.415556	-0.227091
H	2.575819	-1.553692	-2.250511
H	2.450691	-2.987067	0.461677
C	5.187198	0.568327	0.696518
C	4.180942	1.245026	1.388878
H	5.603466	-0.992642	-0.733223
H	6.233055	0.782236	0.895838
H	4.436069	1.981889	2.144926
C	0.070943	0.845452	-0.262409
C	-1.354696	0.876102	-0.349647
C	0.684804	2.103460	-0.510598
C	-2.046443	2.091944	-0.477207
C	-0.000688	3.302236	-0.647897

H	1.759773	2.143466	-0.595391
C	-1.391516	3.308620	-0.585039
H	-3.128159	2.071233	-0.514202
H	0.555705	4.219885	-0.810688
H	-1.959617	4.228985	-0.674060
H	3.874583	-2.536880	-1.553352
H	1.584961	-3.456760	-0.992606
S	-3.569766	-0.594257	0.426997
O	-3.557934	-2.024554	0.765101
O	-3.719953	0.420394	1.475038
C	-4.860885	-0.348919	-0.799104
H	-4.692069	-1.052982	-1.614155
H	-5.815204	-0.548548	-0.308820
H	-4.821752	0.678729	-1.159676
N	-2.147795	-0.296657	-0.415659
H	-1.718512	-1.143551	-0.752827
C	-0.390787	-2.512796	0.272951
H	-1.070626	-2.019992	0.960301
H	-0.957722	-2.902439	-0.585054
H	-0.016254	-3.407000	0.784814

Vibrational frequencies

-43.5745	33.2572	37.1518
75.6422	84.6069	115.0900
134.5795	157.3183	169.4316
193.7399	211.6357	225.8623
239.6874	261.3223	288.1346
299.7638	333.6562	342.7270
351.2203	370.1150	393.0844
415.9739	444.9464	456.4218
461.9562	479.5068	499.6984

510.3833

527.7809

538.4091

TS7

Cartesian coordinates

C	-0.842507	1.451736	-0.351110
C	-1.059120	0.090584	-0.268084
C	-2.503502	-0.242863	0.053293
C	-3.549569	0.446197	-0.584470
C	-3.109880	1.547459	-1.500256
C	-2.031765	2.322608	-0.737806
H	-2.048065	-1.597758	1.673357
C	-2.837224	-1.102887	1.116847
C	-4.880883	0.203623	-0.239708
H	-2.669942	1.145232	-2.423929
H	-2.474019	2.804197	0.148367
C	-5.199453	-0.704607	0.769927
C	-4.166598	-1.339736	1.463757
H	-5.667473	0.750225	-0.753994
H	-6.236505	-0.892057	1.032146
H	-4.392580	-2.016473	2.282833
C	-0.142167	-1.108116	-0.350789
C	1.282524	-1.210447	-0.389130
C	-0.798519	-2.359792	-0.526730
C	1.921393	-2.459336	-0.354923
C	-0.162731	-3.592620	-0.522077
H	-1.869855	-2.362953	-0.658862
C	1.220622	-3.655309	-0.374393
H	3.003005	-2.486818	-0.350041
H	-0.752924	-4.496599	-0.636217
H	1.747903	-4.603069	-0.341686
H	-3.942222	2.199496	-1.781390

H	-1.660578	3.135302	-1.367640
S	3.521915	0.299911	0.247981
O	3.693688	1.754316	0.124103
O	3.432459	-0.344668	1.561863
C	4.894188	-0.433786	-0.665000
H	4.872975	-0.047267	-1.684564
H	5.808635	-0.119305	-0.159042
H	4.810705	-1.519460	-0.656525
N	2.117862	-0.068790	-0.576753
H	2.016567	0.435073	-1.449255
C	0.400146	2.227363	0.087086
C	0.686992	1.882251	1.565159
C	0.330881	3.756173	-0.073801
H	1.267115	1.916534	-0.481594
H	0.834148	0.809122	1.700825
H	1.592920	2.393065	1.903679
H	-0.149071	2.195308	2.200780
H	0.213893	4.064522	-1.117225
H	-0.478987	4.205461	0.509816
H	1.272550	4.183034	0.285251

Vibrational frequencies

-30.8860	43.7249	56.0523
68.8632	80.9867	105.2571
112.0589	123.2200	153.1917
162.2842	176.6899	184.7126
202.7492	234.4753	252.7702
278.5914	285.7220	297.1412
308.4749	324.8464	342.4459
344.2144	359.9269	390.6294
404.1233	419.5946	444.4909

455.2692 465.0090 485.4832

TS8

Cartesian coordinates

C	-0.499982	-0.938490	0.067557
C	0.790649	-0.646676	-0.076347
C	1.894702	-1.110495	1.464653
C	0.984140	-1.427359	2.522125
C	-0.212442	-2.266833	2.192738
C	-1.182436	-1.428791	1.323121
H	3.612448	0.116314	0.955020
C	2.918763	-0.144732	1.747958
C	1.100170	-0.792054	3.758985
H	0.071154	-3.164055	1.632214
H	-1.562367	-0.583882	1.908227
C	2.120077	0.125216	4.010116
C	3.030064	0.447805	2.986618
H	0.374429	-1.019925	4.535908
H	2.199447	0.600066	4.983117
H	3.819409	1.170489	3.171529
C	1.656889	-0.194820	-1.087240
C	1.620793	1.183083	-1.483605
C	2.830929	-0.996423	-1.439690
C	2.706613	1.791065	-2.066311
C	3.979020	-0.272156	-1.931554
C	3.914958	1.060408	-2.238388
H	2.630745	2.817809	-2.407959
H	4.893841	-0.816345	-2.136941
H	4.778806	1.560066	-2.666098
H	-0.731608	-2.589941	3.100286
H	-2.050542	-2.036085	1.053084

S	0.249500	2.912502	0.085540
O	-1.193224	2.907777	0.389778
O	1.218745	2.550948	1.127265
C	0.695186	4.538644	-0.532892
H	0.022742	4.793797	-1.351239
H	0.589475	5.239352	0.296848
H	1.730814	4.503362	-0.871626
N	0.417704	1.934511	-1.288128
H	-0.430762	1.371329	-1.374301
S	-1.471772	-0.926260	-1.473720
C	-3.155673	-0.670432	-0.907592
C	-4.131835	-1.624433	-1.215439
C	-3.516031	0.489162	-0.205520
C	-5.457448	-1.414763	-0.831717
H	-3.856867	-2.526344	-1.753162
C	-4.838250	0.671818	0.191503
H	-2.768096	1.239430	0.031528
C	-5.831711	-0.270968	-0.115989
H	-6.208183	-2.158837	-1.084403
H	-5.107478	1.570696	0.740346
C	-7.256567	-0.065580	0.337643
H	-7.385338	-0.390512	1.377391
H	-7.541010	0.990040	0.291864
H	-7.959431	-0.637668	-0.274298
C	2.879040	-2.380554	-1.242132
C	4.189137	-3.127649	-1.237928
C	1.667383	-3.278941	-1.328375
H	2.250901	-1.921715	0.780840
H	5.005263	-2.552946	-0.792794
H	4.087053	-4.058890	-0.670810

H	4.496196	-3.414214	-2.255296
H	0.757669	-2.751591	-1.610982
H	1.863394	-4.045064	-2.092309
H	1.469331	-3.826294	-0.398349

Vibrational frequencies

-22.8451	21.9104	26.1960
36.3054	45.5652	52.6708
64.4906	71.9944	83.3805
103.2780	107.3902	133.4966
155.8416	175.2675	194.6038
207.4198	239.0744	253.8208
268.3430	277.5681	296.4415
301.8914	308.1877	334.0437
359.2577	378.9422	384.2196
386.0115	421.3812	431.9014

M06-2x TS2S

Cartesian coordinates

C	-1.185474	-2.505013	2.024865
C	-1.496939	-1.403486	1.234174
C	-2.554630	-0.557530	1.559199
C	-3.289693	-0.826474	2.710704
C	-2.960573	-1.914862	3.525955
C	-1.908471	-2.762742	3.187660
C	-0.069749	-3.319213	1.421751
C	0.473729	-2.425053	0.282051
C	-0.595515	-1.325121	0.020141
H	-2.792343	0.296161	0.933500
H	-4.119771	-0.180367	2.979202
H	-3.535658	-2.104831	4.427027
H	-1.662639	-3.615719	3.814339

H	0.702201	-3.590467	2.148239
H	0.671494	-2.981070	-0.630779
H	-0.458134	-4.247288	0.989241
S	-2.174120	-2.844699	-1.652644
O	-1.371558	-4.010784	-1.288238
O	-2.576149	-2.634971	-3.039705
C	-3.653562	-2.890298	-0.672497
C	-3.745790	-3.795271	0.381101
C	-4.680582	-1.997178	-0.961499
C	-4.889801	-3.792249	1.167550
H	-2.931343	-4.484900	0.574938
C	-5.820059	-2.016173	-0.163692
H	-4.595419	-1.297426	-1.789900
C	-5.935278	-2.898445	0.913293
H	-4.969614	-4.488110	1.998108
H	-6.625478	-1.318733	-0.372910
C	-7.142640	-2.867337	1.812183
H	-7.985831	-2.369970	1.329042
H	-7.449325	-3.876175	2.098750
H	-6.912365	-2.319816	2.732464
N	-1.280491	-1.502400	-1.275518
H	-1.797080	-0.659091	-1.548191
S	2.130816	-1.774760	0.804049
C	3.187578	-2.426732	-0.459670
C	4.305926	-3.187822	-0.086476
C	2.928779	-2.111676	-1.808924
C	5.150649	-3.651176	-1.096207
C	3.772154	-2.617447	-2.801970
C	4.878146	-3.374050	-2.431534
H	6.017633	-4.246471	-0.828780

H	3.582826	-2.417144	-3.848381
H	5.536764	-3.756506	-3.204755
C	4.594881	-3.522763	1.353974
H	4.745178	-2.619444	1.952982
H	3.765439	-4.075865	1.804602
H	5.496810	-4.132794	1.424336
O	1.872064	-1.303442	-2.026174
C	1.605775	-0.830266	-3.361333
C	0.852863	0.474953	-3.200636
C	0.821992	-1.872566	-4.142316
H	2.570905	-0.624044	-3.842710
H	1.445213	1.195884	-2.630411
H	0.637068	0.905251	-4.182086
H	-0.094645	0.309935	-2.679698
H	-0.161314	-2.011311	-3.685825
H	0.685453	-1.535631	-5.173384
H	1.340214	-2.834891	-4.160662
H	-0.126526	-0.338593	-0.079431
O	-2.573882	1.092189	-1.278858
S	-3.783117	1.730465	-1.869653
O	-4.529552	0.862763	-2.777594
O	-3.556273	3.112517	-2.307636
C	-4.883481	1.940698	-0.417384
F	-4.292224	2.711352	0.495496
F	-6.024506	2.513986	-0.786424
F	-5.158778	0.767058	0.147201
S	2.344409	0.725996	0.675851
C	4.007506	0.459603	0.126452
C	4.343971	0.573797	-1.224311
C	4.965122	0.039727	1.054684

C	5.625936	0.240322	-1.640945
H	3.597634	0.906309	-1.940822
C	6.241769	-0.299485	0.622147
H	4.689513	-0.047733	2.103660
C	6.584388	-0.220834	-0.731236
H	5.882031	0.313946	-2.694175
H	6.977768	-0.646564	1.342250
C	7.939588	-0.666459	-1.209078
H	8.255725	-0.102132	-2.088996
H	7.904406	-1.725195	-1.488656
H	8.694753	-0.552407	-0.428705
C	2.437879	-0.682696	4.346659
C	2.973332	0.600671	4.311604
C	2.176740	1.694385	3.956859
C	0.829688	1.487493	3.664140
C	0.286091	0.203107	3.705271
C	1.091786	-0.883271	4.039167
H	3.065591	-1.526799	4.617182
H	4.022972	0.758171	4.554520
H	0.206761	2.332172	3.382794
H	-0.764807	0.052183	3.476326
H	0.666743	-1.882163	4.073427
C	2.798202	3.057186	3.787550
C	3.691863	3.108063	2.532788
H	2.021200	3.821236	3.700736
H	3.428300	3.306780	4.647036
C	2.948454	2.948268	1.280833
H	4.471815	2.338279	2.584450
H	4.202170	4.075672	2.468889
C	2.351611	3.059301	0.212998

C	1.712476	3.383502	-1.024879
C	2.483896	3.854324	-2.096147
C	0.326080	3.208089	-1.184989
C	1.881820	4.144883	-3.314239
H	3.553060	3.977421	-1.959158
C	-0.270100	3.511683	-2.407228
C	0.507547	3.972502	-3.466940
H	2.484520	4.501517	-4.142030
H	-1.341539	3.366914	-2.523214
H	0.033448	4.195414	-4.416911
S	-1.015317	3.643637	1.087261
O	0.113955	4.359803	1.667270
O	-1.835142	2.783826	1.930349
C	-2.050470	4.843234	0.272937
H	-1.411795	5.471942	-0.348050
H	-2.525639	5.435197	1.056157
H	-2.792462	4.321733	-0.333134
N	-0.442446	2.641273	-0.125502
H	-1.224625	2.065797	-0.472215

Vibrational frequencies

-229.2380	13.3033	20.3971
23.0609	28.6165	32.8561
33.8094	41.5077	44.4093
47.3127	49.0478	53.3344
55.6707	57.7964	60.0691
63.1254	65.1626	67.5814
69.9168	71.0665	73.1429
75.5302	78.2151	79.7278
83.1545	89.0780	90.9661
93.5891	98.4420	99.6486

M06-2x TS2R

Cartesian coordinates

C	-0.379886	3.346705	-0.104722
C	-0.881395	2.048106	-0.131697
C	-1.765845	1.632569	-1.124855
C	-2.138020	2.551046	-2.103885
C	-1.627258	3.853555	-2.088942
C	-0.748273	4.261811	-1.088326
C	0.531189	3.557713	1.077620
C	0.761698	2.127875	1.626554
C	-0.355897	1.229135	1.027264
H	-2.167129	0.621430	-1.117580
H	-2.831511	2.252242	-2.884037
H	-1.924920	4.554803	-2.862969
H	-0.352867	5.273580	-1.079902
H	1.463795	4.060160	0.806122
H	0.761287	2.081104	2.715526
H	0.036702	4.159020	1.845525
S	-2.391416	1.876669	2.757252
O	-1.609419	3.039628	3.170463
O	-3.101400	1.074984	3.748027
C	-3.577396	2.406894	1.549100
C	-3.501731	3.688408	1.014197
C	-4.507719	1.478346	1.094291
C	-4.372743	4.034689	-0.010199
H	-2.761942	4.388096	1.388329
C	-5.363585	1.839750	0.060600
H	-4.553073	0.488528	1.534528
C	-5.300726	3.114072	-0.510563
H	-4.318063	5.028983	-0.445110

H	-6.083971	1.116699	-0.310693
C	-6.189283	3.490596	-1.666201
H	-6.638684	4.475308	-1.514369
H	-5.606529	3.536579	-2.592428
H	-6.989436	2.761557	-1.807094
N	-1.351217	0.815699	2.030057
H	-1.883089	-0.002459	1.712140
S	2.472190	1.617195	1.125575
C	3.148329	0.879235	2.589101
C	4.380422	1.370669	3.051376
C	2.475060	-0.158767	3.260861
C	4.891068	0.854450	4.243347
C	2.990499	-0.630758	4.473028
C	4.189296	-0.114882	4.952406
H	5.836545	1.229704	4.620500
H	2.474077	-1.397590	5.034977
H	4.585070	-0.489326	5.890851
C	5.149875	2.421847	2.293761
H	5.385608	2.083221	1.279686
H	4.575153	3.347630	2.201059
H	6.086823	2.644169	2.806547
O	1.368216	-0.634316	2.662249
C	0.735428	-1.821822	3.187060
C	0.066129	-2.473173	1.995562
C	-0.231580	-1.467257	4.305553
H	1.524801	-2.485830	3.560757
H	0.800616	-2.723107	1.225403
H	-0.457580	-3.384570	2.294585
H	-0.665744	-1.783482	1.566542
H	-1.038851	-0.839945	3.921570

H	-0.661774	-2.383398	4.718533
H	0.269932	-0.927493	5.113069
H	0.057390	0.277802	0.680353
S	2.279528	0.122818	-0.891981
C	2.658737	1.578439	-1.852159
C	1.644170	2.300085	-2.482856
C	3.991309	1.985618	-1.970276
C	1.972973	3.421608	-3.237588
H	0.606844	1.991754	-2.382426
C	4.301555	3.112675	-2.720938
H	4.771264	1.424846	-1.460500
C	3.289091	3.843277	-3.369854
H	1.178049	3.984729	-3.719151
H	5.336072	3.433375	-2.803791
C	3.665756	5.056024	-4.186379
H	2.759481	5.455889	-4.641212
H	4.140494	5.785412	-3.530089
H	4.369143	4.748497	-4.960184
O	-2.714917	-3.572624	0.279617
S	-3.316852	-2.384065	0.915131
O	-2.755442	-1.115840	0.395470
O	-3.483392	-2.437671	2.364688
C	-5.030575	-2.384847	0.255659
F	-5.643323	-3.520535	0.570734
F	-5.729795	-1.369503	0.764547
F	-5.023624	-2.259298	-1.073159
C	5.780751	-1.292091	0.895700
C	5.685378	-1.600045	-0.457093
C	4.672295	-2.441617	-0.926661
C	3.749737	-2.968394	-0.021581

C	3.848856	-2.665318	1.336208
C	4.865619	-1.833838	1.797511
H	6.572610	-0.640023	1.253423
H	6.405642	-1.186204	-1.160471
H	2.950888	-3.616459	-0.377068
H	3.134227	-3.089775	2.036505
H	4.945926	-1.601410	2.854147
C	4.540895	-2.697121	-2.405620
C	4.028575	-1.446512	-3.141221
H	3.849898	-3.523578	-2.593846
H	5.511982	-2.959166	-2.837412
C	2.640129	-1.117905	-2.793156
H	4.668145	-0.581645	-2.930958
H	4.044405	-1.607777	-4.224262
C	1.412148	-1.048521	-2.841883
C	0.007533	-0.977315	-3.068652
C	-0.482362	-0.129290	-4.073623
C	-0.883419	-1.779203	-2.333134
C	-1.844735	-0.075057	-4.334789
H	0.218061	0.479854	-4.635403
C	-2.246472	-1.723649	-2.610324
C	-2.724911	-0.869265	-3.600415
H	-2.219766	0.585943	-5.108300
H	-2.922208	-2.348958	-2.037990
H	-3.790864	-0.830651	-3.799477
S	0.194177	-4.126916	-1.674773
O	1.091638	-3.982705	-2.814113
O	0.689036	-4.693561	-0.427322
C	-1.231378	-5.057873	-2.191409
H	-1.642237	-4.587613	-3.085693

H	-0.890394	-6.069698	-2.412890
H	-1.951696	-5.048540	-1.372248
N	-0.383775	-2.599944	-1.282635
H	-1.065451	-2.706904	-0.522655

Vibrational frequencies

-237.2933	16.2742	19.7756
22.9963	29.0988	29.9020
33.3946	36.5893	40.7900
43.1896	45.4761	48.7175
49.7909	53.7111	56.5570
58.6538	59.6519	65.5191
69.9505	71.8713	73.8356
75.2782	79.7712	81.9682
82.6099	86.6221	90.4620
95.4533	100.7955	103.0842

ω B97X-D TS2S

Cartesian coordinates

C	-1.184706	-2.694440	1.919038
C	-1.508176	-1.539194	1.218903
C	-2.563576	-0.725486	1.615426
C	-3.296652	-1.089005	2.740620
C	-2.967335	-2.242871	3.456915
C	-1.909156	-3.053753	3.051480
C	-0.049872	-3.433021	1.260626
C	0.466839	-2.454731	0.177238
C	-0.617861	-1.352661	0.011572
H	-2.806907	0.170764	1.057297
H	-4.126291	-0.469958	3.064750
H	-3.542088	-2.511052	4.337967
H	-1.660899	-3.953960	3.605967

H	0.729644	-3.724797	1.969689
H	0.642952	-2.947724	-0.773395
H	-0.409109	-4.345474	0.775542
S	-2.181766	-2.723453	-1.813333
O	-1.370154	-3.914718	-1.575069
O	-2.581038	-2.373258	-3.170749
C	-3.661930	-2.878053	-0.842854
C	-3.744863	-3.867742	0.131991
C	-4.702095	-1.979051	-1.050970
C	-4.886061	-3.943706	0.917617
H	-2.926612	-4.564587	0.269275
C	-5.838170	-2.075437	-0.257680
H	-4.629282	-1.210450	-1.814532
C	-5.942032	-3.044637	0.742838
H	-4.952510	-4.708028	1.685930
H	-6.650325	-1.371782	-0.409592
C	-7.149687	-3.103368	1.640115
H	-8.014171	-2.619530	1.180957
H	-7.417176	-4.136291	1.877925
H	-6.943520	-2.591526	2.586532
N	-1.307952	-1.416251	-1.289157
H	-1.823601	-0.550292	-1.477623
S	2.134824	-1.830021	0.694340
C	3.193116	-2.433030	-0.591354
C	4.312310	-3.202690	-0.239362
C	2.949921	-2.059616	-1.929534
C	5.174326	-3.610207	-1.257108
C	3.812484	-2.511078	-2.930899
C	4.919493	-3.273390	-2.580800
H	6.045314	-4.207903	-1.007329

H	3.636606	-2.267573	-3.970347
H	5.593114	-3.611666	-3.360591
C	4.598766	-3.592955	1.187663
H	4.794739	-2.714054	1.809107
H	3.753894	-4.124002	1.633910
H	5.476282	-4.240466	1.234187
O	1.890768	-1.257156	-2.126356
C	1.632037	-0.692510	-3.427184
C	0.888038	0.604110	-3.177992
C	0.841792	-1.670631	-4.282724
H	2.597659	-0.461513	-3.893174
H	1.474793	1.270973	-2.542759
H	0.696321	1.111636	-4.126578
H	-0.068812	0.411377	-2.688696
H	-0.142224	-1.841495	-3.841469
H	0.706714	-1.254554	-5.284632
H	1.356138	-2.631363	-4.378718
H	-0.165432	-0.356475	-0.002366
O	-2.543071	1.204207	-1.100548
S	-3.716547	1.823695	-1.776848
O	-4.374209	0.942194	-2.739788
O	-3.476967	3.205843	-2.207082
C	-4.941887	2.017799	-0.407212
F	-4.488492	2.879202	0.505580
F	-6.094586	2.477893	-0.889575
F	-5.168961	0.852941	0.200939
S	2.360767	0.657098	0.707426
C	4.029270	0.450452	0.157763
C	4.370011	0.649097	-1.182057
C	4.996216	0.011985	1.065937

C	5.661152	0.380453	-1.609262
H	3.621092	0.994257	-1.886671
C	6.284493	-0.262144	0.622386
H	4.726182	-0.141482	2.106797
C	6.630149	-0.100805	-0.721565
H	5.917128	0.522498	-2.655008
H	7.025892	-0.622935	1.328470
C	7.998731	-0.476155	-1.220111
H	8.349910	0.223711	-1.983688
H	7.967559	-1.471778	-1.676068
H	8.730444	-0.502239	-0.409840
C	2.444013	-0.991475	4.505109
C	2.911507	0.316377	4.438423
C	2.056516	1.365764	4.088440
C	0.716563	1.082660	3.824644
C	0.240135	-0.224506	3.904060
C	1.102991	-1.264647	4.236699
H	3.121909	-1.796910	4.772236
H	3.957236	0.525831	4.657610
H	0.039472	1.883540	3.542595
H	-0.805663	-0.428606	3.705141
H	0.726640	-2.282558	4.290976
C	2.596176	2.767853	3.947413
C	3.546630	2.924060	2.744005
H	1.776753	3.483348	3.841519
H	3.163754	3.044094	4.841452
C	2.875723	2.818322	1.444616
H	4.356169	2.187730	2.791356
H	4.016049	3.913151	2.769802
C	2.328411	3.070093	0.376098

C	1.735829	3.458781	-0.859422
C	2.549656	3.914037	-1.905747
C	0.344102	3.359949	-1.046314
C	1.985553	4.260575	-3.126630
H	3.619767	3.983966	-1.749513
C	-0.209858	3.709661	-2.274821
C	0.608658	4.152414	-3.309491
H	2.620044	4.608434	-3.933720
H	-1.283283	3.615377	-2.414675
H	0.165285	4.415560	-4.263792
S	-1.020606	3.845422	1.205693
O	0.118338	4.561609	1.764103
O	-1.839815	3.001915	2.067219
C	-2.064058	5.042416	0.395487
H	-1.444304	5.635789	-0.276043
H	-2.494209	5.675397	1.172639
H	-2.841836	4.519421	-0.160364
N	-0.469806	2.833109	-0.004423
H	-1.243887	2.245734	-0.348296

Vibrational frequencies

-271.5529	19.8570	23.3317
27.3532	28.7922	33.0265
36.5717	41.0177	43.0532
44.3843	47.6509	49.8800
53.6338	57.2183	58.9571
60.9531	63.2685	68.8538
71.2533	71.9000	74.0614
77.6040	82.1971	86.5415
89.3441	91.0260	95.6995
99.4632	106.9235	108.6022

ωB97X-D TS2R

Cartesian coordinates

C	-0.607391	3.427721	-0.126845
C	-1.071992	2.118614	-0.116928
C	-1.956771	1.655293	-1.084175
C	-2.391397	2.542709	-2.062691
C	-1.940009	3.865303	-2.069906
C	-1.045273	4.317223	-1.103544
C	0.387475	3.668344	0.977836
C	0.592303	2.273240	1.623917
C	-0.501292	1.334843	1.039060
H	-2.313837	0.630017	-1.056282
H	-3.090029	2.206633	-2.821507
H	-2.289855	4.547766	-2.838248
H	-0.682950	5.340658	-1.123752
H	1.320404	4.092483	0.593613
H	0.517248	2.311033	2.710084
H	-0.006626	4.361401	1.725601
S	-2.570651	1.923593	2.746313
O	-1.881855	3.173936	3.052541
O	-3.191175	1.149089	3.814520
C	-3.824031	2.261799	1.532389
C	-3.949092	3.534807	0.990514
C	-4.621584	1.208855	1.094794
C	-4.887306	3.747663	-0.011300
H	-3.304616	4.335285	1.334172
C	-5.544115	1.436130	0.084017
H	-4.510574	0.219398	1.521234
C	-5.686689	2.704517	-0.486923
H	-4.987585	4.738016	-0.445265

H	-6.156102	0.611728	-0.268514
C	-6.654902	2.938067	-1.616370
H	-7.135625	3.916039	-1.531416
H	-6.130957	2.912391	-2.578222
H	-7.432541	2.171446	-1.641039
N	-1.465277	0.901957	2.060070
H	-1.907584	0.008102	1.828160
S	2.331867	1.727526	1.314169
C	2.783958	0.765046	2.738393
C	3.803040	1.275419	3.562879
C	2.161184	-0.467647	3.017762
C	4.154975	0.550804	4.700805
C	2.550900	-1.177058	4.157323
C	3.530053	-0.656712	4.990303
H	4.926620	0.935099	5.359355
H	2.105827	-2.133221	4.387982
H	3.818849	-1.214025	5.875507
C	4.513468	2.569046	3.254400
H	5.025392	2.519149	2.288644
H	3.816512	3.410696	3.210288
H	5.258422	2.782925	4.022888
O	1.245783	-0.874713	2.127867
C	0.292393	-1.941988	2.363351
C	-0.478261	-1.807441	3.672181
C	0.904086	-3.313635	2.132262
H	-0.411426	-1.758481	1.549104
H	-0.700477	-0.758823	3.879072
H	-1.428547	-2.334788	3.552298
H	0.041051	-2.241388	4.528656
H	1.597024	-3.608095	2.924898

H	0.096879	-4.051584	2.104111
H	1.419303	-3.347371	1.170596
H	-0.057213	0.401976	0.692099
S	2.325279	0.378544	-0.771555
C	2.644620	1.894980	-1.654885
C	1.612325	2.555187	-2.321972
C	3.939882	2.417972	-1.679565
C	1.881601	3.730683	-3.010585
H	0.603158	2.158768	-2.293423
C	4.192682	3.598879	-2.365740
H	4.738140	1.907913	-1.147764
C	3.170432	4.271315	-3.043478
H	1.067824	4.243404	-3.515075
H	5.198690	4.007659	-2.372298
C	3.454140	5.537839	-3.806532
H	2.610390	6.230543	-3.753767
H	4.341954	6.043972	-3.420710
H	3.631474	5.317248	-4.864620
O	-2.412945	-3.700557	-0.068985
S	-3.102582	-2.775561	0.855070
O	-2.610021	-1.387075	0.747882
O	-3.295068	-3.280377	2.212002
C	-4.809835	-2.654275	0.158715
F	-5.354440	-3.861787	0.035774
F	-5.584188	-1.918828	0.961462
F	-4.789850	-2.071852	-1.044008
C	6.057151	-0.753708	1.032907
C	5.938037	-0.985564	-0.332931
C	5.041218	-1.940911	-0.820669
C	4.269062	-2.667234	0.085448

C	4.399089	-2.446831	1.454565
C	5.289163	-1.490657	1.931620
H	6.754992	-0.006024	1.397701
H	6.548964	-0.416989	-1.030812
H	3.556490	-3.402506	-0.281018
H	3.795796	-3.018536	2.151468
H	5.374334	-1.311215	2.997822
C	4.893796	-2.145530	-2.307532
C	4.244605	-0.941846	-3.011121
H	4.298593	-3.039122	-2.514159
H	5.877626	-2.293914	-2.764803
C	2.825653	-0.755082	-2.671571
H	4.791471	-0.020567	-2.784411
H	4.286586	-1.081039	-4.096095
C	1.605882	-0.830875	-2.817009
C	0.210475	-0.852295	-3.075606
C	-0.321130	0.048304	-4.011198
C	-0.636357	-1.773729	-2.430679
C	-1.679691	0.048685	-4.287292
H	0.346048	0.744013	-4.507749
C	-1.999686	-1.757050	-2.710717
C	-2.517571	-0.846173	-3.626248
H	-2.084331	0.750545	-5.007423
H	-2.648299	-2.459632	-2.202421
H	-3.583490	-0.844682	-3.827308
S	0.634199	-4.086854	-2.047530
O	1.414409	-3.744110	-3.228353
O	1.287969	-4.699621	-0.899852
C	-0.723689	-5.129467	-2.544055
H	-1.253812	-4.637092	-3.360099

H	-0.303780	-6.078001	-2.879758
H	-1.380195	-5.269978	-1.684771
N	-0.097224	-2.682272	-1.479044
H	-0.791877	-2.944848	-0.767557

Vibrational frequencies

-294.0920	14.9140	25.4319
27.4509	28.9416	31.6782
33.9423	35.8784	39.3923
42.2880	43.3339	44.3018
47.1381	48.0451	54.0439
56.7237	57.8230	59.3107
62.5953	64.4793	68.2763
70.2830	78.1914	80.2454
81.0285	86.3819	88.2655
96.5741	100.4894	102.0888

TS2S($\Phi_1=-60^\circ/\Phi_2=9^\circ$)

Cartesian coordinates

C	2.698445	1.506056	2.195106
C	2.309371	0.497678	1.306940
C	2.443687	-0.847074	1.637943
C	2.978089	-1.179903	2.884572
C	3.374970	-0.175537	3.775074
C	3.240326	1.175027	3.435641
C	2.472340	2.868086	1.578649
C	1.521306	2.561446	0.394403
C	1.816283	1.089655	0.000597
H	2.173511	-1.614111	0.923870
H	3.102024	-2.224660	3.150918
H	3.793868	-0.446933	4.739839
H	3.554921	1.950526	4.128135

H	2.067186	3.606343	2.275352
H	1.601501	3.251497	-0.440068
H	3.405712	3.278061	1.181171
S	4.187655	1.756683	-1.361102
O	3.898218	3.201778	-1.306348
O	4.747335	1.175336	-2.590643
C	5.283051	1.375106	0.002983
C	5.893100	2.403922	0.718929
C	5.491348	0.035676	0.338620
C	6.699723	2.080175	1.809895
H	5.727533	3.435966	0.431328
C	6.293189	-0.266604	1.431827
H	5.024240	-0.758372	-0.228603
C	6.898177	0.746835	2.191407
H	7.171615	2.876792	2.377996
H	6.434806	-1.307237	1.706698
C	7.707838	0.398204	3.414880
H	8.343368	-0.474649	3.237017
H	8.343051	1.229702	3.731191
H	7.042975	0.149117	4.251132
N	2.759687	0.936281	-1.134469
H	2.899264	-0.057967	-1.365780
S	-0.210558	2.719901	1.076885
C	-1.152866	3.666491	-0.089846
C	-2.038427	4.632365	0.445348
C	-1.109032	3.413873	-1.484345
C	-2.840107	5.362989	-0.434606
C	-1.902755	4.192932	-2.338163
C	-2.762656	5.149565	-1.809252
H	-3.519709	6.109704	-0.036959

H	-1.865675	4.047807	-3.408606
H	-3.380530	5.734557	-2.483584
C	-2.146758	4.882501	1.931380
H	-2.507043	3.996134	2.466283
H	-1.178390	5.145238	2.368019
H	-2.845638	5.697784	2.129809
O	-0.303555	2.408930	-1.900805
C	-0.046914	2.229214	-3.326728
C	0.410761	0.794474	-3.516790
C	0.988107	3.255960	-3.772907
H	-0.992431	2.361072	-3.863280
H	-0.337976	0.095337	-3.144261
H	0.557990	0.603510	-4.584139
H	1.353803	0.620608	-2.998688
H	1.908534	3.123886	-3.196846
H	1.214385	3.125519	-4.835140
H	0.626417	4.277035	-3.621804
H	0.911405	0.601316	-0.364499
O	2.880564	-1.868107	-1.416389
S	3.841454	-2.989215	-1.643108
O	5.233191	-2.554956	-1.884559
O	3.325972	-4.069874	-2.504188
C	3.929075	-3.776346	0.050613
F	2.693829	-3.978323	0.559491
F	4.553258	-4.960219	-0.003704
F	4.598196	-2.987332	0.913531
S	-1.468270	0.394181	1.383950
C	-2.560323	0.713587	0.028892
C	-2.404648	0.043073	-1.192643
C	-3.589728	1.654721	0.183173

C	-3.269246	0.319798	-2.242666
H	-1.621633	-0.695833	-1.308516
C	-4.437802	1.938441	-0.885007
H	-3.720826	2.159861	1.133270
C	-4.286809	1.282098	-2.114906
H	-3.148342	-0.216514	-3.178557
H	-5.217270	2.684594	-0.764091
C	-5.164479	1.626718	-3.290370
H	-5.377225	0.746157	-3.903098
H	-4.660592	2.358434	-3.933675
H	-6.112483	2.068135	-2.971675
C	-0.055426	-2.617946	-2.569788
C	-0.083819	-3.006282	-1.230849
C	-1.276015	-3.442593	-0.635812
C	-2.437969	-3.487152	-1.412162
C	-2.417055	-3.092678	-2.752305
C	-1.226369	-2.655752	-3.335539
H	0.886989	-2.294710	-2.997516
H	0.838814	-2.980436	-0.663594
H	-3.364497	-3.825964	-0.967400
H	-3.337441	-3.119752	-3.327845
H	-1.206174	-2.347997	-4.377137
C	-1.297565	-3.854504	0.819455
C	-0.986350	-2.697509	1.798858
H	-2.267954	-4.287966	1.076251
H	-0.534634	-4.622018	0.996569
C	-2.061104	-1.681075	1.885763
H	-0.048014	-2.210593	1.525149
H	-0.852703	-3.100550	2.809531
C	-3.204898	-1.313099	2.205989

C	-4.411232	-0.688500	2.574846
C	-4.533344	-0.148840	3.875823
C	-5.460550	-0.489341	1.639378
C	-5.649317	0.597572	4.226307
H	-3.726982	-0.306815	4.583073
C	-6.572719	0.269587	2.006950
C	-6.662663	0.818624	3.286275
H	-5.729001	1.016723	5.223321
H	-7.366463	0.431054	1.284550
H	-7.531951	1.410313	3.553687
S	-5.762373	-2.651190	0.048035
O	-4.984551	-3.471130	0.983096
O	-5.633996	-2.822388	-1.402381
C	-7.498433	-2.816101	0.498414
H	-7.615377	-2.525667	1.542978
H	-7.763886	-3.865269	0.361088
H	-8.090419	-2.177880	-0.158019
N	-5.350579	-1.038486	0.334614
H	-5.656713	-0.438753	-0.428033

Vibrational frequencies

-176.1713	15.7344	18.4209
25.5071	28.4895	30.1851
34.4282	36.0575	39.2145
43.1078	43.7118	46.0009
49.0406	51.6273	55.0484
58.1845	60.4066	61.9752
63.5926	67.0682	69.9935
71.2872	73.1668	74.5734
76.3745	79.5376	79.7606
84.2436	87.4892	89.8670

TS2S($\Phi 1=-118^\circ/\Phi 2=-62^\circ$)

Cartesian coordinates

C	-2.524890	0.841932	-2.668094
C	-2.424118	0.379128	-1.351228
C	-2.732819	-0.939414	-1.025162
C	-3.164195	-1.793442	-2.041612
C	-3.268128	-1.336092	-3.360994
C	-2.945325	-0.015356	-3.684515
C	-2.143951	2.301418	-2.756678
C	-1.402016	2.542958	-1.419001
C	-1.953553	1.483611	-0.421437
H	-2.636534	-1.285885	-0.004821
H	-3.414724	-2.822112	-1.805556
H	-3.599890	-2.015425	-4.141225
H	-3.020727	0.336426	-4.709737
H	-1.538061	2.543459	-3.634035
H	-1.474209	3.555495	-1.029607
H	-3.037834	2.930254	-2.780088
S	-4.503681	2.474708	0.141207
O	-4.454584	3.324361	-1.060293
O	-5.061543	3.011995	1.391345
C	-5.410462	0.985100	-0.267406
C	-5.847675	0.778166	-1.574598
C	-5.609591	0.023976	0.726326
C	-6.487879	-0.417664	-1.889595
H	-5.670817	1.535066	-2.329109
C	-6.246644	-1.166481	0.389316
H	-5.246870	0.188881	1.734547
C	-6.686512	-1.409838	-0.919893
H	-6.823044	-0.589405	-2.908439

H	-6.381737	-1.926845	1.152493
C	-7.312199	-2.731310	-1.290984
H	-7.789062	-3.207466	-0.429903
H	-8.060679	-2.614369	-2.080058
H	-6.547309	-3.422072	-1.667356
N	-2.941690	2.038237	0.531233
H	-2.969930	1.514879	1.416473
S	0.410640	2.220653	-1.766563
C	1.267451	3.668493	-1.202921
C	2.211133	4.263633	-2.068097
C	1.079934	4.147096	0.117171
C	2.907385	5.387436	-1.612872
C	1.771726	5.294341	0.530398
C	2.676081	5.900542	-0.337951
H	3.631623	5.862577	-2.266520
H	1.616695	5.708949	1.517145
H	3.212210	6.784779	-0.007024
C	2.507942	3.698994	-3.436327
H	2.957345	2.702672	-3.357339
H	1.601623	3.599016	-4.040936
H	3.209721	4.342640	-3.971009
O	0.247235	3.422304	0.897366
C	0.030148	3.792692	2.289821
C	-0.309296	2.508055	3.025333
C	-1.078113	4.836494	2.361466
H	0.970193	4.189713	2.688303
H	0.455674	1.747045	2.855416
H	-0.375576	2.706493	4.098857
H	-1.270391	2.116374	2.696159
H	-2.001921	4.415112	1.954905

H	-1.252600	5.128128	3.401361
H	-0.818824	5.732788	1.790925
H	-1.173698	1.134800	0.253682
O	-1.289760	-0.709350	1.967614
S	-2.206267	-0.581032	3.126681
O	-3.228742	0.494512	2.966854
O	-1.576193	-0.650141	4.458902
C	-3.236850	-2.137564	3.047753
F	-2.480866	-3.220263	3.320789
F	-4.244155	-2.092203	3.928491
F	-3.763257	-2.311132	1.818670
S	1.224768	0.247111	-0.310573
C	2.840207	0.573489	-0.989662
C	3.618751	1.602888	-0.437802
C	3.346323	-0.188386	-2.051669
C	4.879851	1.874546	-0.962522
H	3.228166	2.195820	0.381430
C	4.623134	0.069166	-2.540459
H	2.756414	-0.996977	-2.463371
C	5.408117	1.106054	-2.010289
H	5.465549	2.688866	-0.545662
H	5.015560	-0.551117	-3.340481
C	6.802924	1.361907	-2.521448
H	7.537485	0.823624	-1.910000
H	7.056967	2.424746	-2.474762
H	6.921721	1.020560	-3.553175
C	7.539493	0.472326	2.735758
C	6.499036	0.074298	1.893872
C	5.729643	-1.058581	2.191006
C	6.024944	-1.783823	3.354121

C	7.063312	-1.388820	4.198864
C	7.824508	-0.257840	3.891726
H	8.128710	1.350682	2.487469
H	6.279778	0.643033	0.994672
H	5.437938	-2.667053	3.594827
H	7.280656	-1.965003	5.093716
H	8.634531	0.049367	4.546728
C	4.580230	-1.469276	1.300740
C	3.230567	-0.940358	1.852207
H	4.722621	-1.081509	0.288920
H	4.518094	-2.557397	1.214879
C	2.095384	-1.351455	0.997637
H	3.265824	0.148642	1.936582
H	3.055550	-1.336066	2.859031
C	1.397599	-2.233024	0.470267
C	0.450657	-3.125627	-0.065343
C	-0.655225	-3.482539	0.736045
C	0.549835	-3.646864	-1.382731
C	-1.646226	-4.320862	0.243619
H	-0.728084	-3.058287	1.726308
C	-0.459819	-4.477188	-1.867588
C	-1.551750	-4.810364	-1.061569
H	-2.498126	-4.564323	0.867839
H	-0.393662	-4.860959	-2.880826
H	-2.327816	-5.456474	-1.459129
S	3.166316	-3.994297	-2.042035
O	3.478297	-4.022378	-0.611623
O	4.026658	-3.289614	-2.997233
C	2.951208	-5.695149	-2.595611
H	2.164106	-6.153681	-1.995689

H	3.902090	-6.205728	-2.435292
H	2.690379	-5.688200	-3.654244
N	1.636722	-3.261371	-2.215815
H	1.403104	-3.196563	-3.204005

Vibrational frequencies

-194.4574	9.1709	10.9671
16.7865	17.7251	20.0713
22.3663	26.7558	29.7757
32.4360	35.1452	36.5740
38.5384	40.8891	42.9437
46.0792	48.8803	50.1507
50.6006	54.7820	57.0794
59.0588	60.6231	68.0924
68.3310	70.8331	72.7467
78.7727	79.6802	81.4507

TS2S($\Phi1=92^\circ/\Phi2=-134^\circ$)

Cartesian coordinates

C	3.600651	0.782749	-2.120144
C	3.251471	0.175817	-0.910749
C	3.887883	0.523547	0.278476
C	4.871673	1.513585	0.250951
C	5.208177	2.141865	-0.955472
C	4.579258	1.776251	-2.149236
C	2.810413	0.190422	-3.263595
C	1.634815	-0.519682	-2.546860
C	2.135257	-0.830735	-1.105653
H	3.643142	0.022950	1.206817
H	5.374964	1.793155	1.171370
H	5.968926	2.916623	-0.964156
H	4.847985	2.260552	-3.083355

H	2.482360	0.929350	-3.998997
H	1.266712	-1.409939	-3.054097
H	3.407838	-0.560561	-3.789772
S	3.810883	-3.037848	-1.517003
O	3.844362	-2.749982	-2.957304
O	3.679990	-4.416522	-1.025359
C	5.264054	-2.316237	-0.768217
C	6.104769	-1.508228	-1.532194
C	5.487569	-2.509474	0.597256
C	7.177037	-0.873826	-0.910290
H	5.907317	-1.368403	-2.587933
C	6.561245	-1.863583	1.200870
H	4.830036	-3.140121	1.185928
C	7.412602	-1.028162	0.462425
H	7.828339	-0.233518	-1.497576
H	6.726228	-1.993696	2.265248
C	8.524025	-0.270458	1.143275
H	8.896209	-0.804606	2.021675
H	9.362390	-0.089572	0.465023
H	8.159970	0.707184	1.482831
N	2.462509	-2.256947	-0.895282
H	2.312682	-2.567257	0.059465
S	0.210855	0.698225	-2.539154
C	-1.256447	-0.245948	-2.884814
C	-2.036262	0.142806	-3.996734
C	-1.675855	-1.287604	-2.024521
C	-3.228206	-0.546256	-4.239068
C	-2.870724	-1.959797	-2.302155
C	-3.636574	-1.579211	-3.398394
H	-3.841007	-0.262312	-5.088490

H	-3.229054	-2.746147	-1.655842
H	-4.577182	-2.088758	-3.577668
C	-1.622633	1.272126	-4.911792
H	-1.569381	2.225951	-4.376179
H	-0.634727	1.095364	-5.349035
H	-2.341295	1.384225	-5.726517
O	-0.879650	-1.551161	-0.957736
C	-1.236427	-2.619083	-0.029994
C	-0.506741	-2.306536	1.262379
C	-0.844170	-3.968511	-0.622359
H	-2.310374	-2.561504	0.168945
H	-0.749514	-1.298762	1.596098
H	-0.821656	-3.001661	2.042711
H	0.575593	-2.398444	1.136826
H	0.231920	-3.988280	-0.819210
H	-1.089522	-4.768248	0.082675
H	-1.368812	-4.167302	-1.559898
H	1.327433	-0.666540	-0.395443
O	-5.017482	-0.368569	-0.604134
S	-6.315780	-1.016269	-0.259941
O	-7.360342	-0.907308	-1.296296
O	-6.757114	-0.755052	1.133023
C	-5.881791	-2.829313	-0.251189
F	-4.783552	-3.052467	0.491280
F	-6.887910	-3.558323	0.252016
F	-5.632275	-3.267215	-1.501795
S	-0.149861	1.545829	-0.126939
C	0.390558	3.168004	-0.624196
C	-0.553101	4.102581	-1.077061
C	1.748722	3.512570	-0.573191

C	-0.134612	5.373879	-1.459609
H	-1.602948	3.832729	-1.120461
C	2.151298	4.785900	-0.966239
H	2.482896	2.788646	-0.240863
C	1.221029	5.736119	-1.413591
H	-0.869673	6.096315	-1.803338
H	3.206343	5.042153	-0.928620
C	1.668954	7.102478	-1.867996
H	0.902170	7.858553	-1.677329
H	1.866686	7.103293	-2.946899
H	2.590841	7.409146	-1.366389
C	4.884597	0.085643	4.429177
C	3.674658	0.593269	3.943892
C	2.669215	-0.267691	3.487570
C	2.905119	-1.651988	3.532893
C	4.107225	-2.160851	4.020433
C	5.104849	-1.290507	4.471414
H	5.652642	0.771195	4.774902
H	3.529949	1.668463	3.920467
H	2.133423	-2.333583	3.183335
H	4.267096	-3.234813	4.047729
H	6.042900	-1.683736	4.851588
C	1.354396	0.212686	2.906404
C	1.210317	1.731386	2.726097
H	1.230690	-0.250198	1.923723
H	0.515641	-0.148353	3.512507
C	-0.066359	2.062170	2.073328
H	2.035560	2.128761	2.124817
H	1.231799	2.246419	3.693344
C	-1.259410	2.379027	1.982670

C	-2.584524	2.804095	1.759598
C	-2.866155	4.186870	1.709488
C	-3.618829	1.866699	1.506932
C	-4.147858	4.630254	1.409363
H	-2.062942	4.891143	1.895053
C	-4.900699	2.330492	1.203264
C	-5.160790	3.700674	1.150697
H	-4.357353	5.693775	1.369676
H	-5.682281	1.605406	1.008506
H	-6.163010	4.042647	0.913045
S	-3.306791	-0.373116	2.958932
O	-2.270626	0.229185	3.810998
O	-3.218631	-1.788962	2.581749
C	-4.907066	-0.086482	3.728113
H	-5.013436	0.982191	3.917564
H	-4.913172	-0.644998	4.665341
H	-5.673127	-0.443582	3.037371
N	-3.335490	0.472295	1.493200
H	-3.916267	-0.031645	0.800768

Vibrational frequencies

-208.7289	9.8040	16.3933
18.6298	22.6609	24.2708
28.7954	29.5248	31.0377
33.9400	37.4359	40.5844
42.0643	46.0261	50.9054
53.4056	55.4598	57.7727
58.6966	60.1578	65.2668
66.9986	73.2666	74.5162
77.6294	81.5287	84.8307
85.6501	88.4016	90.3500

TS2S($\Phi_1=57^\circ/\Phi_2=48^\circ$)

Cartesian coordinates

C	-0.756358	3.038347	1.603179
C	0.304950	2.174546	1.326416
C	1.588658	2.431019	1.807477
C	1.799035	3.583235	2.567656
C	0.740299	4.459213	2.837883
C	-0.544863	4.192066	2.357210
C	-2.031330	2.558000	0.955461
C	-1.699329	1.121502	0.479394
C	-0.147707	1.001673	0.479825
H	2.409901	1.763174	1.575091
H	2.793391	3.801604	2.945466
H	0.918236	5.353419	3.428231
H	-1.364242	4.873844	2.566928
H	-2.901084	2.595863	1.617474
H	-2.125775	0.888766	-0.487795
H	-2.272548	3.179660	0.086671
S	0.052206	1.908041	-2.177480
O	-1.369690	1.706502	-2.514240
O	1.082602	1.589228	-3.179202
C	0.236663	3.608826	-1.660703
C	-0.851916	4.476594	-1.736614
C	1.468767	4.026022	-1.149819
C	-0.710805	5.777654	-1.254924
H	-1.789931	4.131011	-2.155920
C	1.586824	5.326076	-0.674252
H	2.316312	3.350124	-1.105749
C	0.499640	6.214323	-0.701567
H	-1.556880	6.457347	-1.300076

H	2.535190	5.652202	-0.257730
C	0.632822	7.593282	-0.107107
H	1.587409	8.054328	-0.378400
H	-0.175437	8.254231	-0.430446
H	0.601075	7.535773	0.987834
N	0.429609	0.916004	-0.886656
H	1.449831	0.804324	-0.850492
S	-2.364183	-0.138592	1.668889
C	-4.126047	0.142230	1.703428
C	-4.743237	0.133409	2.977085
C	-4.892537	0.351118	0.527078
C	-6.117317	0.377474	3.054314
C	-6.264406	0.610053	0.647481
C	-6.863101	0.623218	1.903320
H	-6.600243	0.381431	4.026178
H	-6.863837	0.775871	-0.234807
H	-7.928738	0.816720	1.979532
C	-3.959290	-0.122499	4.241892
H	-3.484994	-1.108409	4.228688
H	-3.153989	0.607503	4.371682
H	-4.614119	-0.072059	5.114540
O	-4.230302	0.244967	-0.647096
C	-4.642173	0.871122	-1.901445
C	-4.867357	2.371133	-1.750883
C	-5.787620	0.121077	-2.580367
H	-3.739231	0.723097	-2.495922
H	-3.983572	2.844313	-1.317657
H	-5.034551	2.804422	-2.741421
H	-5.733144	2.606492	-1.127711
H	-6.772397	0.391704	-2.192356

H	-5.779358	0.357170	-3.648942
H	-5.645804	-0.955379	-2.464959
H	0.177187	0.057300	0.925988
O	3.181497	0.569843	-0.317327
S	4.484951	1.113415	-0.835644
O	4.438098	2.540030	-1.200649
O	5.159328	0.200726	-1.783115
C	5.530897	1.039584	0.701686
F	5.654276	-0.233787	1.108231
F	6.750900	1.537707	0.467246
F	4.958847	1.749393	1.688157
S	-1.389350	-2.306919	0.637643
C	-2.252540	-2.355930	-0.905970
C	-1.835511	-1.520633	-1.952307
C	-3.317091	-3.250862	-1.111352
C	-2.478158	-1.578119	-3.186120
H	-1.008498	-0.838804	-1.799774
C	-3.932741	-3.314423	-2.355249
H	-3.641415	-3.897364	-0.302474
C	-3.524082	-2.479869	-3.413081
H	-2.144429	-0.921745	-3.983831
H	-4.744009	-4.019134	-2.516370
C	-4.218575	-2.545344	-4.749420
H	-3.607775	-2.102549	-5.540334
H	-5.167512	-1.996860	-4.718063
H	-4.451108	-3.577900	-5.027042
C	-0.859957	-1.833502	4.949319
C	-0.575418	-3.080906	4.391825
C	0.416670	-3.221544	3.410197
C	1.115392	-2.078622	2.996291

C	0.827387	-0.827896	3.548578
C	-0.161280	-0.700227	4.525115
H	-1.620740	-1.747656	5.719533
H	-1.120119	-3.959217	4.730697
H	1.893746	-2.169497	2.248119
H	1.378494	0.047386	3.218609
H	-0.384892	0.272992	4.951623
C	0.717900	-4.581331	2.815005
C	-0.279912	-5.028348	1.712499
H	1.726492	-4.596308	2.392372
H	0.680968	-5.342715	3.602205
C	-0.164016	-4.204133	0.490265
H	-1.304697	-4.992269	2.092739
H	-0.065140	-6.065600	1.432078
C	0.421539	-3.900153	-0.562063
C	0.937304	-3.327634	-1.732817
C	0.329491	-3.573414	-2.983577
C	1.993026	-2.377752	-1.640785
C	0.724980	-2.854479	-4.103740
H	-0.476197	-4.296208	-3.041281
C	2.362456	-1.647593	-2.769077
C	1.720242	-1.878258	-3.988148
H	0.241220	-3.030959	-5.058088
H	3.148180	-0.905076	-2.685902
H	2.010993	-1.295687	-4.855973
S	3.755793	-3.259573	0.185247
O	3.216164	-4.612159	-0.011419
O	4.110713	-2.795471	1.531050
C	5.182566	-3.052678	-0.892612
H	4.872648	-3.288783	-1.911369

H	5.950647	-3.747958	-0.550910
H	5.517872	-2.017371	-0.822575
N	2.611271	-2.153271	-0.386317
H	2.949305	-1.186664	-0.257580

Vibrational frequencies

-176.1713	15.7344	18.4209
25.5071	28.4895	30.1851
34.4282	36.0575	39.2145
43.1078	43.7118	46.0009
49.0406	51.6273	55.0484
58.1845	60.4066	61.9752
63.5926	67.0682	69.9935
71.2872	73.1668	74.5734
76.3745	79.5376	79.7606
84.2436	87.4892	89.8670

TS2R($\Phi_1=120^\circ/\Phi_2=-146^\circ$)

Cartesian coordinates

C	-2.589913	-2.014047	2.558793
C	-2.527062	-1.089428	1.512069
C	-3.146695	0.155436	1.612631
C	-3.842977	0.463792	2.782067
C	-3.912329	-0.460219	3.832629
C	-3.284193	-1.704158	3.728640
C	-1.859083	-3.286408	2.204364
C	-1.030838	-2.889241	0.955812
C	-1.729388	-1.638626	0.343774
H	-3.081076	0.866732	0.800204
H	-4.335353	1.427283	2.876028
H	-4.455795	-0.206050	4.738227
H	-3.334737	-2.417235	4.546907

H	-1.243105	-3.674473	3.020241
H	-0.927210	-3.684154	0.222535
H	-2.569934	-4.067709	1.920891
S	-3.895459	-2.809169	-0.946752
O	-3.743908	-3.994858	-0.087176
O	-4.177840	-2.974920	-2.381506
C	-5.186346	-1.776593	-0.258045
C	-5.792045	-2.133084	0.944955
C	-5.523702	-0.592087	-0.918700
C	-6.749405	-1.283383	1.495099
H	-5.502849	-3.049982	1.444104
C	-6.479205	0.244004	-0.350910
H	-5.030867	-0.310875	-1.842850
C	-7.099526	-0.082233	0.864390
H	-7.220446	-1.551226	2.436496
H	-6.726239	1.176104	-0.849202
C	-8.085302	0.865588	1.501115
H	-8.790603	0.337944	2.149214
H	-7.559649	1.603292	2.120011
H	-8.653998	1.418600	0.748044
N	-2.471493	-1.946804	-0.898159
H	-2.579782	-1.120804	-1.503045
S	0.701173	-2.458852	1.521092
C	1.749974	-3.582120	0.614058
C	2.693074	-4.353922	1.322244
C	1.697008	-3.619922	-0.802556
C	3.551741	-5.187299	0.595627
C	2.541991	-4.495076	-1.497399
C	3.466026	-5.262486	-0.792820
H	4.280740	-5.790267	1.127785

H	2.492154	-4.572521	-2.575163
H	4.125327	-5.929578	-1.339767
C	2.798180	-4.295990	2.827983
H	3.078388	-3.295039	3.173682
H	1.843237	-4.539637	3.304125
H	3.551779	-5.000040	3.187957
O	0.815093	-2.772951	-1.386746
C	0.714326	-2.674643	-2.834293
C	0.308655	-1.241963	-3.144640
C	-0.289328	-3.708272	-3.331526
H	1.706215	-2.858277	-3.262325
H	1.061744	-0.537177	-2.784591
H	0.209170	-1.118123	-4.227034
H	-0.648786	-0.995065	-2.685209
H	-1.277334	-3.491449	-2.916090
H	-0.351144	-3.678314	-4.423588
H	0.007135	-4.717401	-3.030692
H	-0.989287	-0.917366	-0.007707
S	1.676478	-0.326357	0.213929
C	1.526732	0.771660	1.604982
C	0.288882	1.397814	1.819028
C	2.612251	1.054332	2.445208
C	0.143037	2.293355	2.873481
H	-0.534593	1.189969	1.148456
C	2.457798	1.975287	3.476983
H	3.573409	0.589310	2.264524
C	1.225459	2.607770	3.709814
H	-0.821332	2.765168	3.039926
H	3.310093	2.211377	4.107686
C	1.074474	3.629633	4.807955

H	0.079167	3.584817	5.259535
H	1.819972	3.488045	5.595018
H	1.204660	4.642870	4.408688
O	-1.539389	1.844684	-0.764742
S	-2.257619	1.787644	-2.062303
O	-2.736115	0.423650	-2.428125
O	-1.648637	2.543442	-3.171294
C	-3.833239	2.721767	-1.685869
F	-3.594419	4.042285	-1.657848
F	-4.772244	2.474198	-2.614244
F	-4.331930	2.364044	-0.488626
C	1.060836	7.132006	-1.250866
C	1.856701	6.003533	-1.033330
C	1.297994	4.815059	-0.549119
C	-0.081712	4.777627	-0.289498
C	-0.880349	5.897061	-0.519831
C	-0.311053	7.081184	-0.997947
H	1.512707	8.046591	-1.624710
H	2.922804	6.045876	-1.242494
H	-0.538212	3.858710	0.062548
H	-1.949540	5.837250	-0.337157
H	-0.932438	7.953985	-1.176833
C	2.146882	3.579800	-0.335102
C	1.681522	2.437002	-1.275241
H	2.057651	3.240636	0.700647
H	3.205271	3.790405	-0.510431
C	2.450435	1.188750	-1.090068
H	0.620723	2.241839	-1.106959
H	1.796899	2.747407	-2.319535
C	3.487727	0.511345	-1.254196

C	4.470899	-0.471477	-1.452464
C	4.398235	-1.278475	-2.611921
C	5.453889	-0.758573	-0.465616
C	5.255147	-2.356714	-2.777255
H	3.644394	-1.048972	-3.356577
C	6.297731	-1.855051	-0.642891
C	6.192738	-2.653831	-1.782754
H	5.182652	-2.976275	-3.663982
H	7.035856	-2.085402	0.118810
H	6.854992	-3.505405	-1.897587
S	6.104980	1.602175	0.758815
O	5.469951	2.340890	-0.333977
O	5.945669	2.018657	2.154049
C	7.857960	1.447603	0.376831
H	7.953481	0.962953	-0.595624
H	8.267701	2.458318	0.344146
H	8.336272	0.860981	1.161221
N	5.504614	0.001164	0.728759
H	5.876054	-0.505195	1.529345

Vibrational frequencies

-191.8122	11.5047	13.3359
15.8768	19.4220	20.3247
24.6224	26.7939	28.0213
30.3060	33.0004	34.6476
37.1843	40.5958	42.2211
43.2079	47.1361	48.9504
50.6511	52.5179	55.3814
59.3152	62.5235	66.9698
70.1230	74.1944	75.6570
79.7473	81.7560	85.4945

TS2R($\Phi_1=66^\circ/\Phi_2=-165^\circ$)

Cartesian coordinates

C	1.015241	-2.956317	-2.372463
C	1.238022	-1.914689	-1.470320
C	2.211274	-0.947013	-1.702289
C	2.976514	-1.032260	-2.864525
C	2.756047	-2.071812	-3.777820
C	1.776702	-3.040610	-3.538797
C	-0.065286	-3.886692	-1.872092
C	-0.712125	-3.104568	-0.702639
C	0.292813	-1.990671	-0.292575
H	2.382321	-0.161993	-0.978708
H	3.749580	-0.294163	-3.049048
H	3.356173	-2.128130	-4.681383
H	1.613712	-3.845815	-4.249616
H	-0.782770	-4.177382	-2.645004
H	-0.970414	-3.722949	0.147205
H	0.373734	-4.805395	-1.468532
S	1.979914	-3.388838	1.409338
O	1.478460	-4.634893	0.806388
O	2.164748	-3.277364	2.865049
C	3.518920	-2.956046	0.615566
C	3.958759	-3.675197	-0.492892
C	4.204643	-1.822836	1.065482
C	5.100345	-3.239347	-1.165110
H	3.402907	-4.539656	-0.835354
C	5.333376	-1.396506	0.378081
H	3.855153	-1.273554	1.932069
C	5.791540	-2.093685	-0.752551
H	5.440927	-3.785492	-2.039734

H	5.839630	-0.494889	0.707010
C	6.998530	-1.589559	-1.502343
H	7.907750	-1.700490	-0.900447
H	7.147132	-2.129346	-2.441031
H	6.889876	-0.523954	-1.725954
N	0.860919	-2.203879	1.048919
H	1.057738	-1.347261	1.562758
S	-2.296161	-2.299469	-1.275000
C	-3.562198	-3.449942	-0.780261
C	-4.492603	-3.876648	-1.753280
C	-3.656391	-3.888879	0.563955
C	-5.487590	-4.778620	-1.364121
C	-4.652542	-4.809091	0.913228
C	-5.557304	-5.242852	-0.051443
H	-6.206024	-5.124355	-2.100236
H	-4.728594	-5.175095	1.928691
H	-6.330614	-5.951094	0.229523
C	-4.430757	-3.396205	-3.184181
H	-4.538376	-2.308315	-3.249353
H	-3.474571	-3.651566	-3.651777
H	-5.229910	-3.849556	-3.774151
O	-2.768374	-3.356628	1.440064
C	-2.502326	-3.999202	2.722516
C	-1.715726	-2.975958	3.526024
C	-1.738450	-5.302155	2.508606
H	-3.459442	-4.190352	3.221241
H	-2.313385	-2.074602	3.681862
H	-1.459552	-3.392220	4.504129
H	-0.793072	-2.710423	3.003973
H	-0.761855	-5.105589	2.055989

H	-1.578298	-5.795725	3.471587
H	-2.294152	-5.988268	1.863816
H	-0.215488	-1.039181	-0.167724
S	-2.844213	-0.205885	0.136276
C	-1.775086	0.818587	-0.857817
C	-0.594891	1.333279	-0.302240
C	-2.104792	1.119981	-2.185748
C	0.240574	2.136433	-1.063393
H	-0.344767	1.125766	0.730257
C	-1.238803	1.901666	-2.952560
H	-3.023824	0.737096	-2.616852
C	-0.053985	2.419805	-2.407037
H	1.138786	2.538437	-0.612921
H	-1.488555	2.111046	-3.988771
C	0.885143	3.276721	-3.218074
H	0.705365	4.340543	-3.020345
H	1.926110	3.075659	-2.950024
H	0.758554	3.111648	-4.291073
O	4.705503	3.992525	1.026456
S	5.507998	2.848808	0.533515
O	5.605181	1.701841	1.472452
O	6.763367	3.198750	-0.166051
C	4.438986	2.169294	-0.831499
F	4.174485	3.096586	-1.769005
F	5.013507	1.115468	-1.444611
F	3.257302	1.752481	-0.325048
C	1.585998	0.216059	3.231684
C	0.252571	0.452662	3.578807
C	-0.358242	1.684860	3.298117
C	0.402059	2.675106	2.660432

C	1.731699	2.437526	2.298008
C	2.329672	1.207589	2.580765
H	2.042601	-0.735851	3.493797
H	-0.308914	-0.324799	4.090744
H	-0.053493	3.630693	2.422898
H	2.311860	3.207505	1.797941
H	3.366709	1.044240	2.304385
C	-1.789706	1.947215	3.721397
C	-2.842546	0.981017	3.114751
H	-2.072960	2.976401	3.488336
H	-1.859983	1.830080	4.809412
C	-3.294058	1.337080	1.752805
H	-2.461575	-0.041871	3.113766
H	-3.739209	0.985382	3.744968
C	-3.899700	2.034550	0.927046
C	-4.559012	2.719131	-0.113700
C	-5.900293	2.402002	-0.420103
C	-3.872467	3.674594	-0.907601
C	-6.532733	2.994915	-1.504912
H	-6.418049	1.672716	0.192865
C	-4.521733	4.259193	-1.995354
C	-5.839312	3.914810	-2.299230
H	-7.560358	2.738478	-1.738268
H	-3.988083	4.983655	-2.601798
H	-6.329233	4.375213	-3.150888
S	-2.131026	5.091862	0.612848
O	-2.865461	4.691572	1.817976
O	-0.666625	5.159667	0.607615
C	-2.791146	6.678776	0.074967
H	-3.866004	6.569813	-0.074583

H	-2.585249	7.399482	0.867728
H	-2.291277	6.966447	-0.850369
N	-2.523430	3.993937	-0.605629
H	-1.892961	4.077486	-1.398916

Vibrational frequencies

-188.5407	14.4684	18.0015
19.8756	24.2913	27.0591
29.1874	30.2096	35.1719
41.1083	42.5001	45.7860
49.7121	50.5291	52.2844
54.8724	57.7271	58.1493
64.0166	66.4732	69.4478
70.5710	72.0698	75.5515
76.3333	79.0571	83.0262
87.6870	88.9001	93.4161

TS2R(Φ 1=-84°/ Φ 2=-35°)

Cartesian coordinates

C	-0.445043	1.414548	-2.054635
C	0.314833	1.758768	-0.932759
C	-0.258245	2.442194	0.138578
C	-1.619382	2.744293	0.091392
C	-2.389054	2.367985	-1.015166
C	-1.806891	1.707109	-2.099476
C	0.420463	0.775227	-3.114686
C	1.696421	0.368117	-2.336021
C	1.747608	1.286916	-1.078279
H	0.339614	2.748127	0.990713
H	-2.088569	3.244534	0.930082
H	-3.453148	2.571689	-1.032699
H	-2.419691	1.415747	-2.945283

H	-0.058623	-0.063275	-3.626461
H	2.615995	0.423779	-2.915988
H	0.700295	1.510104	-3.875778
S	2.773173	3.622817	-2.239303
O	2.495519	3.073356	-3.573658
O	4.032347	4.327965	-1.958670
C	1.421485	4.695997	-1.779372
C	0.237497	4.671366	-2.516006
C	1.541353	5.471731	-0.623889
C	-0.847792	5.419062	-2.069923
H	0.166115	4.063790	-3.409487
C	0.444282	6.212534	-0.193976
H	2.475156	5.496759	-0.072058
C	-0.768524	6.185274	-0.898739
H	-1.777564	5.390672	-2.629535
H	0.527781	6.814340	0.706233
C	-1.978064	6.925338	-0.387209
H	-2.582960	7.320063	-1.208534
H	-2.617564	6.246417	0.190148
H	-1.698192	7.754044	0.268445
N	2.799728	2.322023	-1.178135
H	3.143807	2.641166	-0.278692
S	1.477335	-1.437330	-1.903892
C	3.054196	-2.229214	-2.095102
C	3.092830	-3.397265	-2.892013
C	4.205314	-1.779380	-1.404314
C	4.312097	-4.067621	-3.021746
C	5.417546	-2.459055	-1.581955
C	5.457421	-3.594986	-2.384423
H	4.362350	-4.960758	-3.635706

H	6.321062	-2.119191	-1.095016
H	6.399637	-4.119643	-2.508985
C	1.867525	-3.937756	-3.589899
H	1.105207	-4.246035	-2.867254
H	1.409568	-3.189491	-4.243482
H	2.129116	-4.808157	-4.195043
O	4.036148	-0.718999	-0.578781
C	5.160314	-0.200413	0.188172
C	4.561949	0.463474	1.417902
C	5.980651	0.748419	-0.678187
H	5.770436	-1.047296	0.520948
H	3.994654	-0.254916	2.014171
H	5.356132	0.880923	2.041891
H	3.892377	1.277399	1.137907
H	5.362575	1.588953	-1.003731
H	6.832669	1.131028	-0.108803
H	6.362833	0.239445	-1.566676
H	2.066438	0.707165	-0.212351
S	0.780098	-1.609052	0.518766
C	1.538687	-3.210521	0.589779
C	0.850273	-4.324934	0.070502
C	2.839912	-3.360029	1.091055
C	1.476284	-5.568005	0.052623
H	-0.153556	-4.208288	-0.323341
C	3.450368	-4.609641	1.063042
H	3.370571	-2.492263	1.454235
C	2.779151	-5.730788	0.538854
H	0.950832	-6.423523	-0.362140
H	4.463369	-4.714100	1.440568
C	3.465694	-7.082857	0.544091

H	2.727481	-7.909798	0.008684
H	4.534494	-6.970895	-0.054739
H	3.685557	-7.406723	1.731144
O	-4.953970	0.322269	-0.265229
S	-4.920205	-0.026383	-1.720705
O	-3.904024	-1.040491	-2.071263
O	-5.035023	1.131957	-2.631340
C	-6.541605	-0.919652	-1.945584
F	-7.571518	-0.131826	-1.601191
F	-6.701412	-1.293188	-3.224490
F	-6.589156	-2.028661	-1.178517
C	2.153975	2.832203	6.160645
C	1.408554	1.913739	5.421368
C	1.547951	1.829725	4.027829
C	2.444412	2.700494	3.396098
C	3.191377	3.624472	4.130532
C	3.050909	3.690138	5.517367
H	2.031286	2.882748	7.238664
H	0.704098	1.259943	5.929342
H	2.554387	2.662332	2.316695
H	3.879651	4.290772	3.618645
H	3.629932	4.406318	6.092612
C	0.737911	0.833182	3.231127
C	1.064174	-0.638296	3.586036
H	0.919047	0.971920	2.163314
H	-0.333235	0.998266	3.388924
C	0.211141	-1.544166	2.804711
H	2.122366	-0.849059	3.403963
H	0.873506	-0.827620	4.648383
C	-0.802721	-2.183576	2.509052

C	-1.937447	-2.856482	2.012438
C	-1.997324	-4.264519	1.989659
C	-2.996484	-2.096719	1.448897
C	-3.074495	-4.907425	1.390798
H	-1.181183	-4.831440	2.423301
C	-4.069969	-2.757273	0.850732
C	-4.101412	-4.152095	0.814164
H	-3.112651	-5.991239	1.365835
H	-4.869461	-2.174327	0.413549
H	-4.941348	-4.649961	0.340026
S	-3.296624	0.142259	2.889169
O	-2.768516	-0.641618	4.014016
O	-2.864164	1.532739	2.708306
C	-5.096367	0.104897	2.959984
H	-5.407437	-0.939445	3.011990
H	-5.400896	0.644981	3.857445
H	-5.478917	0.577136	2.055014
N	-2.914842	-0.678531	1.450887
H	-3.450234	-0.246097	0.681225

Vibrational frequencies

-174.1153	12.9483	15.2566
18.7959	22.6828	24.7153
26.9821	28.1229	29.2590
31.1626	38.5133	38.6616
42.5370	45.2671	46.0312
47.0444	50.8314	51.6202
55.1077	56.7270	62.9360
64.6737	64.8896	69.3118
71.8817	74.0077	75.7715
80.5936	91.5588	91.9524

TS2R($\Phi_1=-102^\circ/\Phi_2=106^\circ$)

Cartesian coordinates

C	3.499396	0.605795	-2.386511
C	3.812066	0.661264	-1.025110
C	4.621631	1.673860	-0.514673
C	5.109151	2.648394	-1.387548
C	4.782029	2.606548	-2.749196
C	3.977871	1.583132	-3.258433
C	2.665009	-0.613912	-2.697222
C	2.158259	-1.064281	-1.306974
C	3.149575	-0.471619	-0.264971
H	4.870067	1.701220	0.541052
H	5.742389	3.445117	-1.009459
H	5.160543	3.375460	-3.415972
H	3.733807	1.548360	-4.316209
H	1.857098	-0.422274	-3.407965
H	2.045722	-2.137943	-1.201691
H	3.289655	-1.411736	-3.113884
S	5.213181	-2.346573	-0.432313
O	4.582371	-2.895866	-1.641755
O	5.771300	-3.233241	0.598478
C	6.492341	-1.206142	-0.936002
C	6.557587	-0.783323	-2.263432
C	7.351825	-0.685659	0.034079
C	7.486268	0.191494	-2.614653
H	5.883678	-1.203994	-2.999400
C	8.273295	0.289731	-0.336590
H	7.302259	-1.038478	1.058936
C	8.344905	0.752837	-1.659011
H	7.534304	0.532856	-3.644261

H	8.944145	0.700824	0.412151
C	9.294157	1.859050	-2.043691
H	9.711721	1.698219	-3.041817
H	8.765450	2.819972	-2.063972
H	10.119664	1.950083	-1.333048
N	4.026556	-1.479060	0.367730
H	4.354224	-1.201691	1.288458
S	0.454983	-0.323996	-1.062356
C	-0.609776	-1.714561	-0.739055
C	-1.828748	-1.781889	-1.449055
C	-0.283258	-2.670542	0.254192
C	-2.686056	-2.856838	-1.187578
C	-1.157035	-3.738769	0.479381
C	-2.345597	-3.821555	-0.242648
H	-3.621713	-2.927141	-1.730312
H	-0.929433	-4.482641	1.227117
H	-3.021963	-4.649007	-0.051120
C	-2.228654	-0.736328	-2.463006
H	-2.372855	0.238713	-1.985775
H	-1.461061	-0.610232	-3.233233
H	-3.171500	-1.009577	-2.935975
O	0.860833	-2.431612	0.946198
C	1.631764	-3.449764	1.653298
C	2.063611	-4.575597	0.721514
C	0.974815	-3.924312	2.952008
H	2.518437	-2.870892	1.916469
H	2.608679	-4.174086	-0.136254
H	2.734431	-5.250017	1.261963
H	1.212651	-5.159374	0.361747
H	0.234053	-4.711979	2.800608

H	1.752608	-4.330656	3.605762
H	0.491026	-3.095062	3.474264
H	2.601092	-0.092680	0.590710
S	-0.179064	1.058856	0.996456
C	1.201669	0.947261	2.094435
C	1.355668	-0.160400	2.945402
C	2.183307	1.953136	2.079885
C	2.494244	-0.276826	3.733973
H	0.599649	-0.933890	2.942806
C	3.313151	1.830321	2.884657
H	2.073397	2.794733	1.404852
C	3.495370	0.711195	3.712361
H	2.617061	-1.147539	4.372120
H	4.074380	2.604872	2.859180
C	4.723196	0.578143	4.576082
H	5.029055	-0.467303	4.674876
H	5.562533	1.149952	4.171596
H	4.523877	0.955243	5.586434
O	-5.307494	0.075801	-1.589554
S	-6.036916	-1.204971	-1.835186
O	-6.357198	-1.965954	-0.605176
O	-5.516267	-2.001209	-2.967409
C	-7.697105	-0.610589	-2.437049
F	-7.561718	0.121634	-3.551466
F	-8.500813	-1.650552	-2.703381
F	-8.293339	0.152138	-1.500079
C	1.284263	3.871794	-1.374147
C	0.599513	4.411623	-0.284310
C	-0.772489	4.180514	-0.109988
C	-1.459095	3.436171	-1.077095

C	-0.779595	2.909188	-2.178201
C	0.594295	3.111848	-2.322736
H	2.353701	4.029552	-1.482157
H	1.140321	5.002732	0.452029
H	-2.520416	3.244611	-0.946783
H	-1.322510	2.323654	-2.914195
H	1.130209	2.680113	-3.162357
C	-1.474438	4.657622	1.142700
C	-1.019417	3.904083	2.422247
H	-2.557140	4.548275	1.035631
H	-1.264647	5.719718	1.314187
C	-1.403864	2.486815	2.448029
H	0.067458	3.983139	2.540339
H	-1.472334	4.377489	3.301584
C	-2.037726	1.460961	2.722631
C	-2.686453	0.211426	2.816675
C	-2.294243	-0.731086	3.788950
C	-3.631406	-0.156205	1.820547
C	-2.794765	-2.026009	3.749047
H	-1.573157	-0.436030	4.543513
C	-4.129319	-1.460659	1.795908
C	-3.698187	-2.389509	2.743260
H	-2.476960	-2.753629	4.488240
H	-4.838570	-1.743527	1.024436
H	-4.082380	-3.403596	2.701847
S	-4.945500	2.123688	1.175850
O	-4.685717	2.513767	2.568061
O	-4.725508	3.092122	0.093500
C	-6.634861	1.516229	1.062211
H	-6.742170	0.687364	1.763100

H	-7.294078	2.342088	1.333927
H	-6.806496	1.188225	0.038799
N	-3.982492	0.771740	0.811452
H	-4.329951	0.357761	-0.068331

Vibrational frequencies

-181.5759	12.2332	17.0026
18.8393	23.1791	25.5531
30.3302	32.2282	33.5488
34.6354	38.5638	40.7511
42.6628	45.0851	48.0989
49.7859	52.1604	53.8359
54.5414	56.3127	59.0303
60.4144	65.0728	65.3855
67.4175	68.0198	71.2922
75.5379	81.9003	82.4340