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SUPPLEMENTARY INFORMATION

Elucidating the Selectivity of Dyotropic Rearrangements of β - Lactones: A Computational Survey

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Computational details

1. Computational methods

The calculations were performed with the Gaussian 16 program package and ORCA 4.2.0 program. The geometry optimizations of the intermediates and transition states were performed using the PBE0 functional with def-TZVP basis set for all atoms. DFT-D3 dispersion correction with Becke-Johnson damping was used during optimization. Higher level of single point electronic energies for those structures were calculated at PWPB95-D3(BJ)/def2-QZVPP level with RI approximation using the corresponding auxiliary basis set and D3-BJ dispersion correction (unless otherwise mentioned for some calculation in the Supporting Information). Solvation effects were accounted using M05-2X functional, which is the method that is used when SMD parameter was developed, and with Pople's 6-31G(d) bases set in Et₂O. The vibrational harmonic frequencies and thermal corrections were calculated using the same level as the optimization; the former confirmed the optimized geometrical structures are the minima of PES, and transition states, the first order saddle points. Intrinsic reaction coordinate (IRC) calculations were performed for the identified transition states to confirm the reaction path proceeding in both directions (reactant and product), in which the Hessian was recomputed every five predictor steps with a step size along the reaction path of 0.05 Bohr. All energies mentioned are solvated Gibbs free energies in Et₂O. Natural Bond Orbitals(NBO) analysis is performed with NBO version 3.1. Reduced density gradient(RDG) analysis is performed with Lu's Muiwfn package and visualized by VMD.

2. Geometries and original energies

2.1 Comparison of three coordination modes

There are three possible coordination modes in this system, namely Type A, B and C. We found that in the substrates, Type A is the most stable coordination mode. Type B comes next and Type C is the most unstable coordination. In the TSs, Type A is still the most stable coordination mode. We give an example of each of the three types (σ , π , n) of migration groups, respectively. As shown in **Fig. S1**. (All results are computed at the level of RI-PWPB95-D3(BJ)/def2-QZVPP//SMD (diethylether)-PBE0-D3(BJ)/def-TZVP). We did not compare three coordination forms for each substrates and transition states for that the amount of work is too large. The relative stability among the three coordination modes may be related to the structure of substrates. In this work, we uniformly adopt the coordination mode of Type A to illustrate the effect of different substitution pattern on the selectivity of the reaction.

In our previous study, we found that the most stable coordination mode in the substrate basically does not change. Type A is always the most stable. However, the relative stability of different coordination modes in the transition states may change with Lewis acid. In our previous work (Guo, Z., Bao, R., Li, Y., Li, Y., Zhang, J., & Tang, Y. *Angew. Chem. Int. Ed.* 2021, 60, 14545-14553.), SnCl₄ is used as promoter. We found that the coordination mode of Type A is still the most stable in SnCl₄-substrate complex and Type C is the most unstable (All attempts to optimize the six coordinated SnCl₄-substrate complex failed). But we find that coordination mode of Type C is more stable in the transition states and Type A is the most unstable now. This may because that four coordination demand of Al(III) has been met in the AlEtCl₂-substrate complex, while Sn(IV) is five coordination and unsaturated in the SnCl₄-substrate complex. In the transition states, the coordination mode of Type C and B can better meet the six coordination demand of Sn(IV).

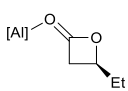
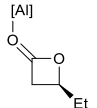
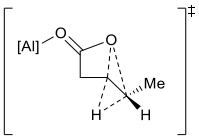
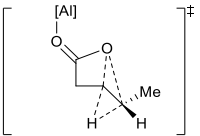
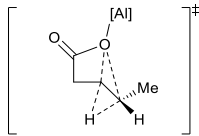
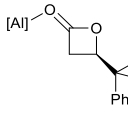
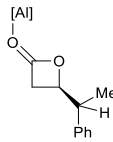
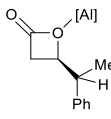
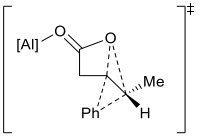
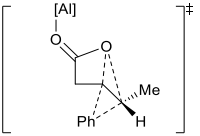
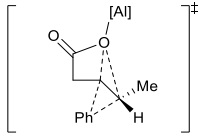
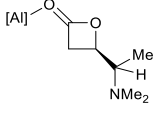
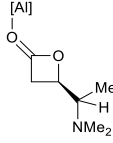
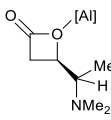
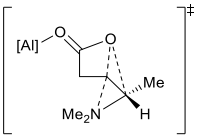
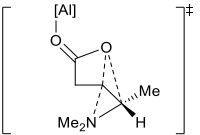
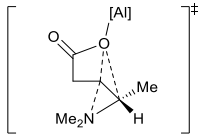
(A)			
Sub_S1			
Type	Type A	Type B	Type C
Relative energy (kJ/mol)	0.0	3.4	28.0
TS_S1			
Type	Type A	Type B	Type C
Relative energy (kJ/mol)	0.0	13.1	9.9
(B)			
Sub_S2			
Type	Type A	Type B	Type C
Relative energy (kJ/mol)	0.0	3.0	27.9
TS_S2			
Type	Type A	Type B	Type C
Relative energy (kJ/mol)	0.0	5.7	8.3
(C)			
Sub_S3			
Type	Type A	Type B	Type C
Relative energy (kJ/mol)	0.0	6.6	27.2
TS_S3			
Type	Type A	Type B	Type C
Relative energy (kJ/mol)	0.0	6.5	13.6

Figure S1. Comparison of three coordination modes of AlEtCl₂

In addition, we also calculated the energy barriers of the transformation among the three coordination types. For AlEtCl_2 , the transformation between Type A and Type B is very easy, with an energy barrier of only 20.7 kJ/mol compared to the most stable Type A complex. However, the formation of Type C complex is very difficult, with an energy barrier of 92.4 kJ/mol. This barrier even exceeds that of many direct dyotropic rearrangements. As shown in **Fig. S2**. We also found that Type C complexes can only be transformed from other types of complexes and can not be generated by the substitution reaction between $\text{AlEtCl}_2(\text{Et}_2\text{O})$ and substrates. As shown in **Fig. S3**. However, the situation is very different when SnCl_4 is used as a catalyst. At this time, the Type C complex can also be easily transformed from the most stable Type A complex, with a barrier of only 45.7 kJ/mol. As shown in **Fig. S4**. This further confirmed that SnCl_4 can catalyze the reaction through Type C complex in the transition states. As can be seen from **Fig. S2** and **Fig. S4**, the geometry of AlEtCl_2 in $\text{TS}_{\text{BC-Al}}$ is close to a plane triangle, while SnCl_4 is an octahedron in $\text{TS}_{\text{BC-Sn}}$.

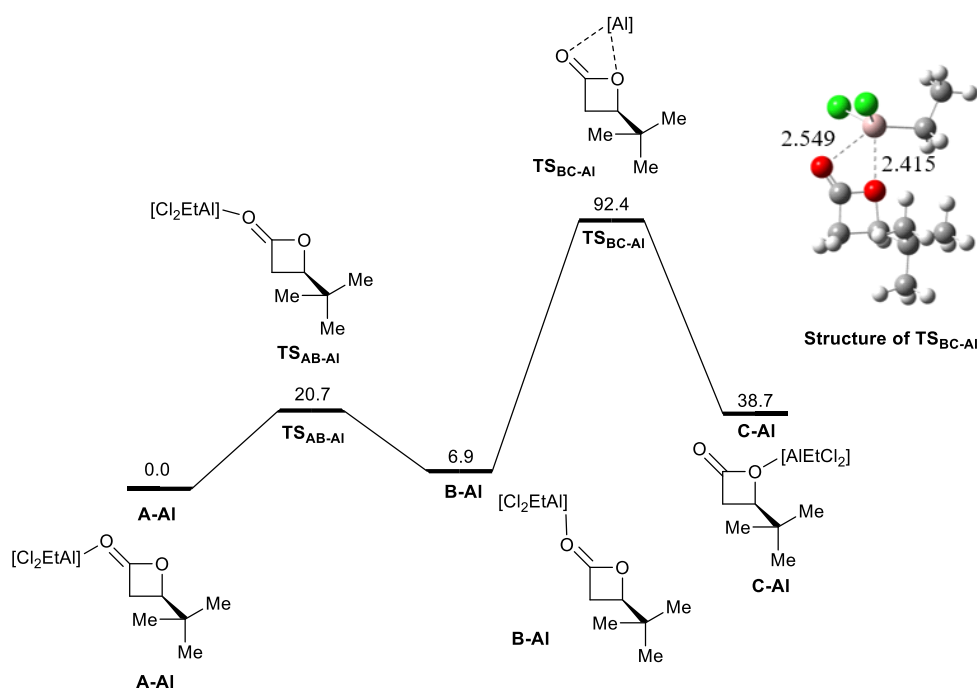


Figure S2. Free energy profile (in kJ/mol) of the transformation among the three coordination types when AlEtCl_2 is used as promoter and the structure of $\text{TS}_{\text{BC-Al}}$.

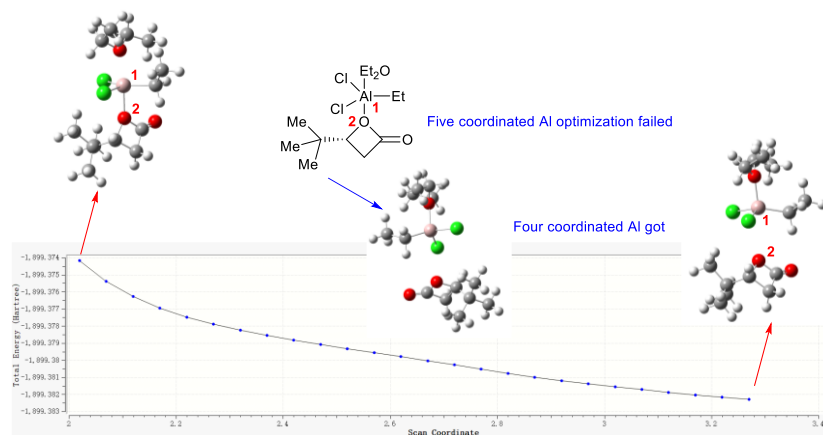


Figure S3. Scanning the $\text{Al}^1\text{-O}^2$ bond from 2.020 to 3.270 Å, the energy decreases monotonically

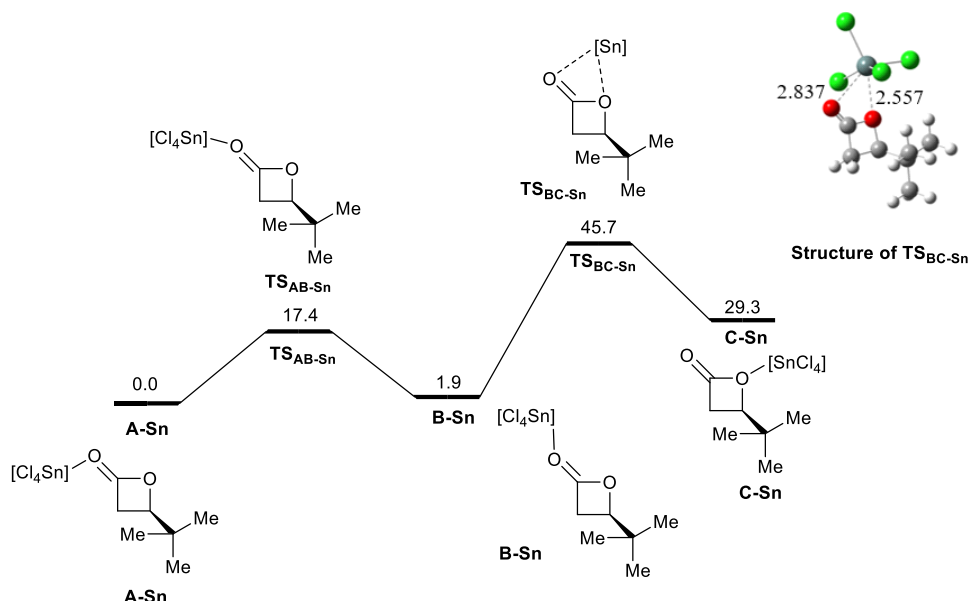


Figure S4. Free energy profile (in kJ/mol) of the transformation among the three coordination types when SnCl₄ is used as promoter and the structure of TS_{BC-Sn}.

For AlEtCl₂, the calculation level is the same as described above. For SnCl₄, calculation is at the level of RI-PWPB95-D3(BJ)/def2-QZVPP//SMD(diethylether)-PBE0-D3(BJ)/def2-SVP. SMD Model is calculated at M05-2X/def2-SVP for Sn, 6-31G* for others level.

2.2 Possibility of AlEtCl⁺ species catalysis

It has been reported that Al⁺ species can be the catalyst (Guo-Jie Jiang, Yi Wang, and Zhi-Xiang Yu *J. Org. Chem.* 2013, 78, 6947-6955). We show the results of Al⁺ species catalysis here as a possibility.

We first calculated the ΔG (in kJ/mol) of all possible pathways for the production of AlEtCl⁺ cation in the reaction system we investigated. There are two reasonable pathways for the production of AlEtCl⁺ cationic species (Fig. S2). That is, equation S1 (substrate substitutes Cl⁻) and equation S2 (Et₂O substitutes Cl⁻). However, the ΔG of these two pathways are all about 88 kJ/mol and the standard equilibrium constant at 298K is about 3.8×10^{-16} , which means that the generation of AlEtCl⁺ species is relatively difficult and its concentration is relatively low.

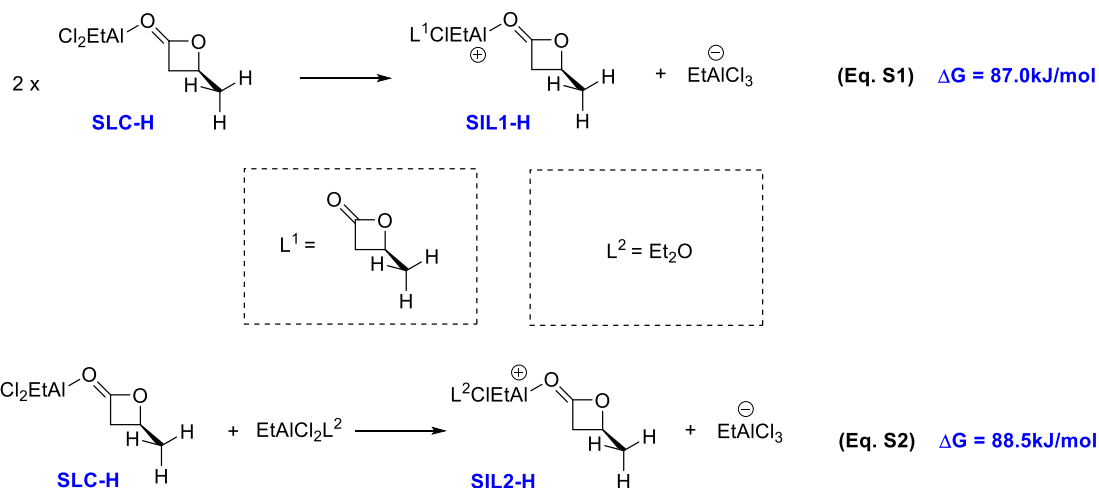
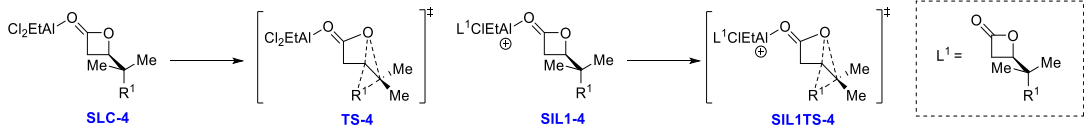


Figure S5. Two reasonable pathways for the production of AlEtCl⁺ cationic species and ΔG

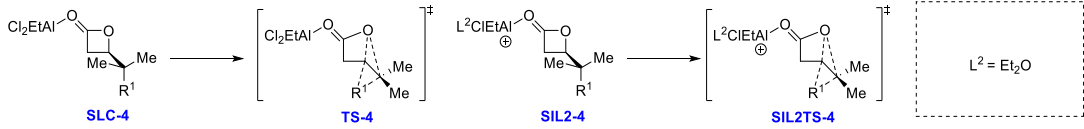
Taking $L^1AlEtCl^+$ and $L^2AlEtCl^+$ as catalytic species, we calculated the energy barrier of some typical dyotropic rearrangement of **SIL1-4** and **SIL2-4** ($R = H, CH_2CH=CH_2, Br, NMe_2, Ph$ and $CH=CH_2$), respectively. As shown in Table S1 and Table S2. Our calculation shows that taking $L^1AlEtCl^+$ and $L^2AlEtCl^+$ as promotor, their barriers are similar and the reaction energy barrier is reduced by about 5-20kJ/mol compared with taking $AlEtCl_2$ as catalyst. However, the intrinsic migration ability obtained with $L^1AlEtCl^+$ and $L^2AlEtCl^+$ as promoters is basically unchanged compared with $AlEtCl_2$ as promotor.

Table S1. Comparison of the energy barrier when $AlEtCl_2$ as catalyst and $L^1AlEtCl^+$ as catalyst



Compound numbering	R^1	$\Delta G^\ddagger$ (kJ/mol)	
		$AlEtCl_2$ as catalyst	$L^1AlEtCl^+$ as catalyst
a	H	86.6	79.8
c	$CH_2CH=CH_2$	90.1	78.3
i	Br	71.9	57.9
l	NMe_2	40.2	28.3
m	Ph	70.8	55.8
n	$CH=CH_2$	67.9	54.2

Table S2. Comparison of the energy barrier when $AlEtCl_2$ as catalyst and $L^2AlEtCl^+$ as catalyst



Compound numbering	R^1	$\Delta G^\ddagger$ (kJ/mol)	
		$AlEtCl_2$ as catalyst	$L^2AlEtCl^+$ as catalyst
a	H	86.6	81.2
c	$CH_2CH=CH_2$	90.1	79.5
i	Br	71.9	52.6
l	NMe_2	40.2	26.0
m	Ph	70.8	55.5
n	$CH=CH_2$	67.9	47.4

In all case, $\Delta G_3 > \Delta G_1 > \Delta G_2$. As shown in **Fig. S6**.

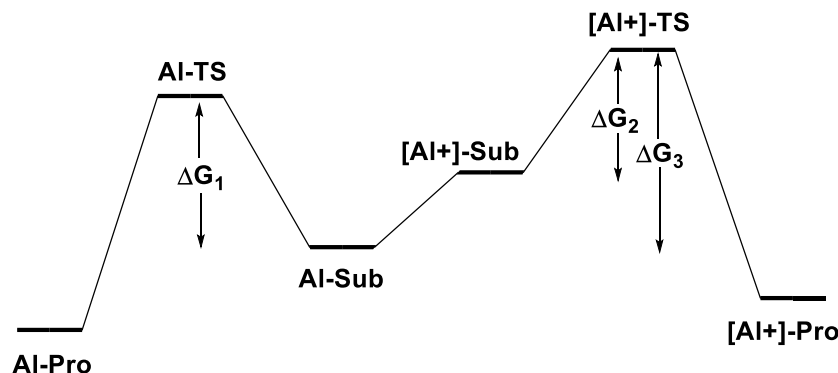


Figure S6. Potential energy surface illustration of Al catalysis and Al + catalysis

2.3 Details of NBO analysis

The definition of NBO second perturbation energy is

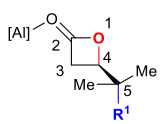
$$\Delta E_{i \rightarrow j}^{(2)} = \eta_i \frac{|\langle \varphi_i | \hat{F} | \varphi_j \rangle|^2}{\varepsilon_j - \varepsilon_i} = \eta_i \frac{|F_{i \rightarrow j}|^2}{\Delta E_{Orb}}$$

$\Delta E_{i \rightarrow j}^{(2)}$ is the interaction energy between orbitals, whose value is determined by three terms. η_i : Number of electrons in donor NBOs. Here, its value is always 2. $\Delta E_{Orb} = \varepsilon_j - \varepsilon_i$: The energy difference between acceptor NBO and donor NBO. $F_{i \rightarrow j} = \langle \varphi_i | \hat{F} | \varphi_j \rangle$. For different σ and π migrating groups, the orientations of σ and π bonds in substrates are basically the same. However, for n migrating groups, it is necessary to ensure that the orientation of lone pair electrons is consistent, based on the optimized structure. Otherwise, there is no control variable. We find that this operation has little effect on the orbital energy (using a.u. as the unit), but it affects the amount which are closely related to the orientation of lone pair electrons. To some extent, $F_{i \rightarrow j}$ reflects the degree of overlap between orbitals. However, it is not always accurate to judge the degree of overlap between orbitals only by $F_{i \rightarrow j}$. Therefore, we further calculated the overlap integral S_{ij} between donor NBOs and acceptor NBOs.

$$S_{ij} = \int |\varphi_i| |\varphi_j| dr.$$

We found that the S_{ij} values of TMS and NMe₂ were significantly greater than those of the same type of migrating groups.

Table S3: Details of NBO analysis and S_{ij} between donor NBOs and acceptor NBOs.

 Acceptor NBO: σ^* (C^4-O^1) Donor NBO: σ (C^5-R^1) for σ migrating groups R^1's localized π orbital for π migrating groups R^1's lone pairs for n migrating groups					
Migrating group	Type	$\Delta E_{i \rightarrow j}^{(2)}$ (kJ/mol)	ΔE_{Orb} (au)	$ F_{i \rightarrow j} $ (au)	S_{ij} (au)
H	σ	31.4	0.66	0.063	0.137
Me	σ	19.9	0.78	0.055	0.126
CH ₂ CH=CH ₂	σ	19.7	0.77	0.054	0.125
CH ₂ C $\equiv$ CH	σ	18.6	0.78	0.053	0.124
COOMe	σ	13.9	0.82	0.047	0.121

COMe	σ	16.4	0.81	0.050	0.121
CHO	σ	17.7	0.82	0.053	0.122
TMS	σ	44.5	0.60	0.072	0.151
Ph	π	4.5	0.42	0.021	0.068
CH=CH ₂	π	5.6	0.45	0.022	0.069
Br	n	13.2	0.46	0.034	0.079
Cl	n	13.3	0.49	0.035	0.079
OMe	n	12.3	0.49	0.034	0.083
NMe ₂	n	14.9	0.44	0.036	0.098

2.4 Energy and coordinates

Specics	Sub-S1-Type B	TS-S1-Type B
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14945	0.14371
(Hartree)		
Solvation Gibbs		
Free Energy	-0.028534	-0.06083
(Hartree)		
Electronic	-1587.86422	-1587.78843
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1587.74331	-1587.70556

Specics	Sub-S1-Type C	TS-S1-Type C
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14993	0.14342
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02404	-0.04935
(Hartree)		
Electronic	-1587.85981	-1587.80083
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1587.73392	-1587.70677

Specics	Sub-S2-Type B	TS-S2-Type B
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	

Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.22310	0.22132
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03294	-0.05250
(Hartree)		
Electronic	-1818.85233	-1818.80191
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1818.66217	-1818.63308
Specics	Sub-S2-Type C	TS-S2-Type C
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.22361	0.22220
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02844	-0.04791
(Hartree)		
Electronic	-1818.84786	-1818.80638
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1818.65269	-1818.63209
Specics	Sub-S3-Type B	TS-S3-Type B
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.21826	0.21693
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02899	-0.04019
(Hartree)		
Electronic	-1721.78753	-1721.75942
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1721.59825	-1721.58267
Specics	Sub-S3-Type C	TS-S3-Type C

Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21757	0.21742
Solvation Gibbs Free Energy (Hartree)	-0.02417	-0.03107
Electronic Energy (Hartree)	-1721.78380	-1721.76631
Imaginaries	0	1
G_{sol}(Hartree)	-1721.59040	-1721.57996
Specics	A-AI	TS_{AB-AI}
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20177	0.20254
Solvation Gibbs Free Energy (Hartree)	-0.02374	-0.02851
Electronic Energy (Hartree)	-1666.47385	-1666.46199
Imaginaries	0	1
G_{sol}(Hartree)	-1666.29583	-1666.28795
Specics	B-AI	TS_{BC-AI}
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20227	0.20224
Solvation Gibbs Free Energy (Hartree)	-0.02769	-0.02593
Electronic Energy (Hartree)	-1666.46780	-1666.43694
Imaginaries	0	1
G_{sol}(Hartree)	-1666.29321	-1666.26063

Specics	C-Al	A-Sn
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP for AlEtCl ₂	
Level	SMD(diethylether)-PBE0-D3(BJ)/def2-SVP for SnCl ₄	
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20344	0.13729
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02689	-0.04869
(Hartree)		
Electronic	-1666.45764	-2479.44806
Energy (Hartree)		
Imaginaires	0	0
G_{sol}(Hartree)	-1666.28110	-2479.35947

Specics	TS _{AB-Sn}	B-Sn
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def2-SVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13794	0.13786
(Hartree)		
Solvation Gibbs		
Free Energy	-0.04838	-0.05119
(Hartree)		
Electronic	-2479.44239	-2479.44543
Energy (Hartree)		
Imaginaires	1	0
G_{sol}(Hartree)	-2479.35283	-2479.35875

Specics	TS _{BC-Sn}	C-Sn
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def2-SVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13821	0.13796
(Hartree)		
Solvation Gibbs		
Free Energy	-0.04666	-0.04528
(Hartree)		
Electronic	-2479.43362	-2479.44098
Energy (Hartree)		
Imaginaires	1	0
G_{sol}(Hartree)	-2479.34207	-2479.34831

Species	SLC-H	SIL1-H	SIL2-H
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP		
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP		
G Correction (Hartree)	0.12279	0.21700	0.25877
Solvation Gibbs Free Energy (Hartree)	-0.02377	-0.07361	-0.07102
Electronic Energy (Hartree)	-1548.57143	-1394.57416	-1321.74261
Imaginaries	0	0	0
G_{sol}(Hartree)	-1548.47241	-1394.43077	-1321.55487

Species	AlEtCl ₃ ⁻	AlEtCl ₂ (Et ₂ O)
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.03235	0.16434
Solvation Gibbs Free Energy (Hartree)	-0.06097	-0.01910
Electronic Energy (Hartree)	-1702.45231	-1475.74234
Imaginaries	0	0
G_{sol}(Hartree)	-1702.48093	-1475.59710

Species	SIL1-4a	SIL1TS-4a
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.32282	0.31950
Solvation Gibbs Free Energy (Hartree)	-0.07288	-0.08336
Electronic Energy (Hartree)	-1551.77615	-1551.73195
Imaginaries	0	1

G_{sol}(Hartree)	-1551.52621	-1551.49582
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Specics	SIL1-4c	SIL1TS-4c
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.43758	0.43597
Solvation Gibbs Free Energy (Hartree)	-0.07431	-0.08162
Electronic Energy (Hartree)	-1785.11581	-1785.07705
Imaginaries	0	1
G_{sol}(Hartree)	-1784.75254	-1784.72270

Specics	SIL1-4i	SIL1TS-4i
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.29874	0.29818
Solvation Gibbs Free Energy (Hartree)	-0.07743	-0.07843
Electronic Energy (Hartree)	-6699.05556	-6699.03196
Imaginaries	0	1
G_{sol}(Hartree)	-6698.83425	-6698.81221

Specics	SIL1-4I	SIL1TS-4I
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.46178	0.46167
Solvation Gibbs Free Energy (Hartree)	-0.07167	-0.07244
Electronic Energy (Hartree)	-1819.62033	-1819.60867

Imaginaries	0	1
G_{sol}(Hartree)	-1819.23022	-1819.21943
Specics	SIL1-4m	SIL1TS-4m
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.47713	0.47682
(Hartree)		
Solvation Gibbs		
Free Energy	-0.07988	-0.08564
(Hartree)		
Electronic	-2013.75106	-2013.72376
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2013.35381	-2013.33257
Specics	SIL1-4n	SIL1TS-4n
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.38602	0.38440
(Hartree)		
Solvation Gibbs		
Free Energy	-0.07194	-0.07723
(Hartree)		
Electronic	-1706.51703	-1706.48948
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1706.20295	-1706.18231
Specics	SIL2-4a	SIL2TS-4a
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.30835	0.30707
(Hartree)		
Solvation Gibbs		
Free Energy	-0.07214	-0.07989
(Hartree)		
Electronic	-1400.34270	-1400.30276

Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1400.10649	-1400.07557
Specics	SIL2-4c	SIL2TS-4c
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.36876	0.36774
(Hartree)		
Solvation Gibbs		
Free Energy	-0.07260	-0.07649
(Hartree)		
Electronic	-1517.01362	-1516.97843
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1516.71747	-1516.68718
Specics	SIL2-4i	SIL2TS-4i
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.30112	0.29493
(Hartree)		
Solvation Gibbs		
Free Energy	-0.07330	-0.07278
(Hartree)		
Electronic	-3973.98663	-3973.96091
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-3973.75881	-3973.73876
Specics	SIL2-4l	SIL2TS-4l
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.38018	0.37810
(Hartree)		
Solvation Gibbs		
Free Energy	-0.07147	-0.07102
(Hartree)		

Electronic Energy (Hartree)	-1534.26545	-1534.25391
Imaginaries	0	1
G_{sol}(Hartree)	-1533.95673	-1533.94683

Specics	SIL2-4m	SIL2TS-4m
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.38970	0.38459
Solvation Gibbs Free Energy (Hartree)	-0.07324	-0.07609
Electronic Energy (Hartree)	-1631.33585	-1631.30675
Imaginaries	0	1
G_{sol}(Hartree)	-1631.01939	-1630.99826

Specics	SIL2-4n	SIL2TS-4n
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.34185	0.33833
Solvation Gibbs Free Energy (Hartree)	-0.07165	-0.07330
Electronic Energy (Hartree)	-1477.71330	-1477.69005
Imaginaries	0	1
G_{sol}(Hartree)	-1477.44310	-1477.42503

Specics	S-1	S-2	AlEtCl₂
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP		
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP		
G Correction (Hartree)	0.08178	0.16861	0.03382
Solvation Gibbs Free Energy	-0.01666	-0.01877	-0.00961

(Hartree)			
Electronic	-2919.36627	-576.71447	-1242.09689
Energy (Hartree)			
Imaginaries	0	0	0
G _{sol} (Hartree)	-2919.30116	-576.56463	-1242.07267

Specics	SLC-1(RCom)	PLC-1	IM-2	PLC-2
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP			
Level				
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP			
Energy Level				
G Correction	0.13881	0.13930	0.22210	0.22611
(Hartree)				
Solvation Gibbs				
Free Energy	-0.02591	-0.02529	-0.05171	-0.02964
(Hartree)				
Electronic	-4161.50886	-4161.53417	-1818.80985	-1818.88716
Energy (Hartree)				
Imaginaries	0	0	0	0
G _{sol} (Hartree)	-4161.39597	-4161.42016	-1818.63945	-1818.69069

Specics	SLC-3a	TS-3a
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15048	0.14170
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02433	-0.04975
(Hartree)		
Electronic	-1587.87075	-1587.80249
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1587.74460	-1587.71054

Specics	SLC-3b	TS-3b
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.17607	0.17216
(Hartree)		
Solvation Gibbs		

Free Energy (Hartree)	-0.02399	-0.04363
Electronic Energy (Hartree)	-1627.17173	-1627.11321
Imaginaries	0	1
G _{sol} (Hartree)	-1627.01965	-1626.98468
Species	SLC-3c	TS-3c
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20586	0.20220
Solvation Gibbs Free Energy (Hartree)	-0.02564	-0.04850
Electronic Energy (Hartree)	-1704.53956	-1704.47747
Imaginaries	0	1
G _{sol} (Hartree)	-1704.35933	-1704.32377
Species	SLC-3d	TS-3d
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.18221	0.17838
Solvation Gibbs Free Energy (Hartree)	-0.02689	-0.05103
Electronic Energy (Hartree)	-1703.29360	-1703.22360
Imaginaries	0	1
G _{sol} (Hartree)	-1703.13829	-1703.09626
Species	SLC-3e	TS-3e
Optimization Level	SMD((diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.15582	0.15190

Solvation Gibbs		
Free Energy	-0.02905	-0.04482
(Hartree)		
Electronic	-1701.17534	-1701.10965
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1701.04857	-1701.00257
Specics	SLC-3f	TS-3f
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18000	0.17914
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02839	-0.04559
(Hartree)		
Electronic	-1740.48970	-1740.42886
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1740.33809	-1740.29531
Specics	SLC-3g	TS-3g
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18610	0.18119
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02706	-0.04184
(Hartree)		
Electronic	-1815.72405	-1815.65101
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1815.56501	-1815.51166
Specics	SLC-3h	TS-3h
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.24177	0.24011

(Hartree)		
Solvation Gibbs		
Free Energy	-0.02411	-0.03860
(Hartree)		
Electronic	-1996.46644	-1996.42718
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1996.24877	-1996.22566
Specics	SLC-3i	TS-3i
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13631	0.13330
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02705	-0.03820
(Hartree)		
Electronic	-4161.50794	-4161.46319
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-4161.39868	-4161.36810
Specics	SLC-3j	TS-3j
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13778	0.13583
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02717	-0.04033
(Hartree)		
Electronic	-2047.45705	-2047.40426
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-2047.34644	-2047.30876
Specics	SLC-3k	TS-3k
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		

G Correction (Hartree)	0.17969	0.17684
Solvation Gibbs Free Energy (Hartree)	-0.02460	-0.03637
Electronic Energy (Hartree)	-1702.37596	-1702.32715
Imaginaries	0	1
G_{sol}(Hartree)	-1702.22087	-1702.18667

Specics	SLC-3l	TS-3l
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21787	0.21701
Solvation Gibbs Free Energy (Hartree)	-0.02513	-0.03261
Electronic Energy (Hartree)	-1721.79349	-1721.76954
Imaginaries	0	1
G_{sol}(Hartree)	-1721.60075	-1721.58515

Specics	SLC-3m	TS-3m
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17946	0.17749
Solvation Gibbs Free Energy (Hartree)	-0.02429	-0.03996
Electronic Energy (Hartree)	-1665.24085	-1665.19537
Imaginaries	0	1
G_{sol}(Hartree)	-1665.08568	-1665.05784

Specics	SLC-3n	TS-3n
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	

Energy Level		
G Correction	0.22384	0.22196
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02880	-0.04207
(Hartree)		
Electronic	-1818.85836	-1818.81513
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1818.66332	-1818.63524

Specics	SLC-3o	TS-3o
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.21194	0.21050
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03091	-0.04371
(Hartree)		
Electronic	-2278.44605	-2278.40186
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2278.26503	-2278.23506

Specics	SLC-3p	TS-3p
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.24803	0.24757
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02932	-0.04119
(Hartree)		
Electronic	-1858.16121	-1858.12150
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1857.94250	-1857.91513

Specics	SLC-3q	TS-3q
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		

Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25286	0.25079
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03006	-0.04036
(Hartree)		
Electronic	-1933.36910	-1933.33380
Energy (Hartree)		
Imaginaires	0	1
G_{sol}(Hartree)	-1933.146295	-1933.12337

Specics	SLC-3r	TS-3r
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.23818	0.23703
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03197	-0.04100
(Hartree)		
Electronic	-1874.21237	-1874.18168
Energy (Hartree)		
Imaginaires	0	1
G_{sol}(Hartree)	-1874.00616	-1873.98564

Specics	SLC-3s	TS-3s
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.22022	0.21835
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03342	-0.04874
(Hartree)		
Electronic	-1911.08807	-1911.03623
Energy (Hartree)		
Imaginaires	0	1
G_{sol}(Hartree)	-1910.90128	-1910.86662

Specics	SLC-3t	TS-3t
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	

Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.22196	0.22037
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03364	-0.04953
(Hartree)		
Electronic	-2023.36037	-2023.30643
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2023.17205	-2023.13558
Specics	SLC-4a	TS-4a
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.17607	0.17065
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02399	-0.04229
(Hartree)		
Electronic	-1627.17173	-1627.11501
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1627.019647	-1626.98665
Specics	SLC-4b	TS-4b
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20177	0.19930
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02374	-0.04112
(Hartree)		
Electronic	-1666.47385	-1666.41944
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1666.29583	-1666.26126
Specics	SLC-4c	TS-4c

Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.23285	0.23054
Solvation Gibbs Free Energy (Hartree)	-0.02536	-0.04034
Electronic Energy (Hartree)	-1743.84084	-1743.78925
Imaginaries	0	1
G_{sol}(Hartree)	-1743.63336	-1743.59906
Specics	SLC-4d	TS-4d
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20934	0.20689
Solvation Gibbs Free Energy (Hartree)	-0.02649	-0.04192
Electronic Energy (Hartree)	-1742.59587	-1742.53867
Imaginaries	0	1
G_{sol}(Hartree)	-1742.41301	-1742.37370
Specics	SLC-4e	TS-4e
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.18329	0.17818
Solvation Gibbs Free Energy (Hartree)	-0.02848	-0.04072
Electronic Energy (Hartree)	-1740.47825	-1740.42012
Imaginaries	0	1
G_{sol}(Hartree)	-1740.32344	-1740.28266

Specics	SLC-4f	TS-4f
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20780	0.20705
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02771	-0.03400
(Hartree)		
Electronic	-1779.79120	-1779.74462
Energy (Hartree)		
Imaginaires	0	1
G_{sol}(Hartree)	-1779.61112	-1779.57157

Specics	SLC-4g	TS-4g
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.21186	0.20978
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02620	-0.03903
(Hartree)		
Electronic	-1855.02581	-1854.95936
Energy (Hartree)		
Imaginaires	0	1
G_{sol}(Hartree)	-1854.84015	-1854.78861

Specics	SLC-4h	TS-4h
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.26628	0.26725
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02385	-0.03250
(Hartree)		
Electronic	-2035.76597	-2035.74589
Energy (Hartree)		
Imaginaires	0	1
G_{sol}(Hartree)	-2035.52353	-2035.51114

Species	SLC-4i	TS-4i
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16343	0.16310
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02696	-0.03467
(Hartree)		
Electronic	-4200.81070	-4200.77528
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4200.67423	-4200.64685

Species	SLC-4j	TS-4j
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16643	0.16069
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02675	-0.03602
(Hartree)		
Electronic	-2086.76128	-2086.71701
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2086.62160	-2086.59234

Species	SLC-4k	TS-4k
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20314	0.20204
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02454	-0.03360
(Hartree)		
Electronic	-1741.67831	-1741.63513
Energy (Hartree)		
Imaginaries	0	1

G_{sol}(Hartree)	-1741.49970	-1741.46669
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Specics	SLC-4l	TS-4l
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.24457	0.24528
Solvation Gibbs Free Energy (Hartree)	-0.02492	-0.03109
Electronic Energy (Hartree)	-1761.09207	-1761.07131
Imaginaries	0	1
G_{sol}(Hartree)	-1760.87241	-1760.85712

Specics	SLC-4m	TS-4m
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20579	0.20408
Solvation Gibbs Free Energy (Hartree)	-0.02423	-0.03743
Electronic Energy (Hartree)	-1704.54179	-1704.50101
Imaginaries	0	1
G_{sol}(Hartree)	-1704.36022	-1704.33436

Specics	SLC-4n	TS-4n
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.25236	0.24976
Solvation Gibbs Free Energy (Hartree)	-0.02870	-0.03978
Electronic Energy (Hartree)	-1858.15904	-1858.11839

Imaginaries	0	1
G_{sol}(Hartree)	-1857.93538	-1857.90842
Specics	SLC-4o	TS-4o
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.23873	0.23761
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03095	-0.04180
(Hartree)		
Electronic	-2317.74686	-2317.70506
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2317.53909	-2317.50925
Specics	SLC-4p	TS-4p
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.27644	0.27422
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02865	-0.03907
(Hartree)		
Electronic	-1897.46292	-1897.42461
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1897.21514	-1897.18946
Specics	SLC-4q	TS-4q
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.28037	0.27785
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02948	-0.03905
(Hartree)		
Electronic	-1972.67084	-1972.63606

Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1972.41995	-1972.39726
Specics	SLC-4r	TS-4r
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.26627	0.26425
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03181	-0.03956
(Hartree)		
Electronic	-1913.51320	-1913.48394
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1913.27874	-1913.25926
Specics	SLC-4s	TS-4s
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.24696	0.24471
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03303	-0.04601
(Hartree)		
Electronic	-1950.38932	-1950.34043
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1950.17540	-1950.14174
Specics	SLC-4t	TS-4t
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25001	0.24828
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03312	-0.04639
(Hartree)		

Electronic Energy (Hartree)	-2062.66194	-2062.61124
Imaginaries	0	1
G _{sol} (Hartree)	-2062.44506	-2062.40934

Specics	SLC-5a	TS-5a
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.15048	0.14287
Solvation Gibbs Free Energy (Hartree)	-0.02433	-0.04799
Electronic Energy (Hartree)	-1587.87075	-1587.80376
Imaginaries	0	1
G _{sol} (Hartree)	-1587.74460	-1587.70888

Specics	SLC-5b	TS-5b
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17607	0.17065
Solvation Gibbs Free Energy (Hartree)	-0.02399	-0.04229
Electronic Energy (Hartree)	-1627.17173	-1627.11501
Imaginaries	0	1
G _{sol} (Hartree)	-1627.01965	-1626.98665

Specics	SLC-5c	TS-5c
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.13631	0.12918
Solvation Gibbs Free Energy	-0.02705	-0.04259

(Hartree)		
Electronic	-4161.50794	-4161.43423
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-4161.39868	-4161.34764
Specics	SLC-5d	TS-5d
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13778	0.13275
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02717	-0.04361
(Hartree)		
Electronic	-2047.45705	-2047.38478
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-2047.34644	-2047.29563
Specics	SLC-5e	TS-5e
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.17969	0.17574
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02460	-0.03884
(Hartree)		
Electronic	-1702.37596	-1702.31850
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1702.22087	-1702.18159
Specics	SLC-5f	TS-5f
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.24177	0.23348
(Hartree)		
Solvation Gibbs		

Free Energy (Hartree)	-0.02411	-0.04381
Electronic Energy (Hartree)	-1996.46644	-1996.40898
Imaginaries	0	1
G _{sol} (Hartree)	-1996.24877	-1996.21931
Specics	SLC-5g	TS-5g
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.22384	0.21936
Solvation Gibbs Free Energy (Hartree)	-0.02880	-0.04423
Electronic Energy (Hartree)	-1818.85836	-1818.80139
Imaginaries	0	1
G _{sol} (Hartree)	-1818.66332	-1818.62626
Specics	SLC-5h	TS-5h
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17945	0.17576
Solvation Gibbs Free Energy (Hartree)	-0.02429	-0.04245
Electronic Energy (Hartree)	-1665.24085	-1665.18309
Imaginaries	0	1
G _{sol} (Hartree)	-1665.08568	-1665.04978
Specics	SLC-5i	TS-5i
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20586	0.20134

Solvation Gibbs		
Free Energy	-0.02564	-0.04412
(Hartree)		
Electronic	-1704.53956	-1704.48127
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1704.35933	-1704.32405
Specics	SLC-5j	TS-5j
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15459	0.14874
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02483	-0.04296
(Hartree)		
Electronic	-1663.99334	-1663.92639
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1663.86358	-1663.82062
Specics	SLC-5k	TS-5k
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18221	0.17777
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02689	-0.04553
(Hartree)		
Electronic	-1703.29360	-1703.23311
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1703.13829	-1703.10087
Specics	SLC-5l	TS-5l
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14523	0.14084

(Hartree)		
Solvation Gibbs		
Free Energy	-0.02927	-0.04861
(Hartree)		
Electronic	-1680.09208	-1680.01160
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1679.97612	-1679.91937
Specics	SLC-5m	TS-5m
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15582	0.14890
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02905	-0.04942
(Hartree)		
Electronic	-1701.17534	-1701.10491
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1701.04857	-1701.00543
Specics	SLC-5n	TS-5n
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18000	0.17622
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02839	-0.05164
(Hartree)		
Electronic	-1740.48970	-1740.41707
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1740.33809	-1740.29249
Specics	SLC-5o	TS-5o
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		

G Correction (Hartree)	0.18610	0.18108
Solvation Gibbs Free Energy (Hartree)	-0.02706	-0.04712
Electronic Energy (Hartree)	-1815.72405	-1815.65292
Imaginaries	0	1
G_{sol}(Hartree)	-1815.56501	-1815.51896

Specics	SLC-6a	TS-6a
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17607	0.17326
Solvation Gibbs Free Energy (Hartree)	-0.02399	-0.04303
Electronic Energy (Hartree)	-1627.17173	-1627.11326
Imaginaries	0	1
G_{sol}(Hartree)	-1627.01965	-1626.98304

Specics	SLC-6b	TS-6b
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20177	0.19930
Solvation Gibbs Free Energy (Hartree)	-0.02374	-0.04112
Electronic Energy (Hartree)	-1666.47385	-1666.41944
Imaginaries	0	1
G_{sol}(Hartree)	-1666.29583	-1666.26126

Specics	SLC-6c	TS-6c
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	

Energy Level		
G Correction	0.16343	0.15931
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02696	-0.04819
(Hartree)		
Electronic	-4200.81070	-4200.73636
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4200.67423	-4200.62523

Specics	SLC-6d	TS-6d
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16643	0.16148
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02675	-0.04542
(Hartree)		
Electronic	-2086.76128	-2086.68985
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2086.62160	-2086.57378

Specics	SLC-6e	TS-6e
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20314	0.20379
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02454	-0.03983
(Hartree)		
Electronic	-1741.67831	-1741.62207
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1741.49970	-1741.45810

Specics	SLC-6f	TS-6f
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		

Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.26628	0.26525
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02385	-0.04154
(Hartree)		
Electronic	-2035.76597	-2035.71407
Energy (Hartree)		
Imaginaires	0	1
G _{sol} (Hartree)	-2035.52353	-2035.49035

Specics	SLC-6g	TS-6g
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25236	0.24673
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02870	-0.04524
(Hartree)		
Electronic	-1858.15904	-1858.10133
Energy (Hartree)		
Imaginaires	0	1
G _{sol} (Hartree)	-1857.93538	-1857.89984

Specics	SLC-6h	TS-6h
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20579	0.20330
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02423	-0.04097
(Hartree)		
Electronic	-1704.54179	-1704.48648
Energy (Hartree)		
Imaginaires	0	1
G _{sol} (Hartree)	-1704.36022	-1704.32414

Specics	SLC-6i	TS-6i
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	

Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.23285	0.22999
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02536	-0.04156
(Hartree)		
Electronic	-1743.84084	-1743.78743
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1743.63336	-1743.59901
Specics	SLC-6j	TS-6j
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18134	0.18012
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02454	-0.04171
(Hartree)		
Electronic	-1703.29646	-1703.23228
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1703.13966	-1703.09387
Specics	SLC-6k	TS-6k
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20934	0.20722
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02649	-0.04334
(Hartree)		
Electronic	-1742.59587	-1742.54066
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1742.41301	-1742.37678
Specics	SLC-6l	TS-6l

Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17185	0.16687
Solvation Gibbs Free Energy (Hartree)	-0.02845	-0.05406
Electronic Energy (Hartree)	-1719.39456	-1719.31350
Imaginaries	0	1
G_{sol}(Hartree)	-1719.25116	-1719.20069

Specics	SLC-6m	TS-6m
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.18329	0.17964
Solvation Gibbs Free Energy (Hartree)	-0.02848	-0.04820
Electronic Energy (Hartree)	-1740.47825	-1740.41611
Imaginaries	0	1
G_{sol}(Hartree)	-1740.32344	-1740.28467

Specics	SLC-6n	TS-6n
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.20780	0.20659
Solvation Gibbs Free Energy (Hartree)	-0.02771	-0.04066
Electronic Energy (Hartree)	-1779.79120	-1779.73779
Imaginaries	0	1
G_{sol}(Hartree)	-1779.61112	-1779.57185

Specics	SLC-6o	TS-6o
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21186	0.21067
Solvation Gibbs Free Energy (Hartree)	-0.02620	-0.04218
Electronic Energy (Hartree)	-1855.02581	-1854.96747
Imaginaries	0	1
G_{sol}(Hartree)	-1854.84015	-1854.79898
Specics	SLC-7a	TS-7a
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.13608	0.13519
Solvation Gibbs Free Energy (Hartree)	-0.03054	-0.03688
Electronic Energy (Hartree)	-4161.50190	-4161.46406
Imaginaries	0	1
G_{sol}(Hartree)	-4161.39636	-4161.36575
Specics	SLC-7b	TS-7b
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.16343	0.16310
Solvation Gibbs Free Energy (Hartree)	-0.02696	-0.03467
Electronic Energy (Hartree)	-4200.81070	-4200.77528
Imaginaries	0	1
G_{sol}(Hartree)	-4200.67423	-4200.64685

Species	SLC-7c	TS-7c
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.12522	0.12194
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02932	-0.03322
(Hartree)		
Electronic	-6735.13634	-6735.09454
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-6735.04043	-6735.00582

Species	SLC-7d	TS-7d
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.12459	0.12382
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02584	-0.03309
(Hartree)		
Electronic	-4621.09081	-4621.04532
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4620.99207	-4620.95459

Species	SLC-7e	TS-7e
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16524	0.16487
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02675	-0.03409
(Hartree)		
Electronic	-4276.01755	-4275.98879
Energy (Hartree)		
Imaginaries	0	1

G_{sol}(Hartree)	-4275.87906	-4275.85800
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Specics	SLC-7f	TS-7f
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.22888	0.22629
Solvation Gibbs Free Energy (Hartree)	-0.02563	-0.03228
Electronic Energy (Hartree)	-4570.10829	-4570.07290
Imaginaries	0	1
G_{sol}(Hartree)	-4569.90503	-4569.87890

Specics	SLC-7g	TS-7g
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21261	0.20905
Solvation Gibbs Free Energy (Hartree)	-0.03087	-0.03821
Electronic Energy (Hartree)	-4392.49507	-4392.45810
Imaginaries	0	1
G_{sol}(Hartree)	-4392.31334	-4392.28726

Specics	SLC-7h	TS-7h
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.16589	0.16508
Solvation Gibbs Free Energy (Hartree)	-0.02695	-0.03448
Electronic Energy (Hartree)	-4238.87907	-4238.84390

Imaginaries	0	1
G_{sol}(Hartree)	-4238.74013	-4238.71330
Specics	SLC-7i	TS-7i
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.19243	0.19321
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02783	-0.03490
(Hartree)		
Electronic	-4278.17984	-4278.14422
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4278.01524	-4277.98591
Specics	SLC-7j	TS-7j
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14289	0.13948
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02660	-0.03332
(Hartree)		
Electronic	-4237.62818	-4237.58664
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4237.51188	-4237.48049
Specics	SLC-7k	TS-7k
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16864	0.16626
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02900	-0.04383
(Hartree)		
Electronic	-4276.93176	-4276.88479

Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4276.79212	-4276.76237
Specics	SLC-7l	TS-7l
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13302	0.12928
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02690	-0.03491
(Hartree)		
Electronic	-4253.72389	-4253.67291
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4253.61777	-4253.57855
Specics	SLC-7m	TS-7m
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14448	0.14000
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02790	-0.04868
(Hartree)		
Electronic	-4274.81413	-4274.75330
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4274.69755	-4274.66198
Specics	SLC-7n	TS-7n
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16922	0.16757
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02882	-0.03857
(Hartree)		

Electronic Energy (Hartree)	-4314.12724	-4314.08067
Imaginaries	0	1
G _{sol} (Hartree)	-4313.98684	-4313.95167

Specics	SLC-7o	TS-7o
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17262	0.17105
Solvation Gibbs Free Energy (Hartree)	-0.02782	-0.03599
Electronic Energy (Hartree)	-4389.35917	-4389.31419
Imaginaries	0	1
G _{sol} (Hartree)	-4389.21437	-4389.17913

Specics	SLC-1b	TS-1b-H
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.25045	0.24668
Solvation Gibbs Free Energy (Hartree)	-0.03108	-0.04661
Electronic Energy (Hartree)	-1858.15454	-1858.09504
Imaginaries	0	1
G _{sol} (Hartree)	-1857.93518	-1857.89497

Specics	TS-1b-Me ¹	TS-1b-Me ²
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.25015	0.24960
Solvation Gibbs Free Energy	-0.04728	-0.05324

(Hartree)		
Electronic	-1858.10080	-1858.08829
Energy (Hartree)		
Imaginaries	1	1
G _{sol} (Hartree)	-1857.89793	-1857.89193
Specics	SLC-1a	TS-1a-H
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25153	0.24553
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02894	-0.04736
(Hartree)		
Electronic	-1858.16017	-1858.10098
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1857.93758	-1857.90281
Specics	TS-1a-Me ¹	TS-1a-Me ²
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.24818	0.24891
(Hartree)		
Solvation Gibbs		
Free Energy	-0.04782	-0.04739
(Hartree)		
Electronic	-1858.10051	-1858.10046
Energy (Hartree)		
Imaginaries	1	1
G _{sol} (Hartree)	-1857.90015	-1857.89894
Specics	SLC-8a	TS-8a-H
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15421	0.14681
(Hartree)		
Solvation Gibbs		

Free Energy (Hartree)	-0.02506	-0.05089
Electronic Energy (Hartree)	-1625.93424	-1625.84945
Imaginaries	0	1
G_{sol}(Hartree)	-1625.80509	-1625.75354

Specics	SLC-8b	TS-8b-H
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.18309	0.17794
Solvation Gibbs Free Energy (Hartree)	-0.02522	-0.04477
Electronic Energy (Hartree)	-1665.23781	-1665.17789
Imaginaries	0	1
G_{sol}(Hartree)	-1665.07994	-1665.04472

Specics	SLC-8c	TS-8c-H
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21108	0.20642
Solvation Gibbs Free Energy (Hartree)	-0.02596	-0.04369
Electronic Energy (Hartree)	-1704.56659	-1704.51162
Imaginaries	0	1
G_{sol}(Hartree)	-1704.38146	-1704.34889

Specics	SLC-8d	TS-8d-H
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction	0.24008	0.23457

(Hartree)		
Solvation Gibbs		
Free Energy	-0.02658	-0.04403
(Hartree)		
Electronic	-1743.87331	-1743.81795
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1743.65980	-1743.62741

Specics	SLC-8e	TS-8e-H
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.26730	0.26229
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02724	-0.04431
(Hartree)		
Electronic	-1783.16132	-1783.10749
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1782.92126	-1782.88951

Specics	SLC-8a	TS-8a-C
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15421	0.15376
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02506	-0.04339
(Hartree)		
Electronic	-1625.93424	-1625.89105
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1625.80509	-1625.78069

Specics	SLC-8b	TS-8b-C
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		

G Correction (Hartree)	0.18309	0.18108
Solvation Gibbs Free Energy (Hartree)	-0.02522	-0.04080
Electronic Energy (Hartree)	-1665.23781	-1665.19175
Imaginaries	0	1
G_{sol}(Hartree)	-1665.07994	-1665.05147

Specics	SLC-8c	TS-8c-C
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21108	0.20877
Solvation Gibbs Free Energy (Hartree)	-0.02596	-0.04424
Electronic Energy (Hartree)	-1704.56659	-1704.51670
Imaginaries	0	1
G_{sol}(Hartree)	-1704.38146	-1704.35216

Specics	SLC-8d	TS-8d-C
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.24008	0.23671
Solvation Gibbs Free Energy (Hartree)	-0.02658	-0.05237
Electronic Energy (Hartree)	-1743.87331	-1743.80415
Imaginaries	0	1
G_{sol}(Hartree)	-1743.65980	-1743.61981

Specics	SLC-8e	TS-8e-C
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	

Energy Level		
G Correction	0.26730	0.26613
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02724	-0.05183
(Hartree)		
Electronic	-1783.16132	-1783.10065
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1782.92126	-1782.88635

Sub-S1-Type B

C	-2.857336	-0.393537	0.498242
C	-2.216332	-1.444127	-0.418559
H	-3.131595	-0.765898	1.484413
H	-2.531113	-1.417079	-1.462592
H	-2.183794	-2.470535	-0.054189
O	-1.501633	0.249662	0.626285
C	-0.981720	-0.664055	-0.148928
O	0.193558	-0.760242	-0.484874
C	-3.864321	0.547059	-0.085254
H	-3.977428	1.402151	0.586937
H	-3.489147	0.928187	-1.040418
Al	1.771196	0.255246	-0.137682
Cl	1.237793	2.208398	-0.903747
Cl	1.853171	0.254381	2.025918
C	3.208341	-0.688077	-1.063804
C	3.446824	-2.120021	-0.583703
H	4.126566	-0.097633	-0.954784
H	2.982386	-0.680505	-2.137905
H	4.263344	-2.608181	-1.127672
H	3.705210	-2.150946	0.479071
H	2.557628	-2.745149	-0.714639
C	-5.200051	-0.154450	-0.278776
H	-5.930816	0.533958	-0.706808
H	-5.110768	-1.007954	-0.956491
H	-5.600236	-0.517978	0.671421

TS-S1-Type B

C	3.328400	0.827484	0.244802
C	2.093523	1.379779	-0.357128
H	3.491224	0.963947	1.312265
H	2.137468	1.406753	-1.447682
H	1.861442	2.376693	0.021558

O	1.350030	-0.579326	0.735741
C	1.008823	0.394747	0.084514
O	-0.171962	0.708715	-0.299551
C	4.312017	0.166314	-0.472753
H	4.476636	1.394319	-0.369459
H	4.124928	0.021774	-1.536155
Al	-1.762702	-0.190963	-0.150406
Cl	-1.478358	-2.100953	-1.174037
Cl	-2.125750	-0.516731	1.977487
C	-3.134746	0.929874	-0.998184
C	-3.296529	2.319654	-0.382657
H	-4.089775	0.390485	-0.959089
H	-2.893092	1.017493	-2.065947
H	-4.071759	2.914376	-0.881048
H	-3.569900	2.260657	0.675671
H	-2.366819	2.895709	-0.438490
C	5.441394	-0.573083	0.149418
H	5.189381	-1.637185	0.104700
H	6.365610	-0.428904	-0.410944
H	5.587778	-0.296700	1.193651

Imaginary vibration frequency: 311.57i

Sub-S1-Type C

C	-2.111520	0.254119	-0.597543
C	-2.513010	1.721876	-0.484575
H	-1.905040	-0.095649	-1.607088
H	-3.359810	1.934716	0.168587
H	-2.619814	2.257388	-1.428355
O	-0.768950	0.623582	0.021198
C	-1.187526	1.968326	0.161992
O	-0.564333	2.835773	0.652981
C	-2.879961	-0.720998	0.238314
H	-3.900348	-0.694454	-0.163095
H	-2.940676	-0.336864	1.262441
Al	1.027454	-0.153171	0.013582
Cl	1.080276	-1.244571	1.873409
Cl	0.808419	-1.484998	-1.674733
C	2.302704	1.308632	-0.194553
H	2.233776	1.964511	0.680389
H	2.004549	1.921543	-1.054340
C	3.741607	0.819104	-0.374412
H	3.847124	0.184280	-1.259492
H	4.445089	1.651056	-0.488742
H	4.078041	0.230646	0.484804

C	-2.353629	-2.143640	0.218153
H	-2.294960	-2.531297	-0.801523
H	-1.360592	-2.215869	0.664996
H	-3.017786	-2.795470	0.789674

TS-S1-Type C

C	2.637574	0.056421	-0.677904
C	2.614643	-1.400326	-0.414464
H	2.501212	0.407258	-1.698252
H	3.058950	-1.654997	0.548421
H	3.118146	-1.962455	-1.203143
O	0.352013	-0.865098	-0.808754
C	1.133015	-1.820103	-0.385831
O	0.809095	-2.916582	-0.015560
C	2.779488	1.018629	0.309881
H	3.825373	0.608108	-0.290277
H	2.908912	0.660115	1.329476
Al	-1.097098	-0.011059	-0.128116
Cl	-2.758895	-1.379548	0.152381
Cl	-0.348130	0.609407	1.850725
C	-1.491995	1.515211	-1.298842
H	-1.753674	1.125705	-2.291609
H	-0.566765	2.090147	-1.442963
C	-2.602040	2.436145	-0.793311
H	-2.356816	2.863767	0.184194
H	-2.796176	3.274714	-1.472495
H	-3.546206	1.895916	-0.673610
C	2.578710	2.471885	0.096351
H	2.522316	2.731891	-0.960909
H	1.625831	2.725328	0.572378
H	3.355356	3.056929	0.590715

Imaginary vibration frequency: 262.41i

Sub-S2-Type B

C	-1.284717	-0.217878	-0.717225
C	-0.812066	1.202390	-0.391070
H	-1.547696	-0.384585	-1.760709
H	-1.190459	1.626583	0.539591
H	-0.866201	1.937051	-1.194201
O	0.137771	-0.681640	-0.533955
C	0.510742	0.540667	-0.259348
O	1.645641	0.917013	0.011241
C	-2.214223	-0.903271	0.251670
H	-1.813342	-0.738032	1.257863

Al	3.318782	0.027959	0.243892
Cl	2.851678	-1.407877	1.796335
Cl	3.597938	-0.947657	-1.668038
C	4.594433	1.432473	0.704405
C	4.768744	2.514922	-0.361268
H	5.559558	0.956177	0.917377
H	4.275280	1.882051	1.653516
H	5.496553	3.277133	-0.060911
H	5.116542	2.094708	-1.309755
H	3.828294	3.035795	-0.568109
C	-3.558337	-0.215107	0.174894
C	-4.351717	-0.306334	-0.968169
C	-4.015540	0.546816	1.246823
C	-5.572950	0.349032	-1.034701
H	-4.021893	-0.900840	-1.814037
C	-5.239064	1.200396	1.184313
H	-3.410316	0.619001	2.145277
C	-6.020396	1.104877	0.041347
H	-6.179307	0.266870	-1.930317
H	-5.582426	1.783484	2.032057
H	-6.976421	1.614234	-0.010262
C	-2.279962	-2.402134	-0.012168
H	-2.644884	-2.615152	-1.019800
H	-1.293248	-2.858083	0.094925
H	-2.954662	-2.879860	0.700543

TS-S2-Type B

C	1.748788	-0.442791	0.328723
C	0.880247	0.654032	-0.184597
H	1.827473	-0.553532	1.404816
H	1.033585	0.866499	-1.242998
H	0.967163	1.578599	0.387988
O	-0.360036	-1.176226	0.457887
C	-0.453918	-0.020741	0.033842
O	-1.519071	0.620504	-0.230958
C	2.535229	-1.328645	-0.483814
H	2.268617	-1.291940	-1.538946
Al	-3.292066	0.129277	-0.142742
Cl	-3.518461	-1.549485	-1.518847
Cl	-3.654328	-0.514936	1.909648
C	-4.339602	1.708054	-0.655448
C	-4.149081	2.922205	0.253698
H	-5.399137	1.423250	-0.681351
H	-4.082174	1.968981	-1.690646

H	-4.749093	3.783907	-0.062935
H	-4.431620	2.697897	1.287067
H	-3.104655	3.250846	0.274520
C	3.632561	-0.263892	-0.220283
C	4.427141	-0.314822	0.933462
C	3.860499	0.739574	-1.173794
C	5.452187	0.596717	1.108052
H	4.249186	-1.078199	1.681335
C	4.889277	1.641971	-0.995133
H	3.240358	0.786458	-2.062172
C	5.683158	1.572383	0.146408
H	6.071096	0.548957	1.996236
H	5.076210	2.403925	-1.742633
H	6.486349	2.287329	0.286665
C	2.795331	-2.724807	0.021278
H	1.927255	-3.345813	-0.207239
H	3.671439	-3.152055	-0.469116
H	2.944169	-2.750203	1.101660

Imaginary vibration frequency: 309.56i

Sub-S2-Type C

C	-0.657300	0.431574	-0.372287
C	-0.875474	1.923348	-0.606805
H	-0.597805	-0.180135	-1.270024
H	-1.633064	2.400758	0.014541
H	-1.003433	2.222580	-1.647488
O	0.767706	0.749209	0.048403
C	0.521970	2.136356	-0.123004
O	1.285720	3.000906	0.100844
C	-1.457805	-0.206162	0.738639
Al	2.467308	-0.227811	-0.008129
Cl	2.739669	-0.837143	2.041883
Cl	1.856563	-1.885508	-1.253619
C	3.807472	0.969190	-0.767792
H	3.948448	1.819354	-0.091340
H	3.418673	1.389813	-1.703680
C	5.145561	0.271644	-1.023870
H	5.040582	-0.565637	-1.720585
H	5.887549	0.955142	-1.450867
H	5.574085	-0.130500	-0.100660
C	-2.905942	-0.192330	0.298566
C	-3.839713	0.590289	0.971858
C	-3.326702	-0.948394	-0.794714
C	-5.167824	0.615577	0.566983

H	-3.524563	1.178551	1.828280
C	-4.652015	-0.920727	-1.204078
H	-2.616323	-1.572167	-1.327696
C	-5.576831	-0.138376	-0.524166
H	-5.884352	1.225191	1.106923
H	-4.964441	-1.515371	-2.055741
H	-6.613372	-0.119777	-0.842435
C	-0.971883	-1.602945	1.099946
H	-1.000159	-2.272646	0.238319
H	0.050154	-1.583620	1.481914
H	-1.611081	-2.022798	1.879123
H	-1.370351	0.442686	1.616968

TS-S2-Type C

C	1.239717	-0.261163	-0.227976
C	1.073362	-1.727028	-0.284275
H	1.105621	0.304354	-1.144875
H	1.553776	-2.254756	0.538868
H	1.382218	-2.159828	-1.236602
O	-0.885112	-0.567863	-0.071931
C	-0.447407	-1.812151	-0.145749
O	-1.098064	-2.813134	-0.105346
C	1.729812	0.460067	0.928010
Al	-2.592781	0.151363	-0.052017
Cl	-3.613964	-0.694443	-1.777356
Cl	-3.507391	-0.532299	1.800151
C	-2.388743	2.102633	-0.156394
H	-1.727047	2.342938	-0.999622
H	-1.865956	2.452013	0.742669
C	-3.711412	2.855735	-0.304616
H	-4.380753	2.659640	0.539070
H	-3.572082	3.941930	-0.357701
H	-4.246655	2.555022	-1.210421
C	3.158037	0.330405	0.353230
C	4.000119	-0.681297	0.827622
C	3.619453	1.208850	-0.632576
C	5.297405	-0.777528	0.361020
H	3.638075	-1.370077	1.582942
C	4.918481	1.102148	-1.101309
H	2.969091	1.984741	-1.019396
C	5.756514	0.112349	-0.605584
H	5.955246	-1.546846	0.748714
H	5.276821	1.792594	-1.855976
H	6.772894	0.030518	-0.974397

C	1.225475	1.868251	1.140421
H	1.168477	2.429430	0.206771
H	0.223855	1.829172	1.570466
H	1.881258	2.400229	1.831482
H	1.674889	-0.143835	1.833960

Imaginary vibration frequency: 190.52i

Sub-S3-Type B

C	-2.047235	-0.798293	-0.105437
C	-1.448929	-0.777872	-1.511621
H	-2.357440	-1.777883	0.254167
H	-1.772845	0.048626	-2.144697
H	-1.459480	-1.713086	-2.070682
O	-0.670155	-0.538021	0.439435
C	-0.184103	-0.525356	-0.774948
O	0.988092	-0.352453	-1.091264
C	-2.994704	0.319601	0.260441
Al	2.574959	0.038033	-0.109229
C	3.989632	0.222329	-1.442143
C	5.363659	0.550105	-0.856224
H	3.689844	1.001047	-2.155186
H	4.040290	-0.708882	-2.020889
H	6.132037	0.646838	-1.631416
H	5.349894	1.491685	-0.298506
H	5.702196	-0.226734	-0.163610
Cl	2.021266	1.837696	0.963056
Cl	2.730632	-1.645985	1.242242
N	-4.201617	0.142378	-0.541188
C	-4.914782	1.386082	-0.747690
H	-5.728678	1.221275	-1.457928
H	-5.354435	1.796975	0.176286
H	-4.243266	2.136106	-1.171745
C	-5.095995	-0.897337	-0.068894
H	-5.598708	-0.645303	0.878132
H	-5.869651	-1.065667	-0.821744
H	-4.563646	-1.840777	0.067524
C	-3.188267	0.420939	1.767650
H	-3.555552	-0.516409	2.192312
H	-2.243737	0.666504	2.257709
H	-3.901805	1.211433	2.009864
H	-2.529570	1.246688	-0.093544

TS-S3-Type B

C	2.318058	0.061364	0.530163
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C	1.504311	1.323256	0.405369
H	2.536255	-0.313769	1.522797
H	1.707478	1.904926	-0.494036
H	1.535747	1.975192	1.278869
O	0.592180	-0.683131	0.380332
C	0.245999	0.525943	0.307076
O	-0.916263	0.977338	0.177071
C	3.191527	-0.417789	-0.552080
Al	-2.566776	0.137439	-0.000593
C	-3.896216	1.560658	-0.211567
C	-5.329726	1.063298	-0.397955
H	-3.601534	2.182641	-1.067069
H	-3.838785	2.217225	0.666589
H	-6.046610	1.884710	-0.512937
H	-5.422998	0.429316	-1.285408
H	-5.662080	0.464867	0.456213
Cl	-2.356267	-1.156597	-1.739263
Cl	-2.800430	-1.052615	1.805917
N	4.208833	0.460267	0.036597
C	4.696410	1.534711	-0.802802
H	5.187309	2.288411	-0.184239
H	5.416635	1.165517	-1.546324
H	3.869562	2.009053	-1.331232
C	5.224586	-0.142302	0.874605
H	5.975238	-0.684354	0.284773
H	5.728069	0.646442	1.436123
H	4.780617	-0.832588	1.591618
C	3.467526	-1.894384	-0.659427
H	3.699593	-2.345721	0.306037
H	2.579715	-2.389710	-1.056992
H	4.295265	-2.081798	-1.346540
H	2.888448	-0.014528	-1.519355

Imaginary vibration frequency: 486.29i

Sub-S3-Type C

C	-1.224816	0.593132	-0.546745
C	-1.381697	2.106549	-0.558864
H	-1.093160	0.120623	-1.517271
H	-2.194850	2.496338	0.052658
H	-1.394629	2.577341	-1.542188
O	0.150770	0.771656	0.055847
C	-0.036473	2.183100	0.087857
O	0.726590	2.963657	0.521615
C	-2.158130	-0.150595	0.386268

H	-2.107408	0.371869	1.348300
Al	1.813207	-0.264349	0.024852
Cl	1.860946	-1.155147	1.988307
Cl	1.281177	-1.713940	-1.487987
C	3.258019	0.967697	-0.424474
H	3.349414	1.710248	0.375997
H	2.980299	1.529056	-1.325532
C	4.597530	0.259828	-0.640930
H	4.545410	-0.468155	-1.456272
H	5.397394	0.965835	-0.889621
H	4.916106	-0.282895	0.254421
N	-3.508058	0.075722	-0.125556
C	-3.866167	-0.747399	-1.265468
H	-4.005015	-1.809631	-1.010788
H	-4.804914	-0.379211	-1.685996
H	-3.108305	-0.682219	-2.048755
C	-4.515184	-0.004870	0.912125
H	-5.482154	0.291997	0.498727
H	-4.628512	-1.017055	1.334627
H	-4.270957	0.681425	1.726214
C	-1.764898	-1.603669	0.601915
H	-1.674726	-2.146835	-0.340135
H	-0.810487	-1.677955	1.125671
H	-2.512853	-2.104953	1.220516

TS-S3-Type C

C	-1.527913	0.517741	-0.452338
C	-1.541781	2.019859	-0.393094
H	-1.394192	0.040026	-1.416292
H	-2.185721	2.433369	0.383040
H	-1.752999	2.508440	-1.344531
O	0.216578	0.777500	-0.034049
C	-0.083579	2.100282	-0.031502
O	0.662342	2.996508	0.199410
C	-2.236282	-0.290262	0.566668
H	-2.326044	0.265239	1.501705
Al	1.849917	-0.166342	-0.003018
Cl	1.948700	-0.927338	2.029478
Cl	1.352845	-1.786792	-1.369613
C	3.343833	0.965134	-0.560714
H	3.438626	1.786325	0.159201
H	3.085719	1.437218	-1.517295
C	4.671109	0.215747	-0.685689
H	4.612362	-0.592996	-1.420755

H	5.489839	0.874667	-0.996644
H	4.968517	-0.237665	0.265106
N	-3.471889	-0.120474	-0.201183
C	-3.882972	-1.214446	-1.055328
H	-4.302948	-2.054320	-0.485198
H	-4.644934	-0.851659	-1.747789
H	-3.043492	-1.583233	-1.645258
C	-4.562103	0.531195	0.491477
H	-5.318812	0.844736	-0.230497
H	-5.035768	-0.136722	1.225996
H	-4.202396	1.417732	1.015832
C	-1.751107	-1.690029	0.846935
H	-1.562826	-2.257605	-0.064287
H	-0.818779	-1.645532	1.412417
H	-2.484696	-2.225439	1.453685

Imaginary vibration frequency: 435.55i

A-Al

C	2.500001	0.805956	0.275581
C	1.229694	0.825057	-0.582573
H	2.899552	1.794666	0.498063
H	1.154779	0.093715	-1.386122
H	0.901345	1.802328	-0.936337
O	1.638979	0.404648	1.449212
C	0.579702	0.408103	0.687247
O	-0.548985	0.124412	1.080252
C	3.599904	-0.195316	-0.005048
Al	-2.172609	-0.039205	0.108279
C	-3.561709	-0.540002	1.381499
C	-4.948454	-0.712405	0.759999
H	-3.594387	0.222550	2.170020
H	-3.252744	-1.468960	1.877305
H	-5.701735	-0.993491	1.504229
H	-5.295196	0.210323	0.284595
H	-4.951774	-1.490149	-0.009948
Cl	-2.338844	1.913294	-0.823189
Cl	-1.625209	-1.509888	-1.392076
C	3.058805	-1.611951	-0.175895
H	2.565285	-1.968952	0.731262
H	2.354105	-1.693373	-1.007013
H	3.887863	-2.291038	-0.387461
C	4.594657	-0.158382	1.153312
H	5.423675	-0.842066	0.955011
H	5.009530	0.844579	1.288224

H	4.125839	-0.464804	2.091889
C	4.280745	0.267477	-1.293178
H	4.669609	1.285412	-1.198236
H	5.121790	-0.391785	-1.520356
H	3.595258	0.239097	-2.144619

TS_{AB-AI}

C	2.533271	0.629232	0.796754
C	1.493085	1.577145	0.187880
H	2.986333	1.001744	1.715018
H	1.509864	1.707352	-0.893465
H	1.372174	2.541362	0.682065
O	1.395792	-0.275265	1.201997
C	0.533738	0.543421	0.659668
O	-0.676851	0.388460	0.644048
C	3.545987	-0.071524	-0.083764
Al	-2.255013	-0.198225	-0.201417
Cl	-1.522865	-1.933776	-1.272331
Cl	-3.486649	-0.754400	1.481852
C	-2.900402	1.275412	-1.312271
C	-3.149954	2.580782	-0.556819
H	-3.821217	0.948228	-1.810864
H	-2.174194	1.436693	-2.119751
H	-3.509736	3.379115	-1.215732
H	-3.898071	2.453456	0.231348
H	-2.239573	2.951354	-0.073825
C	4.256510	-1.133959	0.752463
H	3.558393	-1.899822	1.099551
H	5.025178	-1.628490	0.153822
H	4.742507	-0.690644	1.626489
C	2.898526	-0.722498	-1.302594
H	2.173899	-1.488532	-1.017231
H	2.397833	0.003824	-1.947834
H	3.670657	-1.208698	-1.903224
C	4.542723	0.999681	-0.525715
H	5.012562	1.490262	0.331684
H	5.334027	0.540204	-1.122651
H	4.063842	1.766802	-1.140786

Imaginary vibration frequency: 53.53i

B-AI

C	-2.337864	-0.791379	0.543011
C	-1.594533	-1.813015	-0.328447
H	-2.582148	-1.159955	1.538789

H	-1.889637	-1.880923	-1.374577
H	-1.473167	-2.809829	0.095596
O	-1.041702	-0.030549	0.664540
C	-0.438464	-0.914666	-0.083168
O	0.741796	-0.910314	-0.417031
C	-3.455084	0.053338	-0.030113
Al	2.196239	0.289127	-0.128587
Cl	1.428314	2.141609	-0.946479
Cl	2.309913	0.372003	2.031910
C	3.720228	-0.509002	-1.052404
C	4.128851	-1.890082	-0.539214
H	4.565572	0.185935	-0.974116
H	3.480479	-0.557282	-2.122461
H	4.988527	-2.296042	-1.084249
H	4.403980	-1.861436	0.519403
H	3.315934	-2.616636	-0.638550
C	-3.798267	1.144397	0.982526
H	-2.953544	1.818997	1.142738
H	-4.638416	1.740725	0.618623
H	-4.082115	0.714731	1.947486
C	-3.074509	0.690366	-1.363563
H	-2.203863	1.343432	-1.267184
H	-2.868739	-0.052132	-2.138652
H	-3.906012	1.303431	-1.718736
C	-4.647591	-0.884605	-0.214048
H	-4.939565	-1.352339	0.730610
H	-5.505433	-0.319689	-0.586271
H	-4.430173	-1.676273	-0.936683

TS_{BC-Al}

C	2.103900	-0.441030	-0.789181
C	2.019645	-1.919105	-0.386222
H	2.209511	-0.281472	-1.861571
H	2.576942	-2.217218	0.500411
H	2.171649	-2.640052	-1.188841
O	0.626720	-0.323735	-0.472326
C	0.579395	-1.620116	-0.119027
O	-0.437214	-2.128270	0.257136
C	2.951366	0.528791	0.004448
Al	-1.704153	0.070740	0.021069
Cl	-2.954139	-1.043233	-1.327399
Cl	-2.064771	-0.165744	2.127729
C	-1.412078	1.927234	-0.518785
C	-2.695463	2.757889	-0.495518

H	-0.968855	1.937291	-1.521227
H	-0.666287	2.365625	0.154290
H	-2.515079	3.797219	-0.792289
H	-3.450409	2.355356	-1.177582
H	-3.143336	2.782650	0.502717
C	2.653472	1.944291	-0.484694
H	1.612653	2.219359	-0.299682
H	3.288309	2.662637	0.039644
H	2.847404	2.041735	-1.556747
C	2.687587	0.433417	1.504046
H	1.648766	0.668901	1.748197
H	2.921871	-0.554946	1.907495
H	3.319356	1.154310	2.028002
C	4.406086	0.170760	-0.301312
H	4.614896	0.225460	-1.373677
H	5.071058	0.874591	0.204724
H	4.657513	-0.835196	0.045612

Imaginary vibration frequency: 154.42i

C-Al

C	-1.576571	-0.055035	0.718301
C	-1.875959	-1.521187	1.023850
H	-1.202080	0.520502	1.563828
H	-2.851757	-1.914031	0.746517
H	-1.628241	-1.821593	2.043657
O	-0.383840	-0.505085	-0.098389
C	-0.766691	-1.872345	0.087412
O	-0.260726	-2.799576	-0.421190
C	-2.578071	0.730974	-0.106937
Al	1.452424	0.173755	-0.064239
Cl	2.247697	-1.099042	1.496565
Cl	2.166556	-0.381192	-2.014292
C	1.447126	2.077743	0.378090
H	0.804992	2.259303	1.248268
H	1.007940	2.645891	-0.448573
C	2.862504	2.588417	0.665066
H	3.524080	2.450117	-0.195697
H	2.869251	3.656862	0.906558
H	3.320098	2.063752	1.508938
C	-1.963144	2.062322	-0.526089
H	-1.607802	2.630574	0.337036
H	-1.126293	1.916990	-1.213173
H	-2.712288	2.666851	-1.043025
C	-3.025107	-0.033206	-1.350711

H	-3.541429	-0.965711	-1.110510
H	-3.724712	0.584838	-1.917888
H	-2.183069	-0.261065	-2.009131
C	-3.770348	0.981141	0.817551
H	-3.474709	1.542263	1.708638
H	-4.525537	1.567189	0.288778
H	-4.238155	0.046773	1.139652

A-Sn

C	-3.282959	0.364748	0.779722
C	-1.970342	-0.394891	1.007437
H	-3.735160	0.761382	1.699688
H	-1.832209	-1.354323	0.492626
H	-1.641172	-0.482866	2.051724
O	-2.498498	1.457706	0.149180
C	-1.378726	0.785999	0.306804
O	-0.283418	1.169177	-0.066520
C	-4.346204	-0.196479	-0.152984
Cl	1.325939	-0.043348	2.279439
Cl	0.514504	-1.492777	-1.396787
C	-3.755756	-0.604924	-1.503201
H	-3.312776	0.254250	-2.029203
H	-2.984125	-1.384276	-1.409030
H	-4.550759	-1.011797	-2.146204
C	-5.410594	0.882555	-0.362226
H	-6.206052	0.512733	-1.027139
H	-5.876786	1.175669	0.591905
H	-4.978513	1.784467	-0.822599
C	-4.955049	-1.410934	0.550484
H	-5.367834	-1.143354	1.536388
H	-5.776124	-1.824544	-0.054688
H	-4.211792	-2.210922	0.695948
Sn	1.718948	0.001048	-0.037017
Cl	2.482207	1.984356	-0.998177
Cl	3.758468	-1.195310	-0.010715

TS_{AB-Sn}

C	-3.390692	-0.935810	0.195875
C	-2.409852	-1.489559	-0.844826
H	-4.090843	-1.681807	0.598163
H	-2.249924	-0.914614	-1.765799
H	-2.521276	-2.556057	-1.086312
O	-2.257963	-0.809351	1.144842
C	-1.404697	-1.233236	0.232632

O	-0.202771	-1.341039	0.369193
C	-4.092143	0.394888	-0.041200
Cl	0.637702	0.325461	-2.081101
Cl	0.718631	1.256316	1.759823
C	-3.111174	1.483331	-0.479920
H	-2.328843	1.655010	0.274820
H	-2.619143	1.249888	-1.436336
H	-3.650335	2.432836	-0.617203
C	-4.769373	0.812276	1.265814
H	-5.309180	1.762182	1.131637
H	-5.495879	0.054908	1.601084
H	-4.029553	0.954858	2.068412
C	-5.141072	0.155895	-1.128595
H	-5.855982	-0.629775	-0.836111
H	-5.713636	1.078180	-1.310819
H	-4.676021	-0.142326	-2.081644
Sn	1.670247	0.036761	0.006831
Cl	2.761469	-1.975376	0.453491
Cl	3.566208	1.392134	-0.378825

Imaginary vibration frequency: 33.82i

B-Sn

C	-3.178261	-0.607865	0.614566
C	-2.657655	-1.828067	-0.159655
H	-3.471356	-0.830401	1.650343
H	-3.006413	-1.963082	-1.191777
H	-2.684444	-2.787288	0.375508
O	-1.789569	-0.081500	0.643258
C	-1.350167	-1.116723	-0.036972
O	-0.204693	-1.326959	-0.394958
C	-4.151111	0.369193	-0.027076
Cl	0.401808	1.593622	-1.243974
Cl	1.163822	-0.455168	2.227612
C	-4.199700	1.624961	0.846331
H	-3.217784	2.121148	0.882759
H	-4.927238	2.344493	0.440797
H	-4.500308	1.384933	1.878704
C	-3.725920	0.747936	-1.446221
H	-2.715670	1.184501	-1.465877
H	-3.746663	-0.111624	-2.133770
H	-4.418877	1.501239	-1.850467
C	-5.517943	-0.317337	-0.047206
H	-5.849589	-0.587748	0.968062
H	-6.272905	0.358206	-0.477576

H	-5.503303	-1.234352	-0.657753
Sn	1.649719	0.027947	-0.015761
Cl	2.699139	-1.653439	-1.253231
Cl	3.527420	1.412497	0.382539

TS_{BC-Sn}

C	-2.562542	0.663363	-0.536734
C	-2.538508	2.001243	0.216953
H	-2.566527	0.778705	-1.629738
H	-3.158957	2.064407	1.120837
H	-2.660487	2.907273	-0.391735
O	-1.142932	0.457690	-0.120162
C	-1.105686	1.657423	0.495181
O	-0.114315	2.114351	0.985881
C	-3.465942	-0.477009	-0.101615
Cl	1.249248	1.469385	-1.773919
Cl	3.629110	0.152476	0.494898
C	-3.020276	-1.741318	-0.839409
H	-1.996189	-2.030433	-0.558465
H	-3.686487	-2.581615	-0.591572
H	-3.045669	-1.599229	-1.931530
C	-3.400335	-0.710744	1.407171
H	-2.373519	-0.928700	1.737679
H	-3.775526	0.150759	1.980842
H	-4.026117	-1.575362	1.675033
C	-4.886754	-0.093023	-0.521506
H	-4.957011	0.073058	-1.608292
H	-5.586203	-0.901635	-0.260243
H	-5.228710	0.821993	-0.011990
Sn	1.350977	-0.096605	-0.020262
Cl	0.620558	-0.743094	2.119962
Cl	1.057014	-2.097879	-1.203513

Imaginary vibration frequency: 46.19i

C-Sn

C	-2.296624	0.215394	-0.750782
C	-2.755515	1.675640	-0.749310
H	-2.025528	-0.186913	-1.735277
H	-3.710666	1.923504	-0.270661
H	-2.687117	2.169379	-1.729367
O	-1.047856	0.644995	-0.062382
C	-1.533106	1.939875	0.081351
O	-1.035417	2.815201	0.699260
C	-3.110406	-0.791447	0.058957

Cl	0.676409	-0.414700	2.228340
Cl	0.549756	-1.495491	-1.712959
C	-2.358775	-2.119504	0.151500
H	-2.122575	-2.524789	-0.843473
H	-1.418081	-2.013377	0.711540
H	-2.975685	-2.860466	0.682929
C	-3.397611	-0.279402	1.471497
H	-3.994315	0.645486	1.474758
H	-3.971733	-1.035939	2.027538
H	-2.467012	-0.095969	2.029703
C	-4.419265	-0.998094	-0.708469
H	-4.234131	-1.365086	-1.730696
H	-5.041851	-1.745457	-0.193365
H	-5.005137	-0.068152	-0.779551
Sn	1.314369	-0.101698	0.003013
Cl	1.713584	2.038127	-0.827255
Cl	3.520805	-0.909915	0.181392

SLC-H

C	3.447745	0.398183	0.136200
C	2.181157	0.343635	-0.725351
H	3.902013	1.384914	0.202393
H	2.078200	-0.530800	-1.369024
H	1.909095	1.248591	-1.268350
O	2.565625	0.236389	1.351594
C	1.505726	0.198814	0.590823
O	0.360324	0.077361	1.016249
C	4.436017	-0.712441	0.027698
H	4.995530	-0.590952	-0.903603
H	5.144762	-0.686220	0.857637
H	3.939374	-1.685193	0.008579
Al	-1.302860	-0.023633	0.103489
C	-2.684748	-0.253750	1.459686
C	-4.104518	-0.348227	0.899144
H	-2.613415	0.583235	2.165878
H	-2.448005	-1.154587	2.040000
H	-4.852120	-0.477180	1.689602
H	-4.378973	0.552457	0.341378
H	-4.212543	-1.194611	0.213828
Cl	-1.312585	1.834301	-1.016674
Cl	-0.959333	-1.681932	-1.253655

SIL1-H

C	3.991457	-1.449190	-0.283138
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C	2.754400	-1.152647	0.574279
H	3.945768	-2.391181	-0.825868
H	2.950668	-0.701793	1.548057
H	2.009504	-1.943444	0.664696
O	3.512551	-0.374143	-1.240601
C	2.472879	-0.161986	-0.495863
O	1.599971	0.667527	-0.768895
C	5.338678	-1.128385	0.263646
Al	0.014353	1.255440	-0.021882
C	-0.478476	3.029606	-0.623980
C	-1.953750	3.369899	-0.399315
H	-0.227680	3.116993	-1.687876
H	0.158098	3.757443	-0.107301
H	-2.187031	4.389156	-0.721954
H	-2.613554	2.702456	-0.963099
H	-2.233742	3.297457	0.656202
Cl	0.078335	0.734738	2.058916
O	-1.062612	-0.054600	-0.792073
C	-2.149069	-0.560639	-0.498328
C	-3.140462	-0.468698	0.603116
C	-3.906619	-1.487744	-0.249774
H	-3.589497	0.517087	0.726054
H	-2.768024	-0.836756	1.559922
H	-4.775698	-1.079927	-0.761723
O	-2.756422	-1.436541	-1.238759
C	-4.106333	-2.864320	0.279697
H	5.346102	-0.155319	0.759841
H	6.091171	-1.137043	-0.526971
H	5.605339	-1.894001	0.997097
H	-3.198200	-3.245278	0.752186
H	-4.414529	-3.545011	-0.515660
H	-4.901109	-2.835426	1.029876

SIL2-H

C	4.111516	0.281909	-0.477714
C	3.007124	-0.778215	-0.570113
H	4.474365	0.636652	-1.439803
H	3.075868	-1.602041	0.142373
H	2.764635	-1.154752	-1.564078
O	3.047689	1.265712	-0.024806
C	2.142850	0.340064	-0.115834
O	0.950386	0.524249	0.142947
C	5.177447	0.123039	0.549646
Al	-0.565774	-0.548682	0.253320

C	-0.832723	-1.169746	2.073823
C	-2.239214	-1.709779	2.341905
H	-0.593372	-0.362227	2.775783
H	-0.090380	-1.954079	2.267001
H	-2.342530	-2.079073	3.366872
H	-3.005950	-0.941846	2.200215
H	-2.487700	-2.540784	1.675248
Cl	-0.444972	-1.916176	-1.386845
O	-1.814531	0.740527	-0.247344
C	-2.129394	1.812414	0.699727
H	-3.214554	1.831740	0.805460
H	-1.701529	1.496946	1.652962
C	-1.565521	3.128478	0.245873
H	-1.984987	3.446730	-0.710525
H	-1.820628	3.887820	0.989434
H	-0.478664	3.085429	0.161058
C	-2.717970	0.652796	-1.397723
H	-2.119172	0.249291	-2.212253
H	-2.994948	1.676494	-1.647227
C	-3.910148	-0.207077	-1.090673
H	-3.613907	-1.233149	-0.862916
H	-4.497510	0.189182	-0.259593
H	-4.555001	-0.232319	-1.972872
H	5.726578	1.056439	0.685192
H	4.766116	-0.197657	1.509350
H	5.880719	-0.638151	0.201653

AlEtCl₃

Al	-0.095134	0.000069	-0.120285
C	1.364253	0.005474	-1.443360
C	2.772321	-0.017953	-0.851748
H	1.235862	0.896272	-2.072950
H	1.222706	-0.852593	-2.113580
H	3.555474	0.009371	-1.619892
H	2.944101	0.836378	-0.188704
H	2.939897	-0.919950	-0.254464
Cl	-2.058734	-0.106969	-1.099438
Cl	0.041152	-1.707491	1.256677
Cl	-0.069520	1.820608	1.112404

AlEtCl₂(Et₂O)

Al	0.815387	-0.078648	0.231761
C	1.583420	1.704262	0.477576
C	1.686462	2.536607	-0.800444

H	2.579925	1.570750	0.917319
H	1.005967	2.243518	1.239383
H	2.113877	3.528285	-0.614700
H	2.319973	2.047696	-1.546123
H	0.709227	2.691428	-1.269076
Cl	0.741114	-1.321317	2.006001
Cl	1.537325	-1.209355	-1.463999
O	-1.027305	0.161277	-0.195385
C	-1.789404	-0.603701	-1.172452
H	-2.665645	-0.004148	-1.423174
H	-1.154062	-0.668390	-2.054020
C	-1.836234	0.917358	0.749888
H	-2.708829	0.308481	0.992221
H	-1.236168	1.007671	1.656591
C	-2.161491	-1.964118	-0.650344
H	-2.751259	-2.481822	-1.411447
H	-1.274724	-2.565141	-0.441776
H	-2.764656	-1.900923	0.257921
C	-2.208796	2.265362	0.198668
H	-2.798287	2.183657	-0.717023
H	-2.813974	2.793581	0.940014
H	-1.320170	2.864374	-0.007315

NBO-OMe

C	2.224731	-0.846352	0.646151
C	1.027536	0.044683	0.981680
H	2.628723	-1.401017	1.490720
H	1.015947	1.057827	0.583777
H	0.723080	0.055389	2.028322
O	1.287342	-1.752687	-0.100999
C	0.285562	-0.956481	0.169730
O	-0.863076	-1.146522	-0.217421
C	3.343161	-0.304007	-0.235546
Al	-2.413209	-0.054484	-0.065520
C	-3.897245	-1.059080	-0.833070
C	-5.236017	-0.320271	-0.803233
H	-3.980593	-2.011655	-0.294572
H	-3.634707	-1.321941	-1.865636
H	-6.044621	-0.914817	-1.242497
H	-5.537961	-0.073062	0.219201
H	-5.190175	0.620729	-1.360072
Cl	-2.480895	0.345724	2.064915
Cl	-1.774181	1.733956	-1.116334
O	4.014506	0.584282	0.665797

C	4.117353	1.953161	0.338207
H	4.657116	2.415618	1.165687
H	4.688486	2.121298	-0.580709
H	3.143243	2.445907	0.249165
C	2.821141	0.337353	-1.509918
H	2.315375	-0.418433	-2.113265
H	2.121515	1.155304	-1.334635
H	3.649962	0.721748	-2.105599
C	4.309212	-1.427033	-0.573408
H	5.138066	-1.033578	-1.165535
H	4.715905	-1.865560	0.340389
H	3.815880	-2.212456	-1.151433

NBO-NMe₂

C	1.942553	-0.760584	0.680243
C	0.752947	0.196039	0.832536
H	2.311151	-1.151812	1.625983
H	0.728100	1.081792	0.201290
H	0.471028	0.459778	1.851283
O	0.971232	-1.778494	0.114928
C	-0.014353	-0.939435	0.263982
O	-1.179143	-1.187083	-0.041494
C	3.096980	-0.457150	-0.267504
Al	-2.705537	-0.060355	-0.028518
C	-4.220613	-1.132028	-0.627055
C	-5.544672	-0.368983	-0.686196
H	-4.313609	-1.996220	0.042978
H	-3.979203	-1.544959	-1.614712
H	-6.371584	-1.003556	-1.023705
H	-5.824988	0.029661	0.293708
H	-5.490340	0.480603	-1.373896
Cl	-2.741960	0.644761	2.023044
Cl	-2.054626	1.552178	-1.330166
N	3.772020	0.693927	0.384392
C	3.436490	2.002141	-0.149602
H	3.823059	2.762334	0.533322
H	3.873416	2.191829	-1.142317
H	2.361827	2.156497	-0.219088
C	5.213055	0.603846	0.531616
H	5.756950	0.634297	-0.427014
H	5.546427	1.459798	1.122746
H	5.509163	-0.294270	1.070518
C	3.965371	-1.712842	-0.298055
H	4.312483	-1.997286	0.696803

H	3.375867	-2.542198	-0.694531
H	4.830758	-1.581181	-0.948870
C	2.623700	-0.178785	-1.693482
H	2.177489	-1.077016	-2.123850
H	1.889989	0.626213	-1.758252
H	3.476363	0.096163	-2.317709

SIL1-4a

C	3.624715	-1.604010	-0.298210
C	2.342735	-1.177058	0.426356
H	3.502346	-2.479175	-0.933980
H	2.442442	-0.866037	1.465232
H	1.481115	-1.835961	0.310984
O	3.447987	-0.389606	-1.196854
C	2.373053	-0.061532	-0.552756
O	1.689171	0.930278	-0.828092
C	4.949504	-1.590246	0.414118
Al	0.139141	1.673214	-0.146686
C	-0.201194	3.450025	-0.839666
C	-1.593105	3.998308	-0.514647
H	-0.038514	3.441819	-1.924038
H	0.567573	4.117167	-0.430924
H	-1.714102	5.026308	-0.869592
H	-2.383452	3.407808	-0.988869
H	-1.787944	4.006080	0.562232
Cl	0.140800	1.280195	1.964079
C	5.203072	-0.321288	1.216365
H	5.280292	0.552147	0.563560
H	4.429895	-0.127825	1.963603
H	6.150791	-0.412674	1.750154
C	6.078243	-1.858099	-0.573674
H	7.031019	-1.936717	-0.046350
H	5.919132	-2.788970	-1.124000
H	6.165687	-1.043188	-1.297796
O	-1.021014	0.393525	-0.850140
C	-2.175035	0.047055	-0.581313
C	-3.208726	0.366103	0.436152
C	-4.038675	-0.648944	-0.358965
H	-3.546296	1.402302	0.432860
H	-2.933068	0.059666	1.446649
H	-4.831381	-0.211747	-0.965395
O	-2.838986	-0.829575	-1.270016
C	-4.437245	-1.933648	0.305112
C	-4.879850	-2.966968	-0.719440

H	-5.757665	-2.617659	-1.271162
H	-4.089262	-3.188715	-1.439924
H	-5.149275	-3.899848	-0.219582
C	-5.538948	-1.623857	1.312359
H	-5.824867	-2.534363	1.842473
H	-5.218734	-0.890317	2.056663
H	-6.430127	-1.236096	0.810422
H	4.884654	-2.438793	1.108227
H	-3.561199	-2.312322	0.846200

SIL1TS-4a

C	3.781670	-1.490306	-0.262141
C	2.557958	-0.790170	0.211421
H	3.647488	-2.263060	-1.014993
H	2.668662	-0.289474	1.172771
H	1.692037	-1.454959	0.250744
O	3.314875	0.146462	-1.762851
C	2.428078	0.212209	-0.918158
O	1.458156	1.045514	-0.955776
C	5.068344	-1.375425	0.285286
Al	-0.004737	1.629419	-0.117262
C	-0.504151	3.465804	-0.511179
C	-1.911402	3.845755	-0.046900
H	-0.405702	3.626853	-1.591675
H	0.233953	4.130529	-0.046393
H	-2.144964	4.893013	-0.264557
H	-2.679979	3.242924	-0.542205
H	-2.033444	3.708839	1.032158
Cl	0.042804	1.000808	1.955425
C	5.418772	-0.281703	1.253852
H	5.721108	0.596852	0.677009
H	4.592579	0.001016	1.904535
H	6.264355	-0.584768	1.871395
C	6.218402	-1.987124	-0.469219
H	6.982082	-2.350918	0.218809
H	5.897791	-2.800916	-1.120786
H	6.666196	-1.205104	-1.088166
O	-1.265432	0.457359	-0.874497
C	-2.398592	0.115987	-0.535860
C	-3.340875	0.386627	0.580896
C	-4.246708	-0.580125	-0.189793
H	-3.673285	1.423612	0.630176
H	-2.982558	0.060608	1.556070
H	-5.086553	-0.097350	-0.686877

O	-3.141708	-0.702906	-1.221566
C	-4.619554	-1.913126	0.400884
C	-3.439388	-2.669077	0.995196
H	-2.714690	-2.941337	0.222861
H	-2.921638	-2.102718	1.773059
H	-3.792521	-3.595677	1.451888
C	-5.358057	-2.757507	-0.629687
H	-5.704896	-3.689355	-0.178526
H	-6.228726	-2.231865	-1.029918
H	-4.702342	-3.016529	-1.465728
H	4.502243	-2.259377	0.870701
H	-5.317406	-1.659368	1.209752

Imaginary vibration frequency: 432.18i

SIL1-4c

C	3.724101	-0.742525	-0.855939
C	2.498846	-0.574460	0.052217
H	3.614835	-1.523130	-1.607648
H	2.690785	-0.401587	1.110080
H	1.697189	-1.303220	-0.070949
O	3.331549	0.560476	-1.525606
C	2.309353	0.668416	-0.735763
O	1.510516	1.609028	-0.782145
C	5.123517	-0.701350	-0.281846
Al	0.025507	2.162294	0.167921
C	-0.200681	4.085485	0.122228
C	-1.580327	4.561929	0.583056
H	0.001102	4.433905	-0.897860
H	0.579475	4.534188	0.748744
H	-1.649185	5.654056	0.587145
H	-2.376541	4.199307	-0.075149
H	-1.811388	4.223770	1.597965
Cl	0.015100	1.072597	2.019161
C	5.307559	0.455814	0.695868
H	5.070025	1.414339	0.228285
H	4.698556	0.343786	1.596687
H	6.350423	0.507631	1.012077
C	6.110273	-0.569995	-1.438785
H	7.134796	-0.610999	-1.065082
H	5.983601	-1.381523	-2.161410
H	5.980376	0.380310	-1.962125
O	-1.230197	1.280762	-0.888227
C	-2.374565	0.869024	-0.677441
C	-3.323210	0.802104	0.461778

C	-4.241409	0.152820	-0.581589
H	-3.630585	1.773743	0.848597
H	-2.983024	0.164077	1.276875
H	-5.050050	0.799915	-0.918832
O	-3.115897	0.312304	-1.585355
C	-4.693101	-1.282765	-0.431441
C	-3.538118	-2.210968	-0.067105
H	-2.731998	-2.150445	-0.802600
H	-3.126823	-1.998261	0.923200
H	-3.884505	-3.245441	-0.061140
C	-5.323460	-1.725822	-1.748677
H	-5.721547	-2.737448	-1.653359
H	-6.147745	-1.066345	-2.035009
H	-4.587896	-1.727135	-2.556918
C	5.295081	-2.065738	0.426933
H	5.129150	-2.866856	-0.300929
H	4.516928	-2.155532	1.196056
C	6.628887	-2.255454	1.071256
H	6.864002	-1.601767	1.908537
C	7.517063	-3.166593	0.695939
H	7.321675	-3.843552	-0.131739
H	8.469562	-3.273679	1.204586
C	-5.754018	-1.240189	0.693852
H	-6.546638	-0.540791	0.408698
H	-5.279234	-0.844007	1.600524
C	-6.360159	-2.567597	1.011079
H	-5.696877	-3.316691	1.438306
C	-7.636716	-2.872460	0.817852
H	-8.336319	-2.153670	0.399162
H	-8.031674	-3.849545	1.076346

SIL1TS-4c

C	-3.893979	-0.838516	0.846853
C	-2.731968	-0.222109	0.160862
H	-3.676724	-1.463996	1.709168
H	-2.946406	0.113715	-0.853160
H	-1.866567	-0.888474	0.139203
O	-3.232502	1.065915	2.034825
C	-2.474894	0.957427	1.080843
O	-1.512641	1.767543	0.828664
C	-5.240319	-0.744737	0.450006
Al	-0.119627	2.142642	-0.213527
C	0.239722	4.033843	-0.489479
C	1.610713	4.327767	-1.101863

H	0.136956	4.549764	0.472902
H	-0.550123	4.445058	-1.129852
H	1.766016	5.399319	-1.264022
H	2.425974	3.987861	-0.454066
H	1.736234	3.837031	-2.072165
Cl	-0.115309	0.854284	-1.958209
C	-5.623000	0.310764	-0.557560
H	-5.599541	1.284067	-0.061248
H	-4.959651	0.347716	-1.421645
H	-6.639138	0.137360	-0.911449
C	-6.287905	-0.981697	1.508849
H	-7.210781	-1.342742	1.051135
H	-5.953225	-1.698559	2.260348
H	-6.501130	-0.032860	2.006239
O	1.242824	1.405050	0.853236
C	2.363168	0.964963	0.599336
C	3.194905	0.696960	-0.602839
C	4.227050	0.246869	0.438106
H	3.440626	1.585444	-1.184411
H	2.787788	-0.075198	-1.254218
H	5.053490	0.944424	0.568598
O	3.210901	0.575571	1.508224
C	4.692655	-1.191710	0.492996
C	3.527104	-2.172387	0.403862
H	2.793139	-1.989522	1.192699
H	3.019151	-2.130764	-0.563145
H	3.890911	-3.192254	0.538249
C	5.451674	-1.399349	1.800536
H	5.861793	-2.409973	1.842234
H	6.283468	-0.694826	1.890998
H	4.793494	-1.265903	2.662490
C	-4.901735	-2.259659	-0.270080
H	-5.055488	-3.001776	0.508603
H	-3.893599	-2.366438	-0.683996
C	-5.896003	-2.385626	-1.373889
H	-5.673659	-1.862314	-2.297626
C	-6.990638	-3.124862	-1.256110
H	-7.227511	-3.659631	-0.341344
H	-7.677503	-3.236444	-2.088308
C	5.643795	-1.341120	-0.716875
H	6.450953	-0.606808	-0.624620
H	5.085420	-1.097136	-1.629761
C	6.234775	-2.704249	-0.865745
H	5.543264	-3.513427	-1.090609

C	7.528747	-2.974872	-0.753719
H	8.254742	-2.196398	-0.534229
H	7.911192	-3.982314	-0.881718

Imaginary vibration frequency: 188.11i

SIL1-4i

C	-3.797711	-0.387005	0.901209
C	-2.522227	-0.310889	0.058842
H	-3.755936	-1.091508	1.729075
H	-2.641847	-0.246875	-1.021567
H	-1.742727	-1.031545	0.306676
O	-3.444784	0.978233	1.459912
C	-2.367363	1.003328	0.732744
O	-1.561363	1.935752	0.744131
C	-5.161273	-0.361912	0.246383
Al	0.019855	2.340589	-0.136562
C	0.438590	4.229743	-0.104276
C	1.884786	4.549385	-0.492391
H	0.217803	4.620409	0.896058
H	-0.253615	4.741627	-0.783158
H	2.065245	5.628345	-0.513734
H	2.600512	4.125981	0.219766
H	2.137141	4.163918	-1.484901
Cl	0.031152	1.197864	-1.952480
C	-5.310831	0.670747	-0.847369
H	-5.216495	1.673282	-0.418942
H	-4.574917	0.556798	-1.643999
H	-6.302659	0.594908	-1.293551
C	-6.250717	-0.256348	1.290076
H	-7.234229	-0.351180	0.829154
H	-6.147810	-1.021522	2.061389
H	-6.195421	0.727684	1.765929
O	1.125814	1.351628	1.003757
C	2.246793	0.863131	0.853291
C	3.281336	0.788205	-0.210505
C	4.044591	-0.017782	0.842882
H	3.716631	1.752552	-0.473944
H	2.963616	0.267760	-1.112727
H	4.896225	0.498719	1.279896
O	2.867833	0.187957	1.776662
C	4.317279	-1.492913	0.645864
C	3.130838	-2.292929	0.155723
H	2.355848	-2.301917	0.928026
H	2.702454	-1.909519	-0.771018

H	3.430928	-3.326750	-0.017785
C	4.928839	-2.088569	1.895101
H	5.210287	-3.128672	1.727527
H	5.810259	-1.533333	2.219967
H	4.187800	-2.065542	2.700565
Br	-5.244310	-2.174011	-0.578334
Br	5.698756	-1.458579	-0.788590

SIL1TS-4i

C	-3.934762	-0.256845	0.921027
C	-2.594160	-0.318397	0.185339
H	-4.002881	-0.900382	1.795737
H	-2.618771	-0.350797	-0.902552
H	-1.878424	-1.048812	0.564061
O	-3.548104	1.122943	1.404786
C	-2.417733	1.040727	0.760075
O	-1.571485	1.931982	0.754576
C	-5.238375	-0.206444	0.152258
Al	0.114764	2.119758	-0.035097
C	0.655480	3.984092	-0.033982
C	2.120766	4.218899	-0.408259
H	0.446902	4.406803	0.956437
H	0.001879	4.524392	-0.729618
H	2.365703	5.285212	-0.441543
H	2.801634	3.761266	0.316753
H	2.362719	3.805732	-1.392640
Cl	-0.009093	1.053224	-1.909555
C	-5.249618	0.766108	-1.006037
H	-5.165538	1.786897	-0.621741
H	-4.447673	0.593157	-1.724068
H	-6.197934	0.693332	-1.539071
C	-6.401039	0.019498	1.093113
H	-7.347425	-0.036331	0.554259
H	-6.414823	-0.709268	1.905008
H	-6.318421	1.021402	1.526045
O	1.009725	1.021049	1.094334
C	2.130999	0.426611	1.121263
C	3.194939	0.557093	0.067242
C	4.186720	-0.325979	0.759780
H	3.552340	1.582432	-0.043375
H	2.862904	0.191800	-0.904866
H	4.805532	0.116298	1.532675
O	2.492124	-0.338014	2.027640
C	4.386763	-1.745639	0.491326

C	3.383463	-2.496445	-0.320401
H	2.578242	-2.790527	0.361214
H	2.952900	-1.918338	-1.136419
H	3.827639	-3.407471	-0.721595
C	5.076461	-2.526710	1.562378
H	5.501063	-3.447636	1.162152
H	5.852450	-1.950640	2.066076
H	4.312952	-2.797569	2.299426
Br	-5.358395	-2.060806	-0.570017
Br	5.814743	-0.870500	-0.752413

Imaginary vibration frequency: 352.31i

SIL1-4I

C	3.754915	-0.634220	-0.860110
C	2.469270	-0.538977	-0.039217
H	3.705661	-1.340190	-1.684628
H	2.581887	-0.474085	1.041288
H	1.681645	-1.250431	-0.289039
O	3.419836	0.717771	-1.449197
C	2.336553	0.766286	-0.734578
O	1.540599	1.709411	-0.774362
C	5.105135	-0.646624	-0.149231
Al	-0.009726	2.194461	0.108288
C	-0.318121	4.103906	0.003113
C	-1.733368	4.541865	0.385752
H	-0.077922	4.438696	-1.013230
H	0.414650	4.593193	0.656268
H	-1.836559	5.631164	0.370809
H	-2.481200	4.145395	-0.308369
H	-2.006956	4.208719	1.391714
Cl	-0.014113	1.145799	1.981133
C	5.176763	0.492368	0.863033
H	4.949246	1.443765	0.379465
H	4.493428	0.349786	1.702305
H	6.186775	0.577991	1.263856
C	6.215511	-0.456616	-1.184615
H	7.192621	-0.583266	-0.713229
H	6.135992	-1.170095	-2.007379
H	6.178708	0.550582	-1.605961
O	-1.177448	1.204169	-0.956144
C	-2.307301	0.747151	-0.760827
C	-3.320283	0.740293	0.324570
C	-4.122939	-0.081732	-0.683792
H	-3.714414	1.726301	0.571480

H	-3.008934	0.226055	1.232561
H	-4.949370	0.456181	-1.140312
O	-2.959892	0.049732	-1.642226
C	-4.460979	-1.536373	-0.370641
C	-3.210213	-2.276841	0.092334
H	-2.412586	-2.162449	-0.643788
H	-2.851015	-1.926837	1.061803
H	-3.412025	-3.344936	0.174073
C	-4.989379	-2.210795	-1.638060
H	-5.344560	-3.217357	-1.405706
H	-5.812257	-1.651778	-2.087655
H	-4.196149	-2.302636	-2.383629
N	5.132460	-1.952737	0.538373
C	6.092782	-2.045791	1.623796
H	5.882910	-1.320359	2.407942
H	6.007805	-3.039683	2.068110
H	7.136757	-1.917654	1.294219
C	5.305022	-3.097153	-0.343023
H	6.322969	-3.179682	-0.753819
H	5.102086	-4.006901	0.226353
H	4.603903	-3.078370	-1.177882
N	-5.445092	-1.446267	0.725145
C	-5.597499	-2.662023	1.504447
H	-4.666534	-2.942240	1.994821
H	-6.334310	-2.473808	2.287930
H	-5.955981	-3.519039	0.911218
C	-6.759525	-0.971742	0.321338
H	-7.326443	-1.708588	-0.268016
H	-7.338165	-0.748852	1.220370
H	-6.699710	-0.048696	-0.255888

SIL1TS-4I

C	4.087684	-0.778381	-0.685857
C	2.874330	-0.453022	0.153918
H	3.994777	-1.601154	-1.385412
H	3.081251	-0.046550	1.142791
H	2.152343	-1.264908	0.245139
O	3.386799	0.536005	-1.727161
C	2.484927	0.580383	-0.847828
O	1.500260	1.359211	-0.895463
C	5.481971	-0.481537	-0.266204
Al	0.067417	1.852200	0.097629
C	-0.177941	3.777662	0.176937
C	-1.555715	4.231841	0.662608

H	0.028611	4.193205	-0.816871
H	0.600752	4.185048	0.833734
H	-1.621669	5.321950	0.736804
H	-2.351018	3.915134	-0.019922
H	-1.792405	3.829512	1.652524
Cl	0.050367	0.697105	1.917658
C	5.667717	0.781601	0.553585
H	5.561583	1.644158	-0.106372
H	4.956155	0.893652	1.369920
H	6.674257	0.807351	0.974726
C	6.474595	-0.473290	-1.415425
H	7.497545	-0.489707	-1.033894
H	6.340792	-1.312399	-2.097286
H	6.342340	0.447249	-1.986922
O	-1.244702	1.037804	-0.955639
C	-2.411849	0.704769	-0.745691
C	-3.383625	0.731413	0.378104
C	-4.313018	0.096800	-0.655660
H	-3.643654	1.735560	0.713683
H	-3.109589	0.112336	1.230628
H	-5.082116	0.766729	-1.031415
O	-3.178119	0.163876	-1.648934
C	-4.819987	-1.326508	-0.440000
C	-3.652952	-2.255526	-0.120503
H	-2.886755	-2.179767	-0.893511
H	-3.201411	-2.036730	0.849272
H	-3.988310	-3.292569	-0.109579
C	-5.499963	-1.808838	-1.723133
H	-5.972495	-2.779602	-1.557132
H	-6.263502	-1.109372	-2.069754
H	-4.766453	-1.930175	-2.523597
N	5.425458	-1.737117	0.518138
C	5.530533	-1.673003	1.962425
H	4.848538	-0.935855	2.382018
H	5.253499	-2.645957	2.370920
H	6.550425	-1.438884	2.295860
C	6.042415	-2.920115	-0.048406
H	7.138748	-2.889317	0.002119
H	5.696964	-3.791724	0.509978
H	5.745540	-3.057515	-1.087831
N	-5.722559	-1.218354	0.722874
C	-6.006157	-2.477465	1.388319
H	-5.100161	-2.934241	1.783471
H	-6.664324	-2.272612	2.235125

H	-6.516751	-3.209264	0.741079
C	-6.975413	-0.529747	0.455612
H	-7.665473	-1.109376	-0.176644
H	-7.476215	-0.342133	1.407885
H	-6.813975	0.439456	-0.017199

Imaginary vibration frequency: 466.34i

SIL1-4m

C	-3.828906	0.317458	0.950654
C	-2.467985	0.230214	0.254363
H	-3.849028	-0.128076	1.942825
H	-2.475934	-0.008948	-0.808435
H	-1.699859	-0.354329	0.761973
O	-3.567421	1.799654	1.150290
C	-2.419448	1.682210	0.558325
O	-1.635248	2.623286	0.399387
C	-5.101374	0.040610	0.167868
Al	0.038664	2.794158	-0.374852
C	0.620867	4.634778	-0.521531
C	2.127724	4.776991	-0.750852
H	0.322989	5.169354	0.388504
H	0.069070	5.110460	-1.340476
H	2.423710	5.825182	-0.856159
H	2.705525	4.368514	0.084659
H	2.452726	4.260282	-1.659204
Cl	0.058926	1.444047	-2.044993
C	-5.179900	0.905866	-1.086004
H	-5.256412	1.959207	-0.811212
H	-4.322986	0.787871	-1.752867
H	-6.076772	0.651904	-1.653399
C	-6.307201	0.361572	1.055547
H	-7.230879	0.122581	0.524895
H	-6.294671	-0.206789	1.986812
H	-6.325616	1.425353	1.305989
O	0.966642	1.878271	0.958747
C	2.023203	1.240672	0.987484
C	3.138374	0.916695	0.061632
C	3.663624	0.127944	1.264109
H	3.728080	1.785233	-0.233798
H	2.855555	0.341325	-0.819232
H	4.536567	0.565649	1.743400
O	2.449246	0.608135	2.038482
C	3.739190	-1.388268	1.185894
C	2.393215	-1.987259	0.786065

H	1.662094	-1.826931	1.580371
H	1.989213	-1.572628	-0.140401
H	2.495639	-3.064950	0.648043
C	4.120641	-1.936650	2.563040
H	4.228921	-3.021881	2.513895
H	5.059213	-1.517718	2.929319
H	3.340047	-1.705678	3.292409
C	-5.033752	-1.454810	-0.142419
C	-4.948266	-1.934353	-1.447279
C	-5.024234	-2.382363	0.902529
C	-4.865790	-3.297967	-1.701882
H	-4.956563	-1.247815	-2.284338
C	-4.936703	-3.743009	0.650692
H	-5.093948	-2.044607	1.931091
C	-4.857864	-4.207518	-0.655594
H	-4.809993	-3.647549	-2.727148
H	-4.936242	-4.443493	1.478842
H	-4.795584	-5.271576	-0.855287
C	4.835896	-1.651474	0.154519
C	6.156943	-1.295353	0.434079
C	4.552838	-2.195163	-1.096610
C	7.162343	-1.484663	-0.502060
H	6.414635	-0.868842	1.396816
C	5.559244	-2.389736	-2.034330
H	3.540623	-2.483790	-1.350276
C	6.867352	-2.034758	-1.742213
H	8.181494	-1.204447	-0.258978
H	5.315141	-2.823235	-2.998137
H	7.652926	-2.187263	-2.473944

SIL1TS-4m

C	3.620235	-0.509941	-0.522830
C	2.371946	0.308117	-0.436478
H	4.002268	-0.712320	-1.517637
H	1.797383	0.160914	0.476803
H	1.721432	0.166116	-1.301493
O	4.282932	1.532817	-0.584323
C	3.059027	1.645568	-0.467290
O	2.441229	2.758560	-0.382154
C	4.268662	-1.195486	0.579258
Al	0.782057	3.264127	0.096470
C	0.355250	5.137466	-0.174437
C	-1.137359	5.454523	-0.059420
H	0.734618	5.445509	-1.156216

H	0.920977	5.725120	0.558409
H	-1.336993	6.524281	-0.178224
H	-1.722923	4.937882	-0.827160
H	-1.542185	5.160071	0.913943
Cl	0.355277	2.336081	2.005487
C	4.066626	-0.611483	1.964172
H	4.745748	0.234356	2.082642
H	3.055903	-0.253136	2.156229
H	4.314700	-1.359490	2.719094
C	5.728860	-1.533006	0.335849
H	6.049845	-2.317154	1.023635
H	5.921748	-1.860809	-0.685372
H	6.331559	-0.641632	0.518727
O	-0.201749	2.202566	-1.109984
C	-1.254857	1.568125	-1.064765
C	-2.333395	1.284850	-0.082689
C	-2.910135	0.451879	-1.230429
H	-2.906172	2.165860	0.208457
H	-2.010845	0.744011	0.805434
H	-3.796564	0.879157	-1.694342
O	-1.724519	0.883365	-2.068138
C	-3.000972	-1.059627	-1.092008
C	-1.656547	-1.658665	-0.687714
H	-0.930790	-1.533494	-1.493071
H	-1.243346	-1.214461	0.220850
H	-1.768608	-2.730016	-0.513290
C	-3.407247	-1.653300	-2.443137
H	-3.527242	-2.734873	-2.354376
H	-4.346606	-1.236255	-2.809772
H	-2.635562	-1.456302	-3.191615
C	3.290364	-2.360570	0.221675
C	2.123549	-2.560159	0.975372
C	3.558472	-3.221411	-0.852476
C	1.283296	-3.617901	0.691838
H	1.893565	-1.906160	1.806019
C	2.702816	-4.271815	-1.140074
H	4.444127	-3.079516	-1.458869
C	1.567017	-4.472572	-0.369632
H	0.402098	-3.783115	1.300921
H	2.927120	-4.935078	-1.967192
H	0.899580	-5.297365	-0.593154
C	-4.086026	-1.278857	-0.038549
C	-5.405833	-0.911699	-0.310115
C	-3.795016	-1.796609	1.221502

C	-6.401431	-1.063891	0.642906
H	-5.669636	-0.505184	-1.280096
C	-4.791576	-1.954047	2.176654
H	-2.783493	-2.092185	1.469662
C	-6.098134	-1.587590	1.892532
H	-7.419533	-0.774672	0.406187
H	-4.541279	-2.366641	3.148036
H	-6.876042	-1.710301	2.637935

Imaginary vibration frequency: 347.94i

SIL1-4n

C	3.778862	-0.932983	-0.702967
C	2.456239	-0.793209	0.060490
H	3.773711	-1.704559	-1.470944
H	2.516858	-0.648520	1.137846
H	1.684109	-1.525123	-0.178420
O	3.449163	0.377422	-1.393899
C	2.346105	0.465622	-0.718287
O	1.550892	1.403748	-0.832496
C	5.106875	-0.879224	0.031932
Al	0.013640	1.973960	0.020213
C	-0.305304	3.865877	-0.243526
C	-1.705053	4.329286	0.166016
H	-0.119337	4.103999	-1.297795
H	0.453802	4.418631	0.322744
H	-1.825257	5.409661	0.040455
H	-2.483569	3.853798	-0.439388
H	-1.919717	4.103409	1.214881
Cl	0.030123	1.085733	1.976016
C	5.190850	0.314648	0.986465
H	5.098354	1.261569	0.449506
H	4.431636	0.279076	1.771855
H	6.164727	0.306484	1.479111
C	6.220623	-0.792608	-1.004525
H	7.195921	-0.800980	-0.514164
H	6.183073	-1.627545	-1.708470
H	6.140472	0.136755	-1.572811
O	-1.183546	0.914016	-0.938380
C	-2.321717	0.503134	-0.693596
C	-3.295868	0.574757	0.424181
C	-4.161783	-0.267711	-0.520593
H	-3.653765	1.582417	0.637269
H	-2.953852	0.097888	1.342022
H	-4.998074	0.273365	-0.959347

O	-3.023888	-0.205489	-1.523570
C	-4.538297	-1.694216	-0.162786
C	-3.320791	-2.516568	0.266118
H	-2.598417	-2.608847	-0.548359
H	-2.816369	-2.091608	1.137795
H	-3.646385	-3.522224	0.538146
C	-5.193929	-2.334709	-1.379864
H	-5.518313	-3.350387	-1.144697
H	-6.063481	-1.765963	-1.717395
H	-4.484428	-2.392843	-2.208409
C	-5.475482	-1.561688	1.015543
H	-5.005484	-1.208796	1.932527
C	-6.770206	-1.845831	1.025434
H	-7.295302	-2.210189	0.148899
H	-7.354350	-1.731046	1.932382
C	5.151335	-2.151966	0.845586
H	4.421081	-2.202533	1.652418
C	5.993028	-3.162269	0.677722
H	6.751277	-3.167536	-0.098080
H	5.957802	-4.026918	1.332084

SIL1TS-4n

C	3.766479	-1.059676	-0.535083
C	2.473893	-0.501156	-0.023811
H	3.730315	-1.646111	-1.446717
H	2.464085	-0.284002	1.043720
H	1.611963	-1.125004	-0.268425
O	3.531899	0.773297	-1.573508
C	2.523168	0.747062	-0.858802
O	1.641374	1.665499	-0.835490
C	5.031390	-1.042093	0.179421
Al	0.111473	2.101315	-0.006373
C	-0.413133	3.961487	-0.204063
C	-1.865485	4.261185	0.173018
H	-0.221027	4.264853	-1.240452
H	0.263424	4.568816	0.409577
H	-2.099720	5.326188	0.077379
H	-2.571226	3.725386	-0.471025
H	-2.083475	3.978050	1.207593
Cl	0.099392	1.209029	1.966323
C	5.253819	0.076665	1.177607
H	5.464491	1.005613	0.644788
H	4.396217	0.236288	1.832799
H	6.115085	-0.164552	1.802857

C	6.241003	-1.287699	-0.699549
H	7.093204	-1.587668	-0.087234
H	6.059513	-2.058699	-1.450001
H	6.496064	-0.364098	-1.222984
O	-1.058284	0.983190	-0.966901
C	-2.183228	0.545795	-0.726208
C	-3.182370	0.622637	0.370747
C	-3.995379	-0.291955	-0.554050
H	-3.583111	1.624322	0.526956
H	-2.842297	0.205537	1.317289
H	-4.851798	0.192016	-1.020031
O	-2.851361	-0.217135	-1.542079
C	-4.308749	-1.722150	-0.148591
C	-3.060759	-2.462278	0.340663
H	-2.310337	-2.537496	-0.450015
H	-2.606800	-1.984119	1.212334
H	-3.338515	-3.476357	0.633931
C	-4.897250	-2.442158	-1.355573
H	-5.177643	-3.463182	-1.089033
H	-5.783923	-1.931227	-1.738215
H	-4.163199	-2.495555	-2.162710
C	-5.282570	-1.597734	0.999911
H	-4.861058	-1.174676	1.910618
C	-6.557041	-1.962499	0.992222
H	-7.034606	-2.398125	0.121048
H	-7.171822	-1.844015	1.878190
C	4.458507	-2.300370	0.866851
H	3.988223	-2.124035	1.828588
C	4.466497	-3.524752	0.331773
H	4.898079	-3.732150	-0.641376
H	4.059308	-4.367257	0.880846

Imaginary vibration frequency: 346.50i

SIL2-4a

C	3.262539	-0.934269	0.044112
C	1.999699	-1.155969	0.885112
H	3.770908	-1.852692	-0.244331
H	1.844303	-0.490904	1.732819
H	1.789947	-2.185507	1.177305
O	2.349986	-0.560868	-1.114371
C	1.309701	-0.740032	-0.361894
O	0.151738	-0.565597	-0.754002
C	4.223586	0.173691	0.382237
Al	-1.559818	-0.649196	-0.044212

C	-2.700309	-1.823883	-1.082929
C	-2.244809	-3.285342	-1.016676
H	-2.715039	-1.481334	-2.124640
H	-3.731509	-1.738364	-0.720948
H	-2.899944	-3.938541	-1.601010
H	-1.231997	-3.413509	-1.411508
H	-2.244806	-3.664232	0.009534
Cl	-1.291130	-0.935169	2.063466
C	3.550604	1.512568	0.654615
H	3.044226	1.891500	-0.237336
H	2.829784	1.468505	1.474884
H	4.307064	2.248266	0.934083
C	5.286647	0.296916	-0.702507
H	6.035195	1.038224	-0.415913
H	5.799579	-0.653324	-0.870727
H	4.845768	0.619416	-1.649940
O	-1.945916	1.158004	-0.272385
C	-1.090317	2.216954	0.260367
H	-1.734875	2.896884	0.818760
H	-0.424745	1.731133	0.976648
C	-0.333253	2.905668	-0.839295
H	-1.002345	3.406833	-1.541500
H	0.312747	3.666751	-0.394182
H	0.293238	2.203782	-1.392990
C	-3.270462	1.586458	-0.726493
H	-3.554125	0.874811	-1.501734
H	-3.137397	2.563226	-1.191361
C	-4.254377	1.612992	0.407981
H	-4.372436	0.624226	0.858037
H	-3.959779	2.320627	1.185245
H	-5.226708	1.925269	0.019043
H	4.707832	-0.170442	1.305873

SIL2TS-4a

C	-3.492694	0.548390	-0.438055
C	-2.116086	0.930402	-0.023304
H	-3.855709	0.949231	-1.380984
H	-1.912751	0.804810	1.040644
H	-1.861661	1.950168	-0.320861
O	-2.065073	-0.838372	-1.510627
C	-1.355014	-0.085759	-0.849092
O	-0.077160	-0.125776	-0.838955
C	-4.437327	-0.127528	0.351477
Al	1.345610	0.631867	-0.046388

C	2.098844	2.179162	-0.959023
C	1.100745	3.334589	-1.082642
H	2.446300	1.880938	-1.955873
H	2.990216	2.518268	-0.417793
H	1.546839	4.210000	-1.565450
H	0.229366	3.053029	-1.682994
H	0.733988	3.661780	-0.104585
Cl	0.846900	0.836316	2.047778
C	-4.046851	-0.830147	1.621828
H	-3.711552	-1.838428	1.363119
H	-3.248164	-0.328662	2.166240
H	-4.911940	-0.922514	2.278446
C	-5.692615	-0.619093	-0.318870
H	-6.531960	-0.610437	0.376841
H	-5.944052	-0.027333	-1.199714
H	-5.524462	-1.652586	-0.633105
O	2.494107	-0.841383	-0.154390
C	2.065151	-2.191297	0.200620
H	2.833052	-2.609949	0.852972
H	1.155544	-2.069521	0.789340
C	1.828618	-3.024902	-1.026540
H	2.738991	-3.143454	-1.617657
H	1.501860	-4.020456	-0.714805
H	1.049671	-2.587001	-1.652480
C	3.926625	-0.680956	-0.382883
H	4.018204	0.138837	-1.095158
H	4.270224	-1.593826	-0.870882
C	4.663502	-0.400961	0.897015
H	4.322650	0.527981	1.359124
H	4.550499	-1.212498	1.618842
H	5.728004	-0.296845	0.672081
H	-4.575758	1.039656	0.574089

Imaginary vibration frequency: 371.42i

SIL2-4c

C	2.441261	-0.847154	-0.730726
C	1.331900	-1.256783	0.247062
H	2.894483	-1.680177	-1.266609
H	1.319817	-0.771684	1.221678
H	1.164749	-2.328196	0.364777
O	1.357919	-0.285271	-1.631138
C	0.451297	-0.628668	-0.769217
O	-0.753130	-0.411394	-0.931283
C	3.463077	0.199054	-0.341506

Al	-2.318108	-0.655136	0.038113
C	-3.506899	-1.930217	-0.813041
C	-2.954850	-3.358937	-0.786627
H	-3.690139	-1.615884	-1.847653
H	-4.481224	-1.900620	-0.311415
H	-3.648464	-4.066770	-1.250500
H	-2.007465	-3.440574	-1.328729
H	-2.776620	-3.705644	0.235374
Cl	-1.665745	-0.921322	2.063214
C	2.809061	1.435603	0.268975
H	2.098837	1.892241	-0.424816
H	2.293405	1.218718	1.208267
H	3.570277	2.187178	0.482481
C	4.245858	0.588420	-1.592201
H	5.025154	1.309514	-1.340283
H	4.729056	-0.282777	-2.043622
H	3.592258	1.045299	-2.339384
C	4.383643	-0.511820	0.678159
H	4.780185	-1.425030	0.221746
H	3.775568	-0.814012	1.540015
O	-2.907247	1.105577	-0.098138
C	-2.078033	2.248874	0.282038
H	-2.690077	2.883642	0.923583
H	-1.270398	1.842023	0.892119
C	-1.563825	2.970700	-0.930559
H	-2.376250	3.374801	-1.537923
H	-0.945839	3.809617	-0.600190
H	-0.950229	2.316686	-1.552624
C	-4.317011	1.417044	-0.345247
H	-4.662870	0.663092	-1.052068
H	-4.334934	2.385861	-0.844330
C	-5.109818	1.409722	0.930490
H	-5.102726	0.424847	1.403388
H	-4.735182	2.146223	1.644098
H	-6.146846	1.664476	0.698114
C	5.520611	0.326926	1.162289
H	5.263224	1.209103	1.744975
C	6.799151	0.053492	0.937821
H	7.101501	-0.819888	0.365783
H	7.590957	0.688346	1.321862

SIL2TS-4c

C	2.677502	0.191856	-1.060084
C	1.381109	-0.496645	-0.846323

H	3.039185	0.263474	-2.082450
H	1.240770	-0.870030	0.168371
H	1.216486	-1.310415	-1.557606
O	0.960295	1.692575	-1.516907
C	0.434662	0.652061	-1.142640
O	-0.831206	0.489913	-1.007826
C	3.517629	0.698143	-0.048011
Al	-1.970561	-0.631353	-0.191306
C	-2.596382	-2.126011	-1.270633
C	-1.439734	-3.022018	-1.724201
H	-3.133521	-1.741626	-2.146476
H	-3.324273	-2.718977	-0.704923
H	-1.787246	-3.866127	-2.328483
H	-0.717620	-2.470114	-2.334945
H	-0.894038	-3.441079	-0.872919
Cl	-1.088823	-1.074345	1.737315
C	2.949717	0.855851	1.343018
H	2.246118	1.692268	1.335192
H	2.426244	-0.028475	1.707013
H	3.748629	1.094423	2.045051
C	4.467753	1.803622	-0.439224
H	5.336463	1.802134	0.222262
H	4.801714	1.706862	-1.473682
H	3.954991	2.761599	-0.328816
C	4.341237	-0.771678	-0.270107
H	5.026943	-0.611262	-1.097847
H	3.700255	-1.631065	-0.492823
O	-3.339428	0.595563	0.153513
C	-3.068160	1.925426	0.693224
H	-3.756151	2.075072	1.526661
H	-2.055444	1.884611	1.095086
C	-3.206809	2.976732	-0.370395
H	-4.217329	3.003877	-0.784253
H	-3.001467	3.953848	0.074561
H	-2.493082	2.810529	-1.178536
C	-4.743368	0.197120	0.171874
H	-4.864969	-0.492997	-0.662768
H	-5.322537	1.095984	-0.041797
C	-5.121151	-0.428898	1.485348
H	-4.571796	-1.356262	1.661531
H	-4.940518	0.249375	2.322079
H	-6.187994	-0.665433	1.467330
C	5.057581	-1.019814	1.013963
H	4.473561	-1.425499	1.832886

C	6.355731	-0.787805	1.152243
H	6.957701	-0.387371	0.342235
H	6.865027	-1.017931	2.082139

Imaginary vibration frequency: 185.92i

SIL2-4i

C	-2.477408	1.427990	-0.323331
C	-1.296169	1.480821	0.650104
H	-2.871416	2.401314	-0.615265
H	-1.315824	0.793228	1.493830
H	-0.991421	2.476937	0.974532
O	-1.527791	0.978790	-1.390488
C	-0.544642	0.989389	-0.535606
O	0.605642	0.661284	-0.823723
C	-3.619606	0.464414	-0.114484
Al	2.271868	0.671262	0.011651
C	3.443805	1.944735	-0.865647
C	2.951771	3.389006	-0.730858
H	3.530269	1.675195	-1.925343
H	4.453088	1.854651	-0.447676
H	3.634303	4.093672	-1.215520
H	1.969924	3.529726	-1.194053
H	2.865910	3.692823	0.316549
Cl	1.836897	0.782444	2.106295
C	-4.441031	0.319904	-1.377550
H	-4.860694	1.295561	-1.641516
H	-3.842454	-0.039636	-2.215055
H	-5.267147	-0.373020	-1.216454
C	-4.444119	0.930960	1.067042
H	-5.276307	0.247607	1.236772
H	-3.854610	0.993155	1.982935
H	-4.857496	1.920823	0.849769
O	2.727755	-1.098205	-0.338932
C	1.890292	-2.233301	0.054672
H	2.526497	-2.912053	0.623756
H	1.141401	-1.830326	0.737211
C	1.271311	-2.890361	-1.145016
H	2.026165	-3.289299	-1.825862
H	0.655278	-3.725673	-0.801992
H	0.629914	-2.198540	-1.693563
C	4.113171	-1.445076	-0.668580
H	4.445175	-0.683343	-1.373420
H	4.074251	-2.400642	-1.191349
C	4.969975	-1.494529	0.564342

H	5.022197	-0.520817	1.056474
H	4.604298	-2.230500	1.283137
H	5.984320	-1.779883	0.274814
Br	-2.872460	-1.333074	0.329812

SIL2TS-4i

C	2.643212	0.335100	-0.647766
C	1.402167	-0.402581	-0.250845
H	2.814409	0.495938	-1.706349
H	1.438016	-0.854523	0.741370
H	1.117967	-1.164504	-0.979001
O	1.134638	1.827005	-0.581770
C	0.500546	0.800716	-0.296310
O	-0.746927	0.771866	-0.068435
C	3.639779	0.879762	0.266666
Al	-2.043213	-0.446915	0.269472
C	-2.197585	-0.927870	2.150961
C	-3.518340	-1.611486	2.510979
H	-2.046402	-0.038522	2.774846
H	-1.359785	-1.595808	2.389458
H	-3.554512	-1.902865	3.565575
H	-4.377890	-0.958146	2.330889
H	-3.676605	-2.519676	1.921730
Cl	-1.847205	-2.014964	-1.190214
C	3.332534	0.978132	1.724082
H	2.749143	1.894449	1.865237
H	2.759662	0.136654	2.109159
H	4.252451	1.078190	2.299805
C	4.527371	1.946402	-0.287411
H	5.445419	2.030887	0.294191
H	4.769481	1.786936	-1.338249
H	3.980839	2.891228	-0.198015
O	-3.524677	0.551611	-0.289047
C	-3.944217	1.685453	0.531033
H	-5.026654	1.611329	0.645225
H	-3.490132	1.524300	1.510515
C	-3.511511	2.991455	-0.073310
H	-3.958053	3.152176	-1.056516
H	-3.841832	3.803316	0.579794
H	-2.425361	3.042125	-0.164469
C	-4.415457	0.234198	-1.403587
H	-3.778963	-0.180089	-2.183521
H	-4.820399	1.182564	-1.757359
C	-5.489945	-0.726635	-0.980967

H	-5.066069	-1.679532	-0.657560
H	-6.104819	-0.317697	-0.176191
H	-6.142254	-0.920938	-1.836139
Br	4.445457	-0.992378	-0.176888

Imaginary vibration frequency: 350.30i

SIL2-4l

C	-2.501485	0.753849	-0.623166
C	-1.397316	1.066117	0.385978
H	-2.967298	1.633417	-1.059372
H	-1.369079	0.449065	1.281875
H	-1.262775	2.113889	0.655842
O	-1.423200	0.329529	-1.595927
C	-0.510788	0.608055	-0.713666
O	0.697411	0.468629	-0.925576
C	-3.499496	-0.363305	-0.330509
Al	2.282511	0.687629	0.016524
C	3.456039	1.958680	-0.861185
C	2.885771	3.380542	-0.866147
H	3.642044	1.624455	-1.889123
H	4.430838	1.951339	-0.359657
H	3.570065	4.086816	-1.346034
H	1.937535	3.436917	-1.409831
H	2.702930	3.747871	0.147861
Cl	1.697107	0.936443	2.064324
C	-2.761531	-1.637566	0.069488
H	-2.024129	-1.902889	-0.689715
H	-2.262756	-1.543528	1.036242
H	-3.459176	-2.472642	0.133703
C	-4.318237	-0.641742	-1.592786
H	-5.115066	-1.355596	-1.372461
H	-4.772518	0.266545	-1.993838
H	-3.688657	-1.077508	-2.372093
O	2.860056	-1.076672	-0.148144
C	2.032776	-2.216983	0.243060
H	2.639076	-2.837048	0.904412
H	1.214927	-1.803526	0.835149
C	1.536598	-2.964910	-0.961421
H	2.356230	-3.382875	-1.549180
H	0.912944	-3.795971	-0.621932
H	0.933091	-2.324466	-1.607101
C	4.271136	-1.387833	-0.389824
H	4.614544	-0.642746	-1.107148
H	4.292681	-2.363688	-0.874447

C	5.064445	-1.361165	0.885487
H	5.058731	-0.369583	1.343921
H	4.689991	-2.086740	1.610256
H	6.101264	-1.619530	0.656204
N	-4.289880	0.150408	0.804776
C	-5.012839	-0.865259	1.549403
H	-4.336419	-1.596142	1.989784
H	-5.540106	-0.373802	2.369435
H	-5.764034	-1.398492	0.944182
C	-5.203228	1.231018	0.466975
H	-6.069561	0.899417	-0.125436
H	-5.581894	1.666380	1.394213
H	-4.702945	2.030221	-0.080425

SIL2TS-4I

C	2.811093	0.355086	-0.719785
C	1.641374	-0.582261	-0.525545
H	3.134241	0.529121	-1.740031
H	1.655179	-1.183492	0.383023
H	1.438560	-1.228239	-1.381231
O	1.487546	1.596586	-0.625956
C	0.733788	0.598969	-0.461430
O	-0.508586	0.676550	-0.292234
C	3.857868	0.589150	0.308388
Al	-1.844394	-0.513728	0.073547
C	-1.763909	-1.206415	1.892561
C	-3.060105	-1.867066	2.366940
H	-1.472252	-0.405365	2.582850
H	-0.944831	-1.936182	1.929618
H	-2.962027	-2.280214	3.375874
H	-3.893509	-1.158195	2.392122
H	-3.357386	-2.690343	1.710596
Cl	-1.939662	-1.890808	-1.568261
C	3.377830	0.550578	1.747232
H	2.824579	1.467892	1.954634
H	2.728562	-0.293283	1.974922
H	4.232004	0.515541	2.425799
C	4.655101	1.861919	0.084986
H	5.559723	1.855940	0.696486
H	4.936515	2.006764	-0.957652
H	4.047925	2.716370	0.389036
O	-3.284283	0.656533	-0.161973
C	-3.466103	1.724017	0.819927
H	-4.498223	1.666903	1.168980

H	-2.813905	1.465991	1.656418
C	-3.120636	3.069547	0.247665
H	-3.775592	3.343944	-0.581192
H	-3.246256	3.820379	1.032051
H	-2.084396	3.098610	-0.092353
C	-4.388082	0.484747	-1.106103
H	-3.936493	0.098477	-2.018150
H	-4.777673	1.481467	-1.311613
C	-5.438146	-0.441148	-0.560984
H	-5.034853	-1.439808	-0.380768
H	-5.880406	-0.062001	0.362868
H	-6.237990	-0.531273	-1.300597
N	4.498623	-0.655291	-0.174242
C	4.628916	-1.779505	0.730091
H	3.708321	-1.958684	1.280327
H	4.847413	-2.673784	0.143756
H	5.443803	-1.635408	1.452936
C	5.618654	-0.534695	-1.086134
H	6.539196	-0.216000	-0.579647
H	5.797456	-1.509829	-1.542528
H	5.400059	0.169041	-1.888066

Imaginary vibration frequency: 469.20i

SIL2-4m

C	2.385495	-1.804317	-0.512226
C	1.213159	-1.898850	0.468892
H	2.750507	-2.758890	-0.887389
H	1.258921	-1.261565	1.350424
H	0.890500	-2.904436	0.741638
O	1.411398	-1.266499	-1.537767
C	0.452499	-1.318785	-0.664252
O	-0.702229	-0.950016	-0.897552
C	3.520533	-0.836529	-0.221283
Al	-2.261163	-0.758921	0.094770
C	-3.599035	-2.075894	-0.394850
C	-3.160191	-3.506254	-0.066762
H	-3.818337	-1.985157	-1.465603
H	-4.535834	-1.846422	0.126364
H	-3.930945	-4.236299	-0.332101
H	-2.253693	-3.788115	-0.612097
H	-2.952192	-3.631516	1.000054
Cl	-1.606117	-0.550223	2.125031
C	4.407964	-0.749065	-1.465100
H	4.846784	-1.727020	-1.677482

H	3.858675	-0.432907	-2.352746
H	5.220903	-0.040039	-1.297530
C	4.326614	-1.496096	0.902036
H	5.147384	-0.843247	1.204619
H	3.723693	-1.719062	1.784584
H	4.755611	-2.436276	0.547414
O	-2.663095	0.948454	-0.518350
C	-1.674689	2.026811	-0.564259
H	-2.126037	2.889635	-0.072714
H	-0.835336	1.694987	0.048231
C	-1.260566	2.310315	-1.978822
H	-2.107224	2.612123	-2.598923
H	-0.542326	3.133135	-1.971436
H	-0.779791	1.442003	-2.432124
C	-4.053332	1.369141	-0.703482
H	-4.559756	0.514140	-1.151112
H	-4.037114	2.176743	-1.435338
C	-4.677757	1.785038	0.597852
H	-4.720206	0.954983	1.307041
H	-4.138152	2.615117	1.058105
H	-5.701501	2.114671	0.403766
C	2.973210	0.533780	0.178940
C	2.794211	0.890065	1.516709
C	2.616673	1.469565	-0.795048
C	2.276718	2.129624	1.869197
H	3.069733	0.202633	2.307190
C	2.112864	2.714724	-0.445586
H	2.742077	1.237669	-1.845374
C	1.935878	3.049936	0.889313
H	2.151243	2.377300	2.917586
H	1.866012	3.427186	-1.225037
H	1.545411	4.023653	1.164179

SIL2TS-4m

C	2.328227	0.875076	-0.662235
C	1.141112	-0.007442	-0.438421
H	2.643194	1.013762	-1.690737
H	1.064157	-0.419061	0.568346
H	1.068643	-0.819459	-1.165388
O	0.649690	2.154274	-0.941173
C	0.118647	1.067472	-0.682014
O	-1.139942	0.879329	-0.623577
C	3.199878	1.413284	0.365684
Al	-2.160970	-0.512139	-0.074526

C	-1.689556	-1.116070	1.721329
C	-2.799983	-1.864841	2.460435
H	-1.355273	-0.255190	2.314909
H	-0.810728	-1.767148	1.626192
H	-2.477300	-2.205860	3.449597
H	-3.683303	-1.237114	2.612730
H	-3.126604	-2.750449	1.907378
Cl	-2.245287	-1.961952	-1.657330
C	2.611992	1.586127	1.753472
H	2.017890	2.501484	1.766420
H	1.968708	0.767165	2.072746
H	3.417771	1.690607	2.482101
C	3.963775	2.655988	-0.056815
H	4.837233	2.794956	0.582614
H	4.289566	2.620814	-1.095596
H	3.309473	3.522541	0.053611
O	-3.825940	0.342104	-0.098983
C	-4.056904	1.419676	0.859433
H	-5.029646	1.236863	1.318936
H	-3.294387	1.294258	1.630352
C	-3.967839	2.770238	0.206338
H	-4.733493	2.904164	-0.560217
H	-4.124267	3.536175	0.970201
H	-2.985094	2.925094	-0.241702
C	-4.991143	-0.038890	-0.893977
H	-4.596117	-0.403981	-1.840250
H	-5.549618	0.877510	-1.084980
C	-5.815355	-1.077650	-0.188232
H	-5.246296	-1.995940	-0.029992
H	-6.188020	-0.718779	0.773558
H	-6.679518	-1.320370	-0.811967
C	4.000797	0.086444	0.167312
C	4.945217	-0.031341	-0.862808
C	3.790361	-1.007054	1.020009
C	5.688675	-1.189800	-1.003978
H	5.110537	0.788811	-1.549908
C	4.541580	-2.157834	0.878338
H	3.056925	-0.950725	1.813584
C	5.491090	-2.252618	-0.133392
H	6.423297	-1.262747	-1.797437
H	4.386640	-2.986644	1.559303
H	6.074205	-3.159991	-0.243955

Imaginary vibration frequency: 357.24i

SIL2-4n

C	2.806187	-0.774152	-0.454883
C	1.655921	-1.133908	0.494337
H	3.323830	-1.633581	-0.876341
H	1.564527	-0.555850	1.412152
H	1.524717	-2.194819	0.710407
O	1.758367	-0.349947	-1.467102
C	0.814612	-0.646497	-0.627121
O	-0.384297	-0.495566	-0.875537
C	3.766851	0.352920	-0.117923
Al	-2.017727	-0.681686	-0.014542
C	-3.205095	-1.845884	-1.012533
C	-2.752115	-3.309205	-0.993134
H	-3.267738	-1.485034	-2.046520
H	-4.218720	-1.764573	-0.602900
H	-3.433873	-3.949215	-1.561398
H	-1.757190	-3.433916	-1.432215
H	-2.710381	-3.706010	0.025258
Cl	-1.531794	-1.051771	2.039893
C	3.036498	1.617180	0.343592
H	2.359848	1.991760	-0.428627
H	2.471198	1.458926	1.265505
H	3.771476	2.398123	0.546305
C	4.593986	0.661213	-1.359981
H	5.340741	1.425677	-1.137076
H	5.111131	-0.226164	-1.732972
H	3.954179	1.042056	-2.159170
O	-2.504348	1.114963	-0.107152
C	-1.679578	2.182609	0.455877
H	-2.331722	2.796781	1.077710
H	-0.967814	1.685658	1.116494
C	-0.993233	2.974837	-0.620746
H	-1.704018	3.497515	-1.263006
H	-0.360932	3.728695	-0.144506
H	-0.360394	2.340295	-1.243913
C	-3.846093	1.516152	-0.536753
H	-4.117408	0.817470	-1.327736
H	-3.745960	2.507613	-0.977959
C	-4.822603	1.487075	0.604289
H	-4.926189	0.481357	1.017939
H	-4.536849	2.170740	1.406037
H	-5.800846	1.799670	0.230356
C	4.594341	-0.177147	1.030514
H	4.042164	-0.338561	1.955601

C	5.894276	-0.435580	1.005769
H	6.502431	-0.285845	0.120109
H	6.403231	-0.800014	1.891818

SIL2TS-4n

C	-3.063657	0.154883	-0.604316
C	-1.768934	0.823282	-0.255440
H	-3.516885	0.407926	-1.555868
H	-1.562406	0.886928	0.812445
H	-1.663427	1.814231	-0.701308
O	-1.596405	-1.059046	-1.506331
C	-0.908262	-0.197088	-0.943452
O	0.363942	-0.181196	-0.953421
C	-3.858895	-0.651008	0.308375
Al	1.712322	0.658128	-0.096206
C	2.409395	2.243984	-0.983240
C	1.358637	3.347892	-1.135934
H	2.799633	1.963471	-1.969353
H	3.267400	2.626391	-0.417489
H	1.774311	4.244424	-1.606836
H	0.519829	3.023315	-1.760031
H	0.948348	3.655176	-0.169006
Cl	1.093222	0.809698	1.970061
C	-3.125196	-1.346521	1.438972
H	-2.565344	-2.197984	1.047849
H	-2.436451	-0.686096	1.968100
H	-3.852651	-1.719423	2.162050
C	-4.859743	-1.561044	-0.375671
H	-5.620226	-1.881400	0.338422
H	-5.354264	-1.081240	-1.221105
H	-4.340292	-2.445414	-0.750065
O	2.954059	-0.738975	-0.144509
C	2.601807	-2.102031	0.245743
H	3.356758	-2.435894	0.959030
H	1.652650	-2.024382	0.776629
C	2.498160	-2.999606	-0.954145
H	3.444385	-3.069644	-1.494607
H	2.233244	-4.004610	-0.615255
H	1.721900	-2.652727	-1.637886
C	4.385677	-0.473899	-0.263345
H	4.474218	0.325200	-0.999498
H	4.836043	-1.374675	-0.681212
C	4.989706	-0.092633	1.059336
H	4.550820	0.828093	1.450180

H	4.869194	-0.882368	1.803618
H	6.060227	0.076742	0.918368
C	-4.420259	0.711825	0.768610
H	-3.955729	1.118502	1.660772
C	-5.359538	1.406753	0.120384
H	-5.821221	1.056624	-0.796479
H	-5.711202	2.353295	0.517005

Imaginary vibration frequency: 346.84i

S-1

C	0.685052	1.142988	-0.326449
C	1.385258	0.762121	0.976042
H	0.902662	2.157283	-0.669916
H	0.779386	0.249182	1.722104
H	1.988401	1.541039	1.440938
O	1.525433	0.198510	-1.062018
C	2.169905	-0.167005	0.080164
O	3.052293	-0.956834	0.182877
C	-0.789443	0.900975	-0.500609
H	-1.029664	0.922069	-1.563263
Br	-1.281663	-0.931187	0.049940
C	-1.610283	1.906967	0.268350
H	-1.405589	1.853525	1.339836
H	-1.365368	2.915337	-0.080169
H	-2.676358	1.743430	0.110724

S-2

C	-1.265103	0.308392	-0.492014
C	-1.607448	-1.179629	-0.494518
H	-1.040525	0.723728	-1.475738
H	-1.141660	-1.775011	0.291092
H	-1.536950	-1.696909	-1.450653
O	-2.670336	0.622566	-0.158422
C	-2.995784	-0.694590	-0.158100
O	-4.069574	-1.166928	0.050329
C	-0.307948	0.813087	0.566262
H	-0.633673	0.387700	1.522107
C	1.073913	0.277560	0.273843
C	1.787835	0.697687	-0.848383
C	1.653263	-0.671206	1.112562
C	3.046042	0.181496	-1.123210
H	1.360637	1.440319	-1.514390
C	2.913887	-1.187760	0.842586
H	1.111106	-1.004281	1.992460

C	3.613910	-0.763718	-0.278203
H	3.586897	0.520292	-2.000493
H	3.349685	-1.922640	1.511073
H	4.598518	-1.165225	-0.491817
C	-0.352677	2.333029	0.666028
H	0.329292	2.686285	1.442426
H	-0.062749	2.802800	-0.277644
H	-1.360626	2.671746	0.915210

AlEtCl₂

Al	-0.129521	-0.136869	-0.000041
C	1.397035	-1.335083	-0.000629
C	2.766846	-0.661040	0.000528
H	1.281232	-1.989549	-0.873407
H	1.280995	-1.991816	0.870376
H	3.571204	-1.403265	-0.000601
H	2.908655	-0.025971	-0.877688
H	2.908387	-0.028884	0.880880
Cl	-2.125395	-0.843216	0.000175
Cl	0.051866	1.972365	-0.000082

SLC-1 (RCom)

C	-1.841834	0.690411	0.645856
C	-0.711948	-0.334014	0.522603
H	-2.248079	0.818717	1.647663
H	-0.745456	-0.989901	-0.348254
H	-0.465231	-0.907372	1.415873
O	-0.827814	1.776161	0.414698
C	0.125414	0.880074	0.324755
O	1.303031	1.154216	0.136132
C	-2.896514	0.734138	-0.423712
H	-2.451126	0.545243	-1.401306
Al	2.839592	0.031777	-0.041014
C	4.333987	1.202891	-0.481385
C	5.661692	0.474736	-0.695601
H	4.435711	1.944459	0.321051
H	4.066995	1.771557	-1.381253
H	6.474722	1.165989	-0.943235
H	5.969161	-0.075708	0.198840
H	5.596923	-0.250919	-1.512186
Cl	2.864314	-0.962739	1.883323
Cl	2.178393	-1.356858	-1.570119
Br	-4.031696	-0.837654	-0.079285
C	-3.711147	2.000218	-0.417609

H	-4.188990	2.164634	0.550279
H	-3.054632	2.849095	-0.630820
H	-4.480996	1.968423	-1.189050

PLC-1

C	-2.222999	0.189304	0.399827
C	-0.841808	-0.332100	0.055303
H	-2.303269	0.406469	1.464535
H	-0.831191	-0.925519	-0.866310
H	-0.354032	-0.911034	0.838625
O	-0.925229	1.931300	-0.459658
C	-0.116555	0.940151	-0.233077
O	1.100217	1.132913	-0.283186
C	-2.327696	1.475747	-0.412893
Al	2.616271	0.024337	-0.020235
C	4.195546	1.133785	-0.294039
C	5.519263	0.384071	-0.135648
H	4.150183	1.971446	0.413533
H	4.133647	1.583097	-1.293193
H	6.384461	1.038504	-0.288631
H	5.619306	-0.052226	0.863028
H	5.606338	-0.436983	-0.853911
Cl	2.286175	-0.723289	1.991569
Cl	2.249398	-1.563185	-1.451779
Br	-3.665578	-1.042780	-0.001368
C	-3.176457	2.561471	0.171158
H	-2.857220	2.802999	1.187152
H	-3.130587	3.461243	-0.443640
H	-4.214900	2.224007	0.201408
H	-2.599440	1.260696	-1.449119

IM-2

C	1.807624	1.079414	-0.413274
C	0.408949	0.566309	-0.536601
H	2.187993	1.618296	-1.274317
H	0.108401	-0.003273	0.343768
H	0.305354	-0.094846	-1.400811
O	-0.156427	2.852574	-0.939878
C	-0.559658	1.730421	-0.709225
O	-1.816078	1.422810	-0.604072
C	2.415459	1.379716	0.833019
H	1.883996	1.041544	1.717782
Al	-2.798653	0.006884	-0.078001
C	-4.705367	0.457529	-0.063510

C	-5.629310	-0.680413	0.368779
H	-4.980822	0.803829	-1.068271
H	-4.843895	1.324985	0.595035
H	-6.685967	-0.387629	0.363691
H	-5.533906	-1.548776	-0.290896
H	-5.397136	-1.024654	1.381742
Cl	-2.293128	-1.653252	-1.425372
Cl	-2.024435	-0.548086	1.914028
C	2.934515	-0.007472	0.042433
C	4.155403	0.039338	-0.662432
C	2.534169	-1.207854	0.666307
C	4.939569	-1.086616	-0.752818
H	4.462141	0.959875	-1.144401
C	3.334218	-2.324622	0.583650
H	1.601345	-1.245002	1.216685
C	4.529364	-2.263471	-0.128182
H	5.870007	-1.060215	-1.306704
H	3.032318	-3.245707	1.066852
H	5.153383	-3.147948	-0.197187
C	3.413767	2.461644	1.052119
H	2.861697	3.316036	1.458225
H	4.168550	2.173157	1.784912
H	3.895424	2.786976	0.130762

PLC-2

C	-1.826456	0.669278	0.362552
C	-0.504440	-0.050347	0.104578
H	-1.799397	1.080213	1.376090
H	-0.570781	-0.772329	-0.717770
H	-0.083624	-0.568242	0.965871
O	-0.294030	2.102662	-0.727441
C	0.376021	1.057101	-0.355912
O	1.611229	1.081292	-0.427656
C	-1.744283	1.845210	-0.615810
H	-2.059024	1.539756	-1.616845
Al	2.969548	-0.151701	-0.000497
C	4.672136	0.695559	-0.435711
C	5.899125	-0.162934	-0.126031
H	4.729955	1.645724	0.110538
H	4.659087	0.964145	-1.499735
H	6.834990	0.345650	-0.383101
H	5.954218	-0.419131	0.936538
H	5.882849	-1.105589	-0.681850
Cl	2.598048	-0.556472	2.102089

Cl	2.410195	-1.886647	-1.181432
C	-3.075423	-0.151291	0.209946
C	-4.020039	-0.168618	1.231534
C	-3.326159	-0.882975	-0.949725
C	-5.191966	-0.902336	1.101930
H	-3.832326	0.395938	2.139478
C	-4.495796	-1.616039	-1.081725
H	-2.602552	-0.889755	-1.758971
C	-5.432815	-1.627881	-0.055685
H	-5.915914	-0.908015	1.909535
H	-4.675751	-2.183147	-1.988546
H	-6.345939	-2.203686	-0.158857
C	-2.431021	3.105551	-0.188880
H	-3.502442	2.908756	-0.105033
H	-2.061809	3.439766	0.783331
H	-2.286706	3.901785	-0.920960

SLC-3a

C	3.045006	-0.652169	-0.284382
C	1.849267	-0.302725	0.609212
H	3.475932	-1.634333	-0.094724
H	1.813876	0.721992	0.981768
H	1.594996	-1.003435	1.403818
O	2.080996	-0.802914	-1.433300
C	1.081082	-0.506583	-0.647669
O	-0.089585	-0.463264	-1.015164
C	4.068165	0.406041	-0.554648
H	4.649514	0.116278	-1.434544
H	3.558756	1.345675	-0.791025
Al	-1.676361	0.007925	-0.082433
C	-3.165870	-0.271229	-1.309409
C	-4.534382	0.077380	-0.722395
H	-3.150661	-1.319892	-1.632610
H	-2.981470	0.322421	-2.213736
H	-5.345862	-0.093168	-1.438485
H	-4.757868	-0.522765	0.165074
H	-4.588105	1.127882	-0.420329
Cl	-1.583137	-1.281730	1.660812
Cl	-1.242181	2.050037	0.506086
C	4.982927	0.583371	0.647810
H	5.726936	1.356097	0.446755
H	4.422411	0.885652	1.536678
H	5.516174	-0.341739	0.882315

TS-3a

C	3.099277	-0.297866	0.471250
C	1.638131	-0.073627	0.511354
H	3.485540	-1.260637	0.798983
H	1.371697	0.978752	0.388996
H	1.191966	-0.445910	1.436986
O	1.907479	-1.488834	-1.360022
C	1.102340	-0.883696	-0.670991
O	-0.165544	-0.870309	-0.864264
C	4.018244	0.661105	0.075883
H	3.752576	0.648159	1.292789
Al	-1.629794	-0.078628	-0.137076
C	-3.235346	-0.592894	-1.130344
C	-4.533879	0.022899	-0.609845
H	-3.306870	-1.688243	-1.117173
H	-3.085190	-0.319838	-2.182968
H	-5.407722	-0.290232	-1.193052
H	-4.724884	-0.259251	0.430374
H	-4.502216	1.116594	-0.641873
Cl	-1.626705	-0.695256	1.968662
Cl	-1.191623	2.073591	-0.181458
H	3.611534	1.613120	-0.262726
C	5.462286	0.393268	-0.152624
H	5.607454	0.322352	-1.235127
H	6.078272	1.217367	0.208666
H	5.784953	-0.543741	0.301828

Imaginary vibration frequency: 287.00i

SLC-3b

C	2.771006	0.795665	0.472585
C	1.560165	0.741768	-0.467554
H	3.141977	1.802574	0.657098
H	1.544468	-0.054608	-1.211090
H	1.249914	1.683085	-0.920519
O	1.839658	0.454970	1.609231
C	0.829773	0.410884	0.783500
O	-0.323173	0.157115	1.122327
C	3.887148	-0.204861	0.323559
H	4.489655	-0.129491	1.236143
Al	-1.896465	-0.032490	0.074478
C	-3.363059	-0.400556	1.305530
C	-4.722368	-0.578645	0.627772
H	-3.410297	0.417973	2.035052
H	-3.108683	-1.299228	1.881692

H	-5.520004	-0.782072	1.350786
H	-5.015334	0.315829	0.069419
H	-4.712969	-1.410960	-0.082750
Cl	-1.954546	1.852587	-0.999666
Cl	-1.319606	-1.619427	-1.289517
C	3.408424	-1.641316	0.175236
H	2.764317	-1.949595	1.002007
H	2.865587	-1.795631	-0.761224
H	4.269293	-2.313231	0.163528
C	4.747618	0.225930	-0.859286
H	5.128988	1.243036	-0.736141
H	5.603784	-0.443851	-0.962671
H	4.179813	0.184919	-1.793968

TS-3b

C	-2.732964	0.273864	0.576273
C	-1.324832	-0.183572	0.506857
H	-3.040679	0.876933	1.426099
H	-1.181572	-1.005134	-0.198238
H	-0.915818	-0.467478	1.478593
O	-1.381413	2.051394	-0.155730
C	-0.647029	1.079941	-0.001117
O	0.607969	1.068505	-0.236086
C	-3.704165	-0.042789	-0.398305
H	-3.295330	-0.441990	-1.323256
Al	1.943740	-0.173544	-0.218696
C	3.625966	0.664715	-0.760382
C	4.075059	1.816883	0.139031
H	3.512013	1.016102	-1.794127
H	4.402767	-0.109276	-0.797402
H	5.017304	2.265210	-0.197232
H	3.330921	2.619121	0.168139
H	4.227865	1.485877	1.171074
Cl	1.933541	-0.965791	1.825336
Cl	1.232861	-1.765425	-1.549824
C	-3.935832	-1.281386	0.614174
H	-4.998159	-1.265442	0.849600
H	-3.591204	-2.185724	0.121606
H	-3.431178	-1.251581	1.597023
C	-4.909158	0.838202	-0.568246
H	-5.709387	0.296940	-1.075535
H	-5.280352	1.195220	0.394706
H	-4.639361	1.703630	-1.176876

Imaginary vibration frequency: 180.04i

SLC-3c

C	-2.010025	-1.178714	0.007817
C	-0.668952	-1.140073	-0.731278
H	-2.322583	-2.178125	0.307260
H	-0.597369	-0.493000	-1.604164
H	-0.207889	-2.105433	-0.940771
O	-1.312601	-0.560289	1.198374
C	-0.190802	-0.520597	0.532365
O	0.859199	-0.070377	0.982603
C	-3.162634	-0.338533	-0.473779
Al	2.553674	0.145067	0.149721
C	3.759138	0.888444	1.489712
C	5.182038	1.136273	0.987003
H	3.776714	0.205644	2.348729
H	3.322421	1.824044	1.861417
H	5.828688	1.551333	1.767958
H	5.653178	0.212552	0.637109
H	5.197105	1.840579	0.149511
Cl	2.969565	-1.866185	-0.551117
Cl	2.044116	1.403481	-1.543217
C	-4.323823	-0.425892	0.526841
H	-4.042697	0.075628	1.458656
H	-4.496731	-1.482606	0.766632
C	-5.590159	0.161435	-0.001927
H	-5.972642	-0.283447	-0.920658
C	-6.259551	1.159014	0.560540
H	-7.181838	1.537231	0.131595
H	-5.910037	1.632201	1.474477
C	-2.781796	1.103495	-0.775043
H	-3.646475	1.640020	-1.168401
H	-2.460191	1.624649	0.130597
H	-1.984526	1.181008	-1.517510
H	-3.478850	-0.825965	-1.406442

TS-3c

C	2.474873	-0.857924	0.521586
C	1.035188	-0.506727	0.554626
H	2.835871	-1.559433	1.266766
H	0.795647	0.296097	-0.145353
H	0.713138	-0.198106	1.552567
O	0.807792	-2.817457	0.009164
C	0.240348	-1.753265	0.161506
O	-1.030546	-1.575870	0.019197

C	3.319908	-0.546404	-0.533512
Al	-2.180520	-0.180723	-0.050666
C	-3.993415	-0.808318	-0.440854
C	-5.042358	0.297707	-0.551777
H	-4.282010	-1.523316	0.340605
H	-3.958466	-1.388133	-1.372379
H	-6.042735	-0.094537	-0.769455
H	-5.118868	0.874637	0.375379
H	-4.796060	1.007376	-1.348003
Cl	-1.990098	0.860995	1.875002
Cl	-1.356488	1.171014	-1.580343
C	3.484300	0.691974	0.730096
H	3.413589	0.405721	1.786473
H	4.559877	0.731914	0.549845
C	2.764716	1.950994	0.422511
H	1.826689	2.125371	0.939367
C	3.246940	2.863669	-0.410281
H	2.715179	3.791530	-0.588456
H	4.185656	2.721256	-0.938661
H	2.886733	0.022162	-1.351819
C	4.576561	-1.292390	-0.813921
H	5.319550	-0.657553	-1.298626
H	4.999182	-1.736120	0.089070
H	4.325416	-2.102911	-1.504640

Imaginary vibration frequency: 30.46i

SLC-3d

C	-2.107554	-1.078294	-0.132011
C	-0.792847	-0.886350	-0.894159
H	-2.426409	-2.116660	-0.055547
H	-0.735790	-0.061881	-1.603352
H	-0.358079	-1.785993	-1.330385
O	-1.361911	-0.749056	1.138326
C	-0.260705	-0.571706	0.457936
O	0.810318	-0.245501	0.959867
C	-3.261177	-0.140242	-0.372238
Al	2.496669	0.092408	0.145220
C	3.709238	0.663953	1.560632
C	5.118366	1.010990	1.078059
H	3.754342	-0.131084	2.315681
H	3.260257	1.529122	2.064920
H	5.768565	1.329398	1.900326
H	5.603035	0.155138	0.598207
H	5.105192	1.823954	0.345567

Cl	2.903981	-1.805766	-0.821746
Cl	1.967403	1.564017	-1.359495
C	-4.380112	-0.449402	0.636923
H	-4.047139	-0.177514	1.645021
H	-4.578622	-1.526556	0.649560
C	-5.617878	0.250011	0.341662
C	-6.639833	0.827735	0.082448
H	-7.548315	1.340846	-0.141661
C	-2.876656	1.330747	-0.353177
H	-3.752499	1.942283	-0.575438
H	-2.504458	1.631368	0.629591
H	-2.116407	1.571647	-1.098565
H	-3.626220	-0.403825	-1.372679

TS-3d

C	2.643256	-0.559642	0.553985
C	1.187778	-0.291134	0.716505
H	3.122483	-1.153188	1.325654
H	0.824178	0.411715	-0.033854
H	0.965752	0.127265	1.701326
O	1.051042	-2.671216	0.623376
C	0.442998	-1.619278	0.581212
O	-0.837898	-1.525294	0.439512
C	3.300869	-0.467919	-0.667460
Al	-2.040603	-0.246940	0.008484
C	-3.812856	-1.042084	-0.243342
C	-4.906884	-0.055439	-0.649705
H	-4.093421	-1.551886	0.687593
H	-3.722648	-1.834873	-0.997449
H	-5.881011	-0.541048	-0.781628
H	-5.039409	0.730352	0.100812
H	-4.667433	0.444314	-1.593747
Cl	-1.949520	1.257677	1.602924
Cl	-1.236278	0.706490	-1.808249
C	3.554710	0.975158	0.475493
H	3.725806	0.888746	1.554076
H	4.564771	1.015370	0.057686
C	2.747252	2.101532	0.111219
C	2.057980	3.035794	-0.190575
H	2.763970	0.016010	-1.480798
C	4.536242	-1.203632	-1.000834
H	5.185843	-0.634774	-1.667121
H	5.081143	-1.530909	-0.114828
H	4.209170	-2.097849	-1.545547

H 1.433996 3.862082 -0.454059

Imaginary vibration frequency: 155.94i

SLC-3e

C	-2.469916	0.950608	0.160057
C	-1.132806	0.852139	0.900723
H	-2.819946	1.971430	0.010869
H	-1.036693	0.080155	1.663474
H	-0.712823	1.790907	1.262335
O	-1.753385	0.534990	-1.096084
C	-0.625219	0.451045	-0.438734
O	0.441954	0.127359	-0.946435
C	-3.590984	0.002090	0.502950
Al	2.166262	-0.068421	-0.155579
C	3.380382	-0.647266	-1.565744
C	4.825843	-0.844853	-1.106667
H	3.339906	0.091243	-2.376419
H	2.989277	-1.579850	-1.991731
H	5.476680	-1.170384	-1.925563
H	5.252123	0.079857	-0.705671
H	4.899512	-1.600108	-0.318134
Cl	2.475033	1.906744	0.686124
Cl	1.745234	-1.474810	1.442086
C	-4.749147	0.251175	-0.438826
H	-3.954488	0.361712	1.479274
C	-3.205798	-1.460835	0.594291
H	-4.074456	-2.055316	0.877629
H	-2.850381	-1.839567	-0.365646
H	-2.430818	-1.625425	1.344180
H	-4.997446	1.321301	-0.597580
O	-5.386132	-0.612845	-0.977776

TS-3e

C	2.168683	0.037062	-0.090191
C	1.244158	0.465885	0.973270
H	1.768543	-0.611778	-0.868428
H	1.776861	0.849957	1.846274
H	0.562405	-0.333243	1.262310
O	1.069104	2.727671	0.244857
C	0.461610	1.693380	0.393227
O	-0.780311	1.506695	0.125495
C	3.440201	0.548080	-0.254054
H	3.810260	1.227218	0.515226
Al	-1.939342	0.121065	-0.053800

C	-3.631493	0.754849	-0.802516
C	-4.675894	-0.336186	-1.036948
H	-3.412782	1.275417	-1.743826
H	-4.033803	1.521802	-0.127981
H	-5.607665	0.061961	-1.455159
H	-4.312482	-1.099288	-1.732493
H	-4.936090	-0.851246	-0.106871
Cl	-0.864928	-1.316883	-1.328716
Cl	-2.095684	-0.789906	1.931961
C	4.254956	0.364430	-1.468553
H	3.867341	-0.422233	-2.115697
H	4.204602	1.312881	-2.018971
H	5.305655	0.188354	-1.231555
C	3.457045	-1.091284	0.808486
O	3.812016	-2.068322	0.281199
H	3.426932	-0.823896	1.872671

Imaginary vibration frequency: 257.00i

SLC-3f

C	2.168486	-0.791637	0.539492
C	1.006476	0.184553	0.735478
H	2.552641	-1.231371	1.456660
H	1.031664	1.096632	0.138502
H	0.726804	0.414826	1.763005
O	1.191575	-1.764897	-0.061007
C	0.215144	-0.913099	0.118861
O	-0.950437	-1.133696	-0.193300
C	3.245634	-0.439835	-0.449617
Al	-2.496815	-0.028677	-0.082479
C	-3.963345	-1.014999	-0.905722
C	-5.291573	-0.256965	-0.927944
H	-4.080929	-1.965530	-0.370153
H	-3.665306	-1.282778	-1.927385
H	-6.090975	-0.839926	-1.398457
H	-5.629424	-0.005111	0.082037
H	-5.210650	0.683206	-1.482205
Cl	-2.620546	0.353739	2.046676
Cl	-1.819689	1.762995	-1.104946
C	4.077037	0.701935	0.117449
H	2.779541	-0.088038	-1.378089
C	4.132310	-1.645950	-0.760796
H	4.883219	-1.399594	-1.512450
H	4.646345	-1.992342	0.139325
H	3.528477	-2.467486	-1.150919

O	4.055572	0.955262	1.302045
C	4.889984	1.492369	-0.858155
H	5.340328	0.859402	-1.624938
H	4.218719	2.190995	-1.370759
H	5.657546	2.063833	-0.337535

TS-3f

C	1.898066	0.477316	-0.345989
C	1.069121	1.036898	0.735074
H	1.374725	-0.062567	-1.133987
H	1.667520	1.566254	1.475125
H	0.471557	0.257271	1.215131
O	0.411722	3.208015	-0.007249
C	0.093543	2.045118	0.070646
O	-1.001890	1.540624	-0.396441
C	3.249882	0.665214	-0.471593
H	3.750154	1.235698	0.309440
Al	-2.019017	0.065003	-0.154655
C	-3.751536	0.260642	-1.042794
C	-4.696573	-0.927048	-0.862119
H	-3.570548	0.438608	-2.110813
H	-4.223155	1.177652	-0.666700
H	-5.654515	-0.780169	-1.374481
H	-4.261627	-1.851919	-1.254208
H	-4.922044	-1.104660	0.194158
Cl	-0.830337	-1.630565	-0.911951
Cl	-2.127941	-0.202072	2.022626
C	4.011174	0.402113	-1.717197
H	3.478009	-0.266860	-2.393063
H	4.143197	1.363136	-2.227049
H	5.008006	0.007790	-1.511140
C	3.106811	-1.205257	0.422211
C	3.141584	-1.098011	1.881975
H	3.656978	-0.192099	2.198639
H	2.111722	-1.063842	2.249478
H	3.632388	-1.991698	2.271951
O	3.233062	-2.044228	-0.363153

Imaginary vibration frequency: 121.08i

SLC-3g

C	1.893880	0.677510	-0.783514
C	0.794233	-0.327041	-0.432364
H	2.298778	0.581471	-1.788696
H	0.836372	-0.759722	0.567957

H	0.579419	-1.100900	-1.168222
O	0.838103	1.749412	-0.823946
C	-0.083982	0.868822	-0.529924
O	-1.275002	1.137384	-0.414804
C	2.931436	1.012842	0.255170
Al	-2.747361	0.020663	0.048358
C	-4.333302	1.152904	0.098227
C	-5.622716	0.405702	0.442386
H	-4.433183	1.647891	-0.876021
H	-4.157911	1.956281	0.824870
H	-6.491909	1.072236	0.463796
H	-5.839352	-0.381675	-0.286128
H	-5.561608	-0.074087	1.424101
Cl	-2.652199	-1.495336	-1.499120
Cl	-2.069727	-0.822831	1.929241
C	3.905840	-0.129616	0.467159
H	2.422553	1.148363	1.217321
C	3.693355	2.288794	-0.088414
H	4.420384	2.511317	0.692666
H	4.225868	2.182383	-1.037036
H	3.006027	3.132254	-0.168234
O	4.796873	-0.104672	1.274031
O	3.663738	-1.158271	-0.346453
C	4.533852	-2.290034	-0.216825
H	4.465365	-2.710056	0.787339
H	4.186901	-3.012402	-0.952151
H	5.565446	-2.003254	-0.424285

TS-3g

C	-1.718152	0.619093	0.159804
C	-0.817402	0.017195	-0.834509
H	-1.351192	0.707165	1.181484
H	-1.354928	-0.314838	-1.723764
H	-0.242791	-0.805865	-0.415743
O	-0.415201	2.133039	-1.856674
C	0.106011	1.180422	-1.321952
O	1.369049	1.022831	-1.143371
C	-2.882274	1.301046	-0.169335
H	-3.212411	1.245391	-1.204383
Al	2.439568	0.024831	-0.070019
C	4.270953	0.710973	-0.120720
C	5.266700	-0.056674	0.748307
H	4.247473	1.767388	0.176340
H	4.603750	0.706127	-1.166913

H	6.279614	0.358161	0.687879
H	4.976321	-0.041214	1.803639
H	5.332514	-1.108241	0.451854
Cl	1.465631	0.150942	1.900524
Cl	2.230861	-2.048075	-0.749213
C	-3.550698	2.270694	0.720788
H	-3.236685	2.171495	1.759279
H	-3.238778	3.260180	0.361427
H	-4.636777	2.222801	0.636146
C	-3.282824	-0.458669	0.474267
O	-3.649628	-0.567088	1.591302
O	-3.439796	-1.198427	-0.573197
C	-4.166636	-2.444519	-0.376146
H	-4.184212	-2.914747	-1.354504
H	-3.631202	-3.061330	0.345143
H	-5.174903	-2.224229	-0.027460

Imaginary vibration frequency: 314.53i

SLC-3h

C	-1.566735	0.906037	0.564793
C	-0.449333	-0.142290	0.523081
H	-1.909754	1.155966	1.568152
H	-0.502227	-0.855670	-0.299599
H	-0.207908	-0.656103	1.453079
O	-0.493358	1.956948	0.234515
C	0.416320	1.028229	0.228986
O	1.612004	1.235969	0.024260
C	-2.653337	0.864004	-0.448334
H	-2.210572	0.611379	-1.421044
Al	3.075230	0.035812	-0.063455
C	4.682641	1.100858	-0.355532
C	5.972731	0.282180	-0.421802
H	4.749963	1.845034	0.448281
H	4.551637	1.673820	-1.282225
H	6.853715	0.912741	-0.585203
H	6.144280	-0.275837	0.503886
H	5.945457	-0.448789	-1.235861
Cl	2.924842	-1.009348	1.834285
Cl	2.464088	-1.297241	-1.664464
Si	-3.893495	-0.560203	-0.051434
C	-5.288317	-0.443733	-1.307026
H	-5.958640	-1.301804	-1.197681
H	-5.883598	0.462734	-1.171671
H	-4.903230	-0.449933	-2.331060

C	-3.050183	-2.236807	-0.201777
H	-2.570033	-2.362605	-1.176647
H	-2.297871	-2.398335	0.574489
H	-3.798498	-3.029260	-0.099526
C	-4.558408	-0.333749	1.695635
H	-3.777720	-0.470359	2.449652
H	-4.999262	0.657120	1.836569
H	-5.339523	-1.073770	1.895740
C	-3.376444	2.206129	-0.547191
H	-3.876087	2.464631	0.391293
H	-2.680087	3.014982	-0.785004
H	-4.133707	2.184864	-1.332784

TS-3h

C	2.190112	0.684123	-0.678827
C	0.687224	0.658460	-0.699136
H	2.682114	0.584062	-1.667157
O	1.015363	1.347037	1.547898
C	0.214796	0.906379	0.730524
O	-1.015663	0.665734	1.011951
C	2.755253	1.856275	-0.111798
H	3.820753	1.812002	0.122093
Al	-2.462239	-0.016866	0.153531
C	-3.994746	-0.040408	1.372324
C	-5.288493	-0.578921	0.762248
H	-4.150730	0.981468	1.742182
H	-3.719203	-0.634104	2.253689
H	-6.121027	-0.574957	1.475606
H	-5.603696	0.014787	-0.101683
H	-5.170561	-1.609696	0.413183
Cl	-2.749839	1.243236	-1.618772
Cl	-1.848038	-2.006926	-0.543187
C	2.196461	3.196146	-0.042922
H	2.437015	3.670456	0.912897
H	2.775226	3.766167	-0.791419
H	1.135314	3.274286	-0.259234
Si	2.981242	-1.004245	0.005963
C	4.801301	-0.669653	0.310078
H	4.962296	-0.039408	1.188825
H	5.309626	-1.621919	0.491667
H	5.286916	-0.201348	-0.551318
C	2.107313	-1.585132	1.552604
H	1.042652	-1.763363	1.383431
H	2.555768	-2.540256	1.847545

H	2.216166	-0.879649	2.377140
C	2.730852	-2.222322	-1.395917
H	1.672685	-2.328085	-1.650585
H	3.275063	-1.924625	-2.296543
H	3.094641	-3.209205	-1.094084
H	0.291666	-0.288121	-1.071737
H	0.244903	1.441075	-1.324467

Imaginary vibration frequency: 240.79i

SLC-3i

C	2.016032	1.450464	0.453431
C	0.836399	1.210634	-0.492370
H	2.242047	2.501046	0.638022
H	0.955824	0.433645	-1.246784
H	0.376407	2.097908	-0.926982
O	1.174685	0.956507	1.579138
C	0.175578	0.743399	0.756826
O	-0.911662	0.299238	1.099639
C	3.294122	0.679936	0.293939
H	3.861108	0.736651	1.222865
Al	-2.479381	-0.051049	0.065570
C	-3.797337	-0.820805	1.277310
C	-5.128396	-1.173265	0.611576
H	-3.962488	-0.111388	2.098080
H	-3.357930	-1.714331	1.738390
H	-5.843813	-1.600639	1.322739
H	-5.603574	-0.293022	0.167642
H	-4.996723	-1.905547	-0.190910
Cl	-2.895927	1.919376	-0.741555
Cl	-1.689825	-1.319477	-1.503248
Br	2.930294	-1.244195	0.067924
C	4.094983	1.206152	-0.873003
H	3.546306	1.110995	-1.812396
H	4.322079	2.264062	-0.708623
H	5.037752	0.667726	-0.966606

TS-3i

C	2.091083	0.448540	-0.564516
C	0.706374	-0.038029	-0.332339
H	2.401322	0.678169	-1.579020
H	0.562863	-0.487532	0.653228
H	0.369909	-0.742183	-1.094897
O	0.678551	2.269972	-0.585452
C	-0.041541	1.282630	-0.428443

O	-1.309919	1.315224	-0.348504
C	2.961499	0.875669	0.508035
Al	-2.647759	0.114991	-0.005006
C	-4.371277	1.038330	-0.024250
C	-5.577561	0.146653	0.269431
H	-4.487577	1.516730	-1.005465
H	-4.325419	1.860606	0.701498
H	-6.522032	0.702472	0.245661
H	-5.665164	-0.665650	-0.458962
H	-5.503685	-0.318370	1.257538
Cl	-2.411974	-1.432518	-1.534535
Cl	-2.080461	-0.765125	1.918570
Br	3.573304	-1.046109	0.048122
C	4.008685	1.897570	0.294771
H	4.428268	1.863533	-0.711022
H	3.512512	2.866232	0.430301
H	4.800369	1.820099	1.040080
H	2.542636	0.795027	1.508798

Imaginary vibration frequency: 206.74i

SLC-3j

C	2.528491	1.050938	0.421905
C	1.339905	0.880018	-0.528219
H	2.854957	2.080070	0.568118
H	1.397597	0.066680	-1.250807
H	0.965437	1.787196	-1.002271
O	1.635429	0.680625	1.555611
C	0.629178	0.522956	0.729798
O	-0.495417	0.189473	1.078188
C	3.722203	0.145666	0.307556
H	4.295687	0.198474	1.233231
Al	-2.098151	-0.036769	0.066497
C	-3.455623	-0.710143	1.292218
C	-4.821554	-0.939953	0.643480
H	-3.548550	-0.003244	2.126275
H	-3.085007	-1.644648	1.732137
H	-5.557352	-1.325097	1.357963
H	-5.231477	-0.014324	0.227689
H	-4.762715	-1.661433	-0.177291
Cl	-2.369692	1.963959	-0.726085
Cl	-1.447398	-1.362891	-1.519068
C	4.568564	0.525681	-0.883283
H	4.003346	0.438344	-1.813707
H	4.910595	1.558896	-0.775478

H	5.444655	-0.119561	-0.946452
Cl	3.193660	-1.583133	0.179565

TS-3j

C	2.592896	0.081573	-0.531483
C	1.172859	-0.269977	-0.285198
H	2.917188	0.292222	-1.545195
H	1.008155	-0.719389	0.696771
H	0.763136	-0.928749	-1.052537
O	1.349430	2.037501	-0.502597
C	0.549083	1.115132	-0.347542
O	-0.711289	1.256702	-0.238895
C	3.521426	0.387820	0.538523
Al	-2.149775	0.156457	0.011334
C	-3.784056	1.224453	0.126707
C	-5.064095	0.410769	0.317060
H	-3.858155	1.835039	-0.782485
H	-3.665590	1.937522	0.952905
H	-5.955592	1.045251	0.382137
H	-5.225730	-0.285439	-0.511899
H	-5.029011	-0.187710	1.232919
Cl	-2.071059	-1.238804	-1.673872
Cl	-1.661422	-0.970052	1.826824
C	4.675413	1.287847	0.332053
H	5.070786	1.229260	-0.682281
H	4.298916	2.303063	0.502488
H	5.462473	1.092100	1.060307
H	3.110667	0.327828	1.543369
Cl	3.847984	-1.423748	0.028659

Imaginary vibration frequency: 226.90i

SLC-3k

C	-2.449607	-1.148897	0.440115
C	-1.255893	-0.982846	-0.507164
H	-2.755949	-2.173638	0.637897
H	-1.345245	-0.199087	-1.258048
H	-0.841024	-1.893431	-0.938484
O	-1.569454	-0.697180	1.564254
C	-0.571137	-0.539528	0.735473
O	0.540397	-0.143235	1.071192
C	-3.621446	-0.223745	0.260730
Al	2.139829	0.081071	0.070854
C	3.473276	0.821717	1.285935
C	4.842746	1.053101	0.645656

H	3.568401	0.144984	2.144573
H	3.082389	1.764049	1.690320
H	5.565346	1.469926	1.355979
H	5.270806	0.122171	0.261118
H	4.782037	1.749345	-0.196524
Cl	2.479645	-1.936007	-0.655694
Cl	1.490249	1.340037	-1.570320
O	-3.096017	1.049788	-0.036722
C	-3.979127	2.113724	0.238754
H	-3.442187	3.037134	0.020969
H	-4.878977	2.077096	-0.386256
H	-4.278439	2.117821	1.294670
C	-4.532875	-0.754653	-0.831357
H	-5.373288	-0.076917	-0.987635
H	-3.989558	-0.851129	-1.775018
H	-4.938491	-1.731294	-0.556540
H	-4.166826	-0.187694	1.215459

TS-3k

C	2.571431	-0.408343	0.597027
C	1.188878	0.134688	0.506603
H	2.909740	-0.829827	1.534785
H	1.026866	0.823850	-0.323121
H	0.838778	0.594055	1.432318
O	1.347358	-2.115512	0.192320
C	0.521333	-1.191302	0.239381
O	-0.728384	-1.328493	0.080867
C	3.561687	-0.294699	-0.465741
Al	-2.138287	-0.160114	-0.035972
C	-3.787394	-1.155357	-0.369206
C	-5.038331	-0.286966	-0.503432
H	-3.918090	-1.879687	0.445161
H	-3.645908	-1.754477	-1.278009
H	-5.940111	-0.881977	-0.688222
H	-5.220953	0.299419	0.402564
H	-4.948210	0.424291	-1.330509
Cl	-2.084087	0.956120	1.843817
Cl	-1.543718	1.213641	-1.637037
O	3.854657	0.858226	0.386295
C	3.601268	2.156472	-0.175338
H	4.430438	2.399423	-0.842926
H	2.661591	2.187378	-0.727063
H	3.568448	2.854703	0.658978
C	4.690612	-1.262057	-0.561585

H	4.336123	-2.168033	-1.058458
H	5.501758	-0.837908	-1.156437
H	5.067767	-1.528626	0.427058
H	3.156224	0.024570	-1.425846

Imaginary vibration frequency: 417.63i

SLC-3I

C	2.081049	-0.868857	0.343858
C	0.914332	0.026002	0.755517
H	2.470224	-1.511835	1.131312
H	0.949139	1.049056	0.380192
H	0.623081	0.020936	1.805426
O	1.112882	-1.690047	-0.465621
C	0.131176	-0.910019	-0.094170
O	-1.035961	-1.068228	-0.440762
C	3.146986	-0.257013	-0.534333
H	2.619433	0.312450	-1.307716
Al	-2.576300	-0.016370	-0.073229
C	-4.093331	-0.900492	-0.921272
C	-5.430217	-0.188397	-0.709354
H	-4.148854	-1.927329	-0.537954
H	-3.881707	-0.993372	-1.994008
H	-6.258877	-0.713011	-1.197667
H	-5.681400	-0.109441	0.352887
H	-5.413339	0.829561	-1.110836
Cl	-2.566081	0.056189	2.094956
Cl	-1.976812	1.912027	-0.866736
N	3.856544	0.725613	0.278301
C	4.437250	1.788306	-0.515921
H	4.847018	2.551708	0.149787
H	5.252578	1.446237	-1.175174
H	3.668460	2.258036	-1.133562
C	4.832816	0.165896	1.193146
H	5.724041	-0.238797	0.687792
H	5.165189	0.950160	1.877253
H	4.392887	-0.629513	1.797921
C	4.001544	-1.319732	-1.212659
H	4.468905	-1.987847	-0.485251
H	3.393347	-1.927021	-1.886368
H	4.790170	-0.854092	-1.807717

TS-3I

C	2.136201	0.345124	-0.654107
C	0.874606	-0.396527	-0.304563

H	2.511984	0.267843	-1.667206
H	0.791298	-0.688635	0.742463
H	0.653421	-1.256132	-0.938010
O	0.869047	1.701266	-0.980366
C	0.051836	0.807839	-0.628698
O	-1.192276	0.960434	-0.579129
C	3.110788	0.759475	0.368364
Al	-2.567773	-0.185228	-0.098914
C	-4.244710	0.817223	-0.129695
C	-4.284038	2.016644	0.818112
H	-5.063274	0.125211	0.104392
H	-4.424498	1.145373	-1.161619
H	-5.239278	2.552051	0.770495
H	-4.138273	1.712709	1.859348
H	-3.498647	2.742289	0.584047
Cl	-2.396221	-1.818550	-1.531644
Cl	-1.949951	-0.920160	1.864144
N	3.678229	-0.583854	0.215689
C	3.638969	-1.435309	1.386348
H	3.785004	-2.474703	1.086768
H	4.424434	-1.162384	2.105160
H	2.673215	-1.354824	1.884895
C	4.876483	-0.732625	-0.583160
H	5.770297	-0.376546	-0.054144
H	5.010606	-1.789792	-0.818401
H	4.789233	-0.189129	-1.523772
H	2.648783	0.841185	1.353122
C	3.979710	1.958371	0.091227
H	3.376230	2.862139	0.194796
H	4.798624	2.014954	0.811315
H	4.395973	1.946514	-0.917093

Imaginary vibration frequency: 483.79i

SLC-3m

C	-2.553855	-1.185855	0.371997
C	-1.372302	-0.893970	-0.558390
H	-2.898655	-2.218045	0.361789
H	-1.422406	0.036182	-1.125461
H	-1.028393	-1.712208	-1.190370
O	-1.613951	-1.034119	1.538059
C	-0.627792	-0.770373	0.721726
O	0.515596	-0.515833	1.087947
C	-3.698497	-0.196915	0.423271
Al	2.035846	0.014268	0.075284

C	3.519767	0.193383	1.327364
C	4.837613	0.622705	0.680933
H	3.648840	-0.765800	1.844733
H	3.228122	0.913525	2.102359
H	5.646294	0.713789	1.414475
H	5.169108	-0.095803	-0.075064
H	4.745416	1.592589	0.182424
Cl	2.171122	-1.570622	-1.400921
Cl	1.310661	1.823956	-0.875818
C	-3.206042	1.210011	0.612873
C	-3.326319	2.200575	-0.260904
H	-4.293397	-0.463639	1.306194
C	-4.552317	-0.408742	-0.819013
H	-5.424819	0.246361	-0.795944
H	-3.994348	-0.194343	-1.734396
H	-4.907247	-1.440462	-0.873196
H	-2.707728	1.406678	1.559911
H	-2.934264	3.187232	-0.038140
H	-3.817516	2.076466	-1.220637

TS-3m

C	-2.619447	-0.067383	-0.453957
C	-1.209669	0.348633	-0.211963
H	-3.008805	0.002414	-1.462930
H	-0.987268	0.544068	0.838509
H	-0.896009	1.204923	-0.811510
O	-1.369352	-1.777799	-1.058194
C	-0.552801	-0.930116	-0.678357
O	0.706765	-1.094557	-0.667737
C	-3.526527	-0.470667	0.592253
Al	2.134449	-0.124704	-0.058484
C	3.786027	-1.121846	-0.378433
C	5.056231	-0.428584	0.114183
H	3.859910	-1.321441	-1.455349
H	3.685909	-2.105670	0.098099
H	5.957337	-1.020803	-0.082890
H	5.198763	0.542896	-0.369575
H	5.022544	-0.245277	1.192773
Cl	1.991442	1.792275	-1.105447
Cl	1.670022	0.240425	2.051547
C	-3.771457	1.046285	0.674765
C	-4.560903	1.710032	-0.178264
H	-3.010410	-0.778771	1.500727
C	-4.692669	-1.351750	0.226374

H	-5.447031	-1.327691	1.014516
H	-5.157468	-1.047562	-0.712845
H	-4.341990	-2.378880	0.109890
H	-3.215719	1.576204	1.439308
H	-4.708299	2.779794	-0.074314
H	-5.096213	1.212273	-0.979980

Imaginary vibration frequency: 295.82i

SLC-3n

C	-1.421391	1.299822	0.485162
C	-0.426550	0.142281	0.592820
H	-1.825617	1.650003	1.433521
H	-0.535358	-0.654652	-0.143418
H	-0.264595	-0.281312	1.583748
O	-0.263235	2.199933	0.128279
C	0.559231	1.188505	0.215302
O	1.767177	1.266865	0.009565
C	-2.443143	1.251801	-0.622634
H	-1.911778	0.976607	-1.540305
Al	3.091372	-0.098658	-0.001004
C	4.788253	0.748345	-0.452789
C	5.971491	-0.218449	-0.519286
H	4.986026	1.536099	0.285139
H	4.668254	1.263372	-1.414377
H	6.906494	0.291506	-0.776238
H	6.133832	-0.724217	0.437533
H	5.813809	-0.998106	-1.270925
Cl	2.892205	-0.931430	1.991373
Cl	2.264599	-1.489516	-1.448536
C	-3.414824	0.137634	-0.304504
C	-4.294442	0.235211	0.772830
C	-3.420958	-1.024840	-1.070806
C	-5.162501	-0.804914	1.072357
H	-4.308651	1.132540	1.382857
C	-4.291220	-2.065551	-0.775223
H	-2.740210	-1.113470	-1.912123
C	-5.163939	-1.958415	0.298522
H	-5.841978	-0.713864	1.912950
H	-4.286075	-2.961924	-1.385885
H	-5.844037	-2.770287	0.531773
C	-3.111217	2.605691	-0.824865
H	-3.836589	2.548772	-1.638628
H	-3.638266	2.931135	0.075364
H	-2.373032	3.369325	-1.080239

TS-3n

C	1.715395	1.102358	-0.415263
C	0.436491	0.354998	-0.274583
H	2.041877	1.357494	-1.417634
H	0.306398	-0.107831	0.704117
H	0.285579	-0.399690	-1.048648
O	0.075786	2.602255	-0.607852
C	-0.505503	1.524768	-0.442913
O	-1.769523	1.384674	-0.404819
C	2.591290	1.440417	0.674069
H	2.115410	1.332001	1.647632
Al	-2.908589	-0.003750	-0.062345
C	-4.758211	0.627249	-0.142667
C	-5.810593	-0.451047	0.114899
H	-4.919785	1.082067	-1.128629
H	-4.871593	1.444157	0.581724
H	-6.832463	-0.057969	0.060961
H	-5.740845	-1.264203	-0.614479
H	-5.692182	-0.901216	1.105629
Cl	-2.393841	-1.531795	-1.542711
Cl	-2.278558	-0.750267	1.901149
C	3.258833	0.089908	0.308159
C	4.213719	0.006811	-0.714232
C	2.922161	-1.061019	1.036240
C	4.845689	-1.195888	-0.974243
H	4.468195	0.886910	-1.293116
C	3.561830	-2.255465	0.775128
H	2.174555	-1.001575	1.819715
C	4.521053	-2.323908	-0.231736
H	5.589924	-1.255236	-1.759721
H	3.312933	-3.138653	1.351637
H	5.015649	-3.266318	-0.439599
C	3.441189	2.679985	0.559755
H	2.828172	3.550934	0.799028
H	4.275040	2.635378	1.262194
H	3.835411	2.817121	-0.448068

Imaginary vibration frequency: 305.98i

SLC-3o

C	-0.615783	1.605204	0.567343
C	0.202336	0.312636	0.521846
H	-0.992885	1.874226	1.553025
H	0.015009	-0.344634	-0.328110

H	0.263483	-0.269538	1.440808
O	0.665546	2.369920	0.352275
C	1.338573	1.249840	0.320812
O	2.554265	1.184319	0.166079
C	-1.610002	1.861884	-0.537040
H	-1.114682	1.621870	-1.484011
Al	3.686736	-0.337283	0.006270
C	5.512176	0.322831	-0.173854
C	6.566754	-0.778369	-0.293572
H	5.731747	0.962210	0.690615
H	5.553710	0.981549	-1.050538
H	7.578779	-0.370720	-0.393036
H	6.568624	-1.432336	0.583905
H	6.389301	-1.414158	-1.166479
Cl	3.206995	-1.446132	1.807654
Cl	2.813087	-1.336860	-1.710613
C	-2.752601	0.889360	-0.354239
C	-3.630470	1.007810	0.721547
C	-2.928205	-0.167165	-1.242505
C	-4.661533	0.100385	0.907374
H	-3.520007	1.823093	1.428598
C	-3.956211	-1.083646	-1.074824
H	-2.255546	-0.277913	-2.086979
C	-4.812957	-0.938649	0.002936
H	-5.340607	0.201080	1.745302
H	-4.087561	-1.899685	-1.774969
C	-2.052222	3.319204	-0.561346
H	-2.768567	3.481082	-1.368861
H	-2.529634	3.608371	0.378123
H	-1.199044	3.980862	-0.725957
Cl	-6.112865	-2.086569	0.226685

TS-3o

C	0.937948	1.644790	-0.430002
C	-0.186681	0.694011	-0.225501
H	1.221337	1.872864	-1.451230
H	-0.250060	0.303829	0.790588
H	-0.184879	-0.141195	-0.928610
O	-0.950236	2.802299	-0.744993
C	-1.324280	1.651425	-0.497882
O	-2.540277	1.278591	-0.458157
C	1.729948	2.221188	0.623944
H	1.276193	2.103189	1.606832
Al	-3.391827	-0.293018	-0.069317

C	-5.327518	-0.045613	-0.197824
C	-6.149524	-1.302728	0.086389
H	-5.555130	0.333142	-1.202715
H	-5.616347	0.756995	0.493019
H	-7.227694	-1.123759	0.002306
H	-5.903331	-2.110822	-0.609654
H	-5.965569	-1.684774	1.095549
Cl	-2.554926	-1.741229	-1.482005
Cl	-2.662166	-0.828326	1.928936
C	2.627008	0.988283	0.356773
C	3.588689	0.990501	-0.662657
C	2.496654	-0.144055	1.174232
C	4.427846	-0.092263	-0.836623
H	3.690868	1.846481	-1.318637
C	3.333594	-1.225987	1.011503
H	1.747891	-0.160541	1.958489
C	4.291994	-1.188844	0.003675
H	5.177107	-0.089657	-1.618239
H	3.246916	-2.093232	1.653492
C	2.346229	3.579926	0.410835
H	1.582497	4.341991	0.576368
H	3.160935	3.741412	1.118544
H	2.728897	3.707260	-0.602652
Cl	5.342785	-2.551908	-0.208008

Imaginary vibration frequency: 305.06i

SLC-3p

C	-1.001990	1.451030	0.523272
C	-0.107751	0.209309	0.501011
H	-1.382386	1.723468	1.506671
H	-0.266128	-0.480936	-0.328079
H	-0.001375	-0.343743	1.433879
O	0.232036	2.285337	0.273311
C	0.968065	1.206474	0.260351
O	2.183911	1.208953	0.088738
C	-2.021052	1.619306	-0.574763
H	-1.524828	1.376981	-1.520949
Al	3.419758	-0.232627	0.005189
C	5.180704	0.537514	-0.322967
C	6.306602	-0.493447	-0.415834
H	5.394378	1.257759	0.476940
H	5.130702	1.125247	-1.248354
H	7.279910	-0.025681	-0.600778
H	6.399365	-1.073805	0.507338

H	6.134075	-1.207579	-1.226974
Cl	3.102837	-1.201950	1.919676
Cl	2.563742	-1.450665	-1.574276
C	-3.106845	0.591801	-0.348999
C	-3.985912	0.692942	0.729221
C	-3.229702	-0.503395	-1.196248
C	-4.956436	-0.271278	0.945171
H	-3.918783	1.537390	1.407809
C	-4.205746	-1.467369	-0.979288
H	-2.556422	-0.603588	-2.042439
C	-5.085424	-1.369918	0.094304
H	-5.630212	-0.170507	1.790878
H	-4.283141	-2.311029	-1.658015
C	-2.538558	3.050484	-0.637037
H	-3.272588	3.149526	-1.438899
H	-3.019540	3.343141	0.299505
H	-1.724085	3.751500	-0.832962
C	-6.146903	-2.400192	0.330523
H	-6.096777	-2.793060	1.349858
H	-7.145428	-1.972248	0.198236
H	-6.047334	-3.238123	-0.361629

TS-3p

C	1.312535	1.419595	-0.424693
C	0.132482	0.530300	-0.228955
H	1.614560	1.635993	-1.443048
H	0.056597	0.114491	0.776120
H	0.068632	-0.280997	-0.956347
O	-0.437270	2.700135	-0.671046
C	-0.923938	1.581793	-0.456010
O	-2.169131	1.333491	-0.416499
C	2.156810	1.906128	0.638112
H	1.692211	1.806774	1.618426
Al	-3.171280	-0.158469	-0.068605
C	-5.071622	0.302076	-0.110890
C	-6.014799	-0.867096	0.172735
H	-5.295824	0.736103	-1.093896
H	-5.243309	1.108023	0.614350
H	-7.069337	-0.569629	0.140296
H	-5.886561	-1.673959	-0.555722
H	-5.833978	-1.299610	1.161879
Cl	-2.539961	-1.615143	-1.574155
Cl	-2.444323	-0.860929	1.876628
C	2.970996	0.626177	0.356542

C	3.917308	0.572449	-0.674187
C	2.767576	-0.513057	1.150824
C	4.661657	-0.574288	-0.877083
H	4.078275	1.434218	-1.311431
C	3.518830	-1.647647	0.943369
H	2.028111	-0.489517	1.943979
C	4.477390	-1.700780	-0.076271
H	5.395476	-0.601439	-1.675216
H	3.362298	-2.516352	1.573981
C	2.855491	3.228216	0.446111
H	2.145021	4.036013	0.630994
H	3.685391	3.324368	1.148271
H	3.237928	3.347369	-0.568833
C	5.285853	-2.937210	-0.286925
H	5.843269	-2.896668	-1.223331
H	6.003910	-3.065774	0.529697
H	4.648601	-3.825024	-0.296061

Imaginary vibration frequency: 342.20i

SLC-3q

C	0.623959	1.540297	-0.598246
C	-0.204232	0.258263	-0.489678
H	1.022235	1.744722	-1.591139
H	-0.038866	-0.343423	0.404712
H	-0.247055	-0.382090	-1.370163
O	-0.661355	2.324064	-0.461984
C	-1.339103	1.211316	-0.374425
O	-2.559079	1.160821	-0.242710
C	1.595559	1.860688	0.508476
H	1.077986	1.681394	1.457500
Al	-3.717116	-0.331172	-0.031519
C	-5.527016	0.371772	0.148737
C	-6.600034	-0.701232	0.338977
H	-5.750477	0.974560	-0.740671
H	-5.539808	1.071318	0.994207
H	-7.602182	-0.269504	0.437356
H	-6.630922	-1.395390	-0.506529
H	-6.418148	-1.298943	1.237499
Cl	-3.279573	-1.498070	-1.807263
Cl	-2.857745	-1.307787	1.705990
C	2.736142	0.873032	0.413993
C	3.662399	0.928438	-0.621005
C	2.866704	-0.150688	1.353035
C	4.693215	0.002861	-0.725939

H	3.596361	1.712982	-1.368113
C	3.886163	-1.079029	1.266770
H	2.158576	-0.217110	2.173659
C	4.809310	-1.010307	0.223037
H	5.395942	0.083506	-1.545028
H	3.985301	-1.868288	2.003351
C	2.037886	3.317008	0.452718
H	2.737507	3.528282	1.263518
H	2.536129	3.546914	-0.492384
H	1.183211	3.989385	0.556273
O	5.773355	-1.956156	0.215405
C	6.727244	-1.920884	-0.828784
H	7.301365	-0.988467	-0.817609
H	7.402096	-2.756304	-0.648076
H	6.255122	-2.047777	-1.808661

TS-3q

C	0.898672	1.584993	-0.467595
C	-0.198391	0.605864	-0.204841
H	1.212730	1.721873	-1.496281
H	-0.260492	0.281607	0.834486
H	-0.175162	-0.272993	-0.851390
O	-0.888687	2.676535	-0.828453
C	-1.321439	1.546693	-0.545434
O	-2.548441	1.228364	-0.537576
C	1.698381	2.211317	0.562751
H	1.219910	2.167823	1.540654
Al	-3.455435	-0.304138	-0.095793
C	-5.379534	-0.006774	-0.278586
C	-6.242169	-1.220047	0.069504
H	-5.579750	0.313682	-1.309188
H	-5.655959	0.845456	0.355550
H	-7.313225	-1.016587	-0.044295
H	-6.008762	-2.077135	-0.570079
H	-6.085065	-1.542509	1.103676
Cl	-2.628482	-1.834109	-1.422438
Cl	-2.782935	-0.752107	1.939690
C	2.620394	0.991323	0.417170
C	3.599548	0.925085	-0.580800
C	2.489626	-0.094156	1.302028
C	4.451337	-0.157639	-0.677009
H	3.709040	1.740054	-1.287370
C	3.331258	-1.172973	1.218622
H	1.728585	-0.068063	2.074182

C	4.321752	-1.217143	0.225539
H	5.206389	-0.174453	-1.451575
H	3.246009	-2.003541	1.909214
C	2.291439	3.566712	0.268365
H	1.512911	4.326877	0.355063
H	3.085013	3.795446	0.981928
H	2.702243	3.624604	-0.740857
O	5.090887	-2.307713	0.218932
C	6.108734	-2.417049	-0.767410
H	6.841542	-1.611155	-0.668673
H	6.596880	-3.372305	-0.584799
H	5.684184	-2.413944	-1.775257

Imaginary vibration frequency: 378.85i

SLC-3r

C	-1.015655	1.440450	0.516547
C	-0.114928	0.203784	0.499496
H	-1.400278	1.713161	1.498231
H	-0.267179	-0.487545	-0.329799
H	-0.010273	-0.348813	1.432829
O	0.219041	2.281335	0.272118
C	0.957661	1.205347	0.263067
O	2.174895	1.211575	0.096656
C	-2.032312	1.600329	-0.584221
H	-1.533837	1.350459	-1.527591
Al	3.415923	-0.222643	0.010096
C	5.174532	0.556139	-0.311853
C	6.303227	-0.470360	-0.418671
H	5.387554	1.267533	0.496133
H	5.121460	1.154655	-1.230153
H	7.275029	0.002226	-0.599409
H	6.398970	-1.061504	0.497347
H	6.131443	-1.175238	-1.238025
Cl	3.102712	-1.203565	1.919407
Cl	2.571692	-1.439579	-1.577037
C	-3.116127	0.573398	-0.351234
C	-4.007005	0.682566	0.716054
C	-3.233151	-0.540356	-1.178742
C	-4.976486	-0.276554	0.947232
H	-3.953649	1.538039	1.382250
C	-4.200164	-1.507099	-0.961361
H	-2.556100	-0.652770	-2.020672
C	-5.092126	-1.392892	0.110133
H	-5.659005	-0.166496	1.784458

H	-4.270414	-2.362617	-1.626036
C	-2.546733	3.032004	-0.659289
H	-3.276061	3.126260	-1.466073
H	-3.033924	3.330897	0.272246
H	-1.731162	3.732416	-0.853791
N	-6.022711	-2.378214	0.369754
H	-6.818204	-2.101171	0.923805
H	-6.273130	-2.968009	-0.408700

TS-3r

C	1.283367	1.400070	-0.432624
C	0.142251	0.456208	-0.210211
H	1.592929	1.579432	-1.455793
H	0.099357	0.042873	0.797873
H	0.081854	-0.358334	-0.933552
O	-0.364382	2.609810	-0.619670
C	-0.909163	1.505792	-0.418218
O	-2.159322	1.319449	-0.390612
C	2.168717	1.865021	0.620556
H	1.707823	1.776024	1.604794
Al	-3.207820	-0.154627	-0.065102
C	-5.090670	0.368774	-0.130688
C	-6.076772	-0.771039	0.124933
H	-5.284731	0.820860	-1.111982
H	-5.246574	1.172028	0.601055
H	-7.119923	-0.437178	0.081471
H	-5.965629	-1.572749	-0.611934
H	-5.925061	-1.221478	1.110963
Cl	-2.593054	-1.608862	-1.577071
Cl	-2.515130	-0.880831	1.880071
C	3.015495	0.618659	0.360520
C	3.960199	0.566231	-0.677241
C	2.847523	-0.527640	1.155538
C	4.723438	-0.556175	-0.890808
H	4.107163	1.427532	-1.319243
C	3.605301	-1.653401	0.954156
H	2.119850	-0.516281	1.960570
C	4.562652	-1.695681	-0.079972
H	5.455439	-0.572822	-1.691194
H	3.471755	-2.521402	1.590919
C	2.829547	3.207619	0.420587
H	2.100313	4.002187	0.589228
H	3.652482	3.332799	1.126963
H	3.220346	3.324543	-0.591911

N	5.323540	-2.795352	-0.270308
H	5.116950	-3.645373	0.226561
H	5.909977	-2.870981	-1.084218

Imaginary vibration frequency: 417.51i

SLC-3s

C	-0.760825	1.551432	0.571629
C	0.076085	0.270635	0.520765
H	-1.140026	1.811731	1.558836
H	-0.101905	-0.387085	-0.330980
H	0.148150	-0.312787	1.438172
O	0.505101	2.335283	0.353981
C	1.197416	1.226002	0.319732
O	2.413114	1.181282	0.163914
C	-1.761565	1.798842	-0.530418
H	-1.266733	1.568181	-1.479629
Al	3.570776	-0.323953	0.004123
C	5.386026	0.366317	-0.161939
C	6.460039	-0.716746	-0.274106
H	5.587680	1.008237	0.705026
H	5.423394	1.026742	-1.037494
H	7.465643	-0.291639	-0.364859
H	6.465941	-1.371458	0.602774
H	6.300625	-1.354467	-1.149051
Cl	3.094684	-1.444364	1.798990
Cl	2.715680	-1.327045	-1.719774
C	-2.892671	0.813923	-0.347889
C	-3.763735	0.920869	0.736303
C	-3.060757	-0.236201	-1.247107
C	-4.782209	0.004746	0.919869
H	-3.652370	1.733345	1.445791
C	-4.076990	-1.160367	-1.080169
H	-2.389869	-0.330101	-2.094512
C	-4.941098	-1.041156	0.008515
H	-5.456734	0.093153	1.763104
H	-4.203972	-1.972347	-1.786109
C	-2.223945	3.250390	-0.548246
H	-2.947088	3.405200	-1.350988
H	-2.697683	3.532034	0.395162
H	-1.379345	3.921449	-0.717750
C	-5.990918	-1.986945	0.191580
N	-6.840975	-2.751114	0.341137

TS-3s

C	1.096937	1.600518	-0.425689
C	-0.075363	0.710772	-0.257807
H	1.388069	1.858240	-1.438461
H	-0.176772	0.310537	0.751497
H	-0.092773	-0.114952	-0.972463
O	-0.859044	2.838089	-0.802963
C	-1.204278	1.688448	-0.541852
O	-2.415066	1.287009	-0.485982
C	1.872794	2.154130	0.644052
H	1.412672	2.024019	1.621851
Al	-3.259545	-0.276832	-0.074534
C	-5.196811	-0.039954	-0.202277
C	-6.015216	-1.291740	0.113558
H	-5.429412	0.316002	-1.214317
H	-5.484557	0.777467	0.471545
H	-7.094091	-1.116552	0.030321
H	-5.770626	-2.114808	-0.565289
H	-5.826164	-1.650788	1.130186
Cl	-2.417480	-1.749240	-1.461624
Cl	-2.532571	-0.788181	1.933397
C	2.723356	0.881514	0.348009
C	3.699311	0.878181	-0.657358
C	2.548021	-0.251916	1.155726
C	4.513264	-0.222934	-0.829128
H	3.829543	1.740812	-1.298880
C	3.362120	-1.350130	0.994509
H	1.783415	-0.255709	1.924118
C	4.344659	-1.333276	-0.001107
H	5.274991	-0.230611	-1.598772
H	3.245283	-2.221480	1.626536
C	2.550808	3.486077	0.459183
H	1.822868	4.274677	0.659063
H	3.381221	3.591466	1.158762
H	2.920182	3.625243	-0.557575
C	5.187564	-2.470830	-0.175189
N	5.870141	-3.387507	-0.316505

Imaginary vibration frequency: 208.08i

SLC-3t

C	-0.338701	1.706507	0.555830
C	0.434323	0.385457	0.588375
H	-0.724892	2.038984	1.518129
H	0.229766	-0.313797	-0.223126
H	0.470625	-0.143646	1.540158

O	0.967117	2.414834	0.321502
C	1.603215	1.271806	0.344242
O	2.814570	1.159199	0.191125
C	-1.297584	1.937120	-0.586819
H	-0.786736	1.630235	-1.505647
Al	3.893796	-0.403659	0.034449
C	5.736854	0.193257	-0.179487
C	6.745406	-0.942805	-0.356735
H	6.003967	0.801580	0.693905
H	5.778809	0.872289	-1.040522
H	7.768904	-0.570164	-0.474149
H	6.746560	-1.619500	0.503341
H	6.520388	-1.547979	-1.240331
Cl	3.396627	-1.480062	1.849446
Cl	2.959289	-1.378391	-1.664791
C	-2.483655	1.023100	-0.390673
C	-3.353681	1.205189	0.685014
C	-2.712318	-0.028769	-1.274869
C	-4.431796	0.360663	0.875677
H	-3.194334	2.019314	1.383228
C	-3.789483	-0.881209	-1.103382
H	-2.042530	-0.180615	-2.114171
C	-4.633671	-0.671811	-0.026375
H	-5.110843	0.496164	1.706984
H	-3.974314	-1.696374	-1.790412
C	-1.689412	3.405067	-0.702874
H	-2.374124	3.546244	-1.541005
H	-2.184959	3.761082	0.203482
H	-0.807959	4.025835	-0.875954
N	-5.777355	-1.569044	0.165513
O	-5.952550	-2.450682	-0.653999
O	-6.489604	-1.382914	1.134244

TS-3t

C	0.681873	1.799335	-0.412519
C	-0.431411	0.831112	-0.309129
H	0.981832	2.113181	-1.406873
H	-0.537329	0.398378	0.686174
H	-0.365478	0.024301	-1.042228
O	-1.386248	2.897469	-0.861942
C	-1.629717	1.721807	-0.613155
O	-2.800490	1.209167	-0.584745
C	1.369708	2.382394	0.697189
H	0.892533	2.182998	1.654989

Al	-3.521898	-0.395795	-0.108871
C	-5.466346	-0.345139	-0.313887
C	-6.181669	-1.638167	0.077467
H	-5.691086	-0.092684	-1.358322
H	-5.850749	0.492791	0.281913
H	-7.267765	-1.570259	-0.054352
H	-5.838248	-2.486355	-0.523172
H	-6.001357	-1.896766	1.125665
Cl	-2.508316	-1.874721	-1.369746
Cl	-2.827702	-0.717515	1.950147
C	2.317406	1.176782	0.381179
C	3.322698	1.283747	-0.588558
C	2.205714	0.010129	1.151795
C	4.231174	0.256887	-0.760052
H	3.399741	2.170173	-1.205302
C	3.114820	-1.013328	0.993138
H	1.418136	-0.079772	1.890825
C	4.109444	-0.866233	0.038218
H	5.018368	0.322163	-1.498861
H	3.058033	-1.912638	1.591483
C	1.963559	3.760807	0.580283
H	1.175916	4.489794	0.780763
H	2.760263	3.896455	1.312822
H	2.355979	3.962461	-0.416632
N	5.083823	-1.964375	-0.138038
O	5.939708	-1.822143	-0.986106
O	4.966769	-2.935875	0.578300

Imaginary vibration frequency: 165.09i

SLC-4a

C	2.771006	0.795665	0.472585
C	1.560165	0.741768	-0.467554
H	3.141977	1.802574	0.657098
H	1.544468	-0.054608	-1.211090
H	1.249914	1.683085	-0.920519
O	1.839658	0.454970	1.609231
C	0.829773	0.410884	0.783500
O	-0.323173	0.157115	1.122327
C	3.887148	-0.204861	0.323559
H	4.489655	-0.129491	1.236143
Al	-1.896465	-0.032490	0.074478
C	-3.363059	-0.400556	1.305530
C	-4.722368	-0.578645	0.627772
H	-3.410297	0.417973	2.035052

H	-3.108683	-1.299228	1.881692
H	-5.520004	-0.782072	1.350786
H	-5.015334	0.315829	0.069419
H	-4.712969	-1.410960	-0.082750
Cl	-1.954546	1.852587	-0.999666
Cl	-1.319606	-1.619427	-1.289517
C	3.408424	-1.641316	0.175236
H	2.764317	-1.949595	1.002007
H	2.865587	-1.795631	-0.761224
H	4.269293	-2.313231	0.163528
C	4.747618	0.225930	-0.859286
H	5.128988	1.243036	-0.736141
H	5.603784	-0.443851	-0.962671
H	4.179813	0.184919	-1.793968

TS-4a

C	-2.814416	-0.777512	-0.349217
C	-1.363868	-0.600889	-0.594156
H	-3.202302	-1.792787	-0.343929
H	-1.083510	0.393423	-0.941479
H	-0.965165	-1.346354	-1.284971
O	-1.694425	-1.157340	1.638663
C	-0.838221	-0.850604	0.811389
O	0.407832	-0.738131	1.057669
C	-3.763772	0.250549	-0.266305
H	-3.662379	-0.107063	-1.417044
Al	1.848703	-0.058480	0.165458
C	3.440835	-0.127998	1.298810
C	4.704662	0.433448	0.647029
H	3.603622	-1.171676	1.597370
H	3.223399	0.415180	2.227478
H	5.575727	0.378311	1.310162
H	4.962465	-0.110862	-0.266964
H	4.580633	1.484405	0.367183
Cl	1.987095	-1.230708	-1.679087
Cl	1.212254	1.965888	-0.394348
C	-3.358575	1.692585	-0.155857
H	-3.186353	1.914420	0.901266
H	-2.450044	1.933604	-0.705549
H	-4.164645	2.336325	-0.508171
C	-5.151724	-0.088827	0.202825
H	-5.892607	0.542392	-0.288769
H	-5.398800	-1.138152	0.036231
H	-5.198884	0.110275	1.276861

Imaginary vibration frequency: 412.53i**SLC-4b**

C	2.500001	0.805956	0.275581
C	1.229694	0.825057	-0.582573
H	2.899552	1.794666	0.498063
H	1.154779	0.093715	-1.386122
H	0.901345	1.802328	-0.936337
O	1.638979	0.404648	1.449212
C	0.579702	0.408103	0.687247
O	-0.548985	0.124412	1.080252
C	3.599904	-0.195316	-0.005048
Al	-2.172609	-0.039205	0.108279
C	-3.561709	-0.540002	1.381499
C	-4.948454	-0.712405	0.759999
H	-3.594387	0.222550	2.170020
H	-3.252744	-1.468960	1.877305
H	-5.701735	-0.993491	1.504229
H	-5.295196	0.210323	0.284595
H	-4.951774	-1.490149	-0.009948
Cl	-2.338844	1.913294	-0.823189
Cl	-1.625209	-1.509888	-1.392076
C	3.058805	-1.611951	-0.175895
H	2.565285	-1.968952	0.731262
H	2.354105	-1.693373	-1.007013
H	3.887863	-2.291038	-0.387461
C	4.594657	-0.158382	1.153312
H	5.423675	-0.842066	0.955011
H	5.009530	0.844579	1.288224
H	4.125839	-0.464804	2.091889
C	4.280745	0.267477	-1.293178
H	4.669609	1.285412	-1.198236
H	5.121790	-0.391785	-1.520356
H	3.595258	0.239097	-2.144619

TS-4b

C	-2.603290	-0.771927	-0.111842
C	-1.165309	-0.574408	-0.412902
H	-2.954735	-1.794092	-0.008528
H	-0.930461	0.393328	-0.855901
H	-0.757838	-1.363065	-1.048632
O	-1.414742	-0.943640	1.867840
C	-0.594021	-0.682901	0.990446
O	0.653712	-0.506540	1.189565

C	-3.574327	0.252356	0.001148
Al	2.084087	-0.021735	0.166268
C	3.689764	0.079713	1.278621
C	4.963645	0.466646	0.527693
H	3.824006	-0.892308	1.770804
H	3.497615	0.796249	2.087750
H	5.838469	0.512855	1.186622
H	5.197011	-0.250693	-0.265454
H	4.868599	1.447750	0.051676
Cl	2.164741	-1.518421	-1.431848
Cl	1.484598	1.880237	-0.751284
C	-3.146980	1.673292	0.274860
H	-3.009709	1.800536	1.350889
H	-2.217681	1.946380	-0.224435
H	-3.927912	2.361879	-0.052423
C	-4.859380	-0.142947	0.692048
H	-5.657279	0.556960	0.437204
H	-5.173170	-1.151353	0.412864
H	-4.709205	-0.115349	1.773293
C	-3.665270	-0.017763	-1.608288
H	-3.393194	-1.011268	-1.993779
H	-4.735481	0.071999	-1.797325
H	-3.071678	0.730952	-2.122819

Imaginary vibration frequency: 254.75i

SLC-4c

C	1.896684	-1.469045	-0.012422
C	0.685618	-1.013810	0.809935
H	2.128568	-2.528024	0.096486
H	0.757927	-0.061395	1.332668
H	0.239814	-1.764142	1.463053
O	1.043401	-1.331716	-1.250343
C	0.035263	-0.930978	-0.524045
O	-1.060334	-0.620318	-0.983264
C	3.158881	-0.633654	-0.070139
Al	-2.591446	0.096279	-0.114440
C	-3.936006	0.409594	-1.491106
C	-5.244335	1.004022	-0.967827
H	-4.131868	-0.542218	-2.001061
H	-3.499086	1.070455	-2.250503
H	-5.973001	1.166442	-1.769691
H	-5.718741	0.349204	-0.230375
H	-5.082103	1.970462	-0.480641
Cl	-3.022971	-1.423375	1.372071

Cl	-1.749251	1.840964	0.866037
C	2.832582	0.841279	-0.383255
H	2.135857	1.235475	0.362212
H	2.329543	0.885632	-1.356068
C	4.029424	1.734213	-0.426956
H	4.755691	1.541137	-1.213758
C	4.243630	2.740685	0.410827
H	5.123204	3.370905	0.327767
H	3.542056	2.976379	1.207023
C	3.806459	-0.763353	1.307402
H	4.762577	-0.237270	1.320298
H	3.177952	-0.328693	2.089661
H	3.994484	-1.811136	1.558181
C	4.071946	-1.230908	-1.139229
H	4.253777	-2.291324	-0.943388
H	3.634591	-1.137544	-2.136770
H	5.039912	-0.726967	-1.145446

TS-4c

C	2.159963	-0.927814	0.682688
C	0.794811	-0.357509	0.656206
H	2.401392	-1.582272	1.514876
H	0.680417	0.508494	0.004723
H	0.421378	-0.110242	1.652413
O	0.722208	-2.541445	-0.141234
C	0.037520	-1.545333	0.084668
O	-1.216911	-1.459615	-0.129372
C	3.195641	-0.657032	-0.238436
Al	-2.456054	-0.120833	-0.065016
C	-4.207143	-0.802897	-0.606426
C	-5.331753	0.231754	-0.566956
H	-4.455379	-1.652573	0.042845
H	-4.114809	-1.220406	-1.617317
H	-6.296580	-0.189128	-0.872814
H	-5.465409	0.642965	0.438591
H	-5.125390	1.076740	-1.231474
Cl	-2.368588	0.632705	1.991000
Cl	-1.629748	1.441546	-1.364870
C	3.554386	0.584438	0.860539
H	3.318827	0.337866	1.904927
H	4.641854	0.514622	0.797100
C	3.040433	1.925756	0.497729
H	2.028692	2.178679	0.800011
C	3.782470	2.825452	-0.135048

H	3.395575	3.813785	-0.358065
H	4.803217	2.612829	-0.440462
C	4.336075	-1.649586	-0.237863
H	5.214653	-1.218018	-0.721419
H	4.605273	-1.956069	0.775234
H	4.037166	-2.538371	-0.797974
C	2.867612	-0.114199	-1.603917
H	2.621636	-0.957943	-2.252967
H	2.029661	0.580650	-1.608715
H	3.735771	0.397267	-2.022764

Imaginary vibration frequency: 255.30i

SLC-4d

C	1.910163	-1.110218	0.241980
C	0.731189	-0.380283	0.895729
H	2.232866	-2.002975	0.776818
H	0.774217	0.706822	0.939034
H	0.384449	-0.779369	1.849012
O	0.970216	-1.557673	-0.843538
C	-0.013427	-0.910742	-0.275801
O	-1.154835	-0.867060	-0.723595
C	3.085204	-0.327164	-0.309484
Al	-2.688861	0.052642	-0.070963
C	-4.093021	-0.153023	-1.407395
C	-5.399639	0.561158	-1.058284
H	-4.276100	-1.225315	-1.551515
H	-3.707248	0.215477	-2.366431
H	-6.162669	0.425696	-1.832663
H	-5.824349	0.190214	-0.120381
H	-5.251118	1.638766	-0.938609
Cl	-2.981506	-0.903400	1.852689
Cl	-1.901914	2.053856	0.230759
C	3.846602	0.174247	0.939836
H	4.101038	-0.678482	1.579793
H	3.193459	0.829128	1.527376
C	5.064920	0.896421	0.622306
C	6.073893	1.493420	0.356873
H	6.969699	2.025512	0.126057
C	3.958829	-1.276592	-1.123683
H	4.838490	-0.749998	-1.498720
H	4.300178	-2.120803	-0.517986
H	3.410246	-1.668919	-1.983014
C	2.641574	0.848253	-1.172786
H	2.081819	0.508148	-2.046617

H	2.026417	1.564812	-0.622860
H	3.521176	1.384183	-1.534076

TS-4d

C	2.362249	-0.734142	0.735484
C	0.942027	-0.336963	0.760602
H	2.733885	-1.313353	1.576259
H	0.713872	0.531719	0.141943
H	0.585709	-0.148578	1.775593
O	0.963265	-2.565563	0.015314
C	0.256637	-1.583605	0.205651
O	-1.001499	-1.532065	-0.021565
C	3.287108	-0.432100	-0.287526
Al	-2.273318	-0.227704	-0.045694
C	-3.994405	-0.973639	-0.601540
C	-5.133120	0.043717	-0.673177
H	-4.255190	-1.780880	0.095227
H	-3.860010	-1.457347	-1.577606
H	-6.080980	-0.411676	-0.982795
H	-5.308445	0.521173	0.296109
H	-4.913692	0.844090	-1.386941
Cl	-2.267582	0.625795	1.972641
Cl	-1.461648	1.300927	-1.398535
C	3.514761	0.915540	0.735421
H	3.412881	0.725758	1.813486
H	4.592287	1.008465	0.579545
C	2.784332	2.086568	0.345691
C	2.164021	3.062577	0.024058
C	4.553879	-1.251033	-0.297606
H	5.336333	-0.739920	-0.861207
H	4.914688	-1.454036	0.712728
H	4.347060	-2.206134	-0.785428
H	1.605924	3.927706	-0.260949
C	2.814176	-0.010867	-1.651477
H	2.629632	-0.918221	-2.231417
H	1.900193	0.578627	-1.636265
H	3.591771	0.563175	-2.157546

Imaginary vibration frequency: 213.34i

SLC-4e

C	-2.240474	0.752513	-0.499153
C	-0.934395	1.077194	0.232523
H	-2.609382	1.560815	-1.130669
H	-0.852445	0.766971	1.273450

H	-0.550325	2.090095	0.111949
O	-1.462706	-0.184412	-1.381000
C	-0.362120	0.103275	-0.734892
O	0.733908	-0.381110	-0.992656
C	-3.356917	0.052495	0.245762
Al	2.400012	-0.122489	-0.099826
C	3.723874	-1.227977	-1.006524
C	5.128887	-1.135070	-0.409134
H	3.744275	-0.939075	-2.064933
H	3.373818	-2.267721	-0.987116
H	5.845892	-1.767707	-0.943721
H	5.515352	-0.111786	-0.443227
H	5.143295	-1.448426	0.639298
Cl	2.630475	2.030062	-0.234991
Cl	1.867406	-0.659968	1.934028
C	-4.440917	-0.273006	-0.768494
C	-2.907489	-1.188479	0.995415
H	-3.766229	-1.651617	1.482472
H	-2.471367	-1.932275	0.326551
H	-2.179933	-0.941341	1.770873
H	-4.740626	0.584197	-1.408610
O	-4.979814	-1.339949	-0.881913
C	-3.962159	1.096433	1.195992
H	-4.334001	1.972149	0.657413
H	-4.792640	0.655827	1.750514
H	-3.210659	1.430151	1.915432

TS-4e

C	1.748121	0.139128	-0.109813
C	1.211071	1.192830	0.743824
H	1.025361	-0.567552	-0.520853
H	1.962338	1.864693	1.148154
H	0.595665	0.754895	1.540840
O	0.544473	3.157987	-0.435445
C	0.220893	2.037028	-0.132538
O	-0.869317	1.445953	-0.469066
C	3.081806	-0.065524	-0.459226
Al	-2.001352	0.079343	-0.113131
C	-3.829282	0.544409	-0.628684
C	-4.864336	-0.550664	-0.372663
H	-3.819101	0.811026	-1.693562
H	-4.111877	1.462409	-0.097566
H	-5.871948	-0.252108	-0.684273
H	-4.620619	-1.470289	-0.913935

H	-4.920877	-0.811456	0.688837
Cl	-1.177555	-1.631897	-1.220543
Cl	-1.724738	-0.359906	2.020857
C	3.392489	-1.044600	-1.548494
H	2.599392	-1.780330	-1.682998
H	3.492221	-0.479332	-2.480068
H	4.339199	-1.554429	-1.365197
C	2.895311	-1.050625	1.106967
O	2.839342	-2.213339	1.037184
H	3.100960	-0.401802	1.971467
C	4.166398	0.904546	-0.099509
H	4.202582	1.669912	-0.881582
H	3.996609	1.414121	0.849697
H	5.135829	0.405474	-0.074174

Imaginary vibration frequency: 233.19i

SLC-4f

C	-2.000939	-0.267171	0.998371
C	-0.818914	-0.875072	0.240781
H	-2.392037	-0.899656	1.790621
H	-0.813234	-0.791720	-0.844601
H	-0.538797	-1.886368	0.534825
O	-1.039303	0.703779	1.627414
C	-0.050689	0.183260	0.947624
O	1.106597	0.587627	1.006293
C	-3.101232	0.461629	0.247990
Al	2.637512	0.064610	0.005403
C	4.130346	1.148762	0.635753
C	5.451427	0.875576	-0.084761
H	4.246652	0.978279	1.713572
H	3.854489	2.205535	0.528743
H	6.265610	1.502257	0.295614
H	5.766698	-0.165951	0.031241
H	5.372468	1.068555	-1.159096
Cl	2.721782	-2.067720	0.384794
Cl	1.952990	0.409975	-2.026011
C	-3.909093	-0.617363	-0.476289
C	-4.012162	1.149972	1.272253
H	-4.812176	1.699845	0.774856
H	-4.462036	0.426468	1.956782
H	-3.432839	1.866350	1.859806
O	-3.699750	-1.791137	-0.255860
C	-4.947825	-0.177439	-1.461078
H	-5.468536	0.727985	-1.145854

H	-4.453286	0.045223	-2.412694
H	-5.659912	-0.985632	-1.624455
C	-2.556400	1.492256	-0.741018
H	-1.963077	2.244629	-0.217485
H	-1.936899	1.043490	-1.521077
H	-3.379325	2.013838	-1.230893

TS-4f

C	-1.492286	0.531212	0.272164
C	-1.051664	1.567113	-0.625613
H	-0.713902	-0.025983	0.796773
H	-1.836534	2.244229	-0.951497
H	-0.613792	1.060740	-1.507244
O	0.057723	3.551548	0.055135
C	0.160380	2.355351	-0.047351
O	1.189787	1.651576	0.270073
C	-2.819015	0.103649	0.489406
Al	2.080096	0.093828	0.062736
C	4.013471	0.366796	-0.008233
C	4.831438	-0.915429	-0.160777
H	4.313585	0.899708	0.903080
H	4.230243	1.053405	-0.836626
H	5.909134	-0.718970	-0.195282
H	4.657717	-1.605615	0.670792
H	4.573506	-1.451576	-1.079502
Cl	1.402385	-1.138839	1.754961
Cl	1.219712	-0.841333	-1.733156
C	-3.095807	-0.555244	1.834068
H	-2.249641	-1.137001	2.199847
H	-3.298652	0.238824	2.556271
H	-3.980090	-1.191263	1.779219
C	-2.676389	-1.225113	-0.649568
O	-3.224782	-1.055758	-1.678516
C	-3.945514	0.983456	0.001737
H	-3.986730	1.879705	0.625453
H	-3.824412	1.285910	-1.036562
H	-4.897395	0.459578	0.097433
C	-2.009568	-2.451653	-0.154488
H	-1.809764	-3.102162	-1.005483
H	-1.084666	-2.219470	0.374342
H	-2.677592	-2.966641	0.541122

Imaginary vibration frequency: 68.90i

SLC-4g

C	-1.770896	-0.351563	-0.980966
C	-0.645854	0.537228	-0.444715
H	-2.189068	-0.018091	-1.927959
H	-0.647361	0.768726	0.618954
H	-0.437277	1.438524	-1.020438
O	-0.731028	-1.393374	-1.297992
C	0.208520	-0.619616	-0.819039
O	1.394804	-0.929383	-0.776597
C	-2.831052	-0.917702	-0.053109
Al	2.866019	-0.006845	0.004571
C	4.460632	-1.075800	-0.333527
C	5.747832	-0.475360	0.233808
H	4.555862	-1.215207	-1.417867
H	4.296527	-2.077634	0.083037
H	6.621790	-1.101911	0.024384
H	5.952554	0.513231	-0.188630
H	5.692205	-0.354292	1.320039
Cl	2.746984	1.932505	-0.959381
Cl	2.199670	0.171523	2.061932
C	-3.817038	0.182251	0.328096
C	-3.606861	-2.008762	-0.795424
H	-4.406425	-2.391206	-0.160489
H	-4.050483	-1.625712	-1.718218
H	-2.941004	-2.836513	-1.047537
O	-4.793918	-0.004001	1.003941
O	-3.472116	1.372196	-0.166165
C	-4.340473	2.467999	0.150307
H	-4.386275	2.617898	1.229524
H	-3.902684	3.338325	-0.333411
H	-5.343428	2.283490	-0.236357
C	-2.242772	-1.484052	1.241065
H	-1.545870	-2.295212	1.022029
H	-1.725365	-0.725930	1.833158
H	-3.049229	-1.889238	1.852526

TS-4g

C	-1.425655	0.570144	0.303053
C	-0.758403	0.751084	-0.983766
H	-0.801676	0.197916	1.116776
H	-1.424013	1.054868	-1.786063
H	-0.195617	-0.144100	-1.261216
O	-0.046986	3.032026	-1.027871
C	0.275623	1.905086	-0.741986
O	1.399917	1.550486	-0.225261

C	-2.746486	0.904150	0.630841
Al	2.428694	0.080813	0.035892
C	4.233159	0.601140	0.582201
C	5.169679	-0.568153	0.885474
H	4.147563	1.252444	1.461756
H	4.659511	1.229792	-0.210115
H	6.169841	-0.234259	1.185138
H	4.783678	-1.193337	1.696787
H	5.296464	-1.219431	0.014875
Cl	1.362746	-1.117750	1.544203
Cl	2.311825	-1.041282	-1.843799
C	-3.110859	1.036993	2.078742
H	-2.456606	0.456871	2.727612
H	-2.997656	2.095151	2.334577
H	-4.150396	0.758087	2.252597
C	-2.763855	-0.935460	0.311915
O	-2.778769	-1.661796	1.243242
C	-3.666379	1.577783	-0.337121
H	-3.569218	2.655425	-0.171115
H	-3.433897	1.375195	-1.379067
H	-4.703098	1.305120	-0.135790
O	-3.031047	-1.131407	-0.938361
C	-3.409782	-2.487328	-1.301918
H	-3.573799	-2.454730	-2.374885
H	-2.596384	-3.167051	-1.049819
H	-4.322598	-2.762085	-0.774111

Imaginary vibration frequency: 292.25i

SLC-4h

C	1.460135	0.595176	-0.872827
C	0.319474	-0.369586	-0.525267
H	1.824710	0.494945	-1.894045
H	0.330398	-0.808746	0.470737
H	0.084924	-1.133177	-1.266569
O	0.398876	1.708648	-0.933691
C	-0.525722	0.846501	-0.631754
O	-1.717945	1.128427	-0.510268
C	2.552570	0.892825	0.104839
Al	-3.175843	0.032315	0.000556
C	-4.766810	1.159124	0.048541
C	-6.043633	0.422423	0.455914
H	-4.894348	1.614589	-0.941716
H	-4.576120	1.991744	0.737513
H	-6.915486	1.085768	0.472256

H	-6.275098	-0.395323	-0.233619
H	-5.955120	-0.016318	1.454615
Cl	-3.119937	-1.532367	-1.503459
Cl	-2.479852	-0.769670	1.895989
Si	3.790178	-0.603461	0.081637
C	5.159212	-0.236424	1.318183
H	5.901023	-1.040535	1.283308
H	5.676002	0.700555	1.095716
H	4.777009	-0.183979	2.340902
C	2.926088	-2.204038	0.571664
H	2.408892	-2.116851	1.530977
H	2.204585	-2.535856	-0.179318
H	3.675450	-2.995437	0.675327
C	4.513246	-0.790536	-1.647505
H	3.739583	-0.980323	-2.397372
H	5.073115	0.097314	-1.953069
H	5.203261	-1.639883	-1.667743
C	2.031122	1.100623	1.527260
H	1.300359	1.915354	1.567674
H	1.564507	0.207949	1.950637
H	2.853668	1.379931	2.188633
C	3.294975	2.148935	-0.362076
H	4.154844	2.356103	0.278709
H	3.654814	2.055146	-1.390232
H	2.637533	3.023296	-0.316629

TS-4h

C	-1.599520	-0.722344	-0.774554
C	-0.310098	0.000330	-0.521080
H	-1.885925	-0.829693	-1.816331
H	-0.222099	0.462448	0.461318
H	-0.061617	0.738156	-1.286103
O	-0.219807	-2.216854	-0.876709
C	0.523219	-1.240976	-0.637136
O	1.777240	-1.311401	-0.513286
C	-2.588976	-0.997837	0.189913
Al	3.051410	-0.074668	-0.022773
C	4.811341	-0.924455	-0.007103
C	5.960265	0.008851	0.375516
H	4.991415	-1.354556	-1.000827
H	4.773631	-1.777452	0.682592
H	6.930038	-0.501861	0.371946
H	6.040088	0.853888	-0.315552
H	5.822368	0.428416	1.377040

Cl	2.814742	1.547514	-1.468460
Cl	2.343461	0.647706	1.917348
Si	-3.556995	0.805546	0.015616
C	-5.185217	0.481461	0.885291
H	-5.707115	1.440749	0.970808
H	-5.824666	-0.200414	0.322029
H	-5.045898	0.087531	1.894322
C	-2.584628	2.139092	0.898300
H	-2.339993	1.860670	1.925812
H	-1.662116	2.407511	0.379652
H	-3.210204	3.037160	0.940262
C	-3.829544	1.227811	-1.790125
H	-2.902743	1.520033	-2.290296
H	-4.277632	0.397931	-2.342811
H	-4.519441	2.075545	-1.852355
C	-2.158326	-1.137910	1.639149
H	-1.690023	-2.118089	1.772753
H	-1.445110	-0.379129	1.960390
H	-3.022452	-1.094523	2.304614
C	-3.585387	-2.066640	-0.236985
H	-4.420385	-2.128511	0.460898
H	-3.981003	-1.894083	-1.240817
H	-3.077196	-3.035687	-0.240183

Imaginary vibration frequency: 278.28i

SLC-4i

C	-1.677436	0.162406	-0.801628
C	-0.328273	0.897673	-0.782747
H	-2.085926	0.006666	-1.797426
H	-0.187866	1.677763	-0.035410
H	0.043883	1.234848	-1.749961
O	-0.959564	-1.081396	-0.393655
C	0.181660	-0.438813	-0.377896
O	1.254968	-0.955268	-0.093538
C	-2.732858	0.586080	0.190149
Al	2.993476	-0.178338	0.042799
C	4.213174	-1.604606	0.566962
C	5.669619	-1.162207	0.715575
H	4.137259	-2.408378	-0.176311
H	3.851481	-2.034640	1.509501
H	6.322970	-1.990732	1.010175
H	6.066208	-0.757642	-0.220699
H	5.779145	-0.381176	1.474274
Cl	3.240135	0.679479	-1.933015

Cl	2.629053	1.409467	1.476840
C	-2.266621	0.576302	1.629556
H	-1.912298	-0.406606	1.940346
H	-1.458436	1.300976	1.767197
H	-3.085230	0.870118	2.286816
C	-3.283291	1.931752	-0.235956
H	-3.634602	1.918973	-1.269063
H	-4.112703	2.221877	0.409726
H	-2.500530	2.691301	-0.142329
Br	-4.198109	-0.758150	0.019006

TS-4i

C	1.935412	0.243258	-0.785670
C	0.563966	-0.250776	-0.467567
H	2.264053	0.208086	-1.817649
H	0.404236	-0.526115	0.575215
H	0.265068	-1.088912	-1.098876
O	0.598960	1.903427	-1.229157
C	-0.171930	1.015703	-0.832268
O	-1.427605	1.142344	-0.737029
C	2.834341	0.881532	0.165468
Al	-2.777321	0.093348	-0.060888
C	-4.474094	1.055969	-0.182469
C	-5.673546	0.301227	0.391124
H	-4.652957	1.300264	-1.237534
H	-4.356923	2.020113	0.328957
H	-6.605054	0.872141	0.303510
H	-5.832360	-0.652614	-0.121721
H	-5.535733	0.072993	1.452689
Cl	-2.660744	-1.753712	-1.221825
Cl	-2.106890	-0.352957	1.975764
Br	3.460130	-1.128487	0.140397
C	2.342221	1.248226	1.523613
H	1.813710	2.202571	1.420339
H	1.656641	0.521583	1.955412
H	3.180426	1.402443	2.202867
C	3.909978	1.743721	-0.403636
H	4.270580	1.384821	-1.367477
H	3.467028	2.735296	-0.549542
H	4.742751	1.844895	0.292408

Imaginary vibration frequency: 329.73i

SLC-4j

C	2.294455	1.023091	0.134722
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C	1.057238	0.792829	-0.736126
H	2.632335	2.058071	0.181262
H	1.068829	-0.075645	-1.393436
H	0.667203	1.665513	-1.260248
O	1.456972	0.756259	1.339387
C	0.408711	0.547577	0.580237
O	-0.700742	0.261178	1.010469
C	3.488993	0.104226	0.034794
Al	-2.355088	-0.018124	0.102560
C	-3.635882	-0.624400	1.441014
C	-5.035083	-0.902587	0.889785
H	-3.686579	0.131000	2.235318
H	-3.230781	-1.528130	1.913788
H	-5.724224	-1.245243	1.669488
H	-5.477288	-0.007955	0.440590
H	-5.017243	-1.675022	0.114761
Cl	-2.675264	1.934644	-0.785490
Cl	-1.790537	-1.426779	-1.444462
C	4.200007	0.374684	-1.275682
H	5.060854	-0.287181	-1.375252
H	3.541577	0.219600	-2.131861
H	4.558208	1.407916	-1.290644
C	4.398623	0.269380	1.234045
H	5.259218	-0.394715	1.146979
H	4.761497	1.300484	1.273244
H	3.878066	0.045659	2.165909
Cl	2.890052	-1.627102	0.015907

TS-4j

C	-2.393291	0.303013	-0.706325
C	-0.974910	0.599672	-0.362476
H	-2.755837	0.600561	-1.683105
H	-0.758571	0.636353	0.705178
H	-0.629096	1.528466	-0.818985
O	-1.193720	-1.321353	-1.595577
C	-0.355823	-0.607527	-1.027994
O	0.889626	-0.842317	-0.995688
C	-3.316966	-0.472227	0.115889
Al	2.313514	-0.121057	-0.090413
C	3.938931	-1.113876	-0.530642
C	5.204973	-0.592931	0.149680
H	4.063672	-1.095709	-1.621117
H	3.777161	-2.167506	-0.268887
H	6.093146	-1.175071	-0.121711

H	5.408421	0.447821	-0.121265
H	5.119870	-0.627248	1.240435
Cl	2.328279	1.986759	-0.668863
Cl	1.693504	-0.231428	2.008351
C	-2.827883	-1.189933	1.326231
H	-2.411523	-2.142313	0.981734
H	-2.055844	-0.654555	1.874851
H	-3.661074	-1.408968	1.994005
C	-4.491645	-1.070980	-0.580409
H	-4.838532	-0.456954	-1.411581
H	-4.163547	-2.037447	-0.976641
H	-5.308114	-1.248748	0.119655
Cl	-3.681981	1.394854	0.525759

Imaginary vibration frequency: 347.83i

SLC-4k

C	-2.229690	-1.166387	0.130304
C	-0.992393	-0.903960	-0.733741
H	-2.573318	-2.197679	0.163214
H	-1.029233	-0.026471	-1.376271
H	-0.578584	-1.762709	-1.262208
O	-1.385255	-0.915260	1.343463
C	-0.354294	-0.654113	0.584596
O	0.746319	-0.323757	1.015751
C	-3.379949	-0.185605	0.039527
Al	2.371762	0.050048	0.108695
C	3.664487	0.609423	1.457695
C	5.041599	0.965456	0.895781
H	3.756357	-0.193300	2.200262
H	3.244450	1.468123	1.996812
H	5.739453	1.277951	1.680520
H	5.498726	0.115749	0.379245
H	4.982732	1.785307	0.173205
Cl	2.746888	-1.833901	-0.902700
Cl	1.763319	1.540637	-1.344287
O	-2.748982	1.086243	-0.026263
C	-3.589240	2.217776	-0.026419
H	-2.935594	3.081990	-0.148109
H	-4.303399	2.205994	-0.857106
H	-4.135945	2.327766	0.916117
C	-4.271950	-0.327240	1.264830
H	-4.605782	-1.362027	1.370039
H	-3.737074	-0.039490	2.171923
H	-5.161802	0.297388	1.171471

C	-4.144187	-0.501742	-1.241107
H	-5.001347	0.165050	-1.348096
H	-3.503505	-0.383130	-2.118007
H	-4.525524	-1.525098	-1.219678

TS-4k

C	2.367843	-0.414672	0.811954
C	0.983053	0.132606	0.750660
H	2.720774	-0.813614	1.753573
H	0.799013	0.851516	-0.046660
H	0.645908	0.555533	1.698103
O	1.173250	-2.103604	0.433498
C	0.329670	-1.190855	0.455017
O	-0.909576	-1.346342	0.249914
C	3.362918	-0.308745	-0.259794
Al	-2.293953	-0.167363	-0.015442
C	-3.940298	-1.153337	-0.385628
C	-5.168087	-0.271520	-0.614385
H	-4.121556	-1.840510	0.450927
H	-3.767052	-1.791992	-1.261299
H	-6.070460	-0.859433	-0.817792
H	-5.382722	0.354369	0.257484
H	-5.026942	0.403750	-1.464223
Cl	-2.328073	1.059999	1.792249
Cl	-1.574137	1.093916	-1.658222
O	3.646562	0.884255	0.575236
C	3.360649	2.195179	0.069890
H	4.009856	2.400552	-0.782501
H	2.317012	2.322545	-0.216878
H	3.594460	2.874513	0.888118
C	2.900347	-0.048807	-1.663589
H	3.731360	0.310412	-2.272694
H	2.565199	-0.998938	-2.084418
H	2.075522	0.658163	-1.736743
C	4.527134	-1.251040	-0.171070
H	4.229795	-2.228008	-0.557405
H	5.357331	-0.877754	-0.773883
H	4.860207	-1.369278	0.861067

Imaginary vibration frequency: 434.26i

SLC-4l

C	-1.928405	-0.810744	0.512334
C	-0.751289	-0.699858	-0.454891
H	-2.305394	-1.822053	0.639011

H	-0.760605	0.138009	-1.149642
H	-0.466273	-1.612233	-0.978838
O	-0.966547	-0.570861	1.645056
C	0.020941	-0.467761	0.794196
O	1.183820	-0.247495	1.121194
C	-3.043060	0.230869	0.464044
Al	2.724767	0.019599	0.041271
C	4.224594	0.319597	1.250824
C	5.562852	0.547851	0.546719
H	4.296398	-0.542897	1.925687
H	3.983538	1.178792	1.889531
H	6.380514	0.710257	1.257654
H	5.842974	-0.308139	-0.074958
H	5.529369	1.422914	-0.109680
Cl	2.762366	-1.794755	-1.147524
Cl	2.098881	1.686869	-1.198978
N	-3.740279	-0.040216	-0.808579
C	-4.540429	1.060982	-1.311031
H	-4.985563	0.752503	-2.259395
H	-5.364456	1.347962	-0.636574
H	-3.930864	1.940950	-1.510172
C	-4.543043	-1.252042	-0.814237
H	-5.462071	-1.169238	-0.212943
H	-4.838766	-1.467423	-1.843536
H	-3.981268	-2.115323	-0.456371
C	-3.924135	0.074171	1.705461
H	-4.279186	-0.951189	1.828518
H	-3.369422	0.349228	2.605399
H	-4.792808	0.733150	1.637011
C	-2.446658	1.634714	0.459321
H	-1.768336	1.759134	1.304761
H	-1.902480	1.855123	-0.460570
H	-3.232898	2.381442	0.572737

TS-4l

C	-2.072658	-0.332257	-0.811564
C	-0.767621	0.384939	-0.577831
H	-2.466473	-0.332592	-1.820702
H	-0.642426	0.846726	0.400155
H	-0.511851	1.111809	-1.349237
O	-0.914130	-1.766288	-0.988847
C	-0.028429	-0.903573	-0.729248
O	1.196761	-1.149498	-0.635139
C	-3.077757	-0.575753	0.251672

Al	2.613497	-0.100527	-0.059053
C	4.259016	-1.148449	-0.162706
C	5.513065	-0.401476	0.292571
H	4.380721	-1.490875	-1.198462
H	4.124366	-2.057998	0.436657
H	6.414928	-1.019650	0.217514
H	5.688360	0.496155	-0.308676
H	5.432699	-0.076449	1.334636
Cl	2.531186	1.657149	-1.347316
Cl	1.991605	0.492545	1.949065
N	-3.541384	0.804424	-0.030066
C	-3.402359	1.822364	0.992181
H	-3.515776	2.801798	0.524206
H	-4.165144	1.724582	1.776697
H	-2.420886	1.791886	1.459101
C	-4.726114	0.978975	-0.845875
H	-5.648731	0.740037	-0.300383
H	-4.775669	2.021739	-1.163503
H	-4.683543	0.364777	-1.744331
C	-2.528787	-0.800804	1.647706
H	-3.330511	-0.711780	2.383274
H	-2.132792	-1.815835	1.706858
H	-1.729070	-0.118238	1.929480
C	-4.070733	-1.676039	-0.074834
H	-4.916662	-1.643971	0.615247
H	-4.447456	-1.622019	-1.095584
H	-3.574097	-2.640291	0.044931

Imaginary vibration frequency: 483.32i

SLC-4m

C	-2.334325	-1.010933	0.379506
C	-1.048905	-1.107939	-0.451013
H	-2.714840	-1.965003	0.741908
H	-0.989059	-0.513120	-1.360964
H	-0.668606	-2.113233	-0.632921
O	-1.515248	-0.405692	1.487402
C	-0.444719	-0.461464	0.742892
O	0.659786	-0.056342	1.094772
C	-3.458838	-0.090388	-0.063895
Al	2.277783	0.043500	0.104613
C	3.656187	0.718112	1.307037
C	5.037544	0.849549	0.663828
H	3.707762	0.051539	2.177295
H	3.326793	1.690387	1.694757

H	5.785535	1.230846	1.367715
H	5.404558	-0.113430	0.295480
H	5.021704	1.533988	-0.189986
Cl	2.495852	-1.997585	-0.602378
Cl	1.689406	1.315066	-1.552269
C	-2.896637	1.208069	-0.591698
C	-2.848891	2.364840	0.053821
H	-2.495517	1.160908	-1.602708
H	-2.415777	3.242129	-0.415169
H	-3.233327	2.489244	1.060782
C	-4.181930	-0.816200	-1.201890
H	-3.514151	-0.996224	-2.049059
H	-4.580853	-1.776827	-0.865219
H	-5.016105	-0.206441	-1.555415
C	-4.407738	0.106753	1.114037
H	-4.808402	-0.856283	1.441335
H	-3.911321	0.570827	1.968068
H	-5.245749	0.741884	0.819987

TS-4m

C	-2.422019	0.322897	-0.589359
C	-1.009510	0.592671	-0.192847
H	-2.799317	0.838889	-1.464621
H	-0.780173	0.375742	0.850380
H	-0.689450	1.610353	-0.422717
O	-1.200293	-0.991095	-1.831884
C	-0.369419	-0.409181	-1.121527
O	0.882063	-0.619827	-1.154623
C	-3.372131	-0.474658	0.161832
Al	2.295183	-0.073814	-0.124037
C	3.945855	-0.887132	-0.785157
C	5.199709	-0.510177	0.004010
H	4.065861	-0.604079	-1.838984
H	3.814273	-1.976839	-0.784715
H	6.103200	-0.982537	-0.398562
H	5.371701	0.570777	-0.005047
H	5.120865	-0.811159	1.053447
Cl	2.245790	2.112053	-0.213158
Cl	1.719098	-0.660034	1.907382
C	-3.572255	0.863820	0.910446
C	-4.330409	1.874965	0.473319
C	-4.567905	-0.949664	-0.636830
H	-5.381302	-1.228566	0.035418
H	-4.932134	-0.193091	-1.333016

H	-4.280236	-1.827635	-1.218790
H	-3.004718	0.961412	1.829511
H	-4.433356	2.778271	1.065415
H	-4.881489	1.832182	-0.459664
C	-2.820423	-1.542558	1.084666
H	-2.485622	-2.396887	0.493593
H	-1.983153	-1.191448	1.688918
H	-3.608540	-1.878646	1.760847

Imaginary vibration frequency: 317.60i

SLC-4n

C	-1.752239	-1.872529	0.129783
C	-0.554768	-1.462081	-0.733651
H	-1.970881	-2.939521	0.132442
H	-0.676454	-0.566455	-1.342770
H	-0.070746	-2.253606	-1.305324
O	-0.912550	-1.589961	1.345303
C	0.080674	-1.210437	0.585423
O	1.154308	-0.799703	1.015326
C	-3.026134	-1.042067	0.077107
Al	2.652421	-0.087779	0.087952
C	4.019880	0.299245	1.423639
C	5.309900	0.883552	0.846242
H	4.237583	-0.626088	1.971981
H	3.590857	0.989458	2.161147
H	6.053403	1.091165	1.623764
H	5.776681	0.200829	0.129480
H	5.125596	1.824476	0.318576
Cl	3.088075	-1.665443	-1.339346
Cl	1.772079	1.598561	-0.948476
C	-2.695940	0.447637	0.038325
C	-2.804922	1.192922	-1.135539
C	-2.233756	1.101008	1.183583
C	-2.460948	2.538037	-1.167597
H	-3.164181	0.728691	-2.045324
C	-1.883939	2.442962	1.152391
H	-2.138307	0.561153	2.117603
C	-1.995277	3.168946	-0.024625
H	-2.554576	3.091365	-2.095805
H	-1.520679	2.921658	2.055295
H	-1.717920	4.216860	-0.050766
C	-3.750581	-1.516700	-1.184059
H	-4.673051	-0.950512	-1.325943
H	-3.141425	-1.409387	-2.084815

H	-4.015948	-2.571744	-1.083471
C	-3.889820	-1.385207	1.292811
H	-4.123354	-2.453376	1.302447
H	-3.398061	-1.140506	2.234754
H	-4.829480	-0.830755	1.248305

TS-4n

C	1.620144	0.924278	-0.680045
C	0.334636	0.194313	-0.495382
H	1.971907	1.047248	-1.698155
H	0.182523	-0.222407	0.499320
H	0.184641	-0.596363	-1.232754
O	0.024376	2.403194	-1.027715
C	-0.585014	1.364646	-0.744095
O	-1.849751	1.271994	-0.655380
C	2.493881	1.399132	0.371068
Al	-2.999451	-0.043377	-0.110668
C	-4.831960	0.639590	-0.130827
C	-5.888634	-0.351779	0.356167
H	-5.063625	0.964196	-1.153544
H	-4.860499	1.550232	0.481575
H	-6.899988	0.070100	0.328755
H	-5.902939	-1.259045	-0.256069
H	-5.700309	-0.666536	1.387442
Cl	-2.611800	-1.719604	-1.461524
Cl	-2.261560	-0.617725	1.874249
C	3.152831	-0.009197	0.177442
C	4.123629	-0.215314	-0.814917
C	2.799461	-1.080966	1.011539
C	4.747241	-1.443164	-0.941662
H	4.401429	0.590448	-1.482172
C	3.431173	-2.302249	0.883647
H	2.046883	-0.953818	1.777808
C	4.403256	-2.487190	-0.093596
H	5.501346	-1.586247	-1.706739
H	3.161617	-3.116943	1.545466
H	4.890496	-3.450500	-0.195585
C	3.394815	2.553018	-0.027845
H	2.831054	3.482619	0.068318
H	4.262539	2.601437	0.632719
H	3.737893	2.484508	-1.059895
C	1.886124	1.622778	1.741759
H	2.670995	1.619623	2.500193
H	1.405191	2.602505	1.748972

H 1.132321 0.888568 2.021945

Imaginary vibration frequency: 324.49i

SLC-4o

C	-1.195308	-2.560095	0.120517
C	-0.086738	-1.955079	-0.747730
H	-1.232211	-3.648658	0.123702
H	-0.356073	-1.097195	-1.363725
H	0.523220	-2.657146	-1.315741
O	-0.413218	-2.136374	1.332214
C	0.499223	-1.593106	0.569253
O	1.484591	-1.001475	0.997296
C	-2.592035	-1.957720	0.075345
Al	2.828266	-0.012073	0.084060
C	4.113496	0.565643	1.432073
C	5.287116	1.373155	0.875940
H	4.483592	-0.324771	1.956151
H	3.575557	1.153965	2.186284
H	5.986598	1.678925	1.661830
H	5.860210	0.798884	0.141445
H	4.947881	2.285253	0.375321
Cl	3.523099	-1.449235	-1.387853
Cl	1.652100	1.519697	-0.897320
C	-2.518575	-0.434332	0.046037
C	-2.739929	0.289550	-1.124549
C	-2.185022	0.283064	1.196701
C	-2.631435	1.672301	-1.156111
H	-3.005152	-0.218673	-2.042707
C	-2.067205	1.663896	1.183782
H	-2.006291	-0.232719	2.131472
C	-2.291513	2.347632	0.001639
H	-2.805105	2.214965	-2.077356
H	-1.800169	2.199993	2.086307
C	-3.233417	-2.537872	-1.186652
H	-4.238477	-2.133050	-1.320045
H	-2.656206	-2.325051	-2.089434
H	-3.317952	-3.622893	-1.092800
C	-3.379470	-2.450987	1.291642
H	-3.434089	-3.542896	1.286428
H	-2.927601	-2.143721	2.235399
H	-4.397676	-2.057992	1.259332
Cl	-2.140708	4.088140	-0.028828

TS-4o

C	0.899470	1.448620	-0.685833
C	-0.227432	0.504907	-0.447512
H	1.216591	1.579104	-1.714370
H	-0.306514	0.137577	0.574471
H	-0.218955	-0.348448	-1.127877
O	-0.953518	2.581007	-1.105180
C	-1.352026	1.459104	-0.771022
O	-2.575098	1.121216	-0.693530
C	1.669815	2.137141	0.327068
Al	-3.458265	-0.368724	-0.102814
C	-5.387553	-0.089078	-0.257363
C	-6.242795	-1.274890	0.188584
H	-5.610020	0.162520	-1.302538
H	-5.650429	0.804262	0.323766
H	-7.315932	-1.077360	0.084191
H	-6.023482	-2.172734	-0.397791
H	-6.064022	-1.528643	1.238249
Cl	-2.664593	-2.009926	-1.313220
Cl	-2.723394	-0.649746	1.945026
C	2.580264	0.870920	0.187461
C	3.574274	0.809817	-0.801243
C	2.440750	-0.214443	1.066238
C	4.428193	-0.271253	-0.884495
H	3.690614	1.618098	-1.511738
C	3.292749	-1.296167	0.994812
H	1.674531	-0.211372	1.830056
C	4.280443	-1.315120	0.017546
H	5.198462	-0.306647	-1.644404
H	3.190723	-2.122059	1.687553
C	2.333632	3.420101	-0.137209
H	1.603404	4.228575	-0.073164
H	3.179727	3.663198	0.508261
H	2.677542	3.371763	-1.170174
C	1.039319	2.307878	1.694271
H	1.813651	2.512923	2.435542
H	0.363629	3.164215	1.656501
H	0.459102	1.449736	2.029827
Cl	5.348758	-2.677639	-0.081685

Imaginary vibration frequency: 322.33i

SLC-4p

C	-1.567109	-2.201817	0.116047
C	-0.399005	-1.712400	-0.747081
H	-1.722705	-3.279782	0.114352

H	-0.578809	-0.830078	-1.361018
H	0.138707	-2.473502	-1.312899
O	-0.744520	-1.872532	1.331525
C	0.215726	-1.415319	0.572506
O	1.253480	-0.921774	1.003929
C	-2.886659	-1.444207	0.071293
Al	2.714780	-0.130527	0.085183
C	3.985722	0.455808	1.443387
C	5.237934	1.130955	0.882339
H	4.266505	-0.415289	2.048952
H	3.463776	1.138121	2.126375
H	5.926295	1.447218	1.673920
H	5.795581	0.460887	0.220693
H	4.988395	2.022377	0.298550
Cl	3.339188	-1.745083	-1.224717
Cl	1.740175	1.409400	-1.088229
C	-2.635847	0.060104	0.048978
C	-2.772362	0.814188	-1.115021
C	-2.210926	0.730147	1.198520
C	-2.483822	2.171700	-1.133198
H	-3.110629	0.348015	-2.032171
C	-1.918044	2.084453	1.176413
H	-2.098804	0.193379	2.132600
C	-2.040690	2.832094	0.007827
H	-2.599893	2.725777	-2.059640
H	-1.583543	2.569539	2.088346
C	-3.583207	-1.942472	-1.196297
H	-4.536697	-1.427970	-1.330201
H	-2.982231	-1.786370	-2.095287
H	-3.787510	-3.012472	-1.111508
C	-3.729599	-1.850803	1.281962
H	-3.908509	-2.929508	1.275055
H	-3.249597	-1.596422	2.227608
H	-4.696413	-1.344414	1.246914
C	-1.670199	4.281979	-0.026293
H	-0.596617	4.397000	-0.210199
H	-2.198304	4.810592	-0.822492
H	-1.893474	4.774341	0.922820

TS-4p

C	1.240918	1.239726	-0.702514
C	0.056065	0.358863	-0.484643
H	1.580393	1.362027	-1.725032
H	-0.043271	-0.032067	0.526813

H	0.001209	-0.471820	-1.190170
O	-0.472996	2.497061	-1.072231
C	-0.984656	1.408672	-0.769934
O	-2.233945	1.195930	-0.697297
C	2.067029	1.829856	0.333613
Al	-3.241809	-0.217400	-0.109758
C	-5.140700	0.234320	-0.226306
C	-6.085349	-0.864277	0.261138
H	-5.366453	0.488351	-1.270110
H	-5.308594	1.156084	0.345509
H	-7.139354	-0.575285	0.177039
H	-5.959179	-1.787967	-0.312468
H	-5.904221	-1.114484	1.311231
Cl	-2.617329	-1.906530	-1.351353
Cl	-2.504075	-0.584165	1.922264
C	2.883210	0.508192	0.189043
C	3.879715	0.377757	-0.789362
C	2.651843	-0.578160	1.047512
C	4.640228	-0.772340	-0.873381
H	4.074594	1.187089	-1.481794
C	3.420330	-1.718574	0.959082
H	1.882781	-0.523855	1.806681
C	4.427042	-1.840786	-0.003110
H	5.415637	-0.844708	-1.628535
H	3.238282	-2.536669	1.647925
C	2.825148	3.070687	-0.101447
H	2.153732	3.929142	-0.040035
H	3.675478	3.245163	0.560606
H	3.184424	3.008706	-1.128239
C	1.434920	2.028382	1.697387
H	2.215378	2.170364	2.447225
H	0.818420	2.928543	1.667611
H	0.798169	1.205427	2.018389
C	5.228311	-3.095202	-0.109276
H	4.663804	-3.858115	-0.656328
H	6.164919	-2.928455	-0.642957
H	5.452469	-3.506080	0.877424

Imaginary vibration frequency: 356.74i

SLC-4q

C	-1.307432	-2.521010	0.221817
C	-0.185417	-1.994714	-0.680403
H	-1.372114	-3.606288	0.288772
H	-0.436115	-1.165919	-1.342561

H	0.406346	-2.743235	-1.207028
O	-0.509042	-2.051398	1.407108
C	0.412375	-1.573955	0.613342
O	1.414257	-0.985089	1.008053
C	-2.686157	-1.880835	0.145384
Al	2.809980	-0.105092	0.071195
C	4.152815	0.382664	1.399812
C	5.364115	1.120594	0.828175
H	4.476701	-0.532090	1.912428
H	3.665218	0.997462	2.167198
H	6.094040	1.379093	1.603367
H	5.888953	0.516699	0.081464
H	5.072808	2.054230	0.337061
Cl	3.382613	-1.592651	-1.403651
Cl	1.751422	1.511941	-0.904929
C	-2.570035	-0.367311	0.004157
C	-2.795042	0.282370	-1.212454
C	-2.182613	0.425562	1.082073
C	-2.634895	1.648189	-1.347099
H	-3.102448	-0.281540	-2.084198
C	-2.008225	1.798350	0.964606
H	-2.001991	-0.023876	2.050913
C	-2.228787	2.420241	-0.260637
H	-2.809793	2.134988	-2.299916
H	-1.695951	2.365763	1.831679
C	-3.355220	-2.531938	-1.066820
H	-4.350483	-2.110210	-1.220135
H	-2.782104	-2.396602	-1.987161
H	-3.467928	-3.605270	-0.896911
C	-3.475028	-2.265012	1.399169
H	-3.544714	-3.352892	1.487150
H	-3.016073	-1.883681	2.312146
H	-4.487967	-1.861973	1.336495
O	-2.080760	3.742866	-0.485550
C	-1.591499	4.540575	0.575652
H	-1.515177	5.552878	0.181295
H	-2.277850	4.540392	1.429050
H	-0.601067	4.206675	0.901681

TS-4q

C	0.873723	1.390413	-0.736593
C	-0.219033	0.411229	-0.448887
H	1.227866	1.440319	-1.759473
H	-0.299165	0.103529	0.592887

H	-0.175724	-0.481433	-1.074742
O	-0.893979	2.430341	-1.225455
C	-1.338157	1.331796	-0.848363
O	-2.568334	1.032630	-0.804439
C	1.638501	2.134485	0.253840
Al	-3.498053	-0.396734	-0.126591
C	-5.414405	-0.097790	-0.375862
C	-6.310004	-1.209833	0.169945
H	-5.600051	0.041683	-1.448799
H	-5.673267	0.859055	0.095725
H	-7.374642	-1.003622	0.010099
H	-6.094587	-2.171368	-0.306641
H	-6.168398	-1.349289	1.246319
Cl	-2.687750	-2.138752	-1.171015
Cl	-2.840185	-0.503838	1.960027
C	2.569408	0.893603	0.250360
C	3.556155	0.730063	-0.731884
C	2.444138	-0.111746	1.228015
C	4.409033	-0.356179	-0.730068
H	3.672681	1.470546	-1.513820
C	3.289644	-1.191370	1.244808
H	1.691331	-0.031620	2.001070
C	4.281008	-1.329542	0.263274
H	5.162716	-0.440025	-1.501580
H	3.202373	-1.953888	2.009846
C	2.287985	3.397091	-0.283626
H	1.537775	4.188948	-0.327300
H	3.093935	3.716869	0.379948
H	2.690793	3.270736	-1.288583
C	0.957647	2.404198	1.582163
H	1.704170	2.680927	2.329156
H	0.268237	3.241180	1.459232
H	0.384776	1.562171	1.968149
O	5.049540	-2.416694	0.357778
C	6.061671	-2.621674	-0.618996
H	6.795716	-1.811103	-0.602786
H	6.550070	-3.555596	-0.347862
H	5.631271	-2.715149	-1.620195

Imaginary vibration frequency: 387.69i

SLC-4r

C	-1.529620	-2.210792	0.125283
C	-0.365403	-1.711593	-0.736558
H	-1.669052	-3.291027	0.132898

H	-0.557674	-0.834642	-1.354389
H	0.185787	-2.467605	-1.296106
O	-0.716488	-1.859584	1.342215
C	0.239875	-1.396172	0.582921
O	1.270807	-0.887043	1.013747
C	-2.856721	-1.467853	0.068595
Al	2.724453	-0.095011	0.085058
C	3.989071	0.521982	1.436086
C	5.242430	1.188105	0.867000
H	4.268836	-0.335856	2.060823
H	3.462614	1.217257	2.102340
H	5.926930	1.521769	1.654849
H	5.804179	0.505942	0.221344
H	4.993635	2.067057	0.264270
Cl	3.370434	-1.725857	-1.195994
Cl	1.737178	1.414630	-1.113913
C	-2.630282	0.039040	0.044486
C	-2.762043	0.793254	-1.121675
C	-2.231335	0.726640	1.194027
C	-2.506765	2.153698	-1.148368
H	-3.075883	0.320377	-2.044422
C	-1.968051	2.084152	1.181665
H	-2.116955	0.197093	2.132259
C	-2.096675	2.828652	0.004552
H	-2.617763	2.703665	-2.077712
H	-1.653595	2.580061	2.094739
C	-3.535817	-1.977683	-1.204061
H	-4.495299	-1.476439	-1.345905
H	-2.930040	-1.812674	-2.098259
H	-3.725777	-3.050622	-1.121441
C	-3.703994	-1.887261	1.272118
H	-3.865195	-2.969028	1.267293
H	-3.236660	-1.622633	2.221528
H	-4.678567	-1.396693	1.227493
N	-1.779181	4.168263	-0.027377
H	-2.166241	4.705780	-0.786737
H	-1.788865	4.654387	0.855314

TS-4r

C	1.223435	1.230226	-0.708499
C	0.074751	0.303432	-0.445899
H	1.564245	1.308367	-1.734587
H	0.010739	-0.073678	0.573691
H	0.020790	-0.539066	-1.136963

O	-0.399901	2.420615	-1.024482
C	-0.963489	1.347600	-0.724465
O	-2.215897	1.190059	-0.665127
C	2.098702	1.803252	0.312730
Al	-3.270229	-0.208860	-0.104359
C	-5.151835	0.303281	-0.243963
C	-6.137278	-0.771998	0.213944
H	-5.353752	0.578754	-1.287176
H	-5.299572	1.221689	0.338732
H	-7.180274	-0.448141	0.120564
H	-6.032850	-1.690365	-0.372411
H	-5.978425	-1.043709	1.262297
Cl	-2.668502	-1.891437	-1.362680
Cl	-2.564672	-0.610314	1.928693
C	2.930003	0.507410	0.198128
C	3.901661	0.347053	-0.805533
C	2.730110	-0.572035	1.077213
C	4.653904	-0.798289	-0.907302
H	4.081740	1.143592	-1.517397
C	3.478798	-1.719164	0.989525
H	1.987928	-0.504861	1.862466
C	4.459978	-1.863878	-0.010080
H	5.403366	-0.887545	-1.686592
H	3.314840	-2.527763	1.693688
C	2.829801	3.052230	-0.149783
H	2.145169	3.901735	-0.110386
H	3.676597	3.257388	0.508611
H	3.195769	2.972904	-1.173539
C	1.476469	2.029932	1.678652
H	2.263411	2.186698	2.419166
H	0.854931	2.926440	1.642494
H	0.848106	1.208403	2.021083
N	5.210673	-2.985129	-0.086461
H	4.969846	-3.789830	0.467485
H	5.805950	-3.139855	-0.882674

Imaginary vibration frequency: 421.37i

SLC-4s

C	-1.298361	-2.432501	0.131694
C	-0.166964	-1.858606	-0.728566
H	-1.360395	-3.519687	0.140498
H	-0.407110	-0.996140	-1.350446
H	0.430790	-2.577891	-1.288224
O	-0.520766	-2.019169	1.348818

C	0.415573	-1.506519	0.592561
O	1.412775	-0.940386	1.026434
C	-2.683187	-1.804225	0.067755
Al	2.796920	-0.029793	0.086233
C	4.057173	0.620504	1.423664
C	5.248511	1.385108	0.844894
H	4.408854	-0.238641	2.008938
H	3.507555	1.257283	2.128437
H	5.932798	1.734042	1.626073
H	5.833148	0.763323	0.159877
H	4.927095	2.266955	0.282260
Cl	3.492950	-1.571578	-1.273598
Cl	1.656732	1.443871	-1.020636
C	-2.579530	-0.282808	0.039598
C	-2.782170	0.443238	-1.134282
C	-2.243450	0.423742	1.197737
C	-2.651923	1.820718	-1.161424
H	-3.048483	-0.062918	-2.052757
C	-2.103750	1.798907	1.187249
H	-2.082231	-0.100339	2.130543
C	-2.309018	2.505346	0.002543
H	-2.811676	2.366638	-2.083451
H	-1.836561	2.328587	2.093727
C	-3.320603	-2.372809	-1.201440
H	-4.317287	-1.951416	-1.345861
H	-2.729791	-2.170873	-2.097853
H	-3.424790	-3.455904	-1.107043
C	-3.495374	-2.278171	1.275812
H	-3.579927	-3.367838	1.264400
H	-3.043840	-1.988168	2.225105
H	-4.502278	-1.857777	1.235754
C	-2.169892	3.923112	-0.016762
N	-2.062672	5.070762	-0.031034

TS-4s

C	1.036951	1.405554	-0.677822
C	-0.132150	0.514022	-0.474870
H	1.353448	1.567164	-1.702853
H	-0.244470	0.136188	0.540116
H	-0.143596	-0.329585	-1.167539
O	-0.859598	2.615642	-1.131041
C	-1.242962	1.493469	-0.799624
O	-2.464703	1.139558	-0.714177
C	1.802979	2.063805	0.348670

Al	-3.341029	-0.345359	-0.111154
C	-5.273381	-0.078862	-0.249696
C	-6.116059	-1.259493	0.232662
H	-5.509557	0.148027	-1.297487
H	-5.534810	0.825627	0.314548
H	-7.191524	-1.071080	0.135659
H	-5.897498	-2.169290	-0.335308
H	-5.924249	-1.487945	1.285810
Cl	-2.552683	-1.996885	-1.313669
Cl	-2.593123	-0.617192	1.935591
C	2.667741	0.753040	0.170267
C	3.681486	0.696845	-0.797314
C	2.480916	-0.341041	1.028204
C	4.519831	-0.395833	-0.874231
H	3.824839	1.515935	-1.489701
C	3.317225	-1.433957	0.960390
H	1.692149	-0.336293	1.768113
C	4.340740	-1.459665	0.010070
H	5.309650	-0.430503	-1.614217
H	3.182399	-2.269151	1.636112
C	2.524539	3.325500	-0.083704
H	1.829284	4.161546	0.010701
H	3.384145	3.513067	0.561948
H	2.855302	3.293033	-1.121232
C	5.210281	-2.587841	-0.061173
N	5.915174	-3.496743	-0.119032
C	1.186209	2.214507	1.723167
H	1.969912	2.381206	2.463932
H	0.535277	3.090652	1.708108
H	0.583517	1.365675	2.040600

Imaginary vibration frequency: 254.75i

SLC-4t

C	-0.776332	-2.804157	0.146431
C	0.264155	-2.084266	-0.717780
H	-0.683531	-3.888962	0.166628
H	-0.091055	-1.275640	-1.355952
H	0.963082	-2.719279	-1.262350
O	-0.070285	-2.270922	1.360449
C	0.782612	-1.633176	0.599922
O	1.680960	-0.917406	1.028186
C	-2.236542	-2.381478	0.071173
Al	2.901869	0.196810	0.078980
C	4.022400	1.075550	1.409870

C	5.072441	2.018230	0.820082
H	4.509251	0.299239	2.013761
H	3.368196	1.624332	2.099081
H	5.683023	2.492094	1.596524
H	5.757798	1.490398	0.149733
H	4.611191	2.822528	0.238816
Cl	3.859264	-1.229800	-1.245817
Cl	1.541961	1.439050	-1.065274
C	-2.354544	-0.861236	0.045893
C	-2.651463	-0.171309	-1.130329
C	-2.137532	-0.116314	1.209023
C	-2.724851	1.211008	-1.156345
H	-2.830327	-0.709536	-2.051507
C	-2.201610	1.265096	1.201677
H	-1.910752	-0.613025	2.143026
C	-2.496187	1.911187	0.013803
H	-2.951008	1.740008	-2.072633
H	-2.025640	1.835953	2.103679
C	-2.771515	-3.031404	-1.205964
H	-3.817410	-2.759380	-1.360464
H	-2.205787	-2.740336	-2.093977
H	-2.717793	-4.118455	-1.116057
C	-2.982985	-2.969264	1.271522
H	-2.916841	-4.059981	1.255203
H	-2.580191	-2.623848	2.224258
H	-4.037902	-2.691110	1.227422
N	-2.563653	3.375148	-0.005031
O	-2.830769	3.918756	-1.060025
O	-2.351424	3.967368	1.036131

TS-4t

C	0.641071	1.607503	-0.664447
C	-0.463696	0.626981	-0.542168
H	0.974354	1.842580	-1.669278
H	-0.567955	0.180204	0.445669
H	-0.399533	-0.170792	-1.284472
O	-1.367738	2.687712	-1.146259
C	-1.648979	1.531261	-0.839645
O	-2.835578	1.069309	-0.753949
C	1.304980	2.288198	0.413679
Al	-3.582274	-0.476911	-0.134442
C	-5.532121	-0.364011	-0.231470
C	-6.267241	-1.613043	0.254668
H	-5.808359	-0.146251	-1.271341

H	-5.852317	0.511045	0.348705
H	-7.356197	-1.509887	0.183465
H	-5.989855	-2.496323	-0.329200
H	-6.034082	-1.836671	1.300513
Cl	-2.690530	-2.069114	-1.343947
Cl	-2.776415	-0.682521	1.899572
C	2.283579	1.057866	0.205316
C	3.321444	1.130569	-0.735148
C	2.174136	-0.076907	1.022503
C	4.257223	0.119004	-0.827875
H	3.406948	1.983684	-1.394548
C	3.111063	-1.086229	0.943572
H	1.370778	-0.170314	1.739909
C	4.136396	-0.966294	0.020538
H	5.066115	0.168832	-1.544178
H	3.048390	-1.956493	1.582725
C	1.937765	3.620534	0.064489
H	1.172622	4.392558	0.164651
H	2.752099	3.846634	0.754885
H	2.312335	3.662512	-0.957556
C	0.635543	2.320602	1.770759
H	1.379565	2.497508	2.548926
H	-0.071853	3.151926	1.776112
H	0.078824	1.418788	2.018279
N	5.139499	-2.047155	-0.066191
O	5.051190	-2.958116	0.729985
O	5.989910	-1.953658	-0.926832

Imaginary vibration frequency: 225.97i

SLC-5a

C	3.045006	-0.652169	-0.284382
C	1.849267	-0.302725	0.609212
H	3.475932	-1.634333	-0.094724
H	1.813876	0.721992	0.981768
H	1.594996	-1.003435	1.403818
O	2.080996	-0.802914	-1.433300
C	1.081082	-0.506583	-0.647669
O	-0.089585	-0.463264	-1.015164
C	4.068165	0.406041	-0.554648
H	4.649514	0.116278	-1.434544
H	3.558756	1.345675	-0.791025
Al	-1.676361	0.007925	-0.082433
C	-3.165870	-0.271229	-1.309409
C	-4.534382	0.077380	-0.722395

H	-3.150661	-1.319892	-1.632610
H	-2.981470	0.322421	-2.213736
H	-5.345862	-0.093168	-1.438485
H	-4.757868	-0.522765	0.165074
H	-4.588105	1.127882	-0.420329
Cl	-1.583137	-1.281730	1.660812
Cl	-1.242181	2.050037	0.506086
C	4.982927	0.583371	0.647810
H	5.726936	1.356097	0.446755
H	4.422411	0.885652	1.536678
H	5.516174	-0.341739	0.882315

TS-5a

C	3.188209	-0.803138	0.397117
C	1.725314	-0.631617	0.512208
H	3.593764	-1.809335	0.472137
H	1.430832	0.362823	0.850603
H	1.285800	-1.370729	1.184669
O	1.979223	-1.205406	-1.773313
C	1.191153	-0.868310	-0.907334
O	-0.068270	-0.698916	-1.085187
C	4.106831	0.222523	0.222410
H	3.905234	-0.110284	1.407380
H	5.137749	-0.090025	0.068023
Al	-1.481632	-0.042057	-0.154622
C	-3.077016	-0.012843	-1.286569
C	-4.335675	0.523099	-0.605155
H	-3.252673	-1.032669	-1.652917
H	-2.848073	0.585242	-2.178246
H	-5.204176	0.524711	-1.274063
H	-4.605951	-0.076310	0.269971
H	-4.197690	1.551323	-0.255994
Cl	-1.645512	-1.310159	1.626224
Cl	-0.819397	1.941783	0.527152
C	3.781502	1.649174	-0.035244
H	3.878334	1.801531	-1.115480
H	2.770243	1.928876	0.255703
H	4.501746	2.305222	0.454297

Imaginary vibration frequency: 373.51i

SLC-5b

C	2.771006	0.795665	0.472585
C	1.560165	0.741768	-0.467554
H	3.141977	1.802574	0.657098

H	1.544468	-0.054608	-1.211090
H	1.249914	1.683085	-0.920519
O	1.839658	0.454970	1.609231
C	0.829773	0.410884	0.783500
O	-0.323173	0.157115	1.122327
C	3.887148	-0.204861	0.323559
H	4.489655	-0.129491	1.236143
Al	-1.896465	-0.032490	0.074478
C	-3.363059	-0.400556	1.305530
C	-4.722368	-0.578645	0.627772
H	-3.410297	0.417973	2.035052
H	-3.108683	-1.299228	1.881692
H	-5.520004	-0.782072	1.350786
H	-5.015334	0.315829	0.069419
H	-4.712969	-1.410960	-0.082750
Cl	-1.954546	1.852587	-0.999666
Cl	-1.319606	-1.619427	-1.289517
C	3.408424	-1.641316	0.175236
H	2.764317	-1.949595	1.002007
H	2.865587	-1.795631	-0.761224
H	4.269293	-2.313231	0.163528
C	4.747618	0.225930	-0.859286
H	5.128988	1.243036	-0.736141
H	5.603784	-0.443851	-0.962671
H	4.179813	0.184919	-1.793968

TS-5b

C	-2.814416	-0.777512	-0.349217
C	-1.363868	-0.600889	-0.594156
H	-3.202302	-1.792787	-0.343929
H	-1.083510	0.393423	-0.941479
H	-0.965165	-1.346354	-1.284971
O	-1.694425	-1.157340	1.638663
C	-0.838221	-0.850604	0.811389
O	0.407832	-0.738131	1.057669
C	-3.763772	0.250549	-0.266305
H	-3.662379	-0.107063	-1.417044
Al	1.848703	-0.058480	0.165458
C	3.440835	-0.127998	1.298810
C	4.704662	0.433448	0.647029
H	3.603622	-1.171676	1.597370
H	3.223399	0.415180	2.227478
H	5.575727	0.378311	1.310162
H	4.962465	-0.110862	-0.266964

H	4.580633	1.484405	0.367183
Cl	1.987095	-1.230708	-1.679087
Cl	1.212254	1.965888	-0.394348
C	-3.358575	1.692585	-0.155857
H	-3.186353	1.914420	0.901266
H	-2.450044	1.933604	-0.705549
H	-4.164645	2.336325	-0.508171
C	-5.151724	-0.088827	0.202825
H	-5.892607	0.542392	-0.288769
H	-5.398800	-1.138152	0.036231
H	-5.198884	0.110275	1.276861

Imaginary vibration frequency: 412.53i

SLC-5c

C	2.016032	1.450464	0.453431
C	0.836399	1.210634	-0.492370
H	2.242047	2.501046	0.638022
H	0.955824	0.433645	-1.246784
H	0.376407	2.097908	-0.926982
O	1.174685	0.956507	1.579138
C	0.175578	0.743399	0.756826
O	-0.911662	0.299238	1.099639
C	3.294122	0.679936	0.293939
H	3.861108	0.736651	1.222865
Al	-2.479381	-0.051049	0.065570
C	-3.797337	-0.820805	1.277310
C	-5.128396	-1.173265	0.611576
H	-3.962488	-0.111388	2.098080
H	-3.357930	-1.714331	1.738390
H	-5.843813	-1.600639	1.322739
H	-5.603574	-0.293022	0.167642
H	-4.996723	-1.905547	-0.190910
Cl	-2.895927	1.919376	-0.741555
Cl	-1.689825	-1.319477	-1.503248
Br	2.930294	-1.244195	0.067924
C	4.094983	1.206152	-0.873003
H	3.546306	1.110995	-1.812396
H	4.322079	2.264062	-0.708623
H	5.037752	0.667726	-0.966606

TS-5c

C	1.868919	-0.754627	0.453404
C	0.399168	-0.645811	0.614456
H	2.311708	-1.746849	0.451306

H	0.059340	0.323682	0.978853
H	0.014367	-1.424279	1.275668
O	0.743783	-1.176919	-1.651379
C	-0.098585	-0.887504	-0.814558
O	-1.352699	-0.778648	-1.035945
C	2.730605	0.330997	0.336229
H	2.530204	-0.096427	1.508185
Al	-2.791174	-0.074614	-0.166845
C	-4.366709	-0.124520	-1.323588
C	-5.626996	0.489767	-0.714642
H	-4.553499	-1.170423	-1.599530
H	-4.113865	0.387395	-2.261104
H	-6.484771	0.440744	-1.395319
H	-5.919856	-0.021735	0.207683
H	-5.478943	1.544174	-0.460845
Cl	-2.961468	-1.224626	1.689112
Cl	-2.125901	1.944904	0.390107
C	2.323033	1.754615	0.205573
H	2.299501	1.987937	-0.863169
H	1.329831	1.933783	0.615893
H	3.042952	2.414882	0.687095
Br	4.549380	-0.033731	-0.096146

Imaginary vibration frequency: 574.81i

SLC-5d

C	2.528491	1.050938	0.421905
C	1.339905	0.880018	-0.528219
H	2.854957	2.080070	0.568118
H	1.397597	0.066680	-1.250807
H	0.965437	1.787196	-1.002271
O	1.635429	0.680625	1.555611
C	0.629178	0.522956	0.729798
O	-0.495417	0.189473	1.078188
C	3.722203	0.145666	0.307556
H	4.295687	0.198474	1.233231
Al	-2.098151	-0.036769	0.066497
C	-3.455623	-0.710143	1.292218
C	-4.821554	-0.939953	0.643480
H	-3.548550	-0.003244	2.126275
H	-3.085007	-1.644648	1.732137
H	-5.557352	-1.325097	1.357963
H	-5.231477	-0.014324	0.227689
H	-4.762715	-1.661433	-0.177291
Cl	-2.369692	1.963959	-0.726085

Cl	-1.447398	-1.362891	-1.519068
C	4.568564	0.525681	-0.883283
H	4.003346	0.438344	-1.813707
H	4.910595	1.558896	-0.775478
H	5.444655	-0.119561	-0.946452
Cl	3.193660	-1.583133	0.179565

TS-5d

C	-2.496974	-0.779545	-0.375830
C	-1.034192	-0.658021	-0.584477
H	-2.934564	-1.773650	-0.343220
H	-0.712002	0.315316	-0.953992
H	-0.660722	-1.431559	-1.258128
O	-1.344255	-1.188627	1.677822
C	-0.508736	-0.900136	0.831174
O	0.746394	-0.794254	1.040670
C	-3.370817	0.300927	-0.285552
H	-3.190958	-0.132021	-1.447179
Al	2.168997	-0.075464	0.155411
C	3.763429	-0.142860	1.285060
C	5.004979	0.513860	0.681999
H	3.969999	-1.195844	1.516638
H	3.517931	0.327772	2.245845
H	5.874656	0.448168	1.345969
H	5.289181	0.045887	-0.265829
H	4.838532	1.575786	0.475605
Cl	2.307626	-1.201113	-1.717629
Cl	1.486996	1.948119	-0.361364
Cl	-5.029496	-0.042068	0.143447
C	-2.981457	1.733353	-0.182702
H	-2.967170	1.988974	0.880627
H	-1.991009	1.918230	-0.595568
H	-3.712470	2.367607	-0.682806

Imaginary vibration frequency: 586.82i

SLC-5e

C	-2.449607	-1.148897	0.440115
C	-1.255893	-0.982846	-0.507164
H	-2.755949	-2.173638	0.637897
H	-1.345245	-0.199087	-1.258048
H	-0.841024	-1.893431	-0.938484
O	-1.569454	-0.697180	1.564254
C	-0.571137	-0.539528	0.735473
O	0.540397	-0.143235	1.071192

C	-3.621446	-0.223745	0.260730
Al	2.139829	0.081071	0.070854
C	3.473276	0.821717	1.285935
C	4.842746	1.053101	0.645656
H	3.568401	0.144984	2.144573
H	3.082389	1.764049	1.690320
H	5.565346	1.469926	1.355979
H	5.270806	0.122171	0.261118
H	4.782037	1.749345	-0.196524
Cl	2.479645	-1.936007	-0.655694
Cl	1.490249	1.340037	-1.570320
O	-3.096017	1.049788	-0.036722
C	-3.979127	2.113724	0.238754
H	-3.442187	3.037134	0.020969
H	-4.878977	2.077096	-0.386256
H	-4.278439	2.117821	1.294670
C	-4.532875	-0.754653	-0.831357
H	-5.373288	-0.076917	-0.987635
H	-3.989558	-0.851129	-1.775018
H	-4.938491	-1.731294	-0.556540
H	-4.166826	-0.187694	1.215459

TS-5e

C	2.310542	-0.688109	0.711670
C	0.922320	-0.167879	0.864186
H	2.586453	-1.604726	1.223995
H	0.813456	0.906172	0.717533
H	0.478984	-0.437277	1.824611
O	1.132961	-1.725144	-0.793280
C	0.310761	-0.965581	-0.263708
O	-0.903317	-0.852373	-0.611809
C	3.382003	0.033929	0.150846
H	3.246182	0.371420	1.320737
Al	-2.277123	0.259604	-0.119057
C	-3.864463	-0.143165	-1.186264
C	-4.365859	-1.582572	-1.065489
H	-3.635734	0.089968	-2.234242
H	-4.657589	0.557692	-0.896742
H	-5.256497	-1.764917	-1.677993
H	-3.605334	-2.302508	-1.383724
H	-4.630054	-1.832390	-0.033183
Cl	-2.483825	-0.075968	2.032101
Cl	-1.454271	2.269630	-0.409206
O	4.512399	-0.698960	0.003815

C	5.732895	0.017693	-0.179212
H	5.893440	0.738317	0.628064
H	6.519415	-0.733938	-0.149111
H	5.759416	0.523652	-1.146455
C	3.186064	1.236336	-0.723379
H	3.181347	0.894163	-1.761408
H	2.242573	1.737940	-0.520452
H	3.992247	1.957216	-0.594807

Imaginary vibration frequency: 659.95i

SLC-5f

C	-1.566735	0.906037	0.564793
C	-0.449333	-0.142290	0.523081
H	-1.909754	1.155966	1.568152
H	-0.502227	-0.855670	-0.299599
H	-0.207908	-0.656103	1.453079
O	-0.493358	1.956948	0.234515
C	0.416320	1.028229	0.228986
O	1.612004	1.235969	0.024260
C	-2.653337	0.864004	-0.448334
H	-2.210572	0.611379	-1.421044
Al	3.075230	0.035812	-0.063455
C	4.682641	1.100858	-0.355532
C	5.972731	0.282180	-0.421802
H	4.749963	1.845034	0.448281
H	4.551637	1.673820	-1.282225
H	6.853715	0.912741	-0.585203
H	6.144280	-0.275837	0.503886
H	5.945457	-0.448789	-1.235861
Cl	2.924842	-1.009348	1.834285
Cl	2.464088	-1.297241	-1.664464
Si	-3.893495	-0.560203	-0.051434
C	-5.288317	-0.443733	-1.307026
H	-5.958640	-1.301804	-1.197681
H	-5.883598	0.462734	-1.171671
H	-4.903230	-0.449933	-2.331060
C	-3.050183	-2.236807	-0.201777
H	-2.570033	-2.362605	-1.176647
H	-2.297871	-2.398335	0.574489
H	-3.798498	-3.029260	-0.099526
C	-4.558408	-0.333749	1.695635
H	-3.777720	-0.470359	2.449652
H	-4.999262	0.657120	1.836569
H	-5.339523	-1.073770	1.895740

C	-3.376444	2.206129	-0.547191
H	-3.876087	2.464631	0.391293
H	-2.680087	3.014982	-0.785004
H	-4.133707	2.184864	-1.332784

TS-5f

C	-1.591199	-0.680802	-0.550727
C	-0.116595	-0.568264	-0.592361
H	-2.010016	-1.680071	-0.650316
H	0.232038	0.426314	-0.874923
H	0.321339	-1.295485	-1.279170
O	-0.429879	-1.252534	1.666526
C	0.372728	-0.887401	0.827811
O	1.635902	-0.752407	1.032954
C	-2.489054	0.364708	-0.362524
H	-2.294288	-0.027333	-1.545913
Al	3.066637	-0.060734	0.162160
C	4.659933	-0.142030	1.296108
C	5.931344	0.405446	0.647944
H	4.811194	-1.187222	1.595893
H	4.446072	0.403327	2.224446
H	6.800516	0.342012	1.313084
H	6.185610	-0.142352	-0.264969
H	5.819121	1.457357	0.366461
Cl	3.238638	-1.197247	-1.706594
Cl	2.453791	1.981821	-0.379366
C	-2.012052	1.766658	-0.154211
H	-1.809890	1.884993	0.915672
H	-1.090395	2.001672	-0.687636
H	-2.776060	2.492700	-0.432105
Si	-4.360254	-0.004699	0.018008
C	-4.535396	0.487736	1.816066
H	-5.547271	0.255517	2.162336
H	-3.827943	-0.060390	2.444087
H	-4.369158	1.558249	1.959433
C	-4.674295	-1.829330	-0.255847
H	-5.726059	-2.041932	-0.040197
H	-4.486849	-2.134271	-1.289222
H	-4.070662	-2.451072	0.410639
C	-5.383145	1.066550	-1.127893
H	-6.446773	0.915541	-0.920144
H	-5.167156	2.129359	-0.991588
H	-5.209165	0.810556	-2.176787

Imaginary vibration frequency: 473.78i

SLC-5g

C	-1.421391	1.299822	0.485162
C	-0.426550	0.142281	0.592820
H	-1.825617	1.650003	1.433521
H	-0.535358	-0.654652	-0.143418
H	-0.264595	-0.281312	1.583748
O	-0.263235	2.199933	0.128279
C	0.559231	1.188505	0.215302
O	1.767177	1.266865	0.009565
C	-2.443143	1.251801	-0.622634
H	-1.911778	0.976607	-1.540305
Al	3.091372	-0.098658	-0.001004
C	4.788253	0.748345	-0.452789
C	5.971491	-0.218449	-0.519286
H	4.986026	1.536099	0.285139
H	4.668254	1.263372	-1.414377
H	6.906494	0.291506	-0.776238
H	6.133832	-0.724217	0.437533
H	5.813809	-0.998106	-1.270925
Cl	2.892205	-0.931430	1.991373
Cl	2.264599	-1.489516	-1.448536
C	-3.414824	0.137634	-0.304504
C	-4.294442	0.235211	0.772830
C	-3.420958	-1.024840	-1.070806
C	-5.162501	-0.804914	1.072357
H	-4.308651	1.132540	1.382857
C	-4.291220	-2.065551	-0.775223
H	-2.740210	-1.113470	-1.912123
C	-5.163939	-1.958415	0.298522
H	-5.841978	-0.713864	1.912950
H	-4.286075	-2.961924	-1.385885
H	-5.844037	-2.770287	0.531773
C	-3.111217	2.605691	-0.824865
H	-3.836589	2.548772	-1.638628
H	-3.638266	2.931135	0.075364
H	-2.373032	3.369325	-1.080239

TS-5g

C	1.426900	-0.144955	0.843045
C	-0.041331	0.046215	0.879707
H	1.838213	-0.979052	1.405858
H	-0.375533	1.049536	0.615902
H	-0.471427	-0.229642	1.844775

O	0.470695	-1.606867	-0.676262
C	-0.453559	-0.960808	-0.185101
O	-1.680368	-1.086364	-0.504984
C	2.358148	0.726851	0.256529
H	2.203452	1.025207	1.419178
Al	-3.226184	-0.185864	-0.137505
C	-4.710969	-0.977407	-1.134083
C	-6.061061	-0.295055	-0.914047
H	-4.776893	-2.038332	-0.859951
H	-4.451560	-0.963274	-2.200568
H	-6.865984	-0.768819	-1.487801
H	-6.359195	-0.321735	0.138820
H	-6.033045	0.758295	-1.210378
Cl	-3.426573	-0.278355	2.040920
Cl	-2.767212	1.893623	-0.665252
C	3.761320	0.242913	0.093725
C	3.997211	-1.071384	-0.302172
C	4.833035	1.109874	0.296084
C	5.298687	-1.514836	-0.487240
H	3.161127	-1.736250	-0.490529
C	6.131275	0.658075	0.123076
H	4.653256	2.136223	0.598506
C	6.365500	-0.654336	-0.269519
H	5.477221	-2.535386	-0.806697
H	6.962998	1.332432	0.292984
H	7.382070	-1.003827	-0.411994
C	1.935370	1.882414	-0.608552
H	2.702424	2.656041	-0.610369
H	1.833168	1.510139	-1.631512
H	0.988664	2.325598	-0.303770

Imaginary vibration frequency: 431.82i

SLC-5h

C	-2.553855	-1.185855	0.371997
C	-1.372302	-0.893970	-0.558390
H	-2.898655	-2.218045	0.361789
H	-1.422406	0.036182	-1.125461
H	-1.028393	-1.712208	-1.190370
O	-1.613951	-1.034119	1.538059
C	-0.627792	-0.770373	0.721726
O	0.515596	-0.515833	1.087947
C	-3.698497	-0.196915	0.423271
Al	2.035846	0.014268	0.075284
C	3.519767	0.193383	1.327364

C	4.837613	0.622705	0.680933
H	3.648840	-0.765800	1.844733
H	3.228122	0.913525	2.102359
H	5.646294	0.713789	1.414475
H	5.169108	-0.095803	-0.075064
H	4.745416	1.592589	0.182424
Cl	2.171122	-1.570622	-1.400921
Cl	1.310661	1.823956	-0.875818
C	-3.206042	1.210011	0.612873
C	-3.326319	2.200575	-0.260904
H	-4.293397	-0.463639	1.306194
C	-4.552317	-0.408742	-0.819013
H	-5.424819	0.246361	-0.795944
H	-3.994348	-0.194343	-1.734396
H	-4.907247	-1.440462	-0.873196
H	-2.707728	1.406678	1.559911
H	-2.934264	3.187232	-0.038140
H	-3.817516	2.076466	-1.220637

TS-5h

C	2.487569	-0.880119	0.365303
C	1.047040	-0.620215	0.602095
H	2.802458	-1.919056	0.309958
H	0.820923	0.374703	0.984774
H	0.594084	-1.364646	1.260199
O	1.415194	-1.063776	-1.639640
C	0.540159	-0.784238	-0.819665
O	-0.695393	-0.638492	-1.091958
C	3.517040	0.081313	0.375849
H	3.339619	-0.335686	1.499747
Al	-2.156903	-0.023274	-0.183117
C	-3.726746	-0.041282	-1.348705
C	-5.007111	0.479805	-0.695842
H	-3.876382	-1.070189	-1.700897
H	-3.494854	0.547604	-2.245424
H	-5.865082	0.448376	-1.377314
H	-5.277350	-0.107891	0.187191
H	-4.897342	1.517722	-0.366006
Cl	-2.315464	-1.312135	1.581042
Cl	-1.542047	1.963039	0.514238
C	3.218788	1.551914	0.342659
H	3.174045	1.868452	-0.702274
H	2.268610	1.797590	0.812245
H	4.006507	2.115091	0.841596

C	4.868320	-0.385385	-0.017475
C	5.841148	0.420683	-0.420010
H	5.022703	-1.460850	0.008208
H	5.727893	1.497598	-0.473308
H	6.795951	0.011653	-0.730402

Imaginary vibration frequency: 445.16i

SLC-5i

C	-2.010025	-1.178714	0.007817
C	-0.668952	-1.140073	-0.731278
H	-2.322583	-2.178125	0.307260
H	-0.597369	-0.493000	-1.604164
H	-0.207889	-2.105433	-0.940771
O	-1.312601	-0.560289	1.198374
C	-0.190802	-0.520597	0.532365
O	0.859199	-0.070377	0.982603
C	-3.162634	-0.338533	-0.473779
Al	2.553674	0.145067	0.149721
C	3.759138	0.888444	1.489712
C	5.182038	1.136273	0.987003
H	3.776714	0.205644	2.348729
H	3.322421	1.824044	1.861417
H	5.828688	1.551333	1.767958
H	5.653178	0.212552	0.637109
H	5.197105	1.840579	0.149511
Cl	2.969565	-1.866185	-0.551117
Cl	2.044116	1.403481	-1.543217
C	-4.323823	-0.425892	0.526841
H	-4.042697	0.075628	1.458656
H	-4.496731	-1.482606	0.766632
C	-5.590159	0.161435	-0.001927
H	-5.972642	-0.283447	-0.920658
C	-6.259551	1.159014	0.560540
H	-7.181838	1.537231	0.131595
H	-5.910037	1.632201	1.474477
C	-2.781796	1.103495	-0.775043
H	-3.646475	1.640020	-1.168401
H	-2.460191	1.624649	0.130597
H	-1.984526	1.181008	-1.517510
H	-3.478850	-0.825965	-1.406442

TS-5i

C	-2.125756	-0.755734	-0.126422
C	-0.702962	-0.468543	-0.424719

H	-2.436103	-1.797165	-0.155376
H	-0.504514	0.553630	-0.746630
H	-0.291068	-1.158265	-1.164660
O	-0.884018	-1.093568	1.809636
C	-0.090063	-0.736728	0.942154
O	1.164123	-0.587770	1.118255
C	-3.143676	0.189969	0.050053
H	-3.049614	-0.101369	-1.124466
Al	2.574856	-0.027207	0.105666
C	4.207166	-0.031914	1.183100
C	5.469664	0.391361	0.432461
H	4.337062	-1.039447	1.599080
H	4.045094	0.625573	2.047141
H	6.359417	0.378117	1.072587
H	5.674650	-0.269845	-0.415374
H	5.378898	1.405443	0.030471
Cl	2.598327	-1.385709	-1.612508
Cl	1.968250	1.949195	-0.630737
C	-2.846820	1.650077	0.228109
H	-2.862456	1.860805	1.301113
H	-1.872507	1.940594	-0.160315
H	-3.610456	2.265031	-0.247221
C	-4.492298	-0.310081	0.532840
H	-4.487740	-0.149925	1.618164
H	-4.571442	-1.386785	0.365681
C	-5.663029	0.391470	-0.078855
C	-6.572567	-0.218901	-0.826051
H	-6.513838	-1.282896	-1.040282
H	-7.416018	0.321012	-1.243080
H	-5.763090	1.454766	0.125539

Imaginary vibration frequency: 411.26i

SLC-5j

C	-2.544029	0.417676	0.600111
C	-1.347962	-0.530401	0.493905
H	-2.953556	0.538213	1.601628
H	-1.347447	-1.208507	-0.360424
H	-1.054737	-1.063251	1.398254
O	-1.610433	1.562263	0.339133
C	-0.599174	0.733340	0.261296
O	0.557282	1.083788	0.058117
C	-3.616406	0.341452	-0.464971
Al	2.166660	0.066439	-0.045189
C	3.585670	1.298483	-0.563284

C	4.957109	0.639944	-0.720936
H	3.635648	2.099170	0.185372
H	3.291402	1.784987	-1.501923
H	5.729135	1.360581	-1.012286
H	5.289735	0.171920	0.210718
H	4.943286	-0.142879	-1.485560
Cl	2.259052	-0.789536	1.943821
Cl	1.624131	-1.473310	-1.473264
C	-4.350834	-0.901447	-0.262522
C	-4.953515	-1.923457	-0.073680
H	-3.117478	0.286773	-1.440853
C	-4.531042	1.563928	-0.433397
H	-5.284901	1.488975	-1.217981
H	-5.041707	1.640686	0.528920
H	-3.951973	2.474311	-0.599077
H	-5.491769	-2.831817	0.084055

TS-5j

C	-2.604596	-0.723031	-0.438983
C	-1.147378	-0.555278	-0.620604
H	-3.018081	-1.726262	-0.486705
H	-0.842822	0.448852	-0.914459
H	-0.742689	-1.273436	-1.336704
O	-1.487945	-1.233989	1.592849
C	-0.638825	-0.881706	0.782444
O	0.609844	-0.775301	1.025825
C	-3.528129	0.328180	-0.306000
H	-3.348665	0.003035	-1.480600
Al	2.057580	-0.068007	0.170966
C	3.637370	-0.186225	1.317241
C	4.919697	0.364994	0.694016
H	3.776994	-1.238933	1.595395
H	3.417881	0.340424	2.254937
H	5.780511	0.279244	1.367217
H	5.179491	-0.164795	-0.227864
H	4.819239	1.423820	0.435199
Cl	2.203957	-1.174382	-1.713665
Cl	1.430829	1.977924	-0.325409
C	-3.121185	1.761182	-0.106834
H	-3.033456	1.929050	0.969907
H	-2.165892	1.994348	-0.573561
H	-3.889147	2.427424	-0.497135
C	-4.888146	0.000492	0.012231
C	-6.029604	-0.226685	0.303001

H -7.043688 -0.436117 0.567602

Imaginary vibration frequency: 496.72i

SLC-5k

C	-2.107554	-1.078294	-0.132011
C	-0.792847	-0.886350	-0.894159
H	-2.426409	-2.116660	-0.055547
H	-0.735790	-0.061881	-1.603352
H	-0.358079	-1.785993	-1.330385
O	-1.361911	-0.749056	1.138326
C	-0.260705	-0.571706	0.457936
O	0.810318	-0.245501	0.959867
C	-3.261177	-0.140242	-0.372238
Al	2.496669	0.092408	0.145220
C	3.709238	0.663953	1.560632
C	5.118366	1.010990	1.078059
H	3.754342	-0.131084	2.315681
H	3.260257	1.529122	2.064920
H	5.768565	1.329398	1.900326
H	5.603035	0.155138	0.598207
H	5.105192	1.823954	0.345567
Cl	2.903981	-1.805766	-0.821746
Cl	1.967403	1.564017	-1.359495
C	-4.380112	-0.449402	0.636923
H	-4.047139	-0.177514	1.645021
H	-4.578622	-1.526556	0.649560
C	-5.617878	0.250011	0.341662
C	-6.639833	0.827735	0.082448
H	-7.548315	1.340846	-0.141661
C	-2.876656	1.330747	-0.353177
H	-3.752499	1.942283	-0.575438
H	-2.504458	1.631368	0.629591
H	-2.116407	1.571647	-1.098565
H	-3.626220	-0.403825	-1.372679

TS-5k

C	2.184773	-0.940581	0.354065
C	0.757836	-0.619924	0.580666
H	2.501933	-1.966431	0.525682
H	0.557243	0.437573	0.754556
H	0.332195	-1.201197	1.400977
O	0.931030	-1.582271	-1.543326
C	0.152125	-1.072038	-0.744918
O	-1.097142	-0.904446	-0.946763

C	3.185439	-0.019621	0.034707
H	3.076705	-0.170053	1.246454
Al	-2.456901	-0.020128	-0.113678
C	-4.089203	-0.144450	-1.183708
C	-5.287944	0.609280	-0.607963
H	-4.336037	-1.207294	-1.304159
H	-3.863395	0.222609	-2.193261
H	-6.182065	0.511468	-1.234530
H	-5.553430	0.243307	0.388911
H	-5.080841	1.679534	-0.509360
Cl	-2.591401	-0.923683	1.876869
Cl	-1.683609	2.017876	0.147935
C	2.888077	1.399445	-0.336202
H	2.755972	1.433521	-1.421870
H	1.982372	1.784782	0.127778
H	3.727170	2.044271	-0.076076
C	4.539297	-0.567810	-0.376329
H	4.648347	-1.604739	-0.047291
H	4.539089	-0.584554	-1.472878
C	5.658255	0.225498	0.099546
C	6.582872	0.876521	0.502943
H	7.409356	1.453389	0.855098

Imaginary vibration frequency: 451.14i

SLC-5I

C	-2.639149	-0.978278	0.402182
C	-1.463415	-0.747540	-0.551543
H	-2.940657	-2.017524	0.515723
H	-1.535957	0.110152	-1.221674
H	-1.088120	-1.616543	-1.091575
O	-1.743384	-0.623054	1.539743
C	-0.736723	-0.450879	0.713302
O	0.394267	-0.151531	1.066639
C	-3.853179	-0.077853	0.325516
Al	2.015171	0.026110	0.065822
C	3.316664	0.874991	1.241513
C	4.680128	1.115309	0.591344
H	3.429995	0.251686	2.137347
H	2.892617	1.825307	1.589675
H	5.384914	1.595291	1.279125
H	5.140731	0.179245	0.260716
H	4.599512	1.761258	-0.288324
Cl	2.357022	-2.037119	-0.503599
Cl	1.356223	1.151087	-1.665082

C	-3.464783	1.327464	0.281341
H	-4.438375	-0.221528	1.240069
C	-4.701382	-0.452325	-0.890772
H	-5.595849	0.169019	-0.931699
H	-4.140128	-0.313664	-1.816680
H	-5.008045	-1.497024	-0.815551
N	-3.151293	2.432681	0.232340

TS-5l

C	2.622667	-0.783344	0.420391
C	1.150738	-0.699448	0.496221
H	3.093050	-1.763461	0.439889
H	0.789502	0.249464	0.895402
H	0.748238	-1.505324	1.112145
O	1.435618	-1.120481	-1.827594
C	0.636440	-0.871916	-0.945881
O	-0.630738	-0.747107	-1.102681
C	3.471555	0.312507	0.256773
H	3.177739	-0.142795	1.456172
Al	-2.029942	-0.065124	-0.162543
C	-3.662995	-0.105193	-1.237102
C	-4.894357	0.475119	-0.541503
H	-3.850703	-1.147902	-1.524754
H	-3.472364	0.430672	-2.175664
H	-5.791095	0.423106	-1.169716
H	-5.121864	-0.058390	0.386803
H	-4.748663	1.527102	-0.276533
Cl	-2.135597	-1.244210	1.682151
Cl	-1.345146	1.947532	0.407450
C	3.042642	1.722900	0.065062
H	3.107203	1.914981	-1.012578
H	2.015655	1.892458	0.380530
H	3.719644	2.410880	0.570410
C	4.876889	0.042634	0.078777
N	5.999288	-0.137072	-0.086643

Imaginary vibration frequency: 451.59i

SLC-5m

C	-2.469916	0.950608	0.160057
C	-1.132806	0.852139	0.900723
H	-2.819946	1.971430	0.010869
H	-1.036693	0.080155	1.663474
H	-0.712823	1.790907	1.262335
O	-1.753385	0.534990	-1.096084

C	-0.625219	0.451045	-0.438734
O	0.441954	0.127359	-0.946435
C	-3.590984	0.002090	0.502950
Al	2.166262	-0.068421	-0.155579
C	3.380382	-0.647266	-1.565744
C	4.825843	-0.844853	-1.106667
H	3.339906	0.091243	-2.376419
H	2.989277	-1.579850	-1.991731
H	5.476680	-1.170384	-1.925563
H	5.252123	0.079857	-0.705671
H	4.899512	-1.600108	-0.318134
Cl	2.475033	1.906744	0.686124
Cl	1.745234	-1.474810	1.442086
C	-4.749147	0.251175	-0.438826
H	-3.954488	0.361712	1.479274
C	-3.205798	-1.460835	0.594291
H	-4.074456	-2.055316	0.877629
H	-2.850381	-1.839567	-0.365646
H	-2.430818	-1.625425	1.344180
H	-4.997446	1.321301	-0.597580
O	-5.386132	-0.612845	-0.977776

TS-5m

C	-2.602065	-0.693470	-0.261495
C	-1.128359	-0.703011	-0.388718
H	-3.124817	-1.645117	-0.191303
H	-0.735888	0.188270	-0.880303
H	-0.791364	-1.577789	-0.948480
O	-1.343844	-0.988085	1.962358
C	-0.572108	-0.796348	1.041907
O	0.701662	-0.676739	1.158376
C	-3.389868	0.448170	-0.162975
H	-3.172404	-0.117081	-1.317553
Al	2.085508	-0.073870	0.149879
C	3.746057	-0.090571	1.183929
C	4.974005	0.407349	0.421721
H	3.914338	-1.115836	1.538446
H	3.593330	0.513245	2.087718
H	5.884049	0.378846	1.032184
H	5.167030	-0.197304	-0.470034
H	4.846703	1.440706	0.083757
Cl	2.123481	-1.342393	-1.637283
Cl	1.439324	1.926899	-0.501797
C	-2.885286	1.839791	-0.094652

H	-2.850238	2.102372	0.969691
H	-1.880353	1.952982	-0.495805
H	-3.569385	2.532788	-0.586536
C	-4.870594	0.238081	0.108298
O	-5.521079	-0.621044	-0.412267
H	-5.284888	0.954604	0.838328

Imaginary vibration frequency: 210.43i

SLC-5n

C	2.168486	-0.791637	0.539492
C	1.006476	0.184553	0.735478
H	2.552641	-1.231371	1.456660
H	1.031664	1.096632	0.138502
H	0.726804	0.414826	1.763005
O	1.191575	-1.764897	-0.061007
C	0.215144	-0.913099	0.118861
O	-0.950437	-1.133696	-0.193300
C	3.245634	-0.439835	-0.449617
Al	-2.496815	-0.028677	-0.082479
C	-3.963345	-1.014999	-0.905722
C	-5.291573	-0.256965	-0.927944
H	-4.080929	-1.965530	-0.370153
H	-3.665306	-1.282778	-1.927385
H	-6.090975	-0.839926	-1.398457
H	-5.629424	-0.005111	0.082037
H	-5.210650	0.683206	-1.482205
Cl	-2.620546	0.353739	2.046676
Cl	-1.819689	1.762995	-1.104946
C	4.077037	0.701935	0.117449
H	2.779541	-0.088038	-1.378089
C	4.132310	-1.645950	-0.760796
H	4.883219	-1.399594	-1.512450
H	4.646345	-1.992342	0.139325
H	3.528477	-2.467486	-1.150919
O	4.055572	0.955262	1.302045
C	4.889984	1.492369	-0.858155
H	5.340328	0.859402	-1.624938
H	4.218719	2.190995	-1.370759
H	5.657546	2.063833	-0.337535

TS-5n

C	2.264988	-0.735847	0.378546
C	0.786555	-0.712532	0.462954
H	2.741475	-1.705686	0.268226

H	0.392833	0.202118	0.906968
H	0.414204	-1.560497	1.041804
O	1.053763	-1.088238	-1.872941
C	0.266749	-0.848340	-0.977655
O	-1.002425	-0.709135	-1.129814
C	3.086171	0.385631	0.307635
H	2.834990	-0.256517	1.449118
Al	-2.401543	-0.068644	-0.169612
C	-4.027970	-0.062642	-1.257199
C	-5.264327	0.495824	-0.553034
H	-4.217184	-1.091934	-1.588883
H	-3.825008	0.509519	-2.171658
H	-6.153977	0.476302	-1.193261
H	-5.506160	-0.074508	0.349441
H	-5.115488	1.534792	-0.242312
Cl	-2.519304	-1.325309	1.624202
Cl	-1.741212	1.922679	0.493617
C	2.583967	1.777107	0.327396
H	2.430677	2.068455	-0.718495
H	1.628271	1.874389	0.838276
H	3.319037	2.456740	0.754557
C	4.582793	0.188409	0.004115
O	5.167551	1.145877	-0.427788
C	5.201314	-1.153902	0.190036
H	4.899466	-1.625441	1.128160
H	4.888681	-1.809700	-0.629903
H	6.284475	-1.051214	0.157597

Imaginary vibration frequency: 179.10i

SLC-5o

C	1.893880	0.677510	-0.783514
C	0.794233	-0.327041	-0.432364
H	2.298778	0.581471	-1.788696
H	0.836372	-0.759722	0.567957
H	0.579419	-1.100900	-1.168222
O	0.838103	1.749412	-0.823946
C	-0.083982	0.868822	-0.529924
O	-1.275002	1.137384	-0.414804
C	2.931436	1.012842	0.255170
Al	-2.747361	0.020663	0.048358
C	-4.333302	1.152904	0.098227
C	-5.622716	0.405702	0.442386
H	-4.433183	1.647891	-0.876021
H	-4.157911	1.956281	0.824870

H	-6.491909	1.072236	0.463796
H	-5.839352	-0.381675	-0.286128
H	-5.561608	-0.074087	1.424101
Cl	-2.652199	-1.495336	-1.499120
Cl	-2.069727	-0.822831	1.929241
C	3.905840	-0.129616	0.467159
H	2.422553	1.148363	1.217321
C	3.693355	2.288794	-0.088414
H	4.420384	2.511317	0.692666
H	4.225868	2.182383	-1.037036
H	3.006027	3.132254	-0.168234
O	4.796873	-0.104672	1.274031
O	3.663738	-1.158271	-0.346453
C	4.533852	-2.290034	-0.216825
H	4.465365	-2.710056	0.787339
H	4.186901	-3.012402	-0.952151
H	5.565446	-2.003254	-0.424285

TS-5o

C	-1.856863	-0.969568	-0.292033
C	-0.380939	-0.845202	-0.302883
H	-2.300589	-1.930072	-0.040156
H	-0.022057	-0.078986	-0.993025
H	0.084522	-1.790613	-0.585592
O	-0.745253	-0.405467	2.015425
C	0.072742	-0.478646	1.120948
O	1.337608	-0.281947	1.260470
C	-2.740993	0.095080	-0.419187
H	-2.351291	-0.724158	-1.443376
Al	2.770678	0.030665	0.197082
C	4.343489	0.458644	1.280176
C	5.616811	0.732532	0.480329
H	4.509734	-0.372848	1.977528
H	4.099350	1.325446	1.907862
H	6.472833	0.964429	1.124749
H	5.900763	-0.129076	-0.132101
H	5.490298	1.579462	-0.201591
Cl	2.998518	-1.755094	-1.055145
Cl	2.110155	1.662347	-1.126684
C	-2.342760	1.498754	-0.634156
H	-2.447612	1.993848	0.339363
H	-1.306241	1.599615	-0.949437
H	-3.010375	2.005698	-1.330357
C	-4.214430	-0.257420	-0.227916

O	-4.653054	-1.359522	-0.411014
O	-4.876344	0.798842	0.181249
C	-6.274177	0.601452	0.470581
H	-6.632578	1.563353	0.826710
H	-6.802491	0.304599	-0.435749
H	-6.391446	-0.161661	1.240006

Imaginary vibration frequency: 337.30i

SLC-6a

C	2.771006	0.795665	0.472585
C	1.560165	0.741768	-0.467554
H	3.141977	1.802574	0.657098
H	1.544468	-0.054608	-1.211090
H	1.249914	1.683085	-0.920519
O	1.839658	0.454970	1.609231
C	0.829773	0.410884	0.783500
O	-0.323173	0.157115	1.122327
C	3.887148	-0.204861	0.323559
H	4.489655	-0.129491	1.236143
Al	-1.896465	-0.032490	0.074478
C	-3.363059	-0.400556	1.305530
C	-4.722368	-0.578645	0.627772
H	-3.410297	0.417973	2.035052
H	-3.108683	-1.299228	1.881692
H	-5.520004	-0.782072	1.350786
H	-5.015334	0.315829	0.069419
H	-4.712969	-1.410960	-0.082750
Cl	-1.954546	1.852587	-0.999666
Cl	-1.319606	-1.619427	-1.289517
C	3.408424	-1.641316	0.175236
H	2.764317	-1.949595	1.002007
H	2.865587	-1.795631	-0.761224
H	4.269293	-2.313231	0.163528
C	4.747618	0.225930	-0.859286
H	5.128988	1.243036	-0.736141
H	5.603784	-0.443851	-0.962671
H	4.179813	0.184919	-1.793968

TS-6a

C	-2.914312	-0.798851	0.163720
C	-1.484469	-0.648426	-0.197988
H	-3.260983	-1.790084	0.437825
H	-1.267377	0.246528	-0.782301
H	-1.092533	-1.519150	-0.727527

O	-1.623316	-0.687479	2.131357
C	-0.854164	-0.556878	1.184507
O	0.403824	-0.360043	1.287667
C	-3.866883	0.246960	0.160180
H	-4.764468	0.009904	0.724152
Al	1.773091	0.000032	0.140653
C	3.441686	0.215383	1.138331
C	4.665954	0.522767	0.276333
H	3.610216	-0.702353	1.716745
H	3.295251	1.009985	1.881305
H	5.579534	0.630154	0.872568
H	4.852264	-0.269234	-0.455890
H	4.539130	1.453010	-0.286434
Cl	1.773974	-1.665150	-1.285123
Cl	1.113280	1.788830	-0.947960
C	-3.469391	1.694148	0.239408
H	-3.260445	1.950492	1.280168
H	-2.584978	1.923157	-0.355871
H	-4.290240	2.323479	-0.108000
C	-4.072603	-0.295086	-1.349326
H	-3.595296	-1.249996	-1.631766
H	-5.140129	-0.477967	-1.453064
H	-3.672418	0.459164	-2.021179

Imaginary vibration frequency: 198.66i

SLC-6b

C	2.500001	0.805956	0.275581
C	1.229694	0.825057	-0.582573
H	2.899552	1.794666	0.498063
H	1.154779	0.093715	-1.386122
H	0.901345	1.802328	-0.936337
O	1.638979	0.404648	1.449212
C	0.579702	0.408103	0.687247
O	-0.548985	0.124412	1.080252
C	3.599904	-0.195316	-0.005048
Al	-2.172609	-0.039205	0.108279
C	-3.561709	-0.540002	1.381499
C	-4.948454	-0.712405	0.759999
H	-3.594387	0.222550	2.170020
H	-3.252744	-1.468960	1.877305
H	-5.701735	-0.993491	1.504229
H	-5.295196	0.210323	0.284595
H	-4.951774	-1.490149	-0.009948
Cl	-2.338844	1.913294	-0.823189

Cl	-1.625209	-1.509888	-1.392076
C	3.058805	-1.611951	-0.175895
H	2.565285	-1.968952	0.731262
H	2.354105	-1.693373	-1.007013
H	3.887863	-2.291038	-0.387461
C	4.594657	-0.158382	1.153312
H	5.423675	-0.842066	0.955011
H	5.009530	0.844579	1.288224
H	4.125839	-0.464804	2.091889
C	4.280745	0.267477	-1.293178
H	4.669609	1.285412	-1.198236
H	5.121790	-0.391785	-1.520356
H	3.595258	0.239097	-2.144619

TS-6b

C	-2.603290	-0.771927	-0.111842
C	-1.165309	-0.574408	-0.412902
H	-2.954735	-1.794092	-0.008528
H	-0.930461	0.393328	-0.855901
H	-0.757838	-1.363065	-1.048632
O	-1.414742	-0.943640	1.867840
C	-0.594021	-0.682901	0.990446
O	0.653712	-0.506540	1.189565
C	-3.574327	0.252356	0.001148
Al	2.084087	-0.021735	0.166268
C	3.689764	0.079713	1.278621
C	4.963645	0.466646	0.527693
H	3.824006	-0.892308	1.770804
H	3.497615	0.796249	2.087750
H	5.838469	0.512855	1.186622
H	5.197011	-0.250693	-0.265454
H	4.868599	1.447750	0.051676
Cl	2.164741	-1.518421	-1.431848
Cl	1.484598	1.880237	-0.751284
C	-3.146980	1.673292	0.274860
H	-3.009709	1.800536	1.350889
H	-2.217681	1.946380	-0.224435
H	-3.927912	2.361879	-0.052423
C	-4.859380	-0.142947	0.692048
H	-5.657279	0.556960	0.437204
H	-5.173170	-1.151353	0.412864
H	-4.709205	-0.115349	1.773293
C	-3.665270	-0.017763	-1.608288
H	-3.393194	-1.011268	-1.993779

H	-4.735481	0.071999	-1.797325
H	-3.071678	0.730952	-2.122819

Imaginary vibration frequency: 254.75i

SLC-6c

C	-1.677436	0.162406	-0.801628
C	-0.328273	0.897673	-0.782747
H	-2.085926	0.006666	-1.797426
H	-0.187866	1.677763	-0.035410
H	0.043883	1.234848	-1.749961
O	-0.959564	-1.081396	-0.393655
C	0.181660	-0.438813	-0.377896
O	1.254968	-0.955268	-0.093538
C	-2.732858	0.586080	0.190149
Al	2.993476	-0.178338	0.042799
C	4.213174	-1.604606	0.566962
C	5.669619	-1.162207	0.715575
H	4.137259	-2.408378	-0.176311
H	3.851481	-2.034640	1.509501
H	6.322970	-1.990732	1.010175
H	6.066208	-0.757642	-0.220699
H	5.779145	-0.381176	1.474274
Cl	3.240135	0.679479	-1.933015
Cl	2.629053	1.409467	1.476840
C	-2.266621	0.576302	1.629556
H	-1.912298	-0.406606	1.940346
H	-1.458436	1.300976	1.767197
H	-3.085230	0.870118	2.286816
C	-3.283291	1.931752	-0.235956
H	-3.634602	1.918973	-1.269063
H	-4.112703	2.221877	0.409726
H	-2.500530	2.691301	-0.142329
Br	-4.198109	-0.758150	0.019006

TS-6c

C	-2.006667	-1.401842	-0.103252
C	-0.567741	-1.094354	-0.254580
H	-2.282037	-2.421306	0.149187
H	-0.388974	-0.144387	-0.762560
H	-0.049225	-1.882450	-0.804999
O	-0.716637	-1.326741	2.104853
C	-0.000293	-1.025545	1.167922
O	1.225306	-0.651490	1.268961

C	-3.044297	-0.475709	-0.030710
Al	2.532834	-0.030806	0.174920
C	4.130043	0.420118	1.212200
C	5.294244	0.964973	0.385093
H	4.445791	-0.476554	1.761074
H	3.840450	1.149542	1.979795
H	6.167763	1.206993	1.001756
H	5.624277	0.244027	-0.369611
H	5.015742	1.879021	-0.148924
Cl	2.836995	-1.615488	-1.314434
Cl	1.635911	1.673977	-0.881424
C	-2.892498	-1.024163	-1.662240
H	-2.608740	-2.051399	-1.925723
H	-3.962607	-0.984753	-1.867923
H	-2.310324	-0.300875	-2.218980
Br	-2.621922	1.386017	0.037048
C	-4.363883	-0.823375	0.576698
H	-5.169876	-0.230200	0.144844
H	-4.571844	-1.886161	0.435167
H	-4.312163	-0.620717	1.648537

Imaginary vibration frequency: 240.08i

SLC-6d

C	2.294455	1.023091	0.134722
C	1.057238	0.792829	-0.736126
H	2.632335	2.058071	0.181262
H	1.068829	-0.075645	-1.393436
H	0.667203	1.665513	-1.260248
O	1.456972	0.756259	1.339387
C	0.408711	0.547577	0.580237
O	-0.700742	0.261178	1.010469
C	3.488993	0.104226	0.034794
Al	-2.355088	-0.018124	0.102560
C	-3.635882	-0.624400	1.441014
C	-5.035083	-0.902587	0.889785
H	-3.686579	0.131000	2.235318
H	-3.230781	-1.528130	1.913788
H	-5.724224	-1.245243	1.669488
H	-5.477288	-0.007955	0.440590
H	-5.017243	-1.675022	0.114761
Cl	-2.675264	1.934644	-0.785490
Cl	-1.790537	-1.426779	-1.444462
C	4.200007	0.374684	-1.275682
H	5.060854	-0.287181	-1.375252

H	3.541577	0.219600	-2.131861
H	4.558208	1.407916	-1.290644
C	4.398623	0.269380	1.234045
H	5.259218	-0.394715	1.146979
H	4.761497	1.300484	1.273244
H	3.878066	0.045659	2.165909
Cl	2.890052	-1.627102	0.015907

TS-6d

C	-2.360064	-0.872363	-0.171205
C	-0.875148	-0.912491	-0.255297
H	-2.881316	-1.782867	0.102864
H	-0.470139	-0.122970	-0.889239
H	-0.535169	-1.869875	-0.655115
O	-1.114026	-0.857469	2.108377
C	-0.344567	-0.753284	1.172924
O	0.918382	-0.524526	1.281699
C	-3.093645	0.310837	-0.153043
Al	2.280118	-0.025141	0.196864
C	3.882711	0.355191	1.252826
C	5.084936	0.845396	0.446655
H	4.146926	-0.555457	1.806071
H	3.614516	1.096297	2.017020
H	5.958438	1.043052	1.078873
H	5.392542	0.111528	-0.305001
H	4.859660	1.773431	-0.088260
Cl	2.501898	-1.640150	-1.268792
Cl	1.501351	1.719160	-0.908532
C	-2.520260	1.684135	-0.106892
H	-2.469658	1.984436	0.942504
H	-1.514506	1.718870	-0.525315
H	-3.161736	2.387773	-0.637169
C	-3.016292	-0.336678	-1.766360
H	-2.881002	-1.397781	-2.018800
H	-4.057420	-0.134838	-2.011663
H	-2.295761	0.275939	-2.294952
Cl	-4.728412	0.211037	0.487953

Imaginary vibration frequency: 260.00i

SLC-6e

C	-2.229690	-1.166387	0.130304
C	-0.992393	-0.903960	-0.733741
H	-2.573318	-2.197679	0.163214
H	-1.029233	-0.026471	-1.376271

H	-0.578584	-1.762709	-1.262208
O	-1.385255	-0.915260	1.343463
C	-0.354294	-0.654113	0.584596
O	0.746319	-0.323757	1.015751
C	-3.379949	-0.185605	0.039527
Al	2.371762	0.050048	0.108695
C	3.664487	0.609423	1.457695
C	5.041599	0.965456	0.895781
H	3.756357	-0.193300	2.200262
H	3.244450	1.468123	1.996812
H	5.739453	1.277951	1.680520
H	5.498726	0.115749	0.379245
H	4.982732	1.785307	0.173205
Cl	2.746888	-1.833901	-0.902700
Cl	1.763319	1.540637	-1.344287
O	-2.748982	1.086243	-0.026263
C	-3.589240	2.217776	-0.026419
H	-2.935594	3.081990	-0.148109
H	-4.303399	2.205994	-0.857106
H	-4.135945	2.327766	0.916117
C	-4.271950	-0.327240	1.264830
H	-4.605782	-1.362027	1.370039
H	-3.737074	-0.039490	2.171923
H	-5.161802	0.297388	1.171471
C	-4.144187	-0.501742	-1.241107
H	-5.001347	0.165050	-1.348096
H	-3.503505	-0.383130	-2.118007
H	-4.525524	-1.525098	-1.219678

TS-6e

C	-2.235624	-0.874676	0.216552
C	-0.807506	-0.776307	-0.179118
H	-2.572303	-1.771328	0.726010
H	-0.604358	-0.045221	-0.961910
H	-0.387605	-1.738424	-0.478211
O	-1.103092	-0.228681	2.036128
C	-0.247673	-0.325694	1.152532
O	0.991002	-0.079166	1.306667
C	-3.244455	0.063852	-0.111724
Al	2.419199	0.064567	0.173144
C	4.025958	0.535048	1.182987
C	5.288611	0.689935	0.335287
H	4.180592	-0.235048	1.949906
H	3.825267	1.463509	1.732868

H	6.166587	0.946910	0.939107
H	5.528441	-0.232486	-0.202953
H	5.175024	1.477119	-0.416723
Cl	2.517759	-1.862162	-0.862990
Cl	1.769851	1.558185	-1.296484
C	-2.906560	1.498297	-0.416583
H	-2.881371	2.056978	0.521036
H	-1.934883	1.588096	-0.899674
H	-3.652616	1.942722	-1.075338
C	-3.273631	-0.831542	-1.494567
H	-3.040797	-1.901033	-1.426361
H	-4.336792	-0.783265	-1.735761
H	-2.652225	-0.362894	-2.250524
O	-4.381112	-0.151652	0.637015
C	-5.538677	0.577489	0.259161
H	-6.351975	0.178509	0.863343
H	-5.430730	1.644516	0.468934
H	-5.786245	0.437147	-0.799209

Imaginary vibration frequency: 383.53i

SLC-6f

C	1.460135	0.595176	-0.872827
C	0.319474	-0.369586	-0.525267
H	1.824710	0.494945	-1.894045
H	0.330398	-0.808746	0.470737
H	0.084924	-1.133177	-1.266569
O	0.398876	1.708648	-0.933691
C	-0.525722	0.846501	-0.631754
O	-1.717945	1.128427	-0.510268
C	2.552570	0.892825	0.104839
Al	-3.175843	0.032315	0.000556
C	-4.766810	1.159124	0.048541
C	-6.043633	0.422423	0.455914
H	-4.894348	1.614589	-0.941716
H	-4.576120	1.991744	0.737513
H	-6.915486	1.085768	0.472256
H	-6.275098	-0.395323	-0.233619
H	-5.955120	-0.016318	1.454615
Cl	-3.119937	-1.532367	-1.503459
Cl	-2.479852	-0.769670	1.895989
Si	3.790178	-0.603461	0.081637
C	5.159212	-0.236424	1.318183
H	5.901023	-1.040535	1.283308
H	5.676002	0.700555	1.095716

H	4.777009	-0.183979	2.340902
C	2.926088	-2.204038	0.571664
H	2.408892	-2.116851	1.530977
H	2.204585	-2.535856	-0.179318
H	3.675450	-2.995437	0.675327
C	4.513246	-0.790536	-1.647505
H	3.739583	-0.980323	-2.397372
H	5.073115	0.097314	-1.953069
H	5.203261	-1.639883	-1.667743
C	2.031122	1.100623	1.527260
H	1.300359	1.915354	1.567674
H	1.564507	0.207949	1.950637
H	2.853668	1.379931	2.188633
C	3.294975	2.148935	-0.362076
H	4.154844	2.356103	0.278709
H	3.654814	2.055146	-1.390232
H	2.637533	3.023296	-0.316629

TS-6f

C	-1.489344	0.643451	-0.680022
C	-0.014731	0.675844	-0.559480
H	-1.885937	0.702069	-1.689898
H	0.332650	0.944358	0.438513
H	0.441213	1.353680	-1.284258
O	-0.420928	-1.543783	-1.283556
C	0.421677	-0.753736	-0.891123
O	1.667328	-1.030111	-0.740766
C	-2.400257	0.477567	0.370920
Al	3.140039	-0.219070	-0.058983
C	4.679203	-1.424564	-0.152784
C	5.982010	-0.840196	0.392547
H	4.811716	-1.725564	-1.200170
H	4.424035	-2.344795	0.388603
H	6.818621	-1.545070	0.320992
H	6.276594	0.063216	-0.150815
H	5.887770	-0.560451	1.446649
Cl	3.378340	1.636440	-1.205944
Cl	2.569864	0.355746	1.984907
Si	-4.111565	-0.352041	-0.000144
C	-3.932833	-2.143131	0.514959
H	-3.094926	-2.617527	-0.002475
H	-3.774975	-2.240954	1.591904
H	-4.844029	-2.692376	0.258906
C	-4.477536	-0.196805	-1.833479

H	-5.472557	-0.608632	-2.029212
H	-4.483683	0.840140	-2.181704
H	-3.763492	-0.764859	-2.435642
C	-5.395333	0.547243	1.031080
H	-6.368405	0.062151	0.907181
H	-5.149682	0.523170	2.096185
H	-5.507044	1.591507	0.726897
C	-1.864344	0.204081	1.756949
H	-1.505499	-0.826226	1.810437
H	-1.036690	0.860984	2.032289
H	-2.650751	0.327020	2.504235
C	-2.526297	2.100533	0.049580
H	-3.322018	2.315209	-0.655692
H	-2.752550	2.441054	1.061263
H	-1.622911	2.660651	-0.228061

Imaginary vibration frequency: 53.00i

SLC-6g

C	-1.752239	-1.872529	0.129783
C	-0.554768	-1.462081	-0.733651
H	-1.970881	-2.939521	0.132442
H	-0.676454	-0.566455	-1.342770
H	-0.070746	-2.253606	-1.305324
O	-0.912550	-1.589961	1.345303
C	0.080674	-1.210437	0.585423
O	1.154308	-0.799703	1.015326
C	-3.026134	-1.042067	0.077107
Al	2.652421	-0.087779	0.087952
C	4.019880	0.299245	1.423639
C	5.309900	0.883552	0.846242
H	4.237583	-0.626088	1.971981
H	3.590857	0.989458	2.161147
H	6.053403	1.091165	1.623764
H	5.776681	0.200829	0.129480
H	5.125596	1.824476	0.318576
Cl	3.088075	-1.665443	-1.339346
Cl	1.772079	1.598561	-0.948476
C	-2.695940	0.447637	0.038325
C	-2.804922	1.192922	-1.135539
C	-2.233756	1.101008	1.183583
C	-2.460948	2.538037	-1.167597
H	-3.164181	0.728691	-2.045324
C	-1.883939	2.442962	1.152391
H	-2.138307	0.561153	2.117603

C	-1.995277	3.168946	-0.024625
H	-2.554576	3.091365	-2.095805
H	-1.520679	2.921658	2.055295
H	-1.717920	4.216860	-0.050766
C	-3.750581	-1.516700	-1.184059
H	-4.673051	-0.950512	-1.325943
H	-3.141425	-1.409387	-2.084815
H	-4.015948	-2.571744	-1.083471
C	-3.889820	-1.385207	1.292811
H	-4.123354	-2.453376	1.302447
H	-3.398061	-1.140506	2.234754
H	-4.829480	-0.830755	1.248305

TS-6g

C	-1.344122	0.868798	-0.065194
C	0.133667	0.904536	0.047681
H	-1.802144	1.488903	-0.829221
H	0.515723	0.603818	1.022987
H	0.546220	1.882609	-0.207946
O	-0.441170	-0.535363	-1.687223
C	0.500828	-0.111311	-1.022950
O	1.718702	-0.461895	-1.175171
C	-2.215548	0.111555	0.760860
Al	3.277965	-0.169099	-0.275321
C	4.732832	-1.176361	-1.108304
C	6.092354	-1.009325	-0.429687
H	4.798446	-0.874289	-2.161564
H	4.447106	-2.236173	-1.122146
H	6.879329	-1.590939	-0.923647
H	6.417329	0.035904	-0.430785
H	6.063177	-1.332435	0.615767
Cl	3.533745	2.006048	-0.286034
Cl	2.833001	-0.759591	1.792838
C	-3.613117	-0.070379	0.214943
C	-4.181032	-1.338160	0.142583
C	-4.344636	1.019639	-0.255622
C	-5.451205	-1.511408	-0.392187
H	-3.638202	-2.205551	0.494843
C	-5.611827	0.846509	-0.788399
H	-3.933690	2.022935	-0.204364
C	-6.170873	-0.422764	-0.858696
H	-5.875467	-2.507997	-0.442814
H	-6.165001	1.707523	-1.146765
H	-7.162717	-0.560010	-1.274664

C	-2.094531	1.483736	1.657495
H	-1.366799	1.310331	2.442869
H	-1.845647	2.427616	1.149903
H	-3.112007	1.616963	2.023119
C	-1.650179	-1.052540	1.539788
H	-1.519977	-1.911477	0.880100
H	-0.680588	-0.817564	1.976023
H	-2.329254	-1.328747	2.347109

Imaginary vibration frequency: 259.66i

SLC-6h

C	-2.334325	-1.010933	0.379506
C	-1.048905	-1.107939	-0.451013
H	-2.714840	-1.965003	0.741908
H	-0.989059	-0.513120	-1.360964
H	-0.668606	-2.113233	-0.632921
O	-1.515248	-0.405692	1.487402
C	-0.444719	-0.461464	0.742892
O	0.659786	-0.056342	1.094772
C	-3.458838	-0.090388	-0.063895
Al	2.277783	0.043500	0.104613
C	3.656187	0.718112	1.307037
C	5.037544	0.849549	0.663828
H	3.707762	0.051539	2.177295
H	3.326793	1.690387	1.694757
H	5.785535	1.230846	1.367715
H	5.404558	-0.113430	0.295480
H	5.021704	1.533988	-0.189986
Cl	2.495852	-1.997585	-0.602378
Cl	1.689406	1.315066	-1.552269
C	-2.896637	1.208069	-0.591698
C	-2.848891	2.364840	0.053821
H	-2.495517	1.160908	-1.602708
H	-2.415777	3.242129	-0.415169
H	-3.233327	2.489244	1.060782
C	-4.181930	-0.816200	-1.201890
H	-3.514151	-0.996224	-2.049059
H	-4.580853	-1.776827	-0.865219
H	-5.016105	-0.206441	-1.555415
C	-4.407738	0.106753	1.114037
H	-4.808402	-0.856283	1.441335
H	-3.911321	0.570827	1.968068
H	-5.245749	0.741884	0.819987

TS-6h

C	-2.327699	0.879018	-0.326554
C	-0.876426	0.900131	-0.015774
H	-2.695566	1.609176	-1.040700
H	-0.612749	0.434653	0.933827
H	-0.458839	1.908412	-0.043955
O	-1.232808	-0.228575	-2.007939
C	-0.367852	0.084609	-1.191046
O	0.865513	-0.224212	-1.280915
C	-3.288755	0.019417	0.269639
Al	2.312943	-0.116683	-0.173999
C	3.872961	-0.920456	-1.037077
C	5.148806	-0.898636	-0.195431
H	4.041273	-0.399902	-1.988772
H	3.617622	-1.953433	-1.306640
H	5.998642	-1.356648	-0.714652
H	5.443626	0.123337	0.062921
H	5.019119	-1.440255	0.746899
Cl	2.513514	2.013717	0.293009
Cl	1.655263	-1.126658	1.659916
C	-2.839370	-1.248120	0.950538
H	-2.699863	-2.029768	0.201615
H	-1.901554	-1.120892	1.489071
H	-3.596335	-1.579970	1.662225
C	-3.329846	1.269193	1.342220
H	-2.990906	2.262159	1.011559
H	-4.393769	1.382971	1.544779
H	-2.747911	0.976733	2.210519
C	-4.587863	-0.046875	-0.464903
H	-4.881034	0.871093	-0.970251
C	-5.361409	-1.118633	-0.541031
H	-5.109603	-2.058764	-0.063232
H	-6.286527	-1.087606	-1.105597

Imaginary vibration frequency: 284.31i

SLC-6i

C	1.896684	-1.469045	-0.012422
C	0.685618	-1.013810	0.809935
H	2.128568	-2.528024	0.096486
H	0.757927	-0.061395	1.332668
H	0.239814	-1.764142	1.463053
O	1.043401	-1.331716	-1.250343
C	0.035263	-0.930978	-0.524045
O	-1.060334	-0.620318	-0.983264

C	3.158881	-0.633654	-0.070139
Al	-2.591446	0.096279	-0.114440
C	-3.936006	0.409594	-1.491106
C	-5.244335	1.004022	-0.967827
H	-4.131868	-0.542218	-2.001061
H	-3.499086	1.070455	-2.250503
H	-5.973001	1.166442	-1.769691
H	-5.718741	0.349204	-0.230375
H	-5.082103	1.970462	-0.480641
Cl	-3.022971	-1.423375	1.372071
Cl	-1.749251	1.840964	0.866037
C	2.832582	0.841279	-0.383255
H	2.135857	1.235475	0.362212
H	2.329543	0.885632	-1.356068
C	4.029424	1.734213	-0.426956
H	4.755691	1.541137	-1.213758
C	4.243630	2.740685	0.410827
H	5.123204	3.370905	0.327767
H	3.542056	2.976379	1.207023
C	3.806459	-0.763353	1.307402
H	4.762577	-0.237270	1.320298
H	3.177952	-0.328693	2.089661
H	3.994484	-1.811136	1.558181
C	4.071946	-1.230908	-1.139229
H	4.253777	-2.291324	-0.943388
H	3.634591	-1.137544	-2.136770
H	5.039912	-0.726967	-1.145446

TS-6i

C	1.917765	1.117632	0.312432
C	0.467328	1.065072	-0.000716
H	2.260648	1.917286	0.962314
H	0.226702	0.540545	-0.925218
H	0.008769	2.055244	-0.026221
O	0.848020	0.095485	2.071933
C	-0.014561	0.297547	1.218102
O	-1.227919	-0.083418	1.305477
C	2.905330	0.233190	-0.195198
Al	-2.650148	-0.164392	0.164430
C	-4.173770	-1.000336	1.061809
C	-5.422689	-1.149540	0.193189
H	-4.406980	-0.409368	1.957061
H	-3.853252	-1.982873	1.431714
H	-6.252314	-1.620332	0.733267

H	-5.782620	-0.179955	-0.165292
H	-5.226783	-1.763313	-0.691707
Cl	-2.981756	1.902297	-0.479012
Cl	-1.884441	-1.272584	-1.568302
C	2.495755	-1.107621	-0.753683
H	2.386296	-1.817338	0.069344
H	1.557922	-1.073435	-1.306770
H	3.273484	-1.484060	-1.419224
C	4.197566	0.194507	0.618505
H	4.434290	1.212627	0.948404
H	3.995791	-0.397963	1.515114
C	2.952799	1.373691	-1.350804
H	2.495217	2.354597	-1.136592
H	4.010314	1.592598	-1.489787
H	2.463322	0.977362	-2.234988
C	5.362862	-0.381027	-0.116645
C	6.030354	-1.458306	0.273290
H	5.678831	0.139555	-1.019871
H	5.751106	-2.005523	1.169611
H	6.883303	-1.829082	-0.285395

Imaginary vibration frequency: 249.36i

SLC-6j

C	-2.421880	-1.014525	0.173669
C	-1.169854	-0.862796	-0.694611
H	-2.815769	-2.026299	0.254634
H	-1.150346	-0.016072	-1.380670
H	-0.805389	-1.764744	-1.186018
O	-1.570196	-0.750087	1.377460
C	-0.518980	-0.591285	0.614409
O	0.596948	-0.310365	1.036947
C	-3.540624	0.005730	0.034907
Al	2.227751	-0.000858	0.107184
C	3.569496	0.452609	1.447258
C	4.961032	0.724473	0.873964
H	3.615851	-0.365843	2.176836
H	3.213484	1.328787	2.003935
H	5.686349	0.977721	1.655065
H	5.354638	-0.145995	0.340088
H	4.949514	1.557345	0.164104
Cl	2.483872	-1.871632	-0.961809
Cl	1.652247	1.556480	-1.288373
C	-2.966933	1.350852	-0.021476
C	-2.462072	2.440022	-0.068728

H	-2.016583	3.409097	-0.113314
C	-4.274386	-0.308513	-1.274679
H	-5.096827	0.394811	-1.411873
H	-3.607992	-0.226976	-2.135715
H	-4.686927	-1.319934	-1.240593
C	-4.495079	-0.115483	1.226230
H	-4.911173	-1.125278	1.269139
H	-3.984488	0.096190	2.167031
H	-5.317479	0.593042	1.116119

TS-6j

C	2.425820	0.765426	-0.284719
C	0.966307	0.642780	-0.502420
H	2.851409	1.759809	-0.202368
H	0.662071	-0.315829	-0.923281
H	0.575794	1.445443	-1.130797
O	1.290073	1.067360	1.771033
C	0.447893	0.798560	0.921814
O	-0.800211	0.648079	1.148061
C	3.318705	-0.333794	-0.157771
Al	-2.239089	0.051861	0.200441
C	-3.825523	0.023553	1.343428
C	-5.100348	-0.464251	0.655475
H	-3.975956	1.036243	1.739599
H	-3.604498	-0.604898	2.215839
H	-5.964554	-0.462698	1.329796
H	-5.361260	0.164407	-0.201736
H	-4.989306	-1.486038	0.278918
Cl	-2.376564	1.385364	-1.532865
Cl	-1.609889	-1.914559	-0.550456
C	2.809226	-1.717144	0.181292
H	2.694801	-1.792629	1.263763
H	1.849919	-1.927911	-0.289531
H	3.534223	-2.463059	-0.144713
C	3.346382	-0.076085	-1.779231
H	3.001670	0.901494	-2.159044
H	4.405875	-0.104504	-2.025707
H	2.746690	-0.853718	-2.240103
C	4.602175	-0.025231	0.434846
C	5.663868	0.201936	0.944279
H	6.605068	0.407996	1.405393

Imaginary vibration frequency: 215.44i

SLC-6k

C	1.910163	-1.110218	0.241980
C	0.731189	-0.380283	0.895729
H	2.232866	-2.002975	0.776818
H	0.774217	0.706822	0.939034
H	0.384449	-0.779369	1.849012
O	0.970216	-1.557673	-0.843538
C	-0.013427	-0.910742	-0.275801
O	-1.154835	-0.867060	-0.723595
C	3.085204	-0.327164	-0.309484
Al	-2.688861	0.052642	-0.070963
C	-4.093021	-0.153023	-1.407395
C	-5.399639	0.561158	-1.058284
H	-4.276100	-1.225315	-1.551515
H	-3.707248	0.215477	-2.366431
H	-6.162669	0.425696	-1.832663
H	-5.824349	0.190214	-0.120381
H	-5.251118	1.638766	-0.938609
Cl	-2.981506	-0.903400	1.852689
Cl	-1.901914	2.053856	0.230759
C	3.846602	0.174247	0.939836
H	4.101038	-0.678482	1.579793
H	3.193459	0.829128	1.527376
C	5.064920	0.896421	0.622306
C	6.073893	1.493420	0.356873
H	6.969699	2.025512	0.126057
C	3.958829	-1.276592	-1.123683
H	4.838490	-0.749998	-1.498720
H	4.300178	-2.120803	-0.517986
H	3.410246	-1.668919	-1.983014
C	2.641574	0.848253	-1.172786
H	2.081819	0.508148	-2.046617
H	2.026417	1.564812	-0.622860
H	3.521176	1.384183	-1.534076

TS-6k

C	-2.008919	-0.977491	-0.167492
C	-0.580029	-0.692708	-0.431672
H	-2.299721	-2.020164	-0.082681
H	-0.395970	0.294211	-0.856574
H	-0.118864	-1.445245	-1.074329
O	-0.809855	-1.116517	1.852137
C	-0.012059	-0.791889	0.977775
O	1.224325	-0.542170	1.175099
C	-3.027894	-0.008831	-0.026025

Al	2.628826	0.040029	0.169404
C	4.219373	0.219290	1.293600
C	5.474550	0.685596	0.556444
H	4.404693	-0.749375	1.775727
H	3.981952	0.914350	2.109423
H	6.340947	0.773106	1.222287
H	5.753040	-0.008335	-0.242923
H	5.327973	1.665249	0.090666
Cl	2.807512	-1.425390	-1.449824
Cl	1.923637	1.916202	-0.725998
C	-2.687903	1.426897	0.278480
H	-2.567893	1.539857	1.358184
H	-1.769132	1.754419	-0.206168
H	-3.500874	2.077729	-0.045895
C	-4.295793	-0.511324	0.663417
H	-4.454392	-1.570636	0.435924
H	-4.129612	-0.440618	1.743102
C	-3.091853	-0.263889	-1.637417
H	-2.765156	-1.234167	-2.039504
H	-4.167298	-0.232750	-1.825265
H	-2.542550	0.528079	-2.135207
C	-5.481011	0.242547	0.297237
C	-6.456668	0.862698	-0.029615
H	-7.327921	1.414224	-0.306312

Imaginary vibration frequency: 206.01i

SLC-6I

C	2.400769	-0.951070	-0.099214
C	1.167709	-0.678788	0.766670
H	2.736935	-1.986325	-0.111790
H	1.182219	0.226236	1.374524
H	0.780915	-1.516105	1.347307
O	1.559319	-0.717329	-1.310044
C	0.507311	-0.497998	-0.554998
O	-0.606607	-0.246664	-0.991141
C	3.594073	-0.012770	-0.037015
Al	-2.281079	0.004195	-0.102296
C	-3.515294	0.733053	-1.422510
C	-4.912841	1.027383	-0.875138
H	-3.578553	0.029029	-2.261701
H	-3.071509	1.648918	-1.832972
H	-5.576999	1.439574	-1.642712
H	-5.392950	0.124254	-0.485866
H	-4.880545	1.751994	-0.055686

Cl	-2.647929	-2.002523	0.630866
Cl	-1.731051	1.288450	1.554280
C	3.123778	1.374805	-0.068013
C	4.319109	-0.266744	1.289435
H	5.185672	0.390366	1.369356
H	3.666945	-0.085445	2.145581
H	4.665657	-1.301882	1.319600
N	2.750818	2.462584	-0.090248
C	4.520943	-0.259315	-1.230098
H	5.385822	0.402997	-1.175909
H	4.873106	-1.292734	-1.203564
H	4.009195	-0.083640	-2.177292

TS-6l

C	-2.491998	-0.916412	-0.166625
C	-1.073667	-0.481406	-0.255141
H	-2.673932	-1.949401	0.108098
H	-0.966803	0.505559	-0.713086
H	-0.486010	-1.186784	-0.846124
O	-1.271774	-0.518166	2.120324
C	-0.517767	-0.409143	1.172806
O	0.752588	-0.220080	1.266053
C	-3.569683	-0.057064	0.054146
Al	2.181643	-0.001185	0.176256
C	3.795788	0.294423	1.243875
C	5.069438	0.533783	0.434007
H	3.927319	-0.572916	1.904050
H	3.608748	1.146267	1.910678
H	5.947146	0.690973	1.071947
H	5.296473	-0.313943	-0.220331
H	4.977908	1.415391	-0.208261
Cl	2.243847	-1.816585	-1.062814
Cl	1.659360	1.662919	-1.156588
C	-3.354448	1.365579	-0.006177
C	-3.326160	-0.633923	-1.665676
H	-2.746935	0.091702	-2.223241
H	-3.166973	-1.671811	-1.973322
H	-4.401609	-0.481125	-1.790356
N	-3.219278	2.506545	-0.019546
C	-4.847542	-0.505195	0.671966
H	-5.703754	0.043271	0.280278
H	-4.980691	-1.579042	0.541765
H	-4.762102	-0.294112	1.743140

Imaginary vibration frequency: 220.36i

SLC-6m

C	-2.240474	0.752513	-0.499153
C	-0.934395	1.077194	0.232523
H	-2.609382	1.560815	-1.130669
H	-0.852445	0.766971	1.273450
H	-0.550325	2.090095	0.111949
O	-1.462706	-0.184412	-1.381000
C	-0.362120	0.103275	-0.734892
O	0.733908	-0.381110	-0.992656
C	-3.356917	0.052495	0.245762
Al	2.400012	-0.122489	-0.099826
C	3.723874	-1.227977	-1.006524
C	5.128887	-1.135070	-0.409134
H	3.744275	-0.939075	-2.064933
H	3.373818	-2.267721	-0.987116
H	5.845892	-1.767707	-0.943721
H	5.515352	-0.111786	-0.443227
H	5.143295	-1.448426	0.639298
Cl	2.630475	2.030062	-0.234991
Cl	1.867406	-0.659968	1.934028
C	-4.440917	-0.273006	-0.768494
C	-2.907489	-1.188479	0.995415
H	-3.766229	-1.651617	1.482472
H	-2.471367	-1.932275	0.326551
H	-2.179933	-0.941341	1.770873
H	-4.740626	0.584197	-1.408610
O	-4.979814	-1.339949	-0.881913
C	-3.962159	1.096433	1.195992
H	-4.334001	1.972149	0.657413
H	-4.792640	0.655827	1.750514
H	-3.210659	1.430151	1.915432

TS-6m

C	-2.342820	0.908339	-0.162139
C	-0.880849	0.856061	0.066970
H	-2.729623	1.711200	-0.785858
H	-0.596517	0.293099	0.956611
H	-0.437150	1.852117	0.120814
O	-1.234872	-0.070533	-2.059113
C	-0.394387	0.150334	-1.196919
O	0.843016	-0.158654	-1.281659
C	-3.275321	-0.056554	0.294804
Al	2.293460	-0.101535	-0.180192

C	3.848602	-0.886499	-1.068554
C	5.126521	-0.889033	-0.229664
H	4.015656	-0.342499	-2.007189
H	3.589993	-1.911737	-1.363358
H	5.973641	-1.336773	-0.762075
H	5.425142	0.125422	0.052867
H	4.997541	-1.453139	0.699484
Cl	2.505742	2.012755	0.355898
Cl	1.646577	-1.162882	1.631376
C	-2.841519	-1.400037	0.805465
H	-2.630459	-2.053389	-0.042775
H	-1.949194	-1.337352	1.426561
H	-3.644408	-1.851701	1.388242
C	-3.395427	1.098313	1.433900
H	-2.723153	1.976350	1.365641
H	-4.401454	1.512384	1.402114
H	-3.121343	0.598345	2.359383
C	-4.570501	-0.058524	-0.495022
H	-4.864149	0.927924	-0.905767
O	-5.227483	-1.042382	-0.664091

Imaginary vibration frequency: 94.18i

SLC-6n

C	-2.000939	-0.267171	0.998371
C	-0.818914	-0.875072	0.240781
H	-2.392037	-0.899656	1.790621
H	-0.813234	-0.791720	-0.844601
H	-0.538797	-1.886368	0.534825
O	-1.039303	0.703779	1.627414
C	-0.050689	0.183260	0.947624
O	1.106597	0.587627	1.006293
C	-3.101232	0.461629	0.247990
Al	2.637512	0.064610	0.005403
C	4.130346	1.148762	0.635753
C	5.451427	0.875576	-0.084761
H	4.246652	0.978279	1.713572
H	3.854489	2.205535	0.528743
H	6.265610	1.502257	0.295614
H	5.766698	-0.165951	0.031241
H	5.372468	1.068555	-1.159096
Cl	2.721782	-2.067720	0.384794
Cl	1.952990	0.409975	-2.026011
C	-3.909093	-0.617363	-0.476289
C	-4.012162	1.149972	1.272253

H	-4.812176	1.699845	0.774856
H	-4.462036	0.426468	1.956782
H	-3.432839	1.866350	1.859806
O	-3.699750	-1.791137	-0.255860
C	-4.947825	-0.177439	-1.461078
H	-5.468536	0.727985	-1.145854
H	-4.453286	0.045223	-2.412694
H	-5.659912	-0.985632	-1.624455
C	-2.556400	1.492256	-0.741018
H	-1.963077	2.244629	-0.217485
H	-1.936899	1.043490	-1.521077
H	-3.379325	2.013838	-1.230893

TS-6n

C	-2.101968	0.718833	-0.569851
C	-0.633697	0.883007	-0.422772
H	-2.551877	0.999778	-1.517678
H	-0.299513	0.968895	0.611595
H	-0.247767	1.728910	-0.994296
O	-1.082300	-1.096166	-1.545872
C	-0.178534	-0.425175	-1.046245
O	1.050532	-0.755802	-1.031233
C	-2.967682	0.232237	0.450887
Al	2.532262	-0.168904	-0.133830
C	4.069536	-1.296670	-0.566660
C	5.360270	-0.912223	0.156880
H	4.223211	-1.263763	-1.653021
H	3.804834	-2.336755	-0.336578
H	6.198275	-1.566250	-0.110348
H	5.664957	0.112232	-0.079188
H	5.244465	-0.967262	1.243923
Cl	2.740724	1.935636	-0.695971
Cl	1.914635	-0.222733	1.970766
C	-2.392270	-0.533342	1.621046
H	-2.092887	-1.535156	1.311085
H	-1.519807	-0.033057	2.039347
H	-3.142289	-0.621720	2.408908
C	-3.116745	1.796417	0.729041
H	-2.678176	2.497307	-0.006981
H	-4.189725	1.987768	0.667213
H	-2.641929	2.010678	1.681688
C	-4.277257	-0.355290	-0.110289
O	-5.218664	0.354138	-0.361237
C	-4.268982	-1.828923	-0.335265

H	-5.139665	-2.116022	-0.922398
H	-3.346417	-2.132677	-0.837068
H	-4.298757	-2.347082	0.628173

Imaginary vibration frequency: 222.88i

SLC-6o

C	-1.770896	-0.351563	-0.980966
C	-0.645854	0.537228	-0.444715
H	-2.189068	-0.018091	-1.927959
H	-0.647361	0.768726	0.618954
H	-0.437277	1.438524	-1.020438
O	-0.731028	-1.393374	-1.297992
C	0.208520	-0.619616	-0.819039
O	1.394804	-0.929383	-0.776597
C	-2.831052	-0.917702	-0.053109
Al	2.866019	-0.006845	0.004571
C	4.460632	-1.075800	-0.333527
C	5.747832	-0.475360	0.233808
H	4.555862	-1.215207	-1.417867
H	4.296527	-2.077634	0.083037
H	6.621790	-1.101911	0.024384
H	5.952554	0.513231	-0.188630
H	5.692205	-0.354292	1.320039
Cl	2.746984	1.932505	-0.959381
Cl	2.199670	0.171523	2.061932
C	-3.817038	0.182251	0.328096
C	-3.606861	-2.008762	-0.795424
H	-4.406425	-2.391206	-0.160489
H	-4.050483	-1.625712	-1.718218
H	-2.941004	-2.836513	-1.047537
O	-4.793918	-0.004001	1.003941
O	-3.472116	1.372196	-0.166165
C	-4.340473	2.467999	0.150307
H	-4.386275	2.617898	1.229524
H	-3.902684	3.338325	-0.333411
H	-5.343428	2.283490	-0.236357
C	-2.242772	-1.484052	1.241065
H	-1.545870	-2.295212	1.022029
H	-1.725365	-0.725930	1.833158
H	-3.049229	-1.889238	1.852526

TS-6o

C	-1.742175	1.010591	-0.325594
C	-0.265833	1.012374	-0.209852

H	-2.199466	1.514007	-1.172110
H	0.100019	0.866162	0.806986
H	0.175256	1.924220	-0.616571
O	-0.817681	-0.672167	-1.740502
C	0.099633	-0.172418	-1.100691
O	1.315454	-0.564270	-1.134154
C	-2.624616	0.322066	0.554473
Al	2.831791	-0.222441	-0.183420
C	4.283149	-1.385084	-0.789130
C	5.607888	-1.187183	-0.052545
H	4.423543	-1.223684	-1.865765
H	3.948258	-2.425552	-0.687693
H	6.392876	-1.858991	-0.418678
H	5.982536	-0.164897	-0.164894
H	5.503356	-1.371521	1.021383
Cl	3.196122	1.921815	-0.439309
Cl	2.233655	-0.531214	1.908342
C	-2.107581	-0.744419	1.484126
H	-1.966022	-1.675181	0.934626
H	-1.157128	-0.458986	1.932912
H	-2.825553	-0.922534	2.284573
C	-2.615471	1.799348	1.193688
H	-2.054309	2.585994	0.644416
H	-3.639351	2.165236	1.185436
H	-2.136924	1.720299	2.165102
C	-3.979152	0.070054	-0.100004
O	-4.542847	0.891965	-0.775330
O	-4.419380	-1.143625	0.154530
C	-5.665104	-1.506981	-0.463579
H	-5.858430	-2.528614	-0.146424
H	-6.462109	-0.844233	-0.125171
H	-5.574849	-1.455535	-1.548926

Imaginary vibration frequency: 108.61i

SLC-7a

C	1.806634	1.575759	-0.390531
C	1.117233	1.227092	-1.712737
H	1.883145	2.644727	-0.188122
H	1.583260	0.459296	-2.328544
H	0.808055	2.077243	-2.321356
O	0.612684	1.052009	0.332040
C	0.046549	0.731306	-0.807362
O	-1.045100	0.203570	-0.958277
C	3.074938	0.894112	0.033516

Al	-2.443354	-0.329876	0.242927
Cl	-1.425561	-1.649841	1.616001
Cl	-2.920177	1.563359	1.180516
C	-3.818744	-1.125644	-0.890355
C	-4.429263	-0.180905	-1.925543
H	-4.603984	-1.525057	-0.236456
H	-3.379918	-2.001040	-1.386376
H	-5.195446	-0.674643	-2.533811
H	-4.902895	0.684151	-1.451730
H	-3.673941	0.206741	-2.616704
C	3.391686	1.112621	1.493011
H	4.347199	0.658175	1.754212
H	3.458247	2.187312	1.689473
H	2.616744	0.690251	2.134691
Br	3.004378	-1.039176	-0.354172
H	3.872582	1.271913	-0.608185

TS-7a

C	-2.138477	-0.229306	-0.924208
C	-0.769651	0.211119	-0.549528
H	-2.477310	-0.037179	-1.935918
H	-0.595811	0.287253	0.524703
H	-0.502768	1.162308	-1.012340
O	-0.644030	-1.781481	-1.730570
C	0.033017	-0.929177	-1.153245
O	1.299954	-0.955913	-1.048098
C	-2.968025	-1.092947	-0.106725
Al	2.545313	-0.043712	-0.064261
C	4.326608	-0.775704	-0.401056
C	5.454356	-0.069787	0.351995
H	4.512878	-0.733748	-1.482065
H	4.312505	-1.842743	-0.144337
H	6.436362	-0.506362	0.136362
H	5.510665	0.991487	0.090267
H	5.310565	-0.123181	1.435803
Cl	2.291071	2.053246	-0.634171
Cl	1.821994	-0.265677	1.994132
Br	-3.678346	0.814462	0.254252
C	-2.473006	-1.788803	1.101599
H	-1.974738	-2.698562	0.744612
H	-1.755750	-1.208084	1.679795
H	-3.302749	-2.092738	1.739555
H	-3.779245	-1.578249	-0.642829

Imaginary vibration frequency: 213.48i

SLC-7b

C	-1.677436	0.162406	-0.801628
C	-0.328273	0.897673	-0.782747
H	-2.085926	0.006666	-1.797426
H	-0.187866	1.677763	-0.035410
H	0.043883	1.234848	-1.749961
O	-0.959564	-1.081396	-0.393655
C	0.181660	-0.438813	-0.377896
O	1.254968	-0.955268	-0.093538
C	-2.732858	0.586080	0.190149
Al	2.993476	-0.178338	0.042799
C	4.213174	-1.604606	0.566962
C	5.669619	-1.162207	0.715575
H	4.137259	-2.408378	-0.176311
H	3.851481	-2.034640	1.509501
H	6.322970	-1.990732	1.010175
H	6.066208	-0.757642	-0.220699
H	5.779145	-0.381176	1.474274
Cl	3.240135	0.679479	-1.933015
Cl	2.629053	1.409467	1.476840
C	-2.266621	0.576302	1.629556
H	-1.912298	-0.406606	1.940346
H	-1.458436	1.300976	1.767197
H	-3.085230	0.870118	2.286816
C	-3.283291	1.931752	-0.235956
H	-3.634602	1.918973	-1.269063
H	-4.112703	2.221877	0.409726
H	-2.500530	2.691301	-0.142329
Br	-4.198109	-0.758150	0.019006

TS-7b

C	1.935412	0.243258	-0.785670
C	0.563966	-0.250776	-0.467567
H	2.264053	0.208086	-1.817649
H	0.404236	-0.526115	0.575215
H	0.265068	-1.088912	-1.098876
O	0.598960	1.903427	-1.229157
C	-0.171930	1.015703	-0.832268
O	-1.427605	1.142344	-0.737029
C	2.834341	0.881532	0.165468
Al	-2.777321	0.093348	-0.060888
C	-4.474094	1.055969	-0.182469
C	-5.673546	0.301227	0.391124

H	-4.652957	1.300264	-1.237534
H	-4.356923	2.020113	0.328957
H	-6.605054	0.872141	0.303510
H	-5.832360	-0.652614	-0.121721
H	-5.535733	0.072993	1.452689
Cl	-2.660744	-1.753712	-1.221825
Cl	-2.106890	-0.352957	1.975764
Br	3.460130	-1.128487	0.140397
C	2.342221	1.248226	1.523613
H	1.813710	2.202571	1.420339
H	1.656641	0.521583	1.955412
H	3.180426	1.402443	2.202867
C	3.909978	1.743721	-0.403636
H	4.270580	1.384821	-1.367477
H	3.467028	2.735296	-0.549542
H	4.742751	1.844895	0.292408

Imaginary vibration frequency: 329.73i

SLC-7c

C	-1.191254	-1.027416	0.462064
C	-0.591976	-1.461911	-0.876162
H	-1.410223	-1.836972	1.157646
H	-0.995988	-0.998258	-1.775263
H	-0.481061	-2.537340	-1.015328
O	0.122661	-0.437233	0.829321
C	0.625397	-0.802449	-0.331763
O	1.764295	-0.618057	-0.724352
C	-2.296227	0.003159	0.518794
Al	3.343571	0.179049	0.038382
Cl	2.646577	2.146400	0.590106
Cl	3.624202	-1.075353	1.779227
C	4.691343	0.067447	-1.367752
C	5.021692	-1.351494	-1.831413
H	5.599067	0.565505	-1.005085
H	4.345040	0.673412	-2.214839
H	5.784859	-1.360786	-2.617591
H	5.399315	-1.966989	-1.009462
H	4.141511	-1.861899	-2.235374
C	-2.539856	0.512721	1.914098
H	-3.374170	1.212657	1.934927
H	-2.762339	-0.323827	2.580806
H	-1.645322	1.024614	2.276672
Br	-1.897821	1.511713	-0.665147
Br	-3.875913	-0.949529	-0.152616

TS-7c

C	-1.382737	0.187985	-0.756221
C	0.065604	0.513736	-0.606676
H	-1.797276	0.112324	-1.754610
H	0.346459	0.906625	0.371481
H	0.403408	1.213895	-1.372060
O	-0.246295	-1.719055	-1.080246
C	0.624723	-0.876894	-0.837197
O	1.868513	-1.113418	-0.780499
C	-2.208668	-0.267209	0.347787
Al	3.313212	-0.220021	-0.083606
C	4.902278	-1.348233	-0.224969
C	6.173170	-0.744553	0.372337
H	5.058184	-1.577189	-1.287268
H	4.680452	-2.310135	0.254873
H	7.038897	-1.407856	0.263566
H	6.433517	0.203989	-0.107732
H	6.057871	-0.539925	1.441341
Cl	3.391620	1.661978	-1.190030
Cl	2.655467	0.245516	1.955780
Br	-2.619553	1.793702	0.105815
C	-1.657617	-0.552996	1.694511
H	-1.254256	-1.571216	1.665973
H	-0.851860	0.130455	1.961074
H	-2.436618	-0.514168	2.454895
Br	-3.712712	-1.308707	-0.130783

Imaginary vibration frequency: 317.07i

SLC-7d

C	1.716056	1.250620	0.489661
C	0.521603	1.138937	-0.456614
H	2.038338	2.266811	0.714035
H	0.584419	0.410846	-1.264051
H	0.123402	2.083503	-0.827572
O	0.856876	0.764074	1.597195
C	-0.162106	0.646250	0.771406
O	-1.265943	0.246276	1.103891
C	2.931481	0.366864	0.301580
Al	-2.861648	0.003003	0.066024
C	-4.148554	-0.887840	1.226182
C	-5.501748	-1.159541	0.567116
H	-4.283120	-0.271143	2.123799
H	-3.702546	-1.828347	1.573407

H	-6.198100	-1.659408	1.249242
H	-5.983523	-0.233930	0.237429
H	-5.400115	-1.799901	-0.314435
Cl	-3.275407	2.045998	-0.522562
Cl	-2.093283	-1.104443	-1.629606
C	3.861856	0.402664	1.484469
H	4.746911	-0.204130	1.297198
H	4.172031	1.433435	1.673017
H	3.351215	0.018080	2.369454
Br	2.380106	-1.489404	-0.035295
Cl	3.745737	1.013959	-1.163479

TS-7d

C	-1.772675	-0.079911	-0.775500
C	-0.361767	0.353789	-0.557202
H	-2.154563	-0.126923	-1.788011
H	-0.141492	0.699034	0.453416
H	-0.060398	1.127977	-1.264215
O	-0.503808	-1.855483	-1.164739
C	0.306118	-0.971528	-0.856959
O	1.560903	-1.127241	-0.791743
C	-2.603590	-0.650818	0.270011
Al	2.937261	-0.140796	-0.074984
C	4.625766	-1.099374	-0.292429
C	5.842919	-0.370798	0.278100
H	4.772122	-1.295218	-1.362491
H	4.522612	-2.085571	0.178021
H	6.770141	-0.938098	0.138144
H	5.988473	0.604271	-0.197294
H	5.737152	-0.188899	1.352243
Cl	2.819483	1.789516	-1.092098
Cl	2.287137	0.162376	1.994943
Br	-3.156380	1.398498	0.127955
C	-2.092140	-0.970387	1.624144
H	-1.612021	-1.953169	1.559064
H	-1.358929	-0.242667	1.969069
H	-2.909929	-1.037616	2.341016
Cl	-3.894198	-1.662732	-0.277653

Imaginary vibration frequency: 342.08i

SLC-7e

C	1.659111	1.377587	0.357654
C	0.481067	1.142424	-0.584687
H	1.951417	2.418913	0.491289

H	0.586522	0.346156	-1.319129
H	0.049875	2.033014	-1.042262
O	0.809453	0.968831	1.495668
C	-0.194721	0.734782	0.677886
O	-1.286885	0.323783	1.039463
C	2.906232	0.526259	0.214850
Al	-2.889116	0.001075	0.045923
C	-4.103043	-0.958093	1.231186
C	-5.448487	-1.308827	0.593872
H	-4.258685	-0.349370	2.130751
H	-3.597696	-1.870946	1.571066
H	-6.103701	-1.848947	1.286108
H	-5.988931	-0.413028	0.272711
H	-5.323501	-1.941862	-0.290019
Cl	-3.423597	2.022945	-0.522969
Cl	-2.142156	-1.066260	-1.685140
C	3.827586	0.650784	1.402051
H	4.676327	-0.027357	1.327845
H	4.196699	1.680383	1.453148
H	3.288733	0.422749	2.321499
Br	2.317398	-1.443014	0.154658
O	3.412166	0.886584	-0.993024
C	4.708179	0.411018	-1.337509
H	4.752081	-0.678568	-1.255362
H	4.864929	0.700682	-2.374810
H	5.479887	0.866874	-0.713661

TS-7e

C	-1.689182	-0.036657	-0.858980
C	-0.337379	0.467296	-0.441422
H	-2.037551	0.151262	-1.865508
H	-0.210138	0.663280	0.622457
H	-0.034747	1.357358	-0.994050
O	-0.510356	-1.546458	-1.377477
C	0.361334	-0.773291	-0.906513
O	1.587824	-1.031138	-0.854606
C	-2.624343	-0.741990	0.009761
Al	3.013431	-0.159392	-0.049735
C	4.648890	-1.185695	-0.343550
C	5.905361	-0.538809	0.240793
H	4.771155	-1.336640	-1.423745
H	4.507919	-2.187143	0.082714
H	6.803698	-1.140502	0.062078
H	6.088810	0.448900	-0.193487

H	5.821964	-0.400443	1.323395
Cl	2.974368	1.830893	-0.936736
Cl	2.357400	-0.003924	2.028879
Br	-3.170605	1.481389	0.208952
C	-2.261080	-1.196380	1.373752
H	-1.845054	-2.206388	1.278800
H	-1.517279	-0.553084	1.834927
H	-3.133180	-1.245118	2.023913
O	-3.560293	-1.346322	-0.662779
C	-4.603023	-2.049660	0.032383
H	-5.249500	-2.441161	-0.748330
H	-4.190591	-2.868332	0.621579
H	-5.159880	-1.354524	0.663595

Imaginary vibration frequency: 459.87i

SLC-7f

C	-1.131615	0.703044	-1.035014
C	-0.004839	0.906868	-0.017816
H	-1.427602	1.613842	-1.556457
H	-0.092506	0.368054	0.924241
H	0.310873	1.935353	0.157417
O	-0.131225	0.004464	-1.928676
C	0.806524	0.193279	-1.038939
O	1.969652	-0.168795	-1.179087
C	-2.341202	-0.120698	-0.733849
Al	3.463886	0.068101	-0.022993
C	4.991620	-0.790271	-0.876846
C	6.296068	-0.679358	-0.086220
H	5.116896	-0.349982	-1.874248
H	4.741527	-1.845318	-1.045566
H	7.130847	-1.171195	-0.597632
H	6.585557	0.364314	0.070828
H	6.208953	-1.139967	0.902652
Cl	3.515286	2.231239	0.158345
Cl	2.732885	-0.786931	1.829175
C	-3.057338	-0.506840	-2.016628
H	-3.938517	-1.113510	-1.809111
H	-3.381104	0.397596	-2.541897
H	-2.403598	-1.071671	-2.685010
Br	-1.786046	-1.798929	0.180762
Si	-3.531257	0.825737	0.484789
C	-5.069905	-0.224500	0.694424
H	-4.832094	-1.223248	1.067978
H	-5.733532	0.255227	1.420500

H	-5.622164	-0.327232	-0.242905
C	-3.954697	2.465324	-0.337167
H	-4.699846	2.990171	0.269088
H	-3.082401	3.119892	-0.418998
H	-4.379575	2.328813	-1.335065
C	-2.687670	1.138088	2.131666
H	-2.331069	0.214715	2.593659
H	-1.847169	1.831113	2.043272
H	-3.412806	1.591703	2.815040

TS-7f

C	1.157424	-0.301847	-0.708975
C	-0.295921	-0.600861	-0.558491
H	1.557806	-0.272880	-1.715493
H	-0.585272	-0.979217	0.422102
H	-0.661521	-1.288067	-1.322936
O	0.097107	1.605783	-1.059207
C	-0.807500	0.802930	-0.792784
O	-2.037360	1.102352	-0.719797
C	2.048655	0.068257	0.379008
Al	-3.529735	0.257478	-0.067689
C	-5.066155	1.460240	-0.190920
C	-6.376341	0.873912	0.335025
H	-5.182360	1.757990	-1.241093
H	-4.821424	2.381969	0.352570
H	-7.212062	1.577825	0.248301
H	-6.660973	-0.030775	-0.211360
H	-6.298591	0.596854	1.391102
Cl	-3.691057	-1.581635	-1.236761
Cl	-2.943897	-0.296913	1.969690
Br	2.456521	-1.945547	0.101506
C	1.471701	0.307769	1.736490
H	1.029757	1.310434	1.722256
H	0.692338	-0.399323	2.022096
H	2.249380	0.299719	2.500931
Si	3.632133	1.107845	-0.072425
C	3.143553	2.875958	0.303289
H	3.944388	3.547308	-0.022185
H	2.229511	3.154243	-0.226467
H	2.989170	3.033461	1.373581
C	5.024078	0.514779	1.030284
H	5.343821	-0.499391	0.779124
H	5.886925	1.176161	0.904800
H	4.742130	0.537653	2.086230

C	4.004848	0.855899	-1.889891
H	4.917100	1.407668	-2.137755
H	4.182273	-0.192540	-2.144147
H	3.206270	1.246021	-2.526452

Imaginary vibration frequency: 278.76i

SLC-7g

C	1.347890	-1.486696	0.429820
C	0.022896	-1.159090	1.135248
H	1.711558	-2.501006	0.577612
H	-0.040820	-0.200389	1.650208
H	-0.403867	-1.953516	1.746441
O	0.623396	-1.439778	-0.869736
C	-0.494603	-1.131657	-0.257628
O	-1.554843	-0.924009	-0.832602
C	2.463436	-0.465603	0.554256
Al	-3.225023	-0.281730	-0.168922
C	-4.532009	-0.522746	-1.594982
C	-5.942031	-0.052663	-1.233994
H	-4.548026	-1.584985	-1.870050
H	-4.172651	0.010854	-2.483881
H	-6.649902	-0.203854	-2.056356
H	-6.337481	-0.590529	-0.366792
H	-5.960831	1.013014	-0.985765
Cl	-3.491100	-1.480844	1.621486
Cl	-2.703007	1.742685	0.389898
C	3.097330	-0.669582	1.918355
H	3.932979	0.015181	2.061000
H	2.365076	-0.494096	2.711160
H	3.465274	-1.691038	2.018785
Br	3.838931	-0.999359	-0.795584
C	2.005510	0.948214	0.270824
C	1.897463	1.874527	1.307106
C	1.619919	1.338131	-1.013429
C	1.407902	3.151777	1.067729
H	2.192081	1.610536	2.314487
C	1.128527	2.611134	-1.249606
H	1.721009	0.646082	-1.839950
C	1.018430	3.523618	-0.208770
H	1.330988	3.855925	1.888716
H	0.833192	2.891340	-2.254489
H	0.631548	4.519354	-0.394108

TS-7g

C	-1.048141	0.359733	-0.620801
C	0.417911	0.623370	-0.465953
H	-1.437876	0.328550	-1.628634
H	0.722108	1.032817	0.496453
H	0.805521	1.269806	-1.254906
O	-0.145692	-1.535654	-0.857748
C	0.843590	-0.808469	-0.650774
O	2.037354	-1.217484	-0.605941
C	-1.969253	0.070367	0.473053
Al	3.632768	-0.445152	-0.107089
C	5.061835	-1.772764	-0.228425
C	6.443800	-1.251890	0.167014
H	5.084911	-2.158339	-1.255856
H	4.787317	-2.627673	0.402899
H	7.217543	-2.024219	0.088895
H	6.757290	-0.418184	-0.469097
H	6.457104	-0.887722	1.199154
Cl	3.837660	1.278465	-1.431636
Cl	3.219799	0.296686	1.910154
Br	-2.141794	2.213526	0.151422
C	-1.398011	-0.130194	1.837451
H	-1.090914	-1.178111	1.919075
H	-0.526141	0.492412	2.021878
H	-2.136480	0.073698	2.610569
C	-3.248426	-0.588934	0.138688
C	-3.850344	-0.434704	-1.115517
C	-3.861140	-1.417490	1.081155
C	-5.022406	-1.099135	-1.418410
H	-3.426555	0.229137	-1.860162
C	-5.031895	-2.090682	0.769979
H	-3.420185	-1.559766	2.058457
C	-5.615416	-1.934098	-0.477420
H	-5.478694	-0.964500	-2.392185
H	-5.487044	-2.739866	1.508926
H	-6.533807	-2.457582	-0.718603

Imaginary vibration frequency: 398.76i

SLC-7h

C	-1.729672	-1.247622	0.410472
C	-0.529062	-1.105593	-0.527885
H	-2.034765	-2.275512	0.607700
H	-0.586830	-0.347280	-1.307282
H	-0.123411	-2.034892	-0.928677
O	-0.864893	-0.795667	1.536163

C	0.148720	-0.649610	0.716232
O	1.254481	-0.255066	1.058771
C	-2.963461	-0.389310	0.234252
Al	2.864696	-0.028666	0.057015
C	4.112522	0.926411	1.209934
C	5.476905	1.193011	0.572488
H	4.234605	0.349065	2.135089
H	3.644310	1.873059	1.508086
H	6.148491	1.733498	1.248566
H	5.981418	0.262497	0.294548
H	5.386760	1.793142	-0.338180
Cl	3.327056	-2.086280	-0.444023
Cl	2.153115	1.002624	-1.712275
C	-3.832983	-0.442659	1.469471
H	-4.718192	0.181508	1.350310
H	-4.152631	-1.473905	1.646018
H	-3.282780	-0.098500	2.345222
Br	-2.378034	1.514012	-0.011360
C	-3.625179	-0.793961	-1.044370
C	-4.882683	-1.200293	-1.150562
H	-5.554337	-1.257847	-0.301416
H	-2.997343	-0.749324	-1.930662
H	-5.285388	-1.487495	-2.115521

TS-7h

C	1.763468	-0.009675	-0.830395
C	0.374232	-0.445866	-0.489142
H	2.104845	-0.146956	-1.849297
H	0.197306	-0.653268	0.565712
H	0.054326	-1.311196	-1.071301
O	0.540918	1.624484	-1.397912
C	-0.296735	0.821532	-0.946942
O	-1.538971	1.039498	-0.883444
C	2.682244	0.658222	0.085597
Al	-2.937260	0.163149	-0.064422
C	-4.593576	1.161923	-0.343063
C	-5.834195	0.501539	0.259230
H	-4.730359	1.304660	-1.422740
H	-4.462147	2.168161	0.075022
H	-6.743321	1.088851	0.086682
H	-6.008106	-0.491776	-0.166175
H	-5.736851	0.371708	1.341748
Cl	-2.901735	-1.841751	-0.928338
Cl	-2.271913	0.014793	2.015606

Br	3.213485	-1.434062	0.206676
C	2.190809	1.110358	1.416898
H	1.704808	2.081121	1.273619
H	1.464518	0.427104	1.851881
H	3.012893	1.238589	2.119491
C	3.800466	1.354811	-0.552869
C	4.456786	2.364679	0.009858
H	4.236634	2.727932	1.007064
H	4.051776	1.032284	-1.559188
H	5.241552	2.875321	-0.536427

Imaginary vibration frequency: 388.38i

SLC-7i

C	1.424071	1.254308	0.514716
C	0.266060	1.086227	-0.471602
H	1.712332	2.289086	0.702555
H	0.360084	0.302671	-1.222050
H	-0.120264	2.001473	-0.920522
O	0.511125	0.828268	1.612243
C	-0.467005	0.665821	0.753570
O	-1.588650	0.284644	1.058495
C	2.665303	0.400337	0.411049
Al	-3.153535	0.035010	-0.006104
C	-4.455883	-0.885464	1.114252
C	-5.789697	-1.167810	0.421229
H	-4.619505	-0.281720	2.015841
H	-4.005106	-1.824020	1.460827
H	-6.494679	-1.685979	1.080567
H	-6.276865	-0.244916	0.091691
H	-5.658720	-1.795434	-0.465647
Cl	-3.589567	2.078862	-0.582737
Cl	-2.367113	-1.045322	-1.713270
C	3.481451	0.483978	1.681833
H	4.370095	-0.142534	1.612322
H	3.807802	1.518848	1.828224
H	2.899951	0.175244	2.550949
Br	2.107349	-1.498486	0.167593
C	3.435633	0.854040	-0.831149
H	3.628459	1.926524	-0.711484
H	2.791755	0.737121	-1.709443
C	4.729785	0.144818	-1.058068
C	5.913469	0.742067	-1.049480
H	4.667701	-0.923049	-1.253686
H	6.013603	1.807588	-0.860192

H	6.826747	0.187583	-1.238258
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TS-7i

C	1.576985	0.258824	-0.467634
C	0.161530	-0.212730	-0.512067
H	2.016004	0.638481	-1.381742
H	-0.121463	-0.898876	0.286380
H	-0.098418	-0.664390	-1.470286
O	0.371497	2.049289	-0.270571
C	-0.476169	1.145416	-0.344831
O	-1.727256	1.326665	-0.290361
C	2.382829	0.343846	0.741028
Al	-3.172100	0.209181	-0.084221
C	-4.809555	1.273909	-0.009027
C	-6.090097	0.460027	0.177572
H	-4.871359	1.865525	-0.931696
H	-4.705477	2.003821	0.804070
H	-6.984271	1.093045	0.210571
H	-6.234488	-0.256816	-0.636842
H	-6.069836	-0.115354	1.108469
Cl	-3.041278	-1.181625	-1.764141
Cl	-2.681307	-0.896740	1.741116
Br	2.962498	-1.479960	-0.119174
C	1.750711	0.098815	2.070674
H	1.209668	1.011882	2.341903
H	1.044985	-0.729494	2.075807
H	2.515345	-0.075964	2.827890
C	3.541127	1.308502	0.761842
H	3.114752	2.204654	1.234500
H	4.294472	0.924984	1.453732
C	4.147244	1.673180	-0.552350
C	5.358730	1.289918	-0.930040
H	3.553915	2.307133	-1.207177
H	5.771458	1.586483	-1.888355
H	5.984564	0.670467	-0.293375

Imaginary vibration frequency: 328.96i

SLC-7j

C	1.661163	-1.048741	0.152518
C	0.313577	-1.038790	0.888390
H	2.120402	-2.024912	0.014193
H	0.179837	-0.299800	1.677937
H	-0.060099	-2.011742	1.206073
O	0.949127	-0.663858	-1.090562

C	-0.192975	-0.615081	-0.444486
O	-1.256161	-0.300122	-0.959118
C	2.675085	-0.006416	0.582220
Al	-2.978076	0.009063	-0.192214
C	-4.251269	0.080258	-1.665857
C	-5.697953	0.316946	-1.229326
H	-4.176513	-0.860218	-2.226501
H	-3.932454	0.867975	-2.359856
H	-6.385634	0.344536	-2.081641
H	-6.051111	-0.471066	-0.557000
H	-5.808443	1.266334	-0.696391
Cl	-3.165047	-1.657658	1.185269
Cl	-2.605729	1.829153	0.920774
C	3.300328	-0.423932	1.903047
H	4.069397	0.288718	2.198013
H	2.530270	-0.440246	2.679263
H	3.745981	-1.416383	1.820371
Br	4.100298	0.012149	-0.813247
C	2.083212	1.311628	0.636247
C	1.525099	2.372498	0.699195
H	1.034815	3.319946	0.750983

TS-7j

C	1.836491	0.154760	-0.755532
C	0.439646	-0.322988	-0.533713
H	2.213718	0.213990	-1.768820
H	0.236192	-0.692075	0.471707
H	0.147165	-1.089923	-1.252167
O	0.573127	1.883396	-1.096326
C	-0.243752	0.995013	-0.806268
O	-1.496270	1.157931	-0.744774
C	2.695416	0.690495	0.297171
Al	-2.885298	0.154208	-0.074684
C	-4.569327	1.109214	-0.340509
C	-5.802796	0.375623	0.186626
H	-4.681191	1.309487	-1.413983
H	-4.483973	2.093629	0.137231
H	-6.726469	0.941061	0.018263
H	-5.929990	-0.598013	-0.296949
H	-5.731935	0.189914	1.262988
Cl	-2.730233	-1.764087	-1.109792
Cl	-2.299261	-0.163836	2.010065
Br	3.253435	-1.371866	0.093220
C	2.168370	0.951771	1.668086

H	1.681257	1.932833	1.632942
H	1.439595	0.210657	1.990949
H	2.985279	1.007802	2.386514
C	3.782785	1.498479	-0.127446
C	4.677455	2.224571	-0.465758
H	5.469788	2.873702	-0.772268

Imaginary vibration frequency: 369.45i

SLC-7k

C	1.435438	1.406039	0.338016
C	0.277048	1.076493	-0.606797
H	1.684742	2.466456	0.394980
H	0.393707	0.208847	-1.254912
H	-0.145755	1.914728	-1.160640
O	0.552096	1.081293	1.488952
C	-0.429959	0.784580	0.669997
O	-1.535046	0.409330	1.034136
C	2.706740	0.588796	0.330434
Al	-3.087815	-0.026717	0.006310
C	-4.430920	-0.676823	1.259363
C	-5.756537	-1.070932	0.606170
H	-4.599283	0.101637	2.014244
H	-4.008199	-1.532311	1.801103
H	-6.486562	-1.428922	1.340378
H	-6.215302	-0.226745	0.082195
H	-5.622230	-1.870118	-0.129232
Cl	-3.471394	1.867219	-0.978434
Cl	-2.278010	-1.435416	-1.426654
C	3.521108	0.850819	1.577446
H	4.436548	0.259723	1.567188
H	3.795897	1.910129	1.610550
H	2.955807	0.608135	2.477306
Br	2.234167	-1.338866	0.295338
C	3.459820	0.931768	-0.959853
H	3.610119	2.018793	-0.970792
H	2.843253	0.688459	-1.830308
C	4.750229	0.281299	-1.083624
C	5.822738	-0.247415	-1.192462
H	6.772249	-0.724571	-1.291261

TS-7k

C	-1.700281	-0.759848	0.615399
C	-0.638624	-1.594530	-0.021149
H	-1.865450	-0.874560	1.681052

H	-0.739917	-1.713945	-1.099491
H	-0.560158	-2.580396	0.438775
O	0.202631	0.285907	0.986492
C	0.535272	-0.714414	0.336179
O	1.700597	-1.036506	-0.037030
C	-2.405670	0.327686	-0.044112
Al	3.268699	-0.053807	-0.043074
C	4.629674	-1.172951	-0.902493
C	6.010901	-0.526943	-1.008052
H	4.267092	-1.447410	-1.901962
H	4.699661	-2.115688	-0.343672
H	6.745180	-1.182390	-1.491095
H	5.978032	0.400394	-1.588822
H	6.410279	-0.269710	-0.021948
Cl	2.757813	1.744912	-1.173540
Cl	3.724118	0.458662	2.022895
Br	-3.717880	-1.300756	-0.167299
C	-2.002083	0.783216	-1.401018
H	-1.168096	1.481307	-1.261760
H	-1.671446	-0.024986	-2.049656
H	-2.816776	1.325773	-1.879901
C	-2.985486	1.372614	0.877950
H	-3.283260	0.927064	1.830971
H	-2.143692	2.044286	1.098703
C	-4.082585	2.126993	0.305185
C	-4.998765	2.742297	-0.165938
H	-5.811516	3.295532	-0.582212

Imaginary vibration frequency: 306.36i

SLC-7I

C	-1.800923	1.316958	-0.465785
C	-0.606602	1.210636	0.482944
H	-2.137712	2.331008	-0.680600
H	-0.662656	0.492336	1.299637
H	-0.209814	2.160623	0.842225
O	-0.945089	0.842770	-1.570547
C	0.075941	0.713814	-0.744972
O	1.173554	0.304484	-1.080558
C	-3.011415	0.410303	-0.285754
Al	2.772684	0.007964	-0.054558
C	3.988278	-0.980723	-1.212066
C	5.336110	-1.310847	-0.568902
H	4.140144	-0.397286	-2.128878
H	3.483779	-1.903717	-1.524807

H	5.988578	-1.871288	-1.247275
H	5.877044	-0.405350	-0.277482
H	5.215083	-1.917010	0.334125
Cl	3.291704	2.040334	0.476550
Cl	1.969471	-1.022883	1.672866
C	-3.711023	0.841939	0.914130
C	-3.920814	0.439912	-1.502705
H	-4.793470	-0.192536	-1.345837
H	-4.255237	1.466097	-1.675903
H	-3.376396	0.088572	-2.379397
N	-4.263366	1.218418	1.849518
Br	-2.423877	-1.451730	0.043265

TS-7l

C	1.861490	0.090448	-0.755890
C	0.441168	-0.282501	-0.544088
H	2.226793	0.176255	-1.774319
H	0.213669	-0.641593	0.460602
H	0.110458	-1.031878	-1.264395
O	0.539457	1.987780	-1.058746
C	-0.230395	1.062640	-0.802618
O	-1.495529	1.158413	-0.747711
C	2.691289	0.684015	0.287226
Al	-2.867194	0.143309	-0.078103
C	-4.564605	1.077426	-0.332312
C	-5.787703	0.331520	0.201249
H	-4.683855	1.275742	-1.405407
H	-4.487194	2.063256	0.143819
H	-6.718103	0.886460	0.035018
H	-5.906133	-0.644578	-0.279569
H	-5.710762	0.149277	1.277776
Cl	-2.703697	-1.777452	-1.112207
Cl	-2.266012	-0.176297	2.005596
Br	3.232187	-1.344670	0.109124
C	2.173030	1.026983	1.636946
H	1.693742	2.008770	1.538312
H	1.433076	0.310866	1.990592
H	2.986848	1.117437	2.355860
C	3.806990	1.465033	-0.175443
N	4.682070	2.120174	-0.529813

Imaginary vibration frequency: 201.92i

SLC-7m

C	1.554523	0.156088	-0.932550
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C	0.369996	-0.696336	-0.470640
H	1.950110	-0.108943	-1.912246
H	0.361872	-1.029140	0.566440
H	0.089448	-1.518987	-1.127736
O	0.613132	1.306399	-1.111004
C	-0.393514	0.558470	-0.716768
O	-1.548586	0.948694	-0.648606
C	2.650273	0.518835	0.045381
Al	-3.125441	0.065891	-0.001146
C	-4.609880	1.291148	-0.301229
C	-5.962429	0.773934	0.190979
H	-4.657360	1.507795	-1.375993
H	-4.370565	2.244681	0.185817
H	-6.770440	1.487863	-0.002261
H	-6.239294	-0.164845	-0.298535
H	-5.952952	0.582804	1.268413
Cl	-3.090982	-1.767971	-1.154177
Cl	-2.526243	-0.341824	2.039865
C	3.647351	1.454418	-0.630690
C	2.195758	1.006303	1.392700
H	3.057468	1.238822	2.016386
H	1.618218	1.926947	1.272229
H	1.582118	0.267425	1.907262
H	3.930028	1.161133	-1.659338
O	4.101130	2.426412	-0.098341
Br	3.699630	-1.154709	0.214807

TS-7m

C	1.922590	0.333893	0.495669
C	0.836584	1.218860	0.000431
H	2.043625	0.213037	1.568505
H	0.950790	1.530070	-1.038499
H	0.716922	2.103344	0.626726
O	-0.077834	-0.859615	0.525055
C	-0.351615	0.278751	0.147561
O	-1.496638	0.751479	-0.134106
C	2.626158	-0.634589	-0.319612
Al	-3.160971	-0.046426	-0.162390
Cl	-2.996225	-1.669787	-1.613499
Cl	-3.498416	-0.837313	1.839076
C	-4.439567	1.347548	-0.682403
C	-4.477496	2.557493	0.251391
H	-5.436268	0.892599	-0.745250
H	-4.200487	1.668674	-1.704931

H	-5.204358	3.313432	-0.069248
H	-4.745723	2.268890	1.272570
H	-3.503429	3.054687	0.307428
C	2.279237	-0.929741	-1.726410
H	3.120906	-1.391596	-2.244747
H	1.464879	-1.665561	-1.691269
H	1.929881	-0.061422	-2.282045
Br	3.905965	0.999597	-0.101388
C	3.291672	-1.780352	0.453072
O	3.298273	-1.827252	1.646166
H	3.740219	-2.555882	-0.189530

Imaginary vibration frequency: 195.70i

SLC-7n

C	1.535363	1.158027	0.696082
C	0.371532	1.147103	-0.293706
H	1.838158	2.151990	1.023371
H	0.450868	0.491387	-1.159083
H	0.003226	2.126900	-0.596770
O	0.627354	0.585045	1.726202
C	-0.362203	0.561334	0.861534
O	-1.483572	0.150689	1.123339
C	2.761923	0.298263	0.496282
Al	-3.048379	0.000903	0.035980
C	-4.419993	-0.815594	1.154765
C	-5.763858	-1.020278	0.454176
H	-4.550935	-0.187000	2.044811
H	-4.035808	-1.775910	1.521372
H	-6.507832	-1.477323	1.115923
H	-6.184778	-0.072961	0.103373
H	-5.668067	-1.671633	-0.419965
Cl	-3.347140	2.061650	-0.564920
Cl	-2.298435	-1.145652	-1.641212
C	3.583744	0.886133	-0.660893
C	3.554822	0.167227	1.779277
H	4.432202	-0.463004	1.641657
H	3.886824	1.160709	2.097747
H	2.940344	-0.263585	2.570536
O	3.122267	1.802128	-1.300126
C	4.949652	0.333481	-0.905473
H	5.018169	-0.734069	-0.696450
H	5.241560	0.535713	-1.935254
H	5.651170	0.850663	-0.241667
Br	2.219838	-1.510076	-0.112019

TS-7n

C	-1.590443	0.087155	-0.774236
C	-0.152419	0.398816	-0.576131
H	-1.991570	0.068132	-1.782556
H	0.107098	0.731088	0.430759
H	0.205642	1.141088	-1.291063
O	-0.368736	-1.837017	-1.172346
C	0.448428	-0.967797	-0.868696
O	1.705838	-1.144732	-0.791758
C	-2.457965	-0.461135	0.251581
Al	3.101227	-0.209567	-0.064579
C	4.758755	-1.230245	-0.243893
C	6.000237	-0.519978	0.296096
H	4.896065	-1.471290	-1.305996
H	4.625481	-2.194234	0.263581
H	6.908917	-1.121160	0.176692
H	6.174876	0.430917	-0.216933
H	5.903462	-0.293200	1.362604
Cl	3.094973	1.720247	-1.092708
Cl	2.439543	0.142527	1.997879
Br	-2.884132	1.571467	0.188743
C	-1.917118	-0.903056	1.560134
H	-1.564333	-1.931307	1.414444
H	-1.072576	-0.302269	1.893840
H	-2.681264	-0.916565	2.335746
C	-3.736608	-1.151282	-0.297745
O	-3.920588	-1.154086	-1.484916
C	-4.640408	-1.780120	0.700320
H	-4.132542	-2.624717	1.176731
H	-4.903313	-1.074424	1.493412
H	-5.540889	-2.133666	0.201923

Imaginary vibration frequency: 204.39i

SLC-7o

C	-1.378643	0.404654	-1.242732
C	-0.262334	0.925772	-0.337863
H	-1.689404	1.101493	-2.021994
H	-0.364836	0.744154	0.730024
H	0.057943	1.951593	-0.518560
O	-0.405831	-0.550490	-1.841295
C	0.544777	-0.097373	-1.054786
O	1.694221	-0.513547	-1.063352
C	-2.593204	-0.315291	-0.701360

Al	3.206651	0.034852	-0.026732
C	4.660393	-1.191086	-0.451849
C	5.972001	-0.875761	0.269167
H	4.814468	-1.177008	-1.538209
H	4.332160	-2.209633	-0.209298
H	6.765866	-1.583930	0.007638
H	6.339016	0.124725	0.020234
H	5.854043	-0.912659	1.356528
Cl	3.416911	2.096670	-0.662428
Cl	2.396090	-0.023446	1.981841
C	-3.559260	0.665208	-0.032888
C	-3.286783	-1.113152	-1.780168
H	-4.176754	-1.596606	-1.382010
H	-3.593508	-0.438174	-2.585057
H	-2.618357	-1.869540	-2.190559
O	-4.745708	0.497203	0.017689
Br	-2.053192	-1.547462	0.756763
O	-2.913453	1.707518	0.473883
C	-3.715209	2.673173	1.171366
H	-3.020620	3.437792	1.510351
H	-4.459228	3.103613	0.500411
H	-4.210818	2.205138	2.022569

TS-7o

C	-1.335274	0.293101	-0.755540
C	0.116914	0.502979	-0.537582
H	-1.722242	0.304321	-1.769268
H	0.386235	0.793577	0.479098
H	0.529241	1.236828	-1.231146
O	-0.232442	-1.709597	-1.169420
C	0.633518	-0.893864	-0.855473
O	1.879334	-1.142457	-0.788001
C	-2.239785	-0.221820	0.256115
Al	3.339569	-0.303424	-0.071811
C	4.911486	-1.452407	-0.246824
C	6.199717	-0.863884	0.328297
H	5.045707	-1.681170	-1.312089
H	4.687793	-2.412606	0.235607
H	7.055900	-1.537233	0.205786
H	6.463002	0.081123	-0.157114
H	6.105263	-0.656542	1.398902
Cl	3.469679	1.610974	-1.121024
Cl	2.714484	0.118524	1.988771
Br	-2.538997	1.838156	0.199963

C	-1.757620	-0.706786	1.570742
H	-1.476355	-1.756638	1.424554
H	-0.882321	-0.165501	1.926416
H	-2.546340	-0.675286	2.319938
C	-3.521709	-0.828481	-0.322314
O	-3.776909	-0.802186	-1.494106
O	-4.255610	-1.357085	0.629202
C	-5.487996	-1.972606	0.208511
H	-5.952948	-2.339354	1.119612
H	-6.125482	-1.234901	-0.279667
H	-5.278240	-2.795828	-0.474483

Imaginary vibration frequency: 186.27i

SLC-1b

C	1.363959	1.623209	-0.913050
C	1.295361	0.092386	-1.192133
H	1.423475	2.228580	-1.817818
H	1.286776	-0.109912	-2.266448
O	-0.088444	1.557208	-0.518319
C	-0.106801	0.267704	-0.707207
O	-1.049348	-0.491334	-0.513033
C	2.220677	2.165475	0.194597
H	2.140391	1.494702	1.056055
Al	-2.773880	-0.281753	0.275225
Cl	-2.261998	0.551790	2.208921
Cl	-3.697742	1.202750	-0.999490
C	-3.570441	-2.063792	0.269515
C	-3.751105	-2.677357	-1.119301
H	-4.537619	-2.005964	0.784086
H	-2.945319	-2.715234	0.893625
H	-4.202311	-3.674971	-1.074517
H	-4.396723	-2.060607	-1.751801
H	-2.795663	-2.782584	-1.643206
C	1.746538	3.552940	0.604161
H	0.716946	3.538170	0.967441
H	2.379924	3.941354	1.404950
H	1.803102	4.251229	-0.236768
C	3.670081	2.184465	-0.276243
H	3.791371	2.845186	-1.140102
H	4.313223	2.559035	0.522857
H	4.024950	1.188962	-0.551107
C	2.180898	-0.881646	-0.481600
C	3.215106	-1.494715	-1.184391
C	2.009197	-1.174415	0.869763

C	4.076249	-2.372853	-0.543957
H	3.345663	-1.280352	-2.240272
C	2.869297	-2.055484	1.508824
H	1.199288	-0.723488	1.435002
C	3.906368	-2.652756	0.805344
H	4.878324	-2.843503	-1.101650
H	2.723853	-2.278374	2.559910
H	4.576405	-3.342586	1.306392

TS-1b-H

C	2.251958	-1.611816	0.393065
C	1.055755	-0.713409	0.386156
H	2.021125	-2.627821	0.705716
H	0.493717	-0.890419	1.310686
O	0.974829	-2.121503	-1.472186
C	0.297098	-1.373254	-0.770026
O	-0.936457	-1.122481	-0.950264
C	3.625472	-1.358890	0.246517
H	3.317111	-1.233471	1.408692
Al	-2.398210	-0.396499	-0.136212
C	-3.981892	-1.404835	-0.695762
C	-5.296067	-0.925590	-0.080156
H	-3.816169	-2.462418	-0.451469
H	-4.042268	-1.361581	-1.791094
H	-6.156784	-1.513777	-0.419686
H	-5.275648	-0.988665	1.012548
H	-5.501437	0.119179	-0.333883
Cl	-1.999943	-0.559438	2.021778
Cl	-2.429788	1.709136	-0.679501
C	4.216159	-0.070633	-0.254560
H	4.177110	-0.077145	-1.346933
H	3.695582	0.813796	0.100550
H	5.263524	-0.016807	0.044176
C	4.534965	-2.557123	0.150628
H	5.491825	-2.354093	0.632533
H	4.090787	-3.452819	0.586322
H	4.725117	-2.746969	-0.909184
C	1.229243	0.770241	0.194801
C	1.288980	1.596611	1.312009
C	1.318792	1.331554	-1.075422
C	1.469269	2.964375	1.163041
H	1.183193	1.169171	2.303805
C	1.494229	2.697789	-1.224567
H	1.251486	0.702950	-1.957483

C	1.576685	3.516484	-0.105830
H	1.509908	3.600975	2.039903
H	1.556045	3.125877	-2.218803
H	1.707097	4.586492	-0.224111

Imaginary vibration frequency: 353.83i

TS-1b-Me¹

C	2.150570	-1.627324	0.347727
C	0.967637	-0.708129	0.363045
H	1.987402	-2.631475	0.729615
H	0.433614	-0.806790	1.312647
O	0.646627	-2.241154	-1.387755
C	0.107360	-1.360756	-0.726913
O	-1.090501	-0.955356	-0.889076
C	3.438506	-1.318531	-0.129797
H	3.510437	-0.387156	-0.683844
Al	-2.443050	-0.041886	-0.085208
C	-4.140819	-0.880530	-0.589114
C	-4.246232	-2.362939	-0.231702
H	-4.277222	-0.744123	-1.669938
H	-4.957847	-0.320030	-0.117430
H	-5.206245	-2.799576	-0.531854
H	-3.461583	-2.950572	-0.719247
H	-4.144283	-2.525287	0.846140
Cl	-2.028325	-0.193285	2.072325
Cl	-2.260236	2.037906	-0.696174
C	3.603281	-0.965745	1.445053
H	4.410149	-1.600931	1.802887
H	3.784235	0.103028	1.509820
H	2.758155	-1.169070	2.127631
C	4.350208	-2.413814	-0.604598
H	5.391313	-2.090328	-0.559085
H	4.233491	-3.320721	-0.007966
H	4.109418	-2.651584	-1.642867
C	1.250623	0.746941	0.097815
C	1.221019	1.654238	1.151730
C	1.535234	1.203155	-1.187308
C	1.481991	2.998366	0.928027
H	0.968141	1.308803	2.148509
C	1.796860	2.546205	-1.410739
H	1.531083	0.512257	-2.024878
C	1.772685	3.445721	-0.353053
H	1.442559	3.699307	1.754369
H	2.004385	2.893226	-2.416821

H 1.965424 4.497934 -0.530934

Imaginary vibration frequency: 66.34i

TS-1b-Me²

C	2.197133	-1.899173	0.075592
C	1.049094	-0.928714	0.064744
H	1.865321	-2.931724	0.066919
H	0.444502	-1.136312	0.954140
O	0.694981	-2.016760	-2.030222
C	0.195026	-1.340901	-1.150189
O	-1.018025	-0.914147	-1.160660
C	3.566264	-1.730168	-0.116983
H	4.098053	-2.657557	-0.307513
Al	-2.348631	-0.230177	-0.149373
C	-4.070173	-0.905357	-0.801845
C	-5.289974	-0.394731	-0.035972
H	-4.041183	-2.002653	-0.774961
H	-4.156030	-0.639212	-1.863650
H	-6.232138	-0.790605	-0.433542
H	-5.246657	-0.672555	1.022123
H	-5.359364	0.697023	-0.074317
Cl	-1.928847	-0.878941	1.920245
Cl	-2.184238	1.942078	-0.224663
C	4.329113	-0.499450	-0.469054
H	4.374577	-0.444131	-1.560694
H	3.876669	0.415123	-0.097570
H	5.351602	-0.583160	-0.097381
C	3.175871	-1.737528	1.574526
H	4.106610	-2.245734	1.831499
H	3.145671	-0.703921	1.897014
H	2.402453	-2.341785	2.056612
C	1.355012	0.548452	0.037066
C	1.378158	1.269538	1.226504
C	1.593694	1.211997	-1.163679
C	1.675000	2.625602	1.222445
H	1.141104	0.771821	2.160927
C	1.881902	2.567160	-1.169878
H	1.553677	0.668685	-2.102247
C	1.933345	3.275473	0.024215
H	1.684616	3.177680	2.155691
H	2.059244	3.074755	-2.111553
H	2.153484	4.337289	0.017578

Imaginary vibration frequency: 155.88i

SLC-1a

C	-2.492805	-0.949819	-0.482589
C	-1.346230	-0.213754	0.239691
H	-3.012710	-0.339319	-1.221036
H	-1.252791	-0.524524	1.283014
O	-1.451756	-1.752306	-1.223694
C	-0.495706	-1.091030	-0.630847
O	0.697459	-1.260357	-0.855432
C	-3.414961	-1.819702	0.321057
H	-2.796020	-2.428507	0.991589
Al	2.310407	-0.644044	-0.059334
C	3.670072	-1.962396	-0.531667
C	5.060435	-1.652767	0.024705
H	3.710340	-2.033558	-1.626163
H	3.334571	-2.946663	-0.180883
H	5.799018	-2.409468	-0.262624
H	5.432557	-0.688242	-0.334422
H	5.056560	-1.606812	1.118210
Cl	2.558582	1.339572	-0.873477
Cl	1.769817	-0.543041	2.042714
C	-4.312368	-0.920554	1.163716
H	-4.979255	-1.530336	1.776813
H	-3.736224	-0.278048	1.834534
H	-4.932534	-0.280126	0.529611
C	-4.224342	-2.738073	-0.582428
H	-4.872033	-3.381684	0.017218
H	-4.860642	-2.157654	-1.257595
H	-3.580771	-3.380849	-1.187229
C	-1.187761	1.268914	0.100230
C	-0.941867	2.046182	1.226436
C	-1.264028	1.879581	-1.149757
C	-0.778586	3.418930	1.106469
H	-0.864516	1.573230	2.199192
C	-1.101489	3.250360	-1.268460
H	-1.441446	1.286427	-2.042101
C	-0.858144	4.022904	-0.139917
H	-0.581631	4.015634	1.990081
H	-1.155509	3.715917	-2.246143
H	-0.724004	5.094766	-0.234583

TS-1a-H

C	-2.754415	-0.517199	-0.321648
C	-1.342554	-0.160458	0.005393
H	-3.270160	0.119243	-1.037105

H	-1.001245	-0.631578	0.928441
O	-1.383753	-1.355078	-2.000681
C	-0.637067	-0.842881	-1.170258
O	0.633892	-0.843192	-1.232252
C	-3.525042	-1.502667	0.305129
H	-3.631222	-0.425284	0.873917
Al	2.121613	-0.657736	-0.196637
C	3.519284	-1.848788	-0.879585
C	4.826620	-1.812133	-0.088649
H	3.707807	-1.584570	-1.928382
H	3.120276	-2.871358	-0.899808
H	5.585587	-2.487069	-0.501603
H	5.262080	-0.807946	-0.078512
H	4.673672	-2.102311	0.955808
Cl	2.665767	1.448441	-0.224119
Cl	1.458668	-1.197677	1.832784
C	-2.926513	-2.512542	1.239160
H	-2.571447	-3.353968	0.636961
H	-2.085956	-2.130579	1.816167
H	-3.685952	-2.886410	1.925965
C	-4.867175	-1.845671	-0.276830
H	-5.580960	-2.091105	0.510114
H	-5.265888	-1.041590	-0.896029
H	-4.738983	-2.732751	-0.903303
C	-1.105885	1.327200	0.080697
C	-0.834605	1.920501	1.307973
C	-1.159377	2.115187	-1.066039
C	-0.618216	3.288654	1.390266
H	-0.768815	1.305939	2.199291
C	-0.942375	3.481559	-0.983139
H	-1.349694	1.660367	-2.034024
C	-0.672343	4.070671	0.245728
H	-0.394234	3.741077	2.349871
H	-0.971415	4.086723	-1.882376
H	-0.492947	5.138317	0.307862

Imaginary vibration frequency: 483.56i

TS-1a-Me¹

C	-2.600980	-0.864412	-0.356568
C	-1.257501	-0.335572	0.025703
H	-3.078015	-0.455813	-1.243447
H	-1.005481	-0.632429	1.047066
O	-0.961538	-1.822764	-1.762614
C	-0.370878	-1.132169	-0.939093

O	0.895464	-1.035404	-0.839637
C	-3.274676	-1.871880	0.362357
H	-2.663152	-2.389261	1.097473
Al	2.241026	-0.580058	0.296619
C	3.744523	-1.804784	0.012927
C	4.315065	-1.792993	-1.405346
H	3.412035	-2.817635	0.276006
H	4.531296	-1.556921	0.736848
H	5.153497	-2.489477	-1.525341
H	3.558447	-2.071392	-2.145760
H	4.681482	-0.799716	-1.683174
Cl	2.708421	1.507998	-0.102104
Cl	1.377158	-0.758103	2.313274
C	-3.860022	-0.530661	1.061406
H	-4.939876	-0.597854	0.953166
H	-3.494799	-0.508547	2.083720
H	-3.597146	0.452749	0.625313
C	-4.317661	-2.718316	-0.308522
H	-4.997320	-3.146229	0.430136
H	-4.897282	-2.139267	-1.030527
H	-3.825925	-3.536931	-0.838102
C	-1.121308	1.157806	-0.120381
C	-0.968394	1.949552	1.012034
C	-1.162596	1.757611	-1.376558
C	-0.860242	3.327963	0.892192
H	-0.908921	1.482787	1.989203
C	-1.051305	3.134150	-1.495330
H	-1.258485	1.148675	-2.270564
C	-0.901775	3.921824	-0.360839
H	-0.728280	3.936139	1.780109
H	-1.069423	3.592557	-2.477806
H	-0.805739	4.997747	-0.456146

Imaginary vibration frequency: 113.95i

TS-1a-Me²

C	-2.674212	-1.025916	-0.550825
C	-1.349267	-0.460105	-0.158343
H	-3.244276	-0.477480	-1.294021
H	-0.986708	-0.901230	0.772317
O	-1.061000	-1.554289	-2.216291
C	-0.474450	-0.977472	-1.308382
O	0.784095	-0.777830	-1.262747
C	-3.230236	-2.220428	-0.047376
H	-4.040249	-2.614650	-0.653480

Al	2.154602	-0.362587	-0.144773
C	3.753971	-1.337621	-0.721086
C	4.992958	-1.102762	0.142093
H	3.963530	-1.057877	-1.761893
H	3.510894	-2.408042	-0.746864
H	5.865357	-1.662716	-0.215136
H	5.275980	-0.045530	0.159542
H	4.822864	-1.403057	1.181030
Cl	2.375527	1.802282	-0.185297
Cl	1.469062	-0.969972	1.858333
C	-2.408951	-3.275434	0.635921
H	-1.921811	-3.891571	-0.123007
H	-1.640644	-2.859006	1.287748
H	-3.055373	-3.919917	1.233497
C	-3.859176	-1.111322	0.960600
H	-3.686223	-0.037497	0.758066
H	-4.937530	-1.233021	0.898695
H	-3.423946	-1.301691	1.937489
C	-1.352327	1.043012	-0.035565
C	-1.215546	1.630144	1.217218
C	-1.508758	1.851309	-1.158783
C	-1.235435	3.011450	1.348514
H	-1.066985	1.003891	2.090121
C	-1.524329	3.231139	-1.026806
H	-1.597162	1.405767	-2.145393
C	-1.389516	3.813485	0.227160
H	-1.114993	3.460326	2.328173
H	-1.630595	3.854531	-1.907622
H	-1.393089	4.893202	0.327435

Imaginary vibration frequency: 136.89i

SLC-8a

C	-2.816147	0.997034	-0.074771
C	-1.511886	0.961980	0.733975
H	-3.149284	1.996658	-0.350690
H	-1.485460	0.251987	1.561207
H	-1.085128	1.918525	1.035003
O	-2.050778	0.441872	-1.243699
C	-0.953291	0.423282	-0.532464
O	0.131572	0.043877	-0.961592
Al	1.827584	-0.083212	-0.108489
C	3.071964	-0.813918	-1.419494
C	4.500323	-0.984254	-0.899957
H	3.066654	-0.158802	-2.299859

H	2.678769	-1.779055	-1.763322
H	5.169755	-1.397436	-1.662480
H	4.929405	-0.030194	-0.578577
H	4.538849	-1.658906	-0.039097
Cl	2.149632	1.962184	0.537469
Cl	1.360553	-1.321060	1.610842
C	-3.928315	0.104011	0.343308
C	-4.718102	-0.673172	-0.661265
C	-3.800866	-1.386201	0.289501
H	-4.476472	0.519795	1.183451
H	-4.407590	-0.617232	-1.698015
H	-5.787144	-0.753597	-0.507955
H	-4.238667	-1.953552	1.101381
H	-2.893848	-1.814115	-0.122645

TS-8a-H

C	-2.838880	-0.841845	-0.482156
C	-1.399669	-0.486297	-0.497078
H	-3.130310	-1.880971	-0.623324
H	-1.244036	0.588821	-0.610234
H	-0.863625	-1.004410	-1.295541
O	-1.602734	-1.423571	1.674044
C	-0.843334	-0.932981	0.858231
O	0.415413	-0.749161	1.045461
Al	1.819150	-0.023195	0.156475
C	3.434813	-0.105506	1.257895
C	4.682252	0.488815	0.604486
H	3.613394	-1.155628	1.523226
H	3.226607	0.407124	2.206036
H	5.564381	0.424728	1.252269
H	4.931883	-0.025745	-0.328843
H	4.542139	1.545897	0.357029
Cl	1.953975	-1.140837	-1.728288
Cl	1.182664	2.019054	-0.348526
C	-3.835998	0.076683	-0.291558
C	-5.222882	0.336227	0.062483
C	-4.159415	1.431785	0.124548
H	-3.504840	-0.191849	-1.488988
H	-5.574722	-0.122930	0.980274
H	-5.954148	0.418824	-0.733315
H	-4.218920	2.207827	-0.629990
H	-3.762360	1.740729	1.085920

Imaginary vibration frequency: 403.17i

TS-8a-C

C	-2.625454	0.348175	-0.365638
C	-1.911026	1.054002	0.731268
H	-3.212387	0.978097	-1.028962
H	-1.381905	0.367975	1.391989
H	-2.615415	1.660046	1.301721
O	-1.318102	3.110517	-0.314805
C	-0.920565	2.029975	0.058218
O	0.296446	1.613340	-0.066911
Al	1.385380	0.185303	-0.015932
C	3.259900	0.737441	-0.125200
C	4.270490	-0.408722	-0.104929
H	3.457468	1.427324	0.705737
H	3.384714	1.333459	-1.038485
H	5.305965	-0.053791	-0.165543
H	4.188438	-1.002314	0.811114
H	4.117306	-1.095188	-0.943731
Cl	0.923516	-0.913616	1.840487
Cl	0.729969	-1.087166	-1.685614
C	-2.379156	-0.945067	-0.829039
C	-2.251338	-1.973459	0.186229
C	-3.520847	-1.125831	0.343673
H	-2.772913	-1.218882	-1.801249
H	-1.538546	-1.838762	0.991018
H	-2.370388	-2.988294	-0.170656
H	-4.461584	-1.427112	-0.096217
H	-3.578709	-0.628132	1.303767

Imaginary vibration frequency: 111.27i

SLC-8b

C	-2.438765	1.224789	-0.005437
C	-1.134990	1.064290	0.784731
H	-2.729734	2.255329	-0.204214
H	-1.132368	0.295055	1.558069
H	-0.662318	1.974151	1.153999
O	-1.697077	0.733440	-1.227610
C	-0.606273	0.599920	-0.523874
O	0.459367	0.194846	-0.981018
Al	2.130124	-0.102934	-0.127603
C	3.372079	-0.720044	-1.498200
C	4.779382	-1.020804	-0.980597
H	3.415691	0.041115	-2.287556
H	2.944907	-1.614322	-1.969471
H	5.447475	-1.363856	-1.778283

H	5.242184	-0.136221	-0.532241
H	4.768742	-1.800593	-0.212819
Cl	2.524752	1.834187	0.767748
Cl	1.583251	-1.515269	1.426503
C	-3.588614	0.342890	0.343509
C	-4.678748	0.068813	-0.712619
C	-3.389849	-1.181381	0.488808
H	-4.032816	0.756830	1.254795
C	-4.776448	-1.366976	-0.160783
H	-4.260842	0.078662	-1.721980
H	-5.572066	0.694413	-0.688942
H	-2.595643	-1.553401	-0.163433
H	-3.237262	-1.576196	1.493861
H	-4.887093	-2.176431	-0.882915
H	-5.561480	-1.453281	0.593483

TS-8b-H

C	-2.513861	-1.202296	-0.293165
C	-1.065574	-0.971901	-0.490186
H	-2.863066	-2.206526	-0.063236
H	-0.853556	-0.059625	-1.051100
H	-0.568213	-1.814146	-0.975233
O	-1.418859	-1.022951	1.825119
C	-0.580003	-0.840707	0.950873
O	0.647977	-0.556575	1.163886
Al	2.057803	0.030569	0.172012
C	3.606467	0.332381	1.328520
C	4.860749	0.821384	0.604615
H	3.820408	-0.604058	1.860021
H	3.315325	1.052145	2.104525
H	5.703669	0.975281	1.288355
H	5.191070	0.107013	-0.156075
H	4.685536	1.772927	0.092712
Cl	2.355094	-1.492078	-1.375247
Cl	1.294217	1.829991	-0.827971
C	-3.473276	-0.218794	-0.488060
C	-4.891146	-0.144683	0.039792
C	-3.310207	1.287522	-0.492994
H	-3.301121	-0.813713	-1.524139
C	-4.553056	1.316152	0.432842
H	-5.144929	-0.849501	0.830454
H	-5.633140	-0.191162	-0.757852
H	-2.367398	1.670369	-0.103595
H	-3.513239	1.726429	-1.470216

H	-4.265614	1.391405	1.481114
H	-5.308955	2.063099	0.197351

Imaginary vibration frequency: 391.39i

TS-8b-C

C	2.663809	-1.101142	0.208715
C	1.287126	-0.622942	0.497210
H	2.969174	-2.049291	0.641136
H	1.157216	0.455566	0.403146
H	0.924943	-0.940489	1.476953
O	1.281356	-2.109667	-1.266557
C	0.558110	-1.360757	-0.605687
O	-0.688566	-1.192772	-0.802691
Al	-1.957257	-0.075328	-0.106196
C	-3.662432	-0.346823	-1.023683
C	-4.797129	0.554262	-0.536415
H	-3.945377	-1.401520	-0.911893
H	-3.498353	-0.197157	-2.098658
H	-5.734510	0.371579	-1.074404
H	-5.003392	0.402843	0.527833
H	-4.554279	1.613678	-0.665900
Cl	-1.975947	-0.519633	2.037001
Cl	-1.097365	1.930191	-0.345649
C	3.650995	-0.362435	-0.456568
C	3.374248	1.028398	-1.016030
C	4.004139	0.349089	1.010431
H	4.489767	-0.936645	-0.835417
C	3.593131	1.677531	0.363000
H	2.384967	1.156484	-1.455422
H	4.124135	1.309910	-1.752648
H	3.461552	0.049013	1.910533
H	5.064490	0.166815	1.173112
H	2.690946	2.102283	0.802109
H	4.385070	2.425143	0.395230

Imaginary vibration frequency: 269.56i

SLC-8c

C	-2.127945	1.351554	-0.016756
C	-0.797320	1.256093	0.737170
H	-2.398364	2.361810	-0.320793
H	-0.771451	0.589786	1.599397
H	-0.297886	2.196477	0.970303
O	-1.442123	0.706399	-1.201336
C	-0.329058	0.627168	-0.525313

O	0.708923	0.141525	-0.968386
Al	2.392106	-0.129900	-0.133902
C	3.555499	-0.972100	-1.452716
C	4.970754	-1.260658	-0.950248
H	3.594878	-0.322453	-2.336388
H	3.077415	-1.901530	-1.787190
H	5.593482	-1.730869	-1.719319
H	5.482583	-0.345152	-0.637909
H	4.963330	-1.933614	-0.087255
Cl	2.910488	1.878361	0.503107
Cl	1.831900	-1.311980	1.598434
C	-3.305348	0.555262	0.457129
C	-4.467854	0.569102	-0.554079
C	-3.027217	-0.939436	0.759153
H	-3.619859	1.058720	1.377925
C	-5.141478	-0.786138	-0.376881
H	-4.071489	0.642731	-1.572487
H	-5.137898	1.417509	-0.400457
C	-3.958404	-1.724395	-0.168089
H	-3.266935	-1.149451	1.803761
H	-1.981383	-1.224527	0.619594
H	-5.775383	-0.778002	0.516908
H	-5.769017	-1.062429	-1.226978
H	-4.239362	-2.695220	0.245436
H	-3.464820	-1.905675	-1.128469

TS-8c-H

C	-2.140133	-1.296132	-0.290792
C	-0.724187	-0.940259	-0.551971
H	-2.397480	-2.348228	-0.199084
H	-0.595622	0.055276	-0.979251
H	-0.214055	-1.670530	-1.183510
O	-1.009509	-1.358071	1.712607
C	-0.188038	-1.002384	0.868306
O	1.025453	-0.700570	1.114551
Al	2.398461	0.040329	0.166048
C	3.961224	0.261245	1.321119
C	5.181039	0.873472	0.632719
H	4.218031	-0.722206	1.735840
H	3.665931	0.876557	2.180790
H	6.034968	0.977162	1.312180
H	5.515615	0.262945	-0.211914
H	4.962655	1.870754	0.237898
Cl	2.701454	-1.300242	-1.539182

Cl	1.554365	1.909595	-0.613292
C	-3.191841	-0.379571	-0.316282
C	-4.591692	-0.715998	0.162844
C	-3.018877	1.134090	-0.331603
H	-3.047610	-0.816560	-1.425832
C	-5.362596	0.576231	-0.082607
H	-4.523310	-0.917952	1.236948
H	-5.008963	-1.600512	-0.319713
C	-4.337760	1.657878	0.249842
H	-2.875179	1.488266	-1.355142
H	-2.144285	1.441291	0.243975
H	-5.656807	0.642941	-1.135254
H	-6.267411	0.643495	0.522655
H	-4.600011	2.638264	-0.149282
H	-4.245771	1.753456	1.335411

Imaginary vibration frequency: 401.46i

TS-8c-C

C	2.251486	0.208449	-0.362363
C	0.829156	-0.191988	-0.231956
H	2.616413	0.469783	-1.350985
H	0.611348	-0.690746	0.714635
H	0.480204	-0.817239	-1.056551
O	0.942055	2.123640	-0.399643
C	0.168641	1.175297	-0.283600
O	-1.100909	1.276520	-0.207315
Al	-2.504938	0.129946	-0.007887
C	-4.182813	1.135385	0.018518
C	-5.438255	0.279848	0.186983
H	-4.244802	1.714774	-0.911886
H	-4.122520	1.877720	0.824916
H	-6.354912	0.880977	0.193953
H	-5.539910	-0.450397	-0.622074
H	-5.418012	-0.284886	1.124434
Cl	-2.314525	-1.283137	-1.673413
Cl	-2.061912	-0.969336	1.837034
C	3.161700	0.230871	0.715199
C	3.494270	-1.280673	0.196042
C	4.459030	1.008507	0.572682
H	2.705138	0.197677	1.700118
C	4.988451	-1.220872	-0.118789
H	2.941755	-1.600661	-0.706886
H	3.159161	-1.954689	0.981862
C	5.282509	0.236303	-0.450617

H	4.963665	1.013304	1.541027
H	4.265060	2.045071	0.291671
H	5.533073	-1.513338	0.783171
H	5.257656	-1.912089	-0.917962
H	6.346102	0.472417	-0.397899
H	4.949992	0.467025	-1.467507

Imaginary vibration frequency: 179.15i

SLC-8d

C	-1.753313	-1.465364	-0.125100
C	-0.448125	-1.196630	-0.882307
H	-2.014091	-2.520410	-0.053209
H	-0.436285	-0.375021	-1.596713
H	0.040480	-2.071544	-1.311813
O	-1.023238	-1.106171	1.151241
C	0.060271	-0.851661	0.471023
O	1.107613	-0.451698	0.973567
Al	2.720152	0.125306	0.154434
C	3.961125	0.585556	1.586362
C	5.323402	1.081594	1.099453
H	4.088371	-0.297018	2.226121
H	3.486837	1.346639	2.218849
H	5.992913	1.330151	1.930319
H	5.833049	0.328452	0.490559
H	5.228745	1.980981	0.483132
Cl	3.238649	-1.572445	-1.093421
Cl	2.006261	1.748227	-1.098599
C	-2.958428	-0.595836	-0.353283
C	-4.080127	-0.962635	0.618488
C	-2.671323	0.904343	-0.306124
H	-3.289463	-0.852272	-1.370622
C	-5.339307	-0.150098	0.348979
H	-3.737726	-0.773074	1.643139
H	-4.295254	-2.033947	0.547899
C	-3.934926	1.709951	-0.583462
H	-2.293088	1.166560	0.688628
H	-1.895685	1.181222	-1.025788
C	-5.053551	1.344731	0.381906
H	-6.110718	-0.408576	1.080339
H	-5.737180	-0.420787	-0.637179
H	-3.709187	2.778302	-0.520270
H	-4.265796	1.518897	-1.612005
H	-5.959791	1.909159	0.142356
H	-4.760769	1.634272	1.398887

TS-8d-H

C	1.805583	-1.263959	0.378157
C	0.412610	-0.809335	0.604345
H	2.011633	-2.323415	0.512243
H	0.310513	0.256557	0.806852
H	-0.083679	-1.370740	1.398653
O	0.590067	-1.705121	-1.530768
C	-0.187209	-1.163069	-0.746495
O	-1.408491	-0.896614	-0.997003
Al	-2.738710	0.022769	-0.148623
C	-4.335737	0.064543	-1.276564
C	-5.516376	0.835426	-0.686414
H	-4.630087	-0.972539	-1.483908
H	-4.055319	0.491601	-2.248120
H	-6.390483	0.829424	-1.347839
H	-5.836037	0.412264	0.271120
H	-5.261232	1.883698	-0.501790
Cl	-2.994323	-0.997659	1.772248
Cl	-1.853909	1.987001	0.272075
C	2.918108	-0.442979	0.153960
C	4.221181	-1.084805	-0.262594
C	2.795823	1.028460	-0.152231
H	2.787514	-0.613898	1.344408
C	5.429019	-0.278219	0.194480
H	4.194577	-1.123424	-1.357957
H	4.266142	-2.116955	0.092483
C	4.030234	1.802975	0.296792
H	2.689182	1.096002	-1.241546
H	1.891707	1.456893	0.280737
C	5.314201	1.178913	-0.229085
H	6.335863	-0.729494	-0.215411
H	5.512636	-0.336817	1.286385
H	3.938255	2.838171	-0.040144
H	4.058665	1.829821	1.392744
H	6.178913	1.743401	0.129739
H	5.327179	1.240810	-1.323979

Imaginary vibration frequency: 421.32i

TS-8d-C

C	-1.924614	0.180927	0.735010
C	-0.540821	-0.059665	0.228595
H	-2.013260	0.484148	1.773711
H	-0.551511	-0.680156	-0.673164

H	0.070435	-0.573142	0.971722
O	-0.604582	2.241208	-0.401592
C	0.096155	1.274315	-0.168653
O	1.384850	1.279791	-0.268426
Al	2.762182	0.127423	-0.081945
C	4.450289	1.020659	-0.519389
C	5.694375	0.142774	-0.388598
H	4.544472	1.903917	0.125894
H	4.371983	1.410881	-1.542638
H	6.615303	0.679653	-0.645327
H	5.816375	-0.232506	0.632461
H	5.640385	-0.732472	-1.043904
Cl	2.664872	-0.607292	1.988535
Cl	2.301509	-1.576850	-1.391622
C	-2.908277	0.613272	-0.133816
C	-2.966418	-1.203400	0.603814
C	-4.165996	1.281726	0.229394
H	-2.719866	0.466031	-1.195173
C	-4.122723	-1.588224	-0.356565
H	-3.348431	-1.235582	1.620723
H	-2.164299	-1.919644	0.442960
C	-5.347708	0.629273	-0.480956
H	-4.294955	1.305791	1.314727
H	-4.040586	2.318867	-0.109424
C	-5.430191	-0.845205	-0.129147
H	-4.273734	-2.649094	-0.139647
H	-3.807937	-1.529806	-1.400910
H	-6.267336	1.146765	-0.201717
H	-5.226619	0.748401	-1.562791
H	-6.208848	-1.324551	-0.728105
H	-5.724985	-0.960304	0.920367

Imaginary vibration frequency: 190.23i

SLC-8e

C	1.424990	1.567537	-0.109513
C	0.110340	1.300750	-0.851556
H	1.646223	2.625605	0.022356
H	0.103319	0.518882	-1.608949
H	-0.414604	2.182451	-1.220154
O	0.737522	1.107216	1.159521
C	-0.355068	0.863901	0.490229
O	-1.379944	0.407512	0.991523
Al	-2.996794	-0.154796	0.171285
C	-4.201691	-0.722895	1.595230

C	-5.560815	-1.222023	1.102596
H	-4.337329	0.119170	2.285806
H	-3.699997	-1.507262	2.175965
H	-6.210285	-1.532560	1.928496
H	-6.097478	-0.447712	0.545670
H	-5.456625	-2.082689	0.434674
Cl	-3.572956	1.600973	-0.966838
Cl	-2.273542	-1.685774	-1.186950
C	2.666296	0.765904	-0.408499
C	3.754866	1.112631	0.613604
C	2.380286	-0.726406	-0.570740
H	3.002532	1.157358	-1.380048
C	5.158920	0.710219	0.167608
H	3.733324	2.196789	0.766530
H	3.514312	0.663069	1.583478
C	3.592266	-1.618189	-0.827264
H	1.676706	-0.863814	-1.397182
H	1.878959	-1.099460	0.330228
C	5.587362	-0.708420	0.535630
H	5.224165	0.845717	-0.917801
H	5.885040	1.408135	0.595183
C	4.508397	-1.779324	0.383508
H	3.208346	-2.602590	-1.111083
H	4.158375	-1.254251	-1.692918
H	6.451978	-0.973325	-0.082760
H	5.943557	-0.721852	1.571464
H	4.999663	-2.756374	0.343445
H	3.881099	-1.801251	1.281949

TS-8e-H

C	-1.480819	-1.406065	-0.257142
C	-0.089980	-0.970876	-0.535361
H	-1.672029	-2.476322	-0.253292
H	0.002870	0.049201	-0.907626
H	0.424145	-1.646814	-1.221620
O	-0.288751	-1.546687	1.703571
C	0.491434	-1.101572	0.862597
O	1.698731	-0.766017	1.094929
Al	3.024746	0.062621	0.152401
C	4.598300	0.305402	1.288315
C	5.772771	1.006587	0.605858
H	4.910687	-0.681004	1.654855
H	4.290610	0.868047	2.179228
H	6.633116	1.125669	1.274627

H	6.121497	0.449101	-0.269179
H	5.497069	2.006750	0.256814
Cl	3.342323	-1.204650	-1.605278
Cl	2.103429	1.929505	-0.541305
C	-2.609695	-0.577505	-0.149385
C	-3.900060	-1.226064	0.304662
C	-2.443501	0.916787	-0.009512
H	-2.460072	-0.889091	-1.308323
C	-5.129923	-0.777369	-0.483058
H	-3.783615	-2.309694	0.229885
H	-4.013432	-0.999592	1.369997
C	-3.631031	1.785342	-0.412806
H	-1.556014	1.245215	-0.551459
H	-2.230002	1.085019	1.053382
C	-5.810673	0.485481	0.036106
H	-4.841181	-0.640916	-1.530786
H	-5.858095	-1.592544	-0.482121
C	-4.864392	1.604778	0.467503
H	-3.287682	2.820451	-0.338130
H	-3.880544	1.626574	-1.467828
H	-6.478871	0.855280	-0.748448
H	-6.452765	0.227025	0.884493
H	-5.430526	2.540007	0.494938
H	-4.529084	1.433106	1.496627

Imaginary vibration frequency: 413.28i

TS-8e-C

C	-1.733634	0.896576	0.884959
C	-0.298818	0.548322	0.661666
H	-1.960827	1.598540	1.682870
H	-0.205506	-0.419277	0.157771
H	0.240605	0.463262	1.607265
O	-0.242196	2.524736	-0.680012
C	0.384080	1.592033	-0.216122
O	1.647774	1.396554	-0.423708
Al	2.859487	0.086981	-0.156093
C	4.574372	0.564043	-0.974143
C	5.668301	-0.493488	-0.830914
H	4.908253	1.511883	-0.531898
H	4.397253	0.780580	-2.035704
H	6.611364	-0.187141	-1.298891
H	5.886760	-0.706831	0.220307
H	5.374234	-1.441486	-1.292613
Cl	2.981504	-0.221437	2.016833

Cl	1.951713	-1.731970	-1.007927
C	-2.644367	0.788727	-0.147720
C	-2.673620	-0.494429	1.337254
C	-3.981381	1.402123	-0.206027
H	-2.317264	0.228484	-1.021931
C	-2.871911	-1.771821	0.535390
H	-1.943083	-0.704952	2.124139
H	-3.581385	-0.128483	1.805685
C	-5.038884	0.523267	-0.872496
H	-3.828740	2.304904	-0.816938
H	-4.285253	1.749636	0.784928
C	-3.952522	-1.779680	-0.549270
H	-1.915363	-2.096994	0.117379
H	-3.128020	-2.512345	1.300431
C	-5.177235	-0.890550	-0.310276
H	-5.996412	1.045203	-0.799862
H	-4.807100	0.447201	-1.940149
H	-3.511097	-1.509508	-1.514238
H	-4.277950	-2.816599	-0.663919
H	-6.036237	-1.350152	-0.806079
H	-5.433165	-0.859806	0.755179

Imaginary vibration frequency: 232.00i

(3) Multiple linear regression

We list all training sets and test sets in multiple linear regression, as well as their energy and coordinates. *However, if the energy and coordinate information of the data have been listed above, this part will not repeat.*

Parameters of groups, training set and test set:

Table S4 Parameters of groups involved in multiple linear regression

Groups	ΔE_{Orb} (au)	σ_p	σ_m	A-Value (kJ/mol)
H	0.66	0.00	0.00	0.00
Me	0.78	-0.17	-0.07	7.28
CH ₂ CH=CH ₂	0.77	-0.14	-0.11	7.45
CH ₂ C≡CH	0.78	0.02	0.03	7.12
CN	0.90	0.66	0.56	0.71
CHO	0.82	0.42	0.35	2.34
COMe	0.81	0.50	0.38	4.19
COOMe	0.82	0.45	0.37	5.32
Ph	0.42	-0.01	0.06	11.72
4-PhCl	0.43	0.12	0.15	≈ 11.72
4-PhMe	0.42	-0.03	0.06	≈ 11.72
4-PhOMe	0.42	-0.08	0.05	≈ 11.72

CH=CH ₂	0.45	-0.04	0.06	6.70
C≡CH	0.47	0.23	0.21	5.65
Br	0.46	0.23	0.39	2.01
Cl	0.49	0.23	0.37	2.22
OMe	0.49	-0.27	0.12	2.51

Table S5 Training set (72 data)

n	R ¹	R ²	R ³	$\Delta G^{\ddagger}_{\text{Calc}}$ (kJ/mol)	$\Delta G^{\ddagger}_{\text{Pred}}$ (kJ/mol)
1	H	H	Me	89.4	96.8
2	H	Me	H	93.8	99.8
3	H	Me	Me	86.6	90.4
4	H	Cl	H	141.2	131.2
5	H	Me	Cl	133.4	123.9
6	H	Cl	Me	130.7	121.8
7	H	Br	Me	132.2	122.5
8	H	H	OMe	98.8	100.6
9	H	OMe	H	93.6	101.7
10	H	H	Ph	104.0	108.3
11	H	Me	Ph	96.9	101.9
12	H	H	4-PhCl	103.8	117.0
13	H	Me	4-PhMe	98.1	101.1
14	H	Me	4-PhOMe	92.4	98.8
15	H	CH ₂ CH=CH ₂	H	105.0	99.4
16	H	Me	CH ₂ CH=CH ₂	96.7	89.9
17	H	Me	CH ₂ C≡CH	98.2	101.8
18	H	H	CH=CH ₂	103.1	107.2
19	H	CH=CH ₂	H	105.2	109.9
20	H	Me	CH=CH ₂	94.3	100.7
21	H	CH=CH ₂	Me	94.6	100.5
22	H	Me	C≡CH	112.8	117.3
23	H	Me	CN	149.0	148.3
24	H	CHO	H	146.7	137.9
25	H	Me	COOMe	120.9	132.4
26	Me	H	CH ₂ CH=CH ₂	94.0	105.6
27	Me	CH ₂ CH=CH ₂	H	101.4	108.8
28	Me	Me	Cl	125.5	133.2
29	Me	Br	Me	128.6	131.8

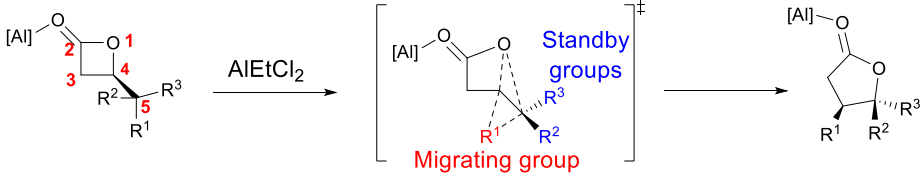
30	Me	Me	OMe	109.2	103.5
31	CH ₂ CH=CH ₂	Me	H	101.0	108.4
32	Br	Me	H	83.2	84.3
33	Br	Me	Me	71.9	74.8
34	Br	Me	Cl	98.4	108.3
35	Br	Me	CH ₂ CH=CH ₂	77.0	74.4
36	Br	Me	CH ₂ C≡CH	78.1	86.3
37	Br	H	H	102.9	90.7
38	Br	H	Me	80.3	81.3
39	Br	H	CH ₂ CH=CH ₂	74.9	80.8
40	Br	CH ₂ CH=CH ₂	H	81.0	83.9
41	Br	H	CH ₂ C≡CH	93.4	92.7
42	Br	CH ₂ C≡CH	H	93.9	95.7
43	Cl	Me	H	102.0	86.6
44	Cl	Me	Me	76.8	77.2
45	Cl	CH ₂ CH=CH ₂	H	100.5	86.2
46	Cl	H	CH=CH ₂	94.2	94.0
47	Cl	CH=CH ₂	H	97.0	96.7
48	Cl	H	CH ₂ C≡CH	105.6	95.1
49	Cl	Ph	H	101.4	100.0
50	Cl	H	Ph	93.3	95.1
51	OMe	Me	H	90.5	87.8
52	OMe	H	Me	89.8	84.7
53	OMe	Me	Me	86.6	78.0
54	Ph	H	H	101.7	87.6
55	Ph	H	Me	73.7	78.2
56	Ph	Me	H	78.3	81.2
57	Ph	Me	Me	70.8	71.7
58	Ph	H	CH ₂ CH=CH ₂	75.2	77.7
59	Ph	CH ₂ CH=CH ₂	H	77.2	80.8
60	Ph	Me	CH=CH ₂	77.5	82.1
61	Ph	OMe	Me	78.0	73.6
62	4-PhOMe	H	H	81.3	87.6
63	CH ₂ C≡CH	H	Me	110.4	106.1
64	CH ₂ C≡CH	Me	H	113.9	109.2
65	CH ₂ C≡CH	Me	Me	103.2	99.7
66	CH=CH ₂	H	H	90.3	90.0
67	CH=CH ₂	H	Me	73.1	80.5
68	CH=CH ₂	H	CH ₂ CH=CH ₂	74.5	80.0
69	COMe	Me	Me	103.8	102.0
70	CHO	Me	Me	107.1	102.8
71	CHO	H	Me	120.8	109.2
72	CHO	Me	H	129.4	112.3

Numbers in green: Calculated energy barrier at the level of RI-PWPB95-D3(BJ)/def2-QZVPP//SMD(diethylether)-PBE0-D3(BJ)/def-TZVP

Numbers in red: The predicted value is higher than the calculated value

Numbers in blue: The predicted value is lower than the calculated value

Table S6 Test set (10 data)

					
n	R ¹	R ²	R ³	$\Delta G_{\text{Calc}}^{\ddagger}$ (kJ/mol)	$\Delta G_{\text{Pred}}^{\ddagger}$ (kJ/mol)
1	H	Me	Br	134.0	124.7
2	H	H	CH ₂ CH=CH ₂	104.5	96.3
3	Me	Me	Br	131.3	134.0
4	Me	H	Ph	103.2	117.6
5	CH ₂ CH=CH ₂	H	Me	97.1	105.3
6	COMe	H	Me	112.3	108.4
7	Cl	H	Me	98.9	83.6
8	Cl	H	CH ₂ C≡CH	105.6	96.4
9	OMe	Me	Ph	84.1	88.6
10	4-PhMe	H	H	94.2	87.6

Numbers in green: Calculated energy barrier at the level of RI-PWPB95-D3(BJ)/def2-QZVPP//SMD(diethylether)-PBE0-D3(BJ)/def-TZVP

Numbers in red: The predicted value is higher than the calculated value

Numbers in blue: The predicted value is lower than the calculated value

Species	SLC-STrain-4	TS-STrain-4
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.11252	0.10552
Solvation Gibbs Free Energy (Hartree)	-0.02728	-0.05058
Electronic Energy (Hartree)	-2008.15248	-2008.06840
Imaginaries	0	1
G_{sol}(Hartree)	-2008.06723	-2008.01346

Specics	SLC-STrain-6	TS-STrain-6
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.13778	0.13265
Solvation Gibbs Free Energy (Hartree)	-0.02717	-0.04638
Electronic Energy (Hartree)	-2047.45705	-2047.38292
Imaginaries	0	1
G_{sol}(Hartree)	-2047.34644	-2047.29665
Specics	SLC-STrain-7	TS-STrain-7
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.13669	0.13082
Solvation Gibbs Free Energy (Hartree)	-0.02768	-0.04509
Electronic Energy (Hartree)	-4161.50687	-4161.43324
Imaginaries	0	1
G_{sol}(Hartree)	-4161.39787	-4161.34751
Specics	SLC-STrain-8	TS-STrain-8
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.15239	0.14830
Solvation Gibbs Free Energy (Hartree)	-0.02356	-0.04250
Electronic Energy (Hartree)	-1663.07013	-1663.00946
Imaginaries	0	1
G_{sol}(Hartree)	-1662.94129	-1662.90366

Species	SLC-STrain-9	TS-STrain-9
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15239	0.14694
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02356	-0.04378
(Hartree)		
Electronic	-1663.07013	-1663.00881
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1662.94129	-1662.90565

Species	SLC-STrain-10	TS-STrain-10
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.19623	0.19171
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03027	-0.05005
(Hartree)		
Electronic	-1779.55578	-1779.49185
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1779.38982	-1779.35020

Species	SLC-STrain-12	TS-STrain-12
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18481	0.17885
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03151	-0.05248
(Hartree)		
Electronic	-2239.14455	-2239.07808
Energy (Hartree)		
Imaginaries	0	1

G_{sol}(Hartree)	-2238.99125	-2238.95171
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Specics	SLC-STrain-13	TS-STrain-13
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.24803	0.24437
Solvation Gibbs Free Energy (Hartree)	-0.02932	-0.04401
Electronic Energy (Hartree)	-1858.16121	-1858.10551
Imaginaries	0	1
G_{sol}(Hartree)	-1857.94250	-1857.90514

Specics	SLC-STrain-14	TS-STrain-14
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.25286	0.24818
Solvation Gibbs Free Energy (Hartree)	-0.03006	-0.04382
Electronic Energy (Hartree)	-1933.36910	-1933.31547
Imaginaries	0	1
G_{sol}(Hartree)	-1933.14630	-1933.11112

Specics	SLC-STrain-15	TS-STrain-15
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17841	0.17323
Solvation Gibbs Free Energy (Hartree)	-0.02630	-0.04783
Electronic Energy (Hartree)	-1665.23877	-1665.17247

Imaginaries	0	1
G_{sol}(Hartree)	-1665.08666	-1665.04706
Specics	SLC-STrain-18	TS-STrain-18
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15051	0.14773
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02476	-0.04742
(Hartree)		
Electronic	-1625.93918	-1625.87446
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1625.81342	-1625.77414
Specics	SLC-STrain-19	TS-STrain-19
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15051	0.14811
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02476	-0.04579
(Hartree)		
Electronic	-1625.93918	-1625.87565
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1625.81342	-1625.77334
Specics	SLC-STrain-21	TS-STrain-21
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.17934	0.17602
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02451	-0.04146
(Hartree)		
Electronic	-1665.24014	-1665.18384

Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1665.08532	-1665.04929
Specics	SLC-STrain-24	TS-STrain-24
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.12937	0.12506
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03025	-0.05057
(Hartree)		
Electronic	-1661.87282	-1661.79230
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1661.77370	-1661.71781
Specics	SLC-STrain-26	TS-STrain-26
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20558	0.20284
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02554	-0.04548
(Hartree)		
Electronic	-1704.53865	-1704.48019
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1704.35862	-1704.32283
Specics	SLC-STrain-27	TS-STrain-27
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.20544	0.20298
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02572	-0.04477

(Hartree)		
Electronic	-1704.54058	-1704.48046
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1704.36086	-1704.32224
Specics	SLC-STrain-29	TS-STrain-29
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16343	0.15931
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02695	-0.04818
(Hartree)		
Electronic	-4200.81070	-4200.73636
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-4200.67423	-4200.62523
Specics	SLC-STrain-37	TS-STrain-37
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.11017	0.10643
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02769	-0.03829
(Hartree)		
Electronic	-4122.20299	-4122.14945
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-4122.12051	-4122.08131
Specics	SLC-STrain-39	TS-STrain-39
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16793	0.16340
(Hartree)		
Solvation Gibbs		

Free Energy (Hartree)	-0.02754	-0.03897
Electronic Energy (Hartree)	-4238.87665	-4238.83216
Imaginarities	0	1
G _{sol} (Hartree)	-4238.73625	-4238.70774
Specics	SLC-STrain-40	TS-STrain-40
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.16676	0.16333
Solvation Gibbs Free Energy (Hartree)	-0.02825	-0.03698
Electronic Energy (Hartree)	-4238.87534	-4238.83232
Imaginarities	0	1
G_{sol}(Hartree)	-4238.73683	-4238.70597
Specics	SLC-STrain-41	TS-STrain-41
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.14312	0.14306
Solvation Gibbs Free Energy (Hartree)	-0.02959	-0.04062
Electronic Energy (Hartree)	-4237.62724	-4237.58056
Imaginarities	0	1
G_{sol}(Hartree)	-4237.51371	-4237.47812
Specics	SLC-STrain-42	TS-STrain-42
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.14175	0.14156

Solvation Gibbs		
Free Energy	-0.03040	-0.03811
(Hartree)		
Electronic	-4237.62597	-4237.58229
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-4237.51462	-4237.47884
Specics	SLC-STrain-43	TS-STrain-43
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.13757	0.13679
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02741	-0.03918
(Hartree)		
Electronic	-2047.45619	-2047.40477
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2047.34603	-2047.30717
Specics	SLC-STrain-45	TS-STrain-45
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.16741	0.16597
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02784	-0.03941
(Hartree)		
Electronic	-2124.82495	-2124.77367
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-2124.68539	-2124.64711
Specics	SLC-STrain-46	TS-STrain-46
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14261	0.14072

(Hartree)		
Solvation Gibbs		
Free Energy	-0.02697	-0.03659
(Hartree)		
Electronic	-2085.52394	-2085.47634
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-2085.40830	-2085.37222

Specics	SLC-STrain-47	TS-STrain-47
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14169	0.14046
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02726	-0.03892
(Hartree)		
Electronic	-2085.52417	-2085.47435
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-2085.40974	-2085.37280

Specics	SLC-STrain-48	TS-STrain-48
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.14582	0.14357
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02854	-0.04254
(Hartree)		
Electronic	-2123.57750	-2123.52104
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-2123.46021	-2123.42000

Specics	SLC-STrain-49	TS-STrain-49
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		

G Correction (Hartree)	0.18660	0.18364
Solvation Gibbs Free Energy (Hartree)	-0.02956	-0.04068
Electronic Energy (Hartree)	-2239.14243	-2239.08974
Imaginaries	0	1
G_{sol}(Hartree)	-2238.98539	-2238.94677

Specics	SLC-STrain-50	TS-STrain-50
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.18800	0.18390
Solvation Gibbs Free Energy (Hartree)	-0.03064	-0.04212
Electronic Energy (Hartree)	-2239.14262	-2239.09150
Imaginaries	0	1
G_{sol}(Hartree)	-2238.98526	-2238.94972

Specics	SLC-STrain-51	TS-STrain-51
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17884	0.17684
Solvation Gibbs Free Energy (Hartree)	-0.02348	-0.03537
Electronic Energy (Hartree)	-1702.37362	-1702.32526
Imaginaries	0	1
G_{sol}(Hartree)	-1702.21826	-1702.18378

Specics	SLC-STrain-54	TS-STrain-54
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	

Energy Level		
G Correction	0.19623	0.19716
(Hartree)		
Solvation Gibbs	-0.03027	-0.04684
Free Energy		
(Hartree)		
Electronic	-1779.55578	-1779.50140
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1779.38982	-1779.35107

Specics	SLC-STrain-56	TS-STrain-56
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.22295	0.22311
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02995	-0.04111
(Hartree)		
Electronic	-1818.85651	-1818.81569
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1818.66351	-1818.63369

Specics	SLC-STrain-58	TS-STrain-58
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25357	0.25246
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03067	-0.04331
(Hartree)		
Electronic	-1896.22612	-1896.18360
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1896.00321	-1895.97445

Specics	SLC-STrain-59	TS-STrain-59
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		

Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25545	0.25289
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03023	-0.04238
(Hartree)		
Electronic	-1896.22817	-1896.18404
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1896.00294	-1895.97353

Specics	SLC-STrain-60	TS-STrain-60
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25419	0.25445
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02952	-0.03979
(Hartree)		
Electronic	-1896.22443	-1896.18490
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1895.99976	-1895.97024

Specics	SLC-STrain-61	TS-STrain-61
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.25390	0.25231
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02864	-0.04126
(Hartree)		
Electronic	-1933.36470	-1933.32079
Energy (Hartree)		
Imaginaries	0	1
G _{sol} (Hartree)	-1933.13944	-1933.10974

Specics	SLC-STrain-62	TS-STrain-62
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	

Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.22638	0.22635
(Hartree)		
Solvation Gibbs		
Free Energy	-0.03122	-0.04532
(Hartree)		
Electronic	-1894.06680	-1894.02169
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1893.87164	-1893.84066
Specics	SLC-STrain-64	TS-STrain-64
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.18219	0.17962
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02722	-0.05103
(Hartree)		
Electronic	-1703.29440	-1703.22360
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1703.13943	-1703.09626
Specics	SLC-STrain-66	TS-STrain-66
Optimization	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Level		
Electronic	RI-PWPB95-D3(BJ)/def2-QZVPP	
Energy Level		
G Correction	0.15051	0.14999
(Hartree)		
Solvation Gibbs		
Free Energy	-0.02476	-0.04939
(Hartree)		
Electronic	-1625.93918	-1625.87964
Energy (Hartree)		
Imaginaries	0	1
G_{sol}(Hartree)	-1625.81342	-1625.77904
Specics	SLC-STrain-68	TS-STrain-68

Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.21080	0.21183
Solvation Gibbs Free Energy (Hartree)	-0.02618	-0.05051
Electronic Energy (Hartree)	-1742.60745	-1742.55581
Imaginaries	0	1
G_{sol}(Hartree)	-1742.42284	-1742.39448

Specics	SLC-STrain-72	TS-STrain-72
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.15519	0.15449
Solvation Gibbs Free Energy (Hartree)	-0.02973	-0.04484
Electronic Energy (Hartree)	-1701.17456	-1701.10946
Imaginaries	0	1
G_{sol}(Hartree)	-1701.04910	-1700.99981

Specics	SLC-STest-2	TS-STest-2
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.17841	0.17388
Solvation Gibbs Free Energy (Hartree)	-0.02630	-0.05142
Electronic Energy (Hartree)	-1665.23877	-1665.16932
Imaginaries	0	1
G_{sol}(Hartree)	-1665.08666	-1665.04686

Specics	SLC-STest-4	TS-STest-4
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.22295	0.22092
Solvation Gibbs Free Energy (Hartree)	-0.02995	-0.04899
Electronic Energy (Hartree)	-1818.85651	-1818.79612
Imaginaries	0	1
G_{sol}(Hartree)	-1818.66351	-1818.62419
Specics	SLC-STest-8	TS-STest-8
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.14582	0.14357
Solvation Gibbs Free Energy (Hartree)	-0.02854	-0.04254
Electronic Energy (Hartree)	-2123.57750	-2123.52104
Imaginaries	0	1
G_{sol}(Hartree)	-2123.46021	-2123.42000
Specics	SLC-STest-9	TS-STest-9
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.25446	0.25161
Solvation Gibbs Free Energy (Hartree)	-0.02802	-0.03639
Electronic Energy (Hartree)	-1933.36173	-1933.31848
Imaginaries	0	1
G_{sol}(Hartree)	-1933.13529	-1933.10326

Species	SLC-STest-10	TS-STest-10
Optimization Level	SMD(diethylether)-PBE0-D3(BJ)/def-TZVP	
Electronic Energy Level	RI-PWPB95-D3(BJ)/def2-QZVPP	
G Correction (Hartree)	0.22287	0.22164
Solvation Gibbs Free Energy (Hartree)	-0.02913	-0.04610
Electronic Energy (Hartree)	-1818.86234	-1818.80826
Imaginaries	0	1
G_{sol}(Hartree)	-1818.66860	-1818.63272

SLC-STrain-4

C	2.794770	1.187716	0.089361
C	1.581215	0.843658	-0.778018
H	3.074582	2.240886	0.085679
H	1.649898	-0.060477	-1.381898
H	1.152764	1.660775	-1.358366
O	1.961077	0.929243	1.299552
C	0.929925	0.636228	0.543965
O	-0.169120	0.322086	0.980286
C	4.021036	0.335021	0.055320
H	4.580550	0.558837	-0.853118
H	4.648093	0.532857	0.923842
Al	-1.819402	-0.050382	0.097150
C	-3.036401	-0.743687	1.452616
C	-4.428234	-1.094825	0.924863
H	-3.114098	-0.000771	2.256444
H	-2.571776	-1.627958	1.907046
H	-5.081390	-1.484460	1.713411
H	-4.928969	-0.221842	0.494970
H	-4.382110	-1.856506	0.140416
Cl	-2.269088	1.886876	-0.765308
Cl	-1.199002	-1.411680	-1.471433
Cl	3.651335	-1.421177	0.050934

TS-STrain-4

C	-2.825774	-1.165597	-0.483053
C	-1.414615	-0.742129	-0.488573
H	-3.081840	-2.218201	-0.594361

H	-1.284894	0.281511	-0.848967
H	-0.804377	-1.405743	-1.103114
O	-1.708653	-1.116804	1.849834
C	-0.925899	-0.804765	0.975008
O	0.310466	-0.511275	1.153632
C	-3.905538	-0.332295	-0.266991
H	-3.551949	-0.632260	-1.486230
H	-4.910385	-0.738717	-0.184580
Al	1.742756	0.012829	0.166995
C	3.287011	0.336607	1.323327
C	4.550224	0.778686	0.584660
H	3.485828	-0.579600	1.894152
H	3.002286	1.092331	2.066849
H	5.392160	0.952884	1.264746
H	4.875325	0.027705	-0.142336
H	4.388118	1.708569	0.030391
Cl	2.022679	-1.592823	-1.302121
Cl	1.057912	1.784533	-0.935611
Cl	-3.761359	1.334546	0.063528

Imaginary vibration frequency: 497.79i

SLC-STrain-6

C	2.528491	1.050938	0.421905
C	1.339905	0.880018	-0.528219
H	2.854957	2.080070	0.568118
H	1.397597	0.066680	-1.250807
H	0.965437	1.787196	-1.002271
O	1.635429	0.680625	1.555611
C	0.629178	0.522956	0.729798
O	-0.495417	0.189473	1.078188
C	3.722203	0.145666	0.307556
H	4.295687	0.198474	1.233231
Al	-2.098151	-0.036769	0.066497
C	-3.455623	-0.710143	1.292218
C	-4.821554	-0.939953	0.643480
H	-3.548550	-0.003244	2.126275
H	-3.085007	-1.644648	1.732137
H	-5.557352	-1.325097	1.357963
H	-5.231477	-0.014324	0.227689
H	-4.762715	-1.661433	-0.177291
Cl	-2.369692	1.963959	-0.726085
Cl	-1.447398	-1.362891	-1.519068
C	4.568564	0.525681	-0.883283
H	4.003346	0.438344	-1.813707

H	4.910595	1.558896	-0.775478
H	5.444655	-0.119561	-0.946452
Cl	3.193660	-1.583133	0.179565

TS-STrain-6

C	2.561157	-0.984471	0.410153
C	1.138534	-0.620803	0.566321
H	2.851021	-2.029409	0.494833
H	0.975642	0.437498	0.776147
H	0.646938	-1.218393	1.336593
O	1.383378	-1.435535	-1.619889
C	0.582193	-0.982181	-0.812522
O	-0.660996	-0.797845	-1.033647
C	3.624350	-0.106707	0.218602
H	3.406938	-0.401988	1.411877
Al	-2.077402	-0.060415	-0.152422
C	-3.671738	-0.133161	-1.282857
C	-4.918894	0.504618	-0.671065
H	-3.867863	-1.185858	-1.524676
H	-3.432891	0.349865	-2.239182
H	-5.789415	0.437262	-1.333862
H	-5.196420	0.023909	0.272405
H	-4.762651	1.565918	-0.453671
Cl	-2.224927	-1.201228	1.714563
Cl	-1.404780	1.959001	0.370357
C	4.991529	-0.558954	-0.161944
H	5.123350	-1.613893	0.079973
H	5.090190	-0.431050	-1.243002
H	5.756667	0.039124	0.331606
Cl	3.311052	1.593368	0.015115

Imaginary vibration frequency: 567.10i

SLC-STrain-7

C	-1.816635	0.496435	-0.664575
C	-0.467278	1.163420	-0.359009
H	-2.230260	0.719939	-1.646438
H	-0.348187	1.577038	0.643140
H	-0.081145	1.857297	-1.105016
O	-1.106495	-0.814609	-0.742228
C	0.038603	-0.228662	-0.493862
O	1.110174	-0.817367	-0.433486
C	-2.837799	0.530708	0.430351
H	-2.396691	0.178604	1.363428

Al	2.856311	-0.183235	0.010335
C	4.045903	-1.725989	-0.030113
C	5.498982	-1.405719	0.323834
H	3.991228	-2.175065	-1.029835
H	3.647921	-2.481698	0.658882
H	6.135913	-2.296455	0.291838
H	5.931729	-0.676195	-0.367624
H	5.585969	-0.984615	1.330173
Cl	3.151039	1.358770	-1.483675
Cl	2.488714	0.742312	1.938182
Br	-4.250461	-0.778446	0.022976
C	-3.427805	1.911962	0.580841
H	-2.638770	2.620995	0.849236
H	-3.897342	2.247776	-0.345868
H	-4.175319	1.924516	1.373840

TS-STrain-7

C	-2.094011	-1.456684	-0.426543
C	-0.679152	-1.068489	-0.572649
H	-2.368792	-2.508345	-0.496286
H	-0.542452	-0.041460	-0.917874
H	-0.138791	-1.744122	-1.237721
O	-0.912179	-1.672436	1.694660
C	-0.144637	-1.218650	0.859183
O	1.063089	-0.866585	1.079876
C	-3.166974	-0.592263	-0.235411
H	-2.932337	-0.886088	-1.429379
Al	2.406310	-0.046745	0.160057
C	3.937167	0.250420	1.340380
C	5.128089	0.944216	0.679484
H	4.246530	-0.720047	1.749535
H	3.590568	0.836988	2.201108
H	5.961858	1.094248	1.375177
H	5.514897	0.364286	-0.164410
H	4.854510	1.929805	0.289745
Cl	2.790751	-1.367179	-1.546222
Cl	1.489885	1.784015	-0.628461
C	-4.530748	-1.063090	0.135070
H	-4.641957	-0.936178	1.215060
H	-5.304725	-0.481668	-0.364961
H	-4.643828	-2.121523	-0.103460
Br	-2.844401	1.265000	-0.002887

Imaginary vibration frequency: 556.07i

SLC-STrain-8

C	2.598190	-0.993113	-0.152017
C	1.451167	-0.387554	0.659278
H	2.978770	-1.942664	0.218406
H	1.511805	0.683788	0.853895
H	1.144646	-0.918653	1.560213
O	1.632509	-1.261825	-1.257482
C	0.659091	-0.741516	-0.549290
O	-0.500756	-0.665681	-0.936238
C	3.685249	-0.071946	-0.627776
H	4.248518	-0.556746	-1.438383
H	3.242045	0.853522	-1.026778
Al	-2.049341	0.048544	-0.082333
C	-3.539770	-0.187692	-1.316235
C	-4.877505	0.329006	-0.784320
H	-3.617749	-1.255040	-1.558922
H	-3.289025	0.315572	-2.258589
H	-5.691812	0.178828	-1.501673
H	-5.166956	-0.178467	0.141074
H	-4.837546	1.400087	-0.563291
Cl	-2.092410	-1.093183	1.760090
Cl	-1.416136	2.079967	0.335716
O	4.497660	0.184918	0.481421
C	5.557100	1.063790	0.171325
H	6.133047	1.212258	1.084662
H	6.213250	0.641230	-0.600437
H	5.181285	2.034740	-0.175972

TS-STrain-8

C	2.540936	-0.492857	0.725900
C	1.160120	0.063081	0.728771
H	2.786109	-1.340860	1.358523
H	1.097453	1.074112	0.320113
H	0.694309	0.046980	1.715490
O	1.331939	-1.790128	-0.617211
C	0.528838	-0.947882	-0.204375
O	-0.702929	-0.903236	-0.510770
C	3.597025	0.160921	0.086560
H	3.427372	0.646005	1.202345
H	3.370737	0.992060	-0.587129
Al	-2.083625	0.254640	-0.181681
C	-3.704860	-0.405487	-1.052600
C	-4.150854	-1.793264	-0.590289
H	-3.530039	-0.407691	-2.136306

H	-4.508116	0.323171	-0.886313
H	-5.058686	-2.130780	-1.103714
H	-3.379350	-2.547394	-0.775217
H	-4.364309	-1.811289	0.483018
Cl	-2.184456	0.367459	2.002506
Cl	-1.342008	2.181633	-0.913222
O	4.774051	-0.454847	-0.049825
C	5.846122	0.399455	-0.463533
H	6.104382	1.104162	0.331319
H	6.693247	-0.252428	-0.664336
H	5.575449	0.940947	-1.373937

Imaginary vibration frequency: 665.08i

SLC-STrain-9

C	2.598190	-0.993113	-0.152017
C	1.451167	-0.387554	0.659278
H	2.978770	-1.942664	0.218406
H	1.511805	0.683788	0.853895
H	1.144646	-0.918653	1.560213
O	1.632509	-1.261825	-1.257482
C	0.659091	-0.741516	-0.549290
O	-0.500756	-0.665681	-0.936238
C	3.685249	-0.071946	-0.627776
H	4.248518	-0.556746	-1.438383
H	3.242045	0.853522	-1.026778
Al	-2.049341	0.048544	-0.082333
C	-3.539770	-0.187692	-1.316235
C	-4.877505	0.329006	-0.784320
H	-3.617749	-1.255040	-1.558922
H	-3.289025	0.315572	-2.258589
H	-5.691812	0.178828	-1.501673
H	-5.166956	-0.178467	0.141074
H	-4.837546	1.400087	-0.563291
Cl	-2.092410	-1.093183	1.760090
Cl	-1.416136	2.079967	0.335716
O	4.497660	0.184918	0.481421
C	5.557100	1.063790	0.171325
H	6.133047	1.212258	1.084662
H	6.213250	0.641230	-0.600437
H	5.181285	2.034740	-0.175972

TS-STrain-9

C	2.535816	-1.169732	0.717567
C	1.273907	-0.387210	0.752007

H	2.581000	-2.144842	1.190816
H	1.416704	0.674739	0.547391
H	0.724170	-0.510839	1.687246
O	1.265016	-1.930689	-0.956171
C	0.570263	-1.074782	-0.400688
O	-0.619259	-0.776254	-0.731856
C	3.756501	-0.651269	0.276393
H	3.675353	-0.502417	1.491588
Al	-1.906228	0.364238	-0.103594
C	-3.520113	0.185149	-1.193628
C	-4.126907	-1.218339	-1.201932
H	-3.272762	0.495048	-2.217294
H	-4.259584	0.913363	-0.837533
H	-5.026078	-1.279653	-1.826100
H	-3.419919	-1.961054	-1.584909
H	-4.412895	-1.539305	-0.195394
Cl	-2.143809	-0.219452	1.995450
Cl	-0.965506	2.338119	-0.147347
H	4.605136	-1.330814	0.168176
O	3.779781	0.495581	-0.406092
C	5.081799	1.062080	-0.585724
H	4.953542	1.908503	-1.256351
H	5.484553	1.407573	0.369862
H	5.758212	0.332781	-1.039539

Imaginary vibration frequency: 672.83i

SLC-STrain-10

C	1.518859	-1.065649	-0.137994
C	0.092597	-1.455633	0.261648
H	1.934316	-1.631161	-0.970140
H	-0.108612	-1.505164	1.332586
H	-0.347719	-2.312712	-0.247195
O	0.958833	0.214032	-0.705782
C	-0.246321	-0.145307	-0.354121
O	-1.249920	0.530766	-0.559522
C	2.510396	-0.798017	0.956890
H	2.720284	-1.766358	1.423218
H	2.041476	-0.168557	1.718976
Al	-3.070440	0.233231	-0.100898
C	-4.095769	1.723691	-0.827667
C	-5.597666	1.644569	-0.550022
H	-3.914400	1.768195	-1.909075
H	-3.685216	2.655116	-0.417674
H	-6.140597	2.496578	-0.973819

H	-6.039649	0.738304	-0.975492
H	-5.809405	1.630532	0.523593
Cl	-3.434929	-1.726600	-0.957768
Cl	-2.950131	0.067413	2.058951
C	3.781046	-0.172366	0.453950
C	4.799797	-0.964906	-0.071010
C	3.945703	1.209900	0.471530
C	5.958564	-0.387841	-0.570488
H	4.687892	-2.045031	-0.081665
C	5.104273	1.789676	-0.027559
H	3.160925	1.837848	0.881105
C	6.113045	0.992410	-0.550868
H	6.745373	-1.017650	-0.971601
H	5.219443	2.867961	-0.005706
H	7.019174	1.444734	-0.938844

TS-STrain-10

C	1.512150	-0.345503	0.664820
C	0.063236	-0.047195	0.670742
H	1.837035	-1.317817	1.023754
H	-0.153458	1.014783	0.536366
H	-0.432729	-0.402794	1.577287
O	0.451213	-1.453448	-1.156851
C	-0.414752	-0.847470	-0.536026
O	-1.658130	-0.843105	-0.830205
C	2.486419	0.592065	0.327091
H	2.232474	0.629933	1.518296
H	2.123966	1.555661	-0.028603
Al	-3.171617	-0.061509	-0.183898
C	-4.714608	-0.588034	-1.264901
C	-6.047446	-0.001922	-0.799281
H	-4.767911	-1.684441	-1.271732
H	-4.517675	-0.295356	-2.304394
H	-6.885708	-0.318236	-1.430872
H	-6.285109	-0.305875	0.225046
H	-6.032391	1.092545	-0.810935
Cl	-3.271087	-0.689874	1.914732
Cl	-2.736502	2.088726	-0.203187
C	3.915885	0.302047	0.115193
C	4.396277	-1.000565	-0.016480
C	4.797743	1.379069	0.028542
C	5.748893	-1.217742	-0.218807
H	3.716432	-1.844664	0.010110
C	6.150352	1.156038	-0.170756

H	4.418884	2.391930	0.117984
C	6.626813	-0.142641	-0.291460
H	6.119041	-2.230176	-0.332818
H	6.832423	1.995925	-0.236594
H	7.684324	-0.318732	-0.454100

Imaginary vibration frequency: 441.10i

SLC-STrain-12

C	-0.672211	1.716774	0.262986
C	0.147670	0.427837	0.374161
H	-1.040437	2.100339	1.212635
H	-0.038625	-0.327863	-0.389511
H	0.212316	-0.038848	1.356659
O	0.603905	2.448219	-0.055941
C	1.281374	1.335756	0.055794
O	2.497124	1.256842	-0.087985
C	-1.666621	1.841624	-0.857562
H	-1.945426	2.893123	-0.965910
H	-1.199712	1.518235	-1.791250
Al	3.662513	-0.243359	0.027480
C	5.463480	0.407783	-0.336981
C	6.548286	-0.667053	-0.254603
H	5.681823	1.218052	0.370275
H	5.466316	0.871174	-1.331688
H	7.545216	-0.262964	-0.462243
H	6.587725	-1.125106	0.738493
H	6.372665	-1.473911	-0.972790
Cl	3.253709	-0.961734	2.032429
Cl	2.775922	-1.595389	-1.420160
C	-2.877163	1.000273	-0.561419
C	-3.831336	1.432113	0.357053
C	-3.046782	-0.240895	-1.167375
C	-4.931383	0.648129	0.666924
H	-3.723191	2.401167	0.833905
C	-4.141975	-1.039115	-0.870177
H	-2.319914	-0.591961	-1.892523
C	-5.072527	-0.584096	0.048548
H	-5.672501	0.992580	1.377738
H	-4.269458	-2.001629	-1.350465
Cl	-6.458017	-1.579581	0.432245

TS-STrain-12

C	0.698385	-0.231637	0.747147
C	-0.754505	0.039066	0.693710

H	1.027990	-1.165906	1.192446
H	-0.984957	1.080224	0.458431
H	-1.264811	-0.241026	1.618595
O	-0.316938	-1.516667	-1.002419
C	-1.199032	-0.873951	-0.445798
O	-2.439209	-0.915817	-0.751264
C	1.663738	0.689449	0.346751
H	1.376711	0.812215	1.529816
H	1.293792	1.616853	-0.088728
Al	-3.974236	-0.104059	-0.200642
C	-5.486138	-0.736434	-1.268593
C	-6.836051	-0.131926	-0.882905
H	-5.527006	-1.830413	-1.187977
H	-5.267668	-0.526062	-2.323604
H	-7.655371	-0.509286	-1.505777
H	-7.094838	-0.355013	0.156978
H	-6.832868	0.958090	-0.983204
Cl	-4.108901	-0.559435	1.940197
Cl	-3.563805	2.043493	-0.385821
C	3.101202	0.411084	0.189983
C	3.604064	-0.887558	0.120297
C	3.974405	1.493433	0.087647
C	4.962186	-1.102269	-0.030564
H	2.939832	-1.743509	0.152908
C	5.334772	1.289957	-0.058351
H	3.587670	2.506142	0.124894
C	5.814357	-0.010080	-0.110474
H	5.354356	-2.109288	-0.098014
H	6.014074	2.129569	-0.135275
Cl	7.524650	-0.278455	-0.295951

Imaginary vibration frequency: 443.60i

SLC-STrain-13

C	-1.001990	1.451030	0.523272
C	-0.107751	0.209309	0.501011
H	-1.382386	1.723468	1.506671
H	-0.266128	-0.480936	-0.328079
H	-0.001375	-0.343743	1.433879
O	0.232036	2.285337	0.273311
C	0.968065	1.206474	0.260351
O	2.183911	1.208953	0.088738
C	-2.021052	1.619306	-0.574763
H	-1.524828	1.376981	-1.520949
Al	3.419758	-0.232627	0.005189

C	5.180704	0.537514	-0.322967
C	6.306602	-0.493447	-0.415834
H	5.394378	1.257759	0.476940
H	5.130702	1.125247	-1.248354
H	7.279910	-0.025681	-0.600778
H	6.399365	-1.073805	0.507338
H	6.134075	-1.207579	-1.226974
Cl	3.102837	-1.201950	1.919676
Cl	2.563742	-1.450665	-1.574276
C	-3.106845	0.591801	-0.348999
C	-3.985912	0.692942	0.729221
C	-3.229702	-0.503395	-1.196248
C	-4.956436	-0.271278	0.945171
H	-3.918783	1.537390	1.407809
C	-4.205746	-1.467369	-0.979288
H	-2.556422	-0.603588	-2.042439
C	-5.085424	-1.369918	0.094304
H	-5.630212	-0.170507	1.790878
H	-4.283141	-2.311029	-1.658015
C	-2.538558	3.050484	-0.637037
H	-3.272588	3.149526	-1.438899
H	-3.019540	3.343141	0.299505
H	-1.724085	3.751500	-0.832962
C	-6.146903	-2.400192	0.330523
H	-6.096777	-2.793060	1.349858
H	-7.145428	-1.972248	0.198236
H	-6.047334	-3.238123	-0.361629

TS-STrain-13

C	1.029608	-0.014215	0.899346
C	-0.444507	0.137129	0.915388
H	1.456477	-0.808994	1.504991
H	-0.804886	1.118107	0.607212
H	-0.878011	-0.112697	1.885924
O	0.151390	-1.557816	-0.556119
C	-0.806424	-0.924808	-0.111572
O	-2.020064	-1.108096	-0.450697
C	1.943585	0.860862	0.288200
H	1.773288	1.206902	1.432158
Al	-3.600611	-0.241046	-0.153483
C	-5.047459	-1.144539	-1.109709
C	-6.422781	-0.499777	-0.937358
H	-5.077057	-2.188805	-0.772440
H	-4.781278	-1.184900	-2.173797

H	-7.206536	-1.037238	-1.483631
H	-6.726036	-0.472111	0.114032
H	-6.431369	0.533546	-1.298317
Cl	-3.822622	-0.209121	2.024666
Cl	-3.205952	1.816294	-0.804136
C	3.358868	0.408244	0.151964
C	3.641102	-0.919520	-0.157824
C	4.409988	1.311374	0.295361
C	4.954361	-1.333150	-0.315728
H	2.829690	-1.625116	-0.301372
C	5.718440	0.886008	0.148927
H	4.207108	2.350066	0.535516
C	6.014113	-0.441802	-0.163076
H	5.159026	-2.368885	-0.566809
H	6.528264	1.596923	0.277526
C	1.491948	1.964411	-0.630367
H	2.239713	2.755693	-0.669074
H	1.397667	1.543741	-1.635031
H	0.535763	2.399967	-0.344242
C	7.429071	-0.885410	-0.362967
H	8.115301	-0.327516	0.277509
H	7.545879	-1.950276	-0.153382
H	7.740600	-0.718295	-1.399475

Imaginary vibration frequency: 445.93i

SLC-STrain-14

C	0.623959	1.540297	-0.598246
C	-0.204232	0.258263	-0.489678
H	1.022235	1.744722	-1.591139
H	-0.038866	-0.343423	0.404712
H	-0.247055	-0.382090	-1.370163
O	-0.661355	2.324064	-0.461984
C	-1.339103	1.211316	-0.374425
O	-2.559079	1.160821	-0.242710
C	1.595559	1.860688	0.508476
H	1.077986	1.681394	1.457500
Al	-3.717116	-0.331172	-0.031519
C	-5.527016	0.371772	0.148737
C	-6.600034	-0.701232	0.338977
H	-5.750477	0.974560	-0.740671
H	-5.539808	1.071318	0.994207
H	-7.602182	-0.269504	0.437356
H	-6.630922	-1.395390	-0.506529
H	-6.418148	-1.298943	1.237499

Cl	-3.279573	-1.498070	-1.807263
Cl	-2.857745	-1.307787	1.705990
C	2.736142	0.873032	0.413993
C	3.662399	0.928438	-0.621005
C	2.866704	-0.150688	1.353035
C	4.693215	0.002861	-0.725939
H	3.596361	1.712982	-1.368113
C	3.886163	-1.079029	1.266770
H	2.158576	-0.217110	2.173659
C	4.809310	-1.010307	0.223037
H	5.395942	0.083506	-1.545028
H	3.985301	-1.868288	2.003351
C	2.037886	3.317008	0.452718
H	2.737507	3.528282	1.263518
H	2.536129	3.546914	-0.492384
H	1.183211	3.989385	0.556273
O	5.773355	-1.956156	0.215405
C	6.727244	-1.920884	-0.828784
H	7.301365	-0.988467	-0.817609
H	7.402096	-2.756304	-0.648076
H	6.255122	-2.047777	-1.808661

TS-STrain-14

C	0.670585	0.196988	0.966884
C	-0.809926	0.289645	0.961442
H	1.125640	-0.509395	1.655355
H	-1.206719	1.219635	0.555763
H	-1.243534	0.116406	1.948377
O	-0.105740	-1.500820	-0.326221
C	-1.106139	-0.879265	0.038196
O	-2.299010	-1.159017	-0.304306
C	1.549096	1.055506	0.280043
H	1.363079	1.507898	1.378406
Al	-3.921155	-0.329501	-0.150489
C	-5.296240	-1.396616	-1.041766
C	-6.703522	-0.803131	-0.978138
H	-5.290633	-2.399809	-0.596088
H	-4.993636	-1.536146	-2.087633
H	-7.443721	-1.429832	-1.488923
H	-7.043614	-0.682703	0.055249
H	-6.744820	0.186390	-1.444276
Cl	-4.216757	-0.058379	2.001385
Cl	-3.579256	1.653630	-1.021139
C	2.980356	0.655894	0.175900

C	3.329667	-0.680736	0.020526
C	3.991828	1.620178	0.188340
C	4.656485	-1.062190	-0.115636
H	2.555021	-1.438352	-0.029587
C	5.313623	1.252947	0.068751
H	3.741946	2.669917	0.301376
C	5.658114	-0.093764	-0.086173
H	4.894687	-2.108395	-0.255302
H	6.103042	1.995303	0.087786
C	1.043833	2.046364	-0.735389
H	1.761049	2.857072	-0.858455
H	0.952465	1.530337	-1.694596
H	0.076691	2.474063	-0.475047
O	6.971108	-0.355556	-0.207879
C	7.369712	-1.705745	-0.375356
H	7.084292	-2.316005	0.487285
H	6.945250	-2.136602	-1.287390
H	8.455054	-1.688837	-0.458612

Imaginary vibration frequency: 464.79i

SLC-STrain-15

C	-2.208617	-1.144821	0.123382
C	-0.878523	-1.178744	-0.634769
H	-2.482918	-2.085301	0.599541
H	-0.859888	-0.649584	-1.588272
H	-0.380531	-2.143817	-0.726182
O	-1.527965	-0.302149	1.177901
C	-0.406559	-0.358133	0.511802
O	0.638018	0.169360	0.882735
C	-3.363718	-0.425939	-0.495233
H	-3.694288	-1.038228	-1.342350
H	-3.020515	0.528002	-0.909137
Al	2.367686	0.201700	0.095797
C	3.499506	1.297803	1.244393
C	4.941650	1.435201	0.753996
H	3.484122	0.865733	2.253039
H	3.037111	2.288684	1.337159
H	5.547399	2.056047	1.423289
H	5.437782	0.462421	0.681593
H	4.988441	1.893106	-0.238890
Cl	2.835115	-1.912998	-0.028622
Cl	1.939944	0.962776	-1.890453
C	-4.520452	-0.200328	0.475288
H	-4.186954	0.414131	1.316446

H	-4.829725	-1.170150	0.884853
C	-5.687652	0.450146	-0.191520
H	-6.131070	-0.099665	-1.021406
C	-6.195515	1.626951	0.150436
H	-7.045523	2.052490	-0.373014
H	-5.780503	2.207303	0.970507

TS-STrain-15

C	2.390186	-1.680372	0.516176
C	1.007829	-1.173568	0.644625
H	2.596031	-2.695960	0.845631
H	0.951995	-0.086232	0.712557
H	0.504537	-1.603079	1.513346
O	0.892471	-2.425498	-1.362507
C	0.297058	-1.657849	-0.626362
O	-0.893284	-1.222727	-0.825009
C	3.473309	-0.956006	0.038717
H	4.406079	-1.507764	-0.064865
H	3.325331	-0.919782	1.274698
Al	-1.988668	0.047771	-0.129767
C	-3.630175	0.170124	-1.187224
C	-4.634314	1.211422	-0.694006
H	-4.096914	-0.823356	-1.204585
H	-3.348469	0.381747	-2.226886
H	-5.537936	1.246035	-1.313697
H	-4.956471	1.005853	0.331708
H	-4.204916	2.218308	-0.696905
Cl	-2.286315	-0.520745	1.965123
Cl	-0.774175	1.882831	-0.128928
C	3.416920	0.405024	-0.576276
H	2.468648	0.905316	-0.376860
H	3.453408	0.215014	-1.658590
C	4.573662	1.265418	-0.172657
H	5.566419	0.864653	-0.368667
C	4.438340	2.459676	0.385062
H	5.303144	3.058272	0.650597
H	3.459741	2.887067	0.585966

Imaginary vibration frequency: 370.39i

SLC-STrain-18

C	-2.849196	-1.237354	0.215658
C	-1.565587	-1.159401	-0.620470
H	-3.174369	-2.247555	0.455914
H	-1.544853	-0.445960	-1.443116

H	-1.137284	-2.110908	-0.935859
O	-2.054525	-0.731232	1.390657
C	-0.985600	-0.643441	0.646551
O	0.100409	-0.235620	1.048366
C	-4.000574	-0.319214	-0.097294
H	-4.658050	-0.294708	0.776534
H	-4.562502	-0.797793	-0.907271
Al	1.724097	0.058435	0.106379
C	3.024188	0.729603	1.395055
C	4.392863	1.051692	0.793386
H	3.129700	-0.014166	2.195025
H	2.602559	1.623389	1.872152
H	5.096229	1.425851	1.545475
H	4.850847	0.169099	0.336209
H	4.320646	1.815528	0.013005
Cl	2.102269	-1.895967	-0.758223
Cl	1.082946	1.421483	-1.455728
C	-3.592065	1.066467	-0.490489
C	-3.640967	2.111735	0.323724
H	-3.224263	1.200149	-1.505570
H	-3.321922	3.096484	-0.001188
H	-4.004112	2.021453	1.344010

TS-STrain-18

C	-2.727398	-0.638420	-0.400261
C	-1.300833	-0.270381	-0.518756
H	-2.992436	-1.691931	-0.447634
H	-1.148226	0.798881	-0.678927
H	-0.792502	-0.827488	-1.310182
O	-1.587796	-1.105179	1.647698
C	-0.761855	-0.682073	0.847702
O	0.489253	-0.562814	1.080522
C	-3.767548	0.289634	-0.341541
H	-3.499961	-0.002400	-1.495178
Al	1.960221	0.008217	0.170342
C	3.553116	-0.152452	1.294200
C	4.856140	0.263134	0.611343
H	3.623949	-1.192683	1.637541
H	3.394804	0.447695	2.199563
H	5.724934	0.159314	1.271707
H	5.055274	-0.342843	-0.278164
H	4.824843	1.307359	0.284484
Cl	2.004914	-1.219974	-1.646677
Cl	1.474853	2.058302	-0.440444

C	-5.159453	-0.069181	-0.061158
C	-6.065300	0.860907	0.217996
H	-5.411342	-1.125582	-0.064053
H	-5.814638	1.917342	0.226031
H	-7.086570	0.590892	0.461213
H	-3.489913	1.339983	-0.262696

Imaginary vibration frequency: 335.71i

SLC-STrain-19

C	-2.849196	-1.237354	0.215658
C	-1.565587	-1.159401	-0.620470
H	-3.174369	-2.247555	0.455914
H	-1.544853	-0.445960	-1.443116
H	-1.137284	-2.110908	-0.935859
O	-2.054525	-0.731232	1.390657
C	-0.985600	-0.643441	0.646551
O	0.100409	-0.235620	1.048366
C	-4.000574	-0.319214	-0.097294
H	-4.658050	-0.294708	0.776534
H	-4.562502	-0.797793	-0.907271
Al	1.724097	0.058435	0.106379
C	3.024188	0.729603	1.395055
C	4.392863	1.051692	0.793386
H	3.129700	-0.014166	2.195025
H	2.602559	1.623389	1.872152
H	5.096229	1.425851	1.545475
H	4.850847	0.169099	0.336209
H	4.320646	1.815528	0.013005
Cl	2.102269	-1.895967	-0.758223
Cl	1.082946	1.421483	-1.455728
C	-3.592065	1.066467	-0.490489
C	-3.640967	2.111735	0.323724
H	-3.224263	1.200149	-1.505570
H	-3.321922	3.096484	-0.001188
H	-4.004112	2.021453	1.344010

TS-STrain-19

C	-2.796652	-1.276457	-0.299306
C	-1.381455	-0.902492	-0.510720
H	-3.041801	-2.334060	-0.262158
H	-1.237563	0.110697	-0.887171
H	-0.872569	-1.600290	-1.179417
O	-1.590087	-1.439099	1.760530
C	-0.814494	-1.039845	0.901228

O	0.411405	-0.740609	1.102680
C	-3.876892	-0.390106	-0.248130
H	-4.838534	-0.829115	0.010777
H	-3.695038	-0.785319	-1.385662
Al	1.760393	0.034963	0.157422
C	3.351337	0.202357	1.283183
C	4.567011	0.814770	0.588011
H	3.600822	-0.795683	1.666443
H	3.082242	0.798132	2.164990
H	5.434664	0.889025	1.253861
H	4.877039	0.221299	-0.277854
H	4.356107	1.824813	0.222567
Cl	2.021219	-1.232086	-1.611538
Cl	0.911444	1.942102	-0.525017
C	-3.782852	1.069500	-0.177424
C	-4.856085	1.798050	0.111923
H	-2.817858	1.539767	-0.330966
H	-4.789072	2.875783	0.207037
H	-5.828841	1.343178	0.274209

Imaginary vibration frequency: 373.71i

SLC-STrain-21

C	2.481779	-1.050598	-0.417094
C	1.340283	-0.650557	0.523764
H	2.830934	-2.073234	-0.285295
H	1.393083	0.338216	0.977998
H	1.044381	-1.388050	1.269768
O	1.485178	-1.062924	-1.545565
C	0.533033	-0.710197	-0.723124
O	-0.633206	-0.532337	-1.062033
C	3.619604	-0.086389	-0.672081
Al	-2.136045	0.029755	-0.041953
C	-3.653361	0.122740	-1.262809
C	-4.962430	0.560330	-0.604156
H	-3.777657	-0.862356	-1.730185
H	-3.394136	0.809474	-2.078590
H	-5.790561	0.601606	-1.320257
H	-5.261727	-0.126079	0.193904
H	-4.875836	1.554779	-0.155549
Cl	-2.204853	-1.478311	1.515872
Cl	-1.416741	1.900142	0.791438
C	4.551720	-0.205766	0.502691
C	4.908591	0.781199	1.313229
H	4.948698	-1.204308	0.678650

H	5.590535	0.602810	2.137860
H	4.550673	1.797571	1.186449
C	3.168081	1.329368	-0.982581
H	2.499725	1.348479	-1.845486
H	2.653852	1.798531	-0.140855
H	4.033494	1.948688	-1.225351
H	4.150648	-0.482754	-1.548201

TS-STrain-21

C	-2.526742	-1.137020	-0.303111
C	-1.091406	-0.872366	-0.570850
H	-2.840380	-2.174417	-0.231697
H	-0.876400	0.105178	-0.999975
H	-0.639663	-1.641079	-1.200890
O	-1.416525	-1.291131	1.681871
C	-0.565622	-0.976082	0.849200
O	0.660448	-0.748275	1.107635
C	-3.561159	-0.178889	-0.304763
H	-3.413408	-0.606344	-1.425659
Al	2.049744	-0.012633	0.173704
C	3.639189	0.093341	1.307475
C	4.865635	0.698621	0.624407
H	3.869247	-0.919152	1.663971
H	3.383580	0.671927	2.204384
H	5.736993	0.734958	1.288428
H	5.159630	0.123538	-0.259321
H	4.675334	1.722950	0.288763
Cl	2.278718	-1.275962	-1.600494
Cl	1.258592	1.919725	-0.502169
C	-3.243236	1.265637	-0.343320
C	-4.919947	-0.613756	0.174473
H	-5.713522	-0.081367	-0.349139
H	-5.059430	-1.686337	0.037589
H	-4.997374	-0.392710	1.241348
C	-4.080274	2.203826	0.081663
H	-2.266131	1.551757	-0.715965
H	-3.782961	3.246188	0.065543
H	-5.066471	1.980553	0.472650

Imaginary vibration frequency: 436.65i

SLC-STrain-24

C	-2.711883	0.816683	-0.068952
C	-1.376068	0.989519	0.657944
H	-3.075609	1.713370	-0.568781

H	-1.290905	0.502284	1.629606
H	-0.964022	1.997504	0.701707
O	-1.993505	-0.009313	-1.101099
C	-0.860682	0.165935	-0.468941
O	0.212982	-0.286075	-0.847470
C	-3.790843	0.030771	0.607371
Al	1.963630	-0.135281	-0.103689
C	3.140053	-1.264713	-1.170619
C	4.597733	-1.256925	-0.707133
H	3.075109	-0.937608	-2.216000
H	2.744229	-2.287966	-1.152329
H	5.230799	-1.899504	-1.328794
H	5.027351	-0.251029	-0.743064
H	4.695410	-1.610536	0.323928
Cl	2.280805	2.007122	-0.196412
Cl	1.617568	-0.728553	1.954472
C	-4.958021	-0.263449	-0.294371
H	-4.174795	0.659032	1.423533
H	-5.271943	0.571524	-0.954158
O	-5.547969	-1.310528	-0.305582
H	-3.408958	-0.893693	1.046699

TS-STrain-24

C	-2.648206	1.434650	0.151310
C	-1.387637	0.738064	0.503577
H	-2.593407	2.444886	-0.247943
H	-1.455253	0.177453	1.441302
H	-0.564899	1.443537	0.596194
O	-2.044812	-0.821935	-1.180689
C	-1.102145	-0.322247	-0.584894
O	0.120398	-0.641244	-0.766050
C	-3.814271	0.724761	-0.105713
H	-3.434086	1.544254	1.080131
H	-4.661157	1.241558	-0.555703
Al	1.760935	-0.168307	-0.113084
C	3.145526	-1.233905	-0.990639
C	4.571663	-0.906505	-0.547958
H	3.047246	-1.097818	-2.075293
H	2.927721	-2.293495	-0.804388
H	5.318245	-1.527991	-1.055708
H	4.828200	0.137088	-0.755543
H	4.705227	-1.059247	0.527676
Cl	1.895845	1.990418	-0.471670
Cl	1.601731	-0.467871	2.049738

C	-4.052535	-0.699860	0.295993
H	-3.368006	-1.141925	1.033629
O	-4.997481	-1.283490	-0.162197

Imaginary vibration frequency: 472.28i

SLC-STrain-26

C	-2.105163	-1.534306	-0.285021
C	-0.877845	-0.973744	-1.010776
H	-2.321815	-2.574006	-0.525547
H	-0.951030	0.025016	-1.438801
H	-0.398621	-1.648538	-1.720620
O	-1.288279	-1.534533	0.987085
C	-0.271179	-1.026772	0.345335
O	0.800080	-0.741536	0.873376
C	-3.360647	-0.711493	-0.153333
Al	2.348312	0.077962	0.135880
C	3.645385	0.261714	1.579734
C	4.955063	0.933267	1.164089
H	3.846818	-0.736672	1.988325
H	3.173530	0.827389	2.393136
H	5.657902	1.018542	2.000178
H	5.463111	0.372763	0.373259
H	4.786299	1.944755	0.781928
Cl	2.846121	-1.276607	-1.483848
Cl	1.516600	1.906518	-0.687520
C	-3.096454	0.697072	0.398754
H	-2.216084	1.144572	-0.071441
H	-2.877853	0.610432	1.469782
C	-4.251166	1.624977	0.203385
H	-5.188315	1.349644	0.683167
C	-4.195723	2.747219	-0.502490
H	-5.061753	3.391862	-0.612148
H	-3.278588	3.066755	-0.991093
C	-4.394262	-1.468259	0.671133
H	-4.589473	-2.456102	0.246062
H	-4.048548	-1.602464	1.700201
H	-5.342992	-0.930438	0.704993
H	-3.729380	-0.614998	-1.183112

TS-STrain-26

C	1.988386	-0.193313	-1.020089
C	0.593267	-0.494738	-0.620639
H	2.183360	0.079601	-2.053555
H	0.533781	-1.017335	0.336648

H	0.042960	-1.060489	-1.375172
O	0.796172	1.827166	-0.752563
C	0.021914	0.910363	-0.496610
O	-1.196410	1.060303	-0.143591
C	3.079641	-0.230790	-0.125441
H	2.802147	-0.281902	0.924634
Al	-2.571661	-0.024531	0.363511
C	-4.152722	1.056041	0.762272
C	-4.660121	1.894563	-0.411296
H	-3.912284	1.706108	1.613601
H	-4.946439	0.387515	1.118752
H	-5.544123	2.487352	-0.148529
H	-3.897745	2.595902	-0.764879
H	-4.936797	1.267203	-1.264436
Cl	-2.817516	-1.422022	-1.308833
Cl	-1.781743	-1.160270	2.064288
C	3.147947	-1.733108	-0.707054
H	4.138461	-1.849055	-1.141527
H	2.919397	-2.413447	0.108121
H	2.453264	-2.003234	-1.525117
C	4.312171	0.602917	-0.401757
H	4.067030	1.640594	-0.159981
H	4.533831	0.560887	-1.474891
C	5.497009	0.159726	0.393846
C	6.128393	0.923634	1.274607
H	5.848598	-0.856540	0.222002
H	6.989304	0.559407	1.825269
H	5.810833	1.943773	1.472870

Imaginary vibration frequency: 151.27i

SLC-STrain-27

C	-1.995194	0.942369	0.480335
C	-0.833409	0.011933	0.844632
H	-2.328531	1.593765	1.287940
H	-0.897651	-1.008126	0.463878
H	-0.501279	0.007621	1.882401
O	-1.028838	1.737845	-0.362501
C	-0.059042	0.928279	-0.033045
O	1.097709	1.047422	-0.426937
C	-3.126864	0.392230	-0.339835
Al	2.626528	-0.033064	-0.097116
C	4.110887	0.751457	-1.088122
C	5.427172	-0.016000	-0.956099
H	4.241978	1.786367	-0.747576

H	3.818757	0.819311	-2.143771
H	6.236586	0.452656	-1.526635
H	5.759055	-0.072262	0.085227
H	5.332643	-1.044454	-1.318061
Cl	2.739405	0.011965	2.068955
Cl	1.927869	-1.983509	-0.743734
C	-3.977706	-0.508258	0.567881
H	-4.458897	0.101969	1.339477
H	-3.320520	-1.221095	1.081206
C	-5.010601	-1.271774	-0.192912
H	-4.633079	-1.943784	-0.963095
C	-6.319035	-1.184122	0.006193
H	-7.021745	-1.771932	-0.575378
H	-6.735536	-0.523347	0.761990
C	-3.943839	1.509920	-0.967048
H	-4.760724	1.097250	-1.561781
H	-4.383012	2.150036	-0.195388
H	-3.331641	2.133706	-1.621548
H	-2.690095	-0.229934	-1.131510

TS-STrain-27

C	-2.139666	-1.571610	0.239079
C	-0.764085	-1.158493	-0.126203
H	-2.278993	-2.584039	0.604378
H	-0.725810	-0.288524	-0.783182
H	-0.193484	-1.969487	-0.583090
O	-0.919119	-1.030579	2.203202
C	-0.184585	-0.826127	1.243193
O	1.006157	-0.367954	1.319093
C	-3.286944	-0.751998	0.145290
H	-4.135328	-1.120529	0.715218
Al	2.288922	0.166787	0.141818
C	3.850100	0.838416	1.110006
C	4.992229	1.325364	0.218405
H	4.206298	0.041523	1.775665
H	3.517472	1.648873	1.771438
H	5.846789	1.692663	0.798452
H	5.364858	0.526942	-0.431068
H	4.672686	2.143529	-0.434781
Cl	2.675313	-1.586174	-1.115930
Cl	1.284777	1.659021	-1.117024
C	-3.204482	0.758855	0.110085
H	-3.016912	1.099177	1.132256
H	-2.354576	1.076735	-0.501441

C	-3.323553	-1.443532	-1.315646
H	-2.671399	-2.316543	-1.498034
H	-4.334179	-1.831040	-1.427432
H	-3.038350	-0.690354	-2.044492
C	-4.464296	1.372659	-0.411151
C	-5.260701	2.157875	0.300702
H	-4.719788	1.149320	-1.445840
H	-5.035356	2.409320	1.333615
H	-6.161836	2.585632	-0.126001

Imaginary vibration frequency: 168.75i

SLC-STrain-29

C	-1.677436	0.162406	-0.801628
C	-0.328273	0.897673	-0.782747
H	-2.085926	0.006666	-1.797426
H	-0.187866	1.677763	-0.035410
H	0.043883	1.234848	-1.749961
O	-0.959564	-1.081396	-0.393655
C	0.181660	-0.438813	-0.377896
O	1.254968	-0.955268	-0.093538
C	-2.732858	0.586080	0.190149
Al	2.993476	-0.178338	0.042799
C	4.213174	-1.604606	0.566962
C	5.669619	-1.162207	0.715575
H	4.137259	-2.408378	-0.176311
H	3.851481	-2.034640	1.509501
H	6.322970	-1.990732	1.010175
H	6.066208	-0.757642	-0.220699
H	5.779145	-0.381176	1.474274
Cl	3.240135	0.679479	-1.933015
Cl	2.629053	1.409467	1.476840
C	-2.266621	0.576302	1.629556
H	-1.912298	-0.406606	1.940346
H	-1.458436	1.300976	1.767197
H	-3.085230	0.870118	2.286816
C	-3.283291	1.931752	-0.235956
H	-3.634602	1.918973	-1.269063
H	-4.112703	2.221877	0.409726
H	-2.500530	2.691301	-0.142329
Br	-4.198109	-0.758150	0.019006

TS-STrain-29

C	-2.006667	-1.401842	-0.103252
C	-0.567741	-1.094354	-0.254580

H	-2.282037	-2.421306	0.149187
H	-0.388974	-0.144387	-0.762560
H	-0.049225	-1.882450	-0.804999
O	-0.716637	-1.326741	2.104853
C	-0.000293	-1.025545	1.167922
O	1.225306	-0.651490	1.268961
C	-3.044297	-0.475709	-0.030710
Al	2.532834	-0.030806	0.174920
C	4.130043	0.420118	1.212200
C	5.294244	0.964973	0.385093
H	4.445791	-0.476554	1.761074
H	3.840450	1.149542	1.979795
H	6.167763	1.206993	1.001756
H	5.624277	0.244027	-0.369611
H	5.015742	1.879021	-0.148924
Cl	2.836995	-1.615488	-1.314434
Cl	1.635911	1.673977	-0.881424
C	-2.892498	-1.024163	-1.662240
H	-2.608740	-2.051399	-1.925723
H	-3.962607	-0.984753	-1.867923
H	-2.310324	-0.300875	-2.218980
Br	-2.621922	1.386017	0.037048
C	-4.363883	-0.823375	0.576698
H	-5.169876	-0.230200	0.144844
H	-4.571844	-1.886161	0.435167
H	-4.312163	-0.620717	1.648537

Imaginary vibration frequency: 240.08i

SLC-STrain-37

C	-1.975625	0.853707	-0.144509
C	-0.608650	1.198851	0.461811
H	-2.375106	1.596485	-0.831136
H	-0.480300	0.985728	1.523847
H	-0.199689	2.179178	0.218310
O	-1.306397	-0.213084	-0.950239
C	-0.145171	0.104575	-0.433153
O	0.908680	-0.444570	-0.726082
C	-2.988012	0.295011	0.794787
H	-3.343932	1.088406	1.451395
H	-2.582130	-0.520953	1.390717
Al	2.684327	-0.161627	-0.082904
C	3.832764	-1.442394	-0.997923
C	5.308902	-1.346116	-0.609251
H	3.717543	-1.294390	-2.079114

H	3.453150	-2.451258	-0.792463
H	5.922903	-2.081322	-1.140821
H	5.722040	-0.358421	-0.835932
H	5.457010	-1.517622	0.461376
Cl	2.973978	1.940431	-0.527260
Cl	2.405161	-0.415321	2.053491
Br	-4.542760	-0.404918	-0.150125

TS-STrain-37

C	-2.250120	0.435241	0.572546
C	-0.922961	0.019864	0.072656
H	-2.378069	0.546308	1.645430
H	-0.963490	-0.430644	-0.923250
H	-0.410564	-0.661353	0.749774
O	-0.840663	2.388740	-0.164568
C	-0.173982	1.364090	-0.073669
O	1.098886	1.326175	-0.108909
C	-3.035003	1.298891	-0.267474
H	-3.724950	2.014848	0.165619
H	-2.811150	1.370767	-1.324343
Al	2.432274	0.078265	-0.023291
C	4.161327	0.966444	-0.236683
C	5.369037	0.030160	-0.201847
H	4.251637	1.725942	0.550720
H	4.143783	1.522574	-1.182947
H	6.316527	0.567958	-0.322556
H	5.428662	-0.515835	0.744941
H	5.321275	-0.718605	-0.998758
Cl	2.136846	-0.905373	1.911925
Cl	1.931697	-1.365731	-1.589690
Br	-3.911829	-0.635374	-0.036720

Imaginary vibration frequency: 209.44i

SLC-STrain-39

C	-1.367379	0.117862	0.897633
C	-0.164108	-0.691446	0.409054
H	-1.696827	-0.110290	1.909771
H	-0.202443	-1.035591	-0.625231
H	0.192647	-1.491173	1.057410
O	-0.474611	1.326210	0.966168
C	0.548416	0.603886	0.576034
O	1.684919	1.040533	0.454728
C	-2.508572	0.364361	-0.047674
Al	3.310405	0.175585	-0.058378

C	4.666490	1.569312	-0.186686
C	6.048780	1.063019	-0.601515
H	4.726863	2.077520	0.784033
H	4.312967	2.326030	-0.898503
H	6.783107	1.873795	-0.661016
H	6.439093	0.327493	0.108582
H	6.023701	0.579290	-1.582811
Cl	3.522831	-1.296177	1.516609
Cl	2.707237	-0.805775	-1.895319
C	-3.448286	1.456963	0.423645
H	-3.882839	1.186201	1.389892
H	-2.824451	2.346617	0.584493
C	-4.517438	1.786354	-0.564222
C	-5.815434	1.746749	-0.301016
H	-4.176595	2.082749	-1.555244
H	-6.552997	2.008121	-1.052405
H	-6.188245	1.450008	0.675478
H	-2.131971	0.569420	-1.051194
Br	-3.431592	-1.365026	-0.196713

TS-STrain-39

C	1.569780	-0.005243	-0.774743
C	0.163323	-0.299461	-0.397369
H	1.847011	-0.027890	-1.823519
H	0.035955	-0.513625	0.666580
H	-0.272779	-1.113392	-0.978366
O	0.319719	1.891670	-1.149179
C	-0.472140	1.036213	-0.749301
O	-1.725257	1.209583	-0.623262
C	2.522447	0.558612	0.154765
Al	-3.137161	0.231788	0.010545
C	-4.772977	1.297777	-0.093218
C	-6.025161	0.593324	0.429054
H	-4.918667	1.597345	-1.139153
H	-4.607437	2.230564	0.461296
H	-6.919445	1.222615	0.353254
H	-6.231957	-0.326206	-0.127514
H	-5.919454	0.311487	1.481427
Cl	-3.136730	-1.587192	-1.205994
Cl	-2.526316	-0.326870	2.038819
Br	2.970724	-1.448833	0.096412
C	3.640022	1.428469	-0.303888
H	3.989104	1.124643	-1.293674
H	3.158888	2.412575	-0.418968

H	2.149212	0.729881	1.163087
C	4.764167	1.515482	0.676193
C	6.012104	1.178598	0.386790
H	4.510676	1.877565	1.670364
H	6.802843	1.259799	1.124751
H	6.290506	0.816960	-0.599265

Imaginary vibration frequency: 193.77i

SLC-STrain-40

C	1.555308	1.333781	-0.312557
C	0.276957	0.927692	-1.048437
H	1.835617	2.379403	-0.443045
H	0.287166	-0.019170	-1.586197
H	-0.191192	1.705436	-1.652477
O	0.814787	1.210321	0.976790
C	-0.268353	0.842417	0.334073
O	-1.326367	0.565913	0.881363
C	2.784178	0.472407	-0.355199
Al	-3.020110	0.051948	0.162975
C	-4.139633	-0.444675	1.679143
C	-5.554407	-0.882749	1.297695
H	-4.181956	0.409485	2.366835
H	-3.632262	-1.246782	2.229932
H	-6.152324	-1.152748	2.175099
H	-6.094929	-0.089339	0.772348
H	-5.542444	-1.754703	0.636511
Cl	-3.565457	1.834706	-0.943775
Cl	-2.454580	-1.515885	-1.221903
H	3.191718	0.537338	-1.365798
C	3.821717	0.899182	0.672474
H	3.971342	1.977690	0.546305
H	3.411793	0.743069	1.675969
C	5.133996	0.198906	0.534419
C	6.267692	0.806943	0.212641
H	5.134415	-0.872327	0.721106
H	7.199371	0.257153	0.130378
H	6.308847	1.876868	0.025460
Br	2.310994	-1.427999	-0.128152

TS-STrain-40

C	-1.696074	-0.840672	0.993266
C	-0.317402	-0.842297	0.438064
H	-1.924678	-1.538879	1.790785
H	-0.226433	-0.393614	-0.552193

H	0.107071	-1.846726	0.402427
O	-0.347426	0.378377	2.412043
C	0.380203	0.003622	1.491315
O	1.618394	0.273582	1.387713
C	-2.687975	0.178678	0.714182
Al	2.877853	0.137193	0.066369
C	4.564291	0.917632	0.673653
C	5.695153	0.861961	-0.353591
H	4.866741	0.401405	1.593988
H	4.373154	1.957902	0.967035
H	6.623172	1.306378	0.024147
H	5.926957	-0.168047	-0.642281
H	5.432949	1.398305	-1.271036
Cl	2.964905	-1.995551	-0.410635
Cl	1.940716	1.158427	-1.632721
Br	-3.184159	-1.396910	-0.524085
C	-2.381099	1.449044	-0.000796
H	-1.948392	2.091448	0.778646
H	-1.607632	1.300216	-0.758479
H	-3.510085	0.224845	1.424129
C	-3.593171	2.101486	-0.588163
C	-4.117754	3.230098	-0.134744
H	-4.039563	1.602842	-1.446121
H	-3.687584	3.760343	0.710324
H	-4.992528	3.670062	-0.601286

Imaginary vibration frequency: 202.77i

SLC-STrain-41

C	1.575332	1.497499	-0.260092
C	0.301385	1.091383	-1.002845
H	1.839097	2.551091	-0.355825
H	0.327920	0.172203	-1.586217
H	-0.191407	1.886771	-1.562678
O	0.847707	1.313056	1.027798
C	-0.228277	0.930414	0.379193
O	-1.269057	0.590119	0.922023
C	2.812451	0.649974	-0.347415
H	3.212614	0.758940	-1.356433
Al	-2.919776	-0.017911	0.168357
C	-4.085708	-0.470302	1.662737
C	-5.467865	-0.975863	1.246344
H	-4.185033	0.416451	2.301469
H	-3.577210	-1.225051	2.275835
H	-6.093788	-1.221633	2.111200

H	-6.010730	-0.229252	0.658542
H	-5.399279	-1.879253	0.632512
Cl	-3.472702	1.683059	-1.057737
Cl	-2.239748	-1.633556	-1.103259
Br	2.379582	-1.257144	-0.170633
C	3.852064	1.060197	0.688457
H	3.985538	2.146360	0.609350
H	3.474426	0.859923	1.695624
C	5.137965	0.413784	0.504390
C	6.205967	-0.111260	0.344484
H	7.152127	-0.585595	0.206980

TS-STrain-41

C	1.637275	-0.093603	-0.707649
C	0.253498	-0.229354	-0.199021
H	1.789386	-0.116176	-1.783868
H	0.214891	-0.497228	0.860466
H	-0.324171	-0.959466	-0.766246
O	0.445674	2.109912	-0.538923
C	-0.331394	1.185380	-0.347897
O	-1.599284	1.306907	-0.249051
C	2.639373	0.597776	0.068034
Al	-3.051084	0.243034	0.042269
C	-4.667350	1.344258	0.085586
C	-5.963243	0.572798	0.333968
H	-4.731161	1.890897	-0.864282
H	-4.532661	2.111685	0.858959
H	-6.841412	1.228585	0.354734
H	-6.141317	-0.176763	-0.443542
H	-5.938178	0.040114	1.289863
Cl	-2.988601	-1.235493	-1.575425
Cl	-2.603060	-0.809708	1.910192
Br	3.004010	-1.480009	0.043290
C	3.721796	1.393914	-0.567519
H	3.937103	1.038203	-1.579336
H	3.268755	2.391978	-0.680604
H	2.400897	0.810019	1.107127
C	4.929099	1.481606	0.230205
C	5.928903	1.534852	0.890865
H	6.820989	1.587146	1.475385

Imaginary vibration frequency: 62.17i

SLC-STrain-42

C	1.407599	-0.272089	0.905548
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C	0.136268	0.591054	0.941945
H	1.738143	-0.644018	1.873983
H	0.134487	1.477265	0.305370
H	-0.272636	0.826504	1.923860
O	0.616034	-1.343450	0.238887
C	-0.466316	-0.604828	0.294984
O	-1.562921	-0.965333	-0.109288
C	2.536775	0.213635	0.045006
H	2.168812	0.507037	-0.938369
Al	-3.237803	-0.040992	-0.139661
C	-4.561715	-1.287852	-0.838140
C	-5.974558	-0.709887	-0.934915
H	-4.562182	-2.179758	-0.198894
H	-4.224858	-1.628055	-1.825449
H	-6.690602	-1.438901	-1.329702
H	-6.347929	-0.389745	0.042684
H	-6.009245	0.163570	-1.593274
Cl	-3.424979	0.561901	1.935054
Cl	-2.736987	1.686558	-1.348994
Br	3.769658	-1.274230	-0.286283
C	3.258492	1.373073	0.721641
H	2.515376	2.140683	0.970333
H	3.694470	1.037883	1.667862
C	4.284116	1.974638	-0.110048
C	5.123347	2.484519	-0.800816
H	5.874027	2.931351	-1.413954

TS-STrain-42

C	-1.728875	-0.860165	0.934467
C	-0.357388	-0.763605	0.378161
H	-1.936571	-1.649768	1.648820
H	-0.287484	-0.185372	-0.545050
H	0.083252	-1.746361	0.202693
O	-0.321253	0.240968	2.489014
C	0.367629	-0.046746	1.513330
O	1.609750	0.208443	1.396415
C	-2.721773	0.189220	0.828788
Al	2.854842	0.124078	0.059749
C	4.550960	0.867010	0.686397
C	5.661277	0.894625	-0.363950
H	4.873995	0.285985	1.559925
H	4.361110	1.881566	1.059922
H	6.595313	1.312864	0.028573
H	5.890315	-0.109284	-0.735190

H	5.379240	1.498534	-1.232152
Cl	2.917742	-1.987174	-0.510275
Cl	1.916040	1.223995	-1.590225
Br	-3.230789	-1.200820	-0.594949
C	-2.409988	1.543249	0.279343
H	-1.941116	2.077115	1.119661
H	-1.662575	1.505887	-0.517961
H	-3.530091	0.148597	1.554231
C	-3.594552	2.253924	-0.161893
C	-4.581974	2.827209	-0.530000
H	-5.454849	3.346370	-0.859788

Imaginary vibration frequency: 107.58i

SLC-STrain-43

C	-2.418273	-0.145985	0.654965
C	-1.123085	-0.927214	0.397720
H	-2.831628	-0.248781	1.656671
H	-1.046275	-1.431689	-0.566371
H	-0.774943	-1.580426	1.196975
O	-1.621341	1.116785	0.605918
C	-0.521959	0.433462	0.405079
O	0.587080	0.938232	0.286673
C	-3.463293	-0.203412	-0.418287
Al	2.291656	0.137535	-0.030231
C	3.579560	1.593190	-0.169468
C	5.016818	1.137852	-0.426301
H	3.530194	2.181265	0.755710
H	3.248790	2.267468	-0.969535
H	5.709723	1.983468	-0.496496
H	5.383396	0.487638	0.373972
H	5.101209	0.574832	-1.360890
Cl	2.466876	-1.199855	1.666651
Cl	1.887033	-1.021030	-1.819576
Cl	-4.672502	1.112282	-0.119956
H	-3.015890	0.028898	-1.385801
C	-4.146604	-1.549724	-0.437777
H	-4.914571	-1.570859	-1.211097
H	-3.417618	-2.333257	-0.662325
H	-4.612725	-1.769387	0.524846

TS-STrain-43

C	-2.654062	0.371743	-0.722041
C	-1.249978	0.497816	-0.258439
H	-2.960595	0.939294	-1.593493

H	-1.084750	0.163506	0.767313
H	-0.878023	1.518993	-0.356362
O	-1.320880	-0.982164	-2.048766
C	-0.565910	-0.431423	-1.247559
O	0.696526	-0.592052	-1.209416
C	-3.597192	-0.613899	-0.219788
Al	2.048263	-0.070962	-0.094195
C	3.745487	-0.821518	-0.710249
C	4.954211	-0.448105	0.147958
H	3.903924	-0.492235	-1.745471
H	3.641417	-1.913034	-0.759737
H	5.886002	-0.881213	-0.233702
H	5.098485	0.636077	0.190622
H	4.838341	-0.794549	1.179781
Cl	1.964906	2.116157	-0.094012
Cl	1.386312	-0.758124	1.880418
Cl	-3.984598	1.014609	0.695494
C	-3.214060	-1.735298	0.665311
H	-2.863478	-2.538096	0.006577
H	-2.417461	-1.486179	1.364129
H	-4.083504	-2.104663	1.209287
H	-4.456440	-0.782500	-0.862427

Imaginary vibration frequency: 229.82i

SLC-STrain-45

C	-1.870871	-1.089855	-0.259363
C	-0.568373	-0.776331	-0.998319
H	-2.199126	-2.126310	-0.335693
H	-0.535684	0.145096	-1.578050
H	-0.125497	-1.598992	-1.559706
O	-1.139945	-0.924820	1.031960
C	-0.034704	-0.643180	0.384014
O	1.031289	-0.387108	0.927479
C	-3.053008	-0.169568	-0.372372
Al	2.735883	0.013848	0.163404
C	3.945779	0.388068	1.644686
C	5.372753	0.732726	1.215538
H	3.952418	-0.483418	2.311457
H	3.519862	1.211006	2.232563
H	6.021901	0.939802	2.073406
H	5.834107	-0.085219	0.653602
H	5.398135	1.617859	0.572474
Cl	3.099455	-1.779610	-1.001907
Cl	2.246318	1.651051	-1.168497

Cl	-2.521673	1.559438	-0.268284
H	-3.455955	-0.290753	-1.380125
C	-4.120861	-0.466793	0.669854
H	-4.331341	-1.540655	0.623466
H	-3.709645	-0.254861	1.662656
C	-5.385966	0.299831	0.461707
C	-6.557953	-0.261808	0.197947
H	-5.315020	1.381918	0.542956
H	-7.452657	0.336382	0.060703
H	-6.669196	-1.339945	0.116077

TS-STrain-45

C	-2.019610	-1.462252	0.332859
C	-0.660855	-1.057212	-0.106455
H	-2.173708	-2.491808	0.635300
H	-0.633570	-0.147289	-0.707432
H	-0.161320	-1.852898	-0.661332
O	-0.723490	-1.057589	2.217071
C	-0.000314	-0.840327	1.245323
O	1.213796	-0.462416	1.312128
C	-3.108731	-0.537246	0.597704
Al	2.468637	0.120533	0.117159
C	4.101436	0.633201	1.062716
C	5.231645	1.123898	0.157830
H	4.438944	-0.229845	1.651141
H	3.842831	1.408115	1.795828
H	6.128521	1.400363	0.724094
H	5.531346	0.357368	-0.563742
H	4.932549	2.004679	-0.419164
Cl	2.704395	-1.530587	-1.298992
Cl	1.460998	1.758920	-0.938619
Cl	-3.400347	-1.222642	-1.151757
C	-2.943138	0.941433	0.656383
H	-2.570684	1.118341	1.676834
H	-2.175801	1.295816	-0.033243
H	-3.917022	-0.947805	1.197107
C	-4.231141	1.671128	0.445546
C	-4.410817	2.567443	-0.513054
H	-5.040288	1.433352	1.133017
H	-3.615967	2.823461	-1.208051
H	-5.357192	3.084115	-0.630877

Imaginary vibration frequency: 222.49i

SLC-STrain-46

C	-2.275779	-0.975902	-0.256083
C	-0.979396	-0.662140	-1.005931
H	-2.635396	-1.998323	-0.368078
H	-0.935988	0.280823	-1.549237
H	-0.567182	-1.472238	-1.607612
O	-1.521166	-0.880247	1.026201
C	-0.419555	-0.598244	0.371365
O	0.660395	-0.391600	0.907220
C	-3.439773	-0.022282	-0.307828
Al	2.372876	-0.015699	0.146681
C	3.604416	0.235885	1.636039
C	5.042635	0.541512	1.215137
H	3.577422	-0.668207	2.257452
H	3.216506	1.044631	2.268179
H	5.704613	0.674339	2.077895
H	5.465296	-0.264127	0.606872
H	5.102793	1.457866	0.619942
Cl	2.665025	-1.762581	-1.106104
Cl	1.935375	1.700056	-1.101032
Cl	-2.861644	1.692658	-0.118771
H	-3.865173	-0.086457	-1.310995
C	-4.467856	-0.316081	0.727356
C	-5.720527	-0.623401	0.423134
H	-4.135687	-0.271497	1.761075
H	-6.066989	-0.656540	-0.605791
H	-6.445281	-0.849742	1.197365

TS-STrain-46

C	-2.444162	-0.857580	0.668628
C	-1.035743	-0.946277	0.189712
H	-2.808342	-1.593689	1.373723
H	-0.850986	-0.459159	-0.768242
H	-0.687844	-1.978271	0.128523
O	-1.202172	0.084061	2.229420
C	-0.390770	-0.213079	1.343014
O	0.847682	0.058111	1.374489
C	-3.334679	0.245815	0.348800
Al	2.185509	0.051981	0.118882
C	3.826424	0.779241	0.893090
C	5.013606	0.823518	-0.069201
H	4.081926	0.182691	1.778332
H	3.608231	1.787492	1.268097
H	5.913335	1.239638	0.398433
H	5.274075	-0.175104	-0.433715

H	4.796539	1.437140	-0.949282
Cl	2.309248	-2.022821	-0.554895
Cl	1.339109	1.234747	-1.523433
Cl	-3.757012	-1.185516	-0.928783
C	-2.887801	1.474382	-0.275672
H	-4.224358	0.316852	0.966751
C	-3.595817	2.590420	-0.115141
H	-1.957383	1.471849	-0.833400
H	-3.252588	3.532523	-0.527028
H	-4.527510	2.597296	0.442585

Imaginary vibration frequency: 377.80i

SLC-STrain-47

C	2.283660	0.893823	0.571428
C	1.115502	0.829111	-0.416285
H	2.639558	1.897744	0.799625
H	1.164583	0.066418	-1.192951
H	0.782727	1.779398	-0.833333
O	1.353404	0.467938	1.653206
C	0.362164	0.407277	0.796102
O	-0.780990	0.090717	1.094511
C	3.455142	-0.039849	0.420395
H	4.024393	-0.056602	1.349909
Al	-2.369213	-0.002517	0.038573
C	-3.753686	-0.766799	1.177661
C	-5.114945	-0.918417	0.497325
H	-3.846904	-0.137457	2.071768
H	-3.400280	-1.742404	1.534858
H	-5.864303	-1.352334	1.168458
H	-5.506789	0.045656	0.158696
H	-5.056852	-1.567555	-0.381780
Cl	-2.587426	2.069859	-0.560846
Cl	-1.709080	-1.176621	-1.659146
C	4.310022	0.376364	-0.724585
Cl	2.870270	-1.744214	0.169984
C	5.583040	0.715878	-0.581996
H	3.831299	0.395423	-1.700404
H	6.076322	0.687857	0.385026
H	6.177307	1.029600	-1.433186

TS-STrain-47

C	-2.340922	0.414428	-0.669431
C	-0.909934	0.661227	-0.337000
H	-2.704979	0.635830	-1.665358

H	-0.717185	0.716861	0.736443
H	-0.511157	1.555625	-0.817365
O	-1.218475	-1.321504	-1.446739
C	-0.345886	-0.605908	-0.938090
O	0.891029	-0.883136	-0.909888
C	-3.239865	-0.263795	0.243811
Al	2.360135	-0.183719	-0.062906
C	3.925763	-1.285793	-0.458659
C	5.212279	-0.836889	0.234351
H	4.068853	-1.296665	-1.546943
H	3.690815	-2.321458	-0.180899
H	6.064625	-1.480202	-0.012821
H	5.488015	0.183743	-0.049084
H	5.107783	-0.847534	1.323852
Cl	2.472677	1.884386	-0.762591
Cl	1.764491	-0.141874	2.044878
C	-4.415372	-0.968574	-0.221826
H	-2.804337	-0.591662	1.184281
Cl	-3.546897	1.663196	0.487319
C	-4.943110	-1.946519	0.510428
H	-5.788069	-2.521579	0.149009
H	-4.536554	-2.212496	1.481090
H	-4.812310	-0.701093	-1.196204

Imaginary vibration frequency: 377.08i

SLC-STrain-48

C	-1.864158	0.510669	-0.859712
C	-0.617835	1.026197	-0.138095
H	-2.187182	1.102177	-1.714767
H	-0.647492	1.005222	0.951918
H	-0.201511	1.970959	-0.486270
O	-1.054068	-0.643577	-1.361509
C	0.009765	-0.177852	-0.747229
O	1.109305	-0.710585	-0.790144
C	-3.013374	0.016894	-0.022173
H	-2.646985	-0.571533	0.819678
Al	2.766817	-0.205248	0.024970
C	4.082331	-1.540209	-0.507821
C	5.487538	-1.287298	0.040621
H	4.106792	-1.576964	-1.604310
H	3.722454	-2.524832	-0.183639
H	6.198811	-2.056007	-0.280704
H	5.883627	-0.323314	-0.293124
H	5.498159	-1.276887	1.134847

Cl	3.010403	1.806439	-0.742760
Cl	2.199785	-0.124647	2.115134
C	-4.021306	-0.777618	-0.837508
H	-4.439153	-0.142676	-1.625017
H	-3.480531	-1.591844	-1.333192
Cl	-3.768524	1.491544	0.689196
C	-5.090183	-1.338488	-0.031921
C	-5.968396	-1.805655	0.640676
H	-6.752097	-2.219319	1.235483

TS-STrain-48

C	-2.010670	0.598224	-0.680805
C	-0.598820	0.556866	-0.235505
H	-2.209161	0.804164	-1.729038
H	-0.496415	0.698671	0.844139
H	0.014125	1.303818	-0.739771
O	-0.984229	-1.706183	-0.839195
C	-0.134652	-0.868391	-0.570307
O	1.123539	-1.094905	-0.538031
C	-2.997643	-0.198122	0.013315
Al	2.640951	-0.238859	-0.006181
C	4.171181	-1.447684	-0.163070
C	5.501818	-0.856552	0.302173
H	4.246960	-1.765349	-1.211176
H	3.944960	-2.358644	0.406076
H	6.332529	-1.563899	0.195905
H	5.767588	0.038083	-0.269817
H	5.464747	-0.561329	1.355526
Cl	2.767936	1.551132	-1.265589
Cl	2.195783	0.419431	2.036804
C	-4.165143	-0.790980	-0.680358
H	-4.417361	-0.220741	-1.578751
H	-3.779928	-1.764155	-1.025611
H	-2.731197	-0.577187	0.995725
Cl	-3.166499	1.762509	0.294352
C	-5.321324	-0.983217	0.172880
C	-6.278685	-1.129482	0.880599
H	-7.132795	-1.265738	1.506784

Imaginary vibration frequency: 71.59i

SLC-STrain-49

C	-1.693076	-1.763048	0.699537
C	-0.542786	-1.581767	-0.293515
H	-1.914733	-2.791596	0.974474

H	-0.689373	-0.887713	-1.119634
H	-0.074922	-2.499436	-0.649642
O	-0.825572	-1.167273	1.759532
C	0.139428	-0.989947	0.888108
O	1.216331	-0.476700	1.158712
C	-2.958583	-0.940364	0.546791
H	-3.531587	-1.035899	1.469483
Al	2.707336	-0.045506	0.046068
C	4.065451	0.726486	1.211836
C	5.352135	1.134671	0.493085
H	4.289877	-0.000034	2.003105
H	3.625323	1.594271	1.719284
H	6.089284	1.564246	1.180357
H	5.829305	0.280314	0.003184
H	5.161351	1.883150	-0.282152
Cl	3.143107	-1.967639	-0.859066
Cl	1.786855	1.254785	-1.421451
C	-2.734730	0.511804	0.237707
C	-2.551356	0.991465	-1.056283
C	-2.650825	1.396851	1.310617
C	-2.271959	2.332584	-1.270881
H	-2.640895	0.319572	-1.902566
C	-2.366870	2.737111	1.094294
H	-2.805840	1.033545	2.321339
C	-2.173725	3.206830	-0.197208
H	-2.128924	2.694623	-2.282720
H	-2.301681	3.415663	1.937493
H	-1.952129	4.254406	-0.368006
Cl	-3.927323	-1.796429	-0.715564

TS-STrain-49

C	-1.595630	-1.894480	0.488259
C	-0.272821	-1.414753	0.016578
H	-1.626745	-2.816312	1.056892
H	-0.310979	-0.676814	-0.782851
H	0.375037	-2.236687	-0.291891
O	-0.575232	-0.870939	2.246866
C	0.216533	-0.782511	1.306177
O	1.355115	-0.219135	1.364370
C	-2.834916	-1.132063	0.443728
Al	2.686490	0.161549	0.168366
C	4.120486	1.141774	1.066399
C	5.297134	1.513839	0.164168
H	4.471541	0.534328	1.910637

H	3.687683	2.046454	1.512674
H	6.079928	2.059449	0.703698
H	5.766889	0.626432	-0.271682
H	4.980723	2.148364	-0.669743
Cl	3.266783	-1.785977	-0.645685
Cl	1.680105	1.267883	-1.434064
Cl	-2.894489	-2.355882	-1.053765
H	-3.589996	-1.494130	1.135366
C	-2.951776	0.289508	0.111792
C	-3.659171	1.064479	1.033282
C	-2.370038	0.894599	-1.003430
C	-3.738421	2.437410	0.868424
H	-4.125354	0.589685	1.889997
C	-2.468457	2.263932	-1.169787
H	-1.873647	0.304643	-1.764023
C	-3.141297	3.037398	-0.230819
H	-4.273662	3.036399	1.595927
H	-2.016434	2.730383	-2.037111
H	-3.208960	4.111063	-0.365440

Imaginary vibration frequency: 322.72i

SLC-STrain-50

C	-1.728505	-1.838754	-0.375634
C	-0.466761	-1.346340	-1.095116
H	-1.988912	-2.881571	-0.539499
H	-0.524221	-0.383802	-1.602338
H	0.040853	-2.081604	-1.719340
O	-0.990472	-1.733855	0.915140
C	0.066772	-1.273132	0.290952
O	1.099220	-0.933440	0.852997
C	-2.936442	-0.936302	-0.424433
H	-3.375852	-1.072163	-1.414055
Al	2.675261	-0.123671	0.141133
C	3.865283	0.215936	1.646876
C	5.183892	0.888875	1.262804
H	4.061770	-0.738312	2.151757
H	3.324997	0.833741	2.375362
H	5.824778	1.066034	2.133493
H	5.758788	0.278408	0.559622
H	5.017614	1.858643	0.783680
Cl	3.296864	-1.603409	-1.317500
Cl	1.843424	1.596698	-0.880895
C	-2.647972	0.517689	-0.198386
C	-2.685767	1.378715	-1.291992

C	-2.282362	1.015396	1.050792
C	-2.344602	2.715688	-1.146184
H	-2.980292	0.998471	-2.265146
C	-1.943270	2.351824	1.194139
H	-2.274171	0.361403	1.914866
C	-1.968294	3.202929	0.096776
H	-2.373609	3.375953	-2.005730
H	-1.656212	2.730143	2.168803
H	-1.697114	4.246352	0.212316
Cl	-4.168443	-1.581569	0.739738

TS-STrain-50

C	-1.298534	0.809933	-0.517950
C	0.160132	0.875949	-0.210937
H	-1.623958	0.950477	-1.540346
H	0.373294	1.027804	0.849566
H	0.684026	1.636374	-0.791528
O	-0.501567	-1.152800	-1.024406
C	0.501721	-0.526153	-0.652837
O	1.679668	-0.991853	-0.641113
C	-2.274716	0.441874	0.487029
Al	3.309604	-0.377992	-0.062001
C	4.661600	-1.761892	-0.343225
C	6.065270	-1.386496	0.131950
H	4.679804	-2.006419	-1.413227
H	4.324762	-2.675652	0.163205
H	6.793101	-2.186370	-0.046694
H	6.438488	-0.493299	-0.378946
H	6.082836	-1.170394	1.204806
Cl	3.624767	1.471900	-1.184184
Cl	2.947529	0.159454	2.028751
H	-1.859130	0.226377	1.467717
Cl	-2.248218	2.425679	0.425063
C	-3.566336	-0.158752	0.207973
C	-4.146519	-0.150346	-1.063937
C	-4.224962	-0.784090	1.270020
C	-5.366879	-0.765892	-1.263969
H	-3.652981	0.335610	-1.897044
C	-5.444679	-1.403831	1.061651
H	-3.768166	-0.788621	2.253974
C	-6.015137	-1.393116	-0.204066
H	-5.816254	-0.763376	-2.250062
H	-5.949699	-1.896112	1.884344
H	-6.970886	-1.877996	-0.369511

Imaginary vibration frequency: 405.66i**SLC-STrain-51**

C	-2.376390	-0.901407	0.533396
C	-1.207280	-0.753876	-0.444161
H	-2.744655	-1.918424	0.648026
H	-1.236299	0.089276	-1.133235
H	-0.897734	-1.656207	-0.970908
O	-1.429138	-0.615487	1.652993
C	-0.440234	-0.493253	0.802187
O	0.714352	-0.241588	1.128365
C	-3.516569	0.094432	0.499979
Al	2.258870	0.039228	0.047529
C	3.746852	0.385686	1.258333
C	5.075515	0.662180	0.553081
H	3.848878	-0.476511	1.929550
H	3.477262	1.233774	1.900390
H	5.888249	0.848385	1.263753
H	5.383306	-0.180852	-0.073228
H	5.011479	1.538877	-0.098796
Cl	2.327698	-1.790997	-1.113397
Cl	1.598290	1.673993	-1.215944
O	-4.267947	-0.323195	-0.619062
C	-5.562908	0.234150	-0.682605
H	-6.083198	-0.265477	-1.500168
H	-6.116425	0.060368	0.249273
H	-5.541456	1.309856	-0.888880
C	-3.083462	1.544983	0.427837
H	-2.408124	1.791286	1.250400
H	-2.587602	1.767447	-0.519590
H	-3.948764	2.203009	0.518694
H	-4.103287	-0.060918	1.418991

TS-STrain-51

C	-2.604285	0.684972	0.745462
C	-1.258453	0.053625	0.648529
H	-2.878789	1.158626	1.678041
H	-1.139024	-0.686848	-0.142515
H	-0.918423	-0.375617	1.592292
O	-1.299525	2.292351	0.242905
C	-0.524656	1.324953	0.305227
O	0.724692	1.383868	0.103705
C	-3.647903	0.591416	-0.271767
Al	2.045587	0.116540	-0.034356

C	3.754507	0.986061	-0.413031
C	4.944956	0.031841	-0.509549
H	3.934806	1.733580	0.370400
H	3.650723	1.554573	-1.346128
H	5.883780	0.557518	-0.718325
H	5.089881	-0.526435	0.420652
H	4.806673	-0.706309	-1.305880
Cl	1.961851	-0.976987	1.857434
Cl	1.305944	-1.223428	-1.604154
O	-3.967585	-0.524005	0.632390
C	-3.779114	-1.873318	0.177865
H	-4.486478	-2.079642	-0.626229
H	-2.761142	-2.066445	-0.157298
H	-4.001348	-2.497713	1.041370
C	-3.340791	0.291483	-1.701159
H	-4.241469	-0.041721	-2.219436
H	-3.017057	1.224388	-2.168671
H	-2.553142	-0.447671	-1.838278
H	-4.440352	1.327854	-0.160573

Imaginary vibration frequency: 426.01i

SLC-STrain-54

C	1.518859	-1.065649	-0.137994
C	0.092597	-1.455633	0.261648
H	1.934316	-1.631161	-0.970140
H	-0.108612	-1.505164	1.332586
H	-0.347719	-2.312712	-0.247195
O	0.958833	0.214032	-0.705782
C	-0.246321	-0.145307	-0.354121
O	-1.249920	0.530766	-0.559522
C	2.510396	-0.798017	0.956890
H	2.720284	-1.766358	1.423218
H	2.041476	-0.168557	1.718976
Al	-3.070440	0.233231	-0.100898
C	-4.095769	1.723691	-0.827667
C	-5.597666	1.644569	-0.550022
H	-3.914400	1.768195	-1.909075
H	-3.685216	2.655116	-0.417674
H	-6.140597	2.496578	-0.973819
H	-6.039649	0.738304	-0.975492
H	-5.809405	1.630532	0.523593
Cl	-3.434929	-1.726600	-0.957768
Cl	-2.950131	0.067413	2.058951
C	3.781046	-0.172366	0.453950

C	4.799797	-0.964906	-0.071010
C	3.945703	1.209900	0.471530
C	5.958564	-0.387841	-0.570488
H	4.687892	-2.045031	-0.081665
C	5.104273	1.789676	-0.027559
H	3.160925	1.837848	0.881105
C	6.113045	0.992410	-0.550868
H	6.745373	-1.017650	-0.971601
H	5.219443	2.867961	-0.005706
H	7.019174	1.444734	-0.938844

TS-STrain-54

C	1.867939	-0.973670	0.345168
C	0.513768	-0.363609	0.147586
H	1.937995	-1.616494	1.218631
H	0.530285	0.520146	-0.495518
H	0.050319	-0.066721	1.088405
O	0.217985	-2.330207	-1.167791
C	-0.335342	-1.407175	-0.578345
O	-1.610406	-1.253516	-0.559214
C	2.415650	-1.544536	-0.844461
H	3.073405	-2.405124	-0.820483
H	2.230194	-1.079965	-1.803412
Al	-2.798539	0.002800	-0.006497
C	-4.609040	-0.529421	-0.529523
C	-5.701810	0.473419	-0.160519
H	-4.822131	-1.503122	-0.069142
H	-4.613172	-0.708134	-1.612623
H	-6.699538	0.136145	-0.465158
H	-5.739054	0.649912	0.919184
H	-5.532940	1.445089	-0.635428
Cl	-2.524042	0.190364	2.162139
Cl	-2.111480	1.873610	-0.927657
C	3.174695	-0.167575	0.191317
C	4.326471	-0.633869	0.851620
C	3.236877	1.025487	-0.550422
C	5.495501	0.096696	0.804571
H	4.278403	-1.563540	1.408755
C	4.410107	1.748967	-0.590532
H	2.361593	1.386200	-1.077585
C	5.535631	1.287275	0.086039
H	6.377782	-0.256681	1.324718
H	4.453180	2.675415	-1.150511
H	6.455243	1.860756	0.049484

Imaginary vibration frequency: 317.77i

SLC-STrain-56

C	1.391303	-0.948230	-0.458690
C	-0.032558	-1.403327	-0.122744
H	1.786373	-1.335800	-1.396400
H	-0.218797	-1.664064	0.919962
H	-0.493680	-2.136030	-0.784361
O	0.836792	0.423602	-0.738335
C	-0.366978	0.007339	-0.451290
O	-1.368376	0.716049	-0.498458
C	2.408241	-0.926773	0.652283
H	1.927672	-0.477327	1.528426
Al	-3.175783	0.312381	-0.067487
C	-4.222858	1.923766	-0.395424
C	-5.713183	1.774840	-0.085720
H	-4.083248	2.215202	-1.444145
H	-3.793546	2.739002	0.200605
H	-6.269238	2.698083	-0.282451
H	-6.174299	0.987303	-0.689727
H	-5.883315	1.514752	0.963603
Cl	-3.568251	-1.400958	-1.340016
Cl	-2.985887	-0.348954	1.991044
C	3.596266	-0.070701	0.280401
C	3.807832	1.144486	0.924209
C	4.486514	-0.463495	-0.717772
C	4.886578	1.950480	0.584983
H	3.118411	1.463249	1.699818
C	5.563627	0.340532	-1.060884
H	4.343683	-1.408300	-1.232495
C	5.767581	1.550628	-0.409656
H	5.036555	2.894130	1.098392
H	6.247746	0.020378	-1.839434
H	6.610492	2.178378	-0.677334
C	2.785898	-2.366814	0.991919
H	1.909515	-2.940691	1.303823
H	3.236100	-2.875812	0.136567
H	3.508202	-2.378511	1.809656

TS-STrain-56

C	1.723750	1.120524	-0.709719
C	0.472740	0.346331	-0.481257
H	2.060384	1.219482	-1.734343
H	0.341843	-0.014586	0.538140

H	0.358855	-0.492830	-1.169937
O	0.033225	2.509019	-1.127840
C	-0.509767	1.450961	-0.792903
O	-1.767490	1.281374	-0.702287
C	2.570169	1.661993	0.325128
H	3.222195	2.448984	-0.050009
Al	-2.834339	-0.078373	-0.104133
C	-4.710019	0.467810	-0.194859
C	-5.705199	-0.584921	0.292883
H	-4.934051	0.744566	-1.233235
H	-4.823241	1.391069	0.388038
H	-6.743358	-0.239302	0.226904
H	-5.636154	-1.506713	-0.293307
H	-5.523775	-0.857512	1.337355
Cl	-2.306052	-1.796451	-1.352648
Cl	-2.095940	-0.490383	1.920923
C	3.312741	0.308637	0.170096
C	4.313901	0.189799	-0.804658
C	3.024676	-0.781607	1.001834
C	5.038368	-0.981299	-0.918961
H	4.523841	1.030548	-1.457945
C	3.756301	-1.947783	0.884236
H	2.249317	-0.707385	1.754164
C	4.758282	-2.049952	-0.075358
H	5.819192	-1.064665	-1.665823
H	3.542836	-2.784215	1.539302
H	5.322650	-2.971306	-0.166927
C	1.992435	1.985755	1.679125
H	2.794144	2.080142	2.413176
H	1.465275	2.939526	1.617717
H	1.284175	1.238584	2.037281

Imaginary vibration frequency: 311.25i

SLC-STrain-58

C	-1.372285	-0.437277	-0.848372
C	-0.023008	0.040620	-0.444349
H	-1.638234	-0.358933	-1.896746
H	0.085468	0.192498	0.630009
H	0.292059	0.945942	-0.966394
O	0.061908	-2.062365	-1.373601
C	0.766166	-1.167448	-0.894482
O	2.030624	-1.231650	-0.771547
C	-2.372922	-0.925948	0.059442
H	-1.979687	-1.155090	1.048980

Al	3.315197	-0.167710	-0.022179
C	5.056813	-1.044093	-0.179104
C	6.221808	-0.271128	0.438573
H	5.249418	-1.226392	-1.244397
H	4.979053	-2.037775	0.280892
H	7.176870	-0.797634	0.327767
H	6.342909	0.713324	-0.024321
H	6.070767	-0.102840	1.509535
Cl	3.146475	1.746228	-1.071291
Cl	2.622320	0.146917	2.034392
C	-2.832209	0.553613	0.051216
C	-3.669821	1.055553	-0.954918
C	-2.426902	1.393317	1.099067
C	-4.123607	2.360365	-0.887129
H	-3.973689	0.422254	-1.780242
C	-2.888739	2.692006	1.161821
H	-1.768184	1.008739	1.869582
C	-3.735464	3.175930	0.168360
H	-4.778876	2.744037	-1.660203
H	-2.589375	3.332723	1.982870
H	-4.091176	4.199083	0.217247
C	-3.361136	-1.967717	-0.432821
H	-2.834126	-2.924943	-0.455095
H	-3.649117	-1.743748	-1.465265
C	-4.570742	-2.060614	0.437877
C	-4.915096	-3.143598	1.121461
H	-5.191313	-1.168234	0.499618
H	-5.807235	-3.163313	1.738708
H	-4.320025	-4.052290	1.084398

TS-STrain-58

C	-1.372285	-0.437277	-0.848372
C	-0.023008	0.040620	-0.444349
H	-1.638234	-0.358933	-1.896746
H	0.085468	0.192498	0.630009
H	0.292059	0.945942	-0.966394
O	0.061908	-2.062365	-1.373601
C	0.766166	-1.167448	-0.894482
O	2.030624	-1.231650	-0.771547
C	-2.372922	-0.925948	0.059442
H	-1.979687	-1.155090	1.048980
Al	3.315197	-0.167710	-0.022179
C	5.056813	-1.044093	-0.179104
C	6.221808	-0.271128	0.438573

H	5.249418	-1.226392	-1.244397
H	4.979053	-2.037775	0.280892
H	7.176870	-0.797634	0.327767
H	6.342909	0.713324	-0.024321
H	6.070767	-0.102840	1.509535
Cl	3.146475	1.746228	-1.071291
Cl	2.622320	0.146917	2.034392
C	-2.832209	0.553613	0.051216
C	-3.669821	1.055553	-0.954918
C	-2.426902	1.393317	1.099067
C	-4.123607	2.360365	-0.887129
H	-3.973689	0.422254	-1.780242
C	-2.888739	2.692006	1.161821
H	-1.768184	1.008739	1.869582
C	-3.735464	3.175930	0.168360
H	-4.778876	2.744037	-1.660203
H	-2.589375	3.332723	1.982870
H	-4.091176	4.199083	0.217247
C	-3.361136	-1.967717	-0.432821
H	-2.834126	-2.924943	-0.455095
H	-3.649117	-1.743748	-1.465265
C	-4.570742	-2.060614	0.437877
C	-4.915096	-3.143598	1.121461
H	-5.191313	-1.168234	0.499618
H	-5.807235	-3.163313	1.738708
H	-4.320025	-4.052290	1.084398

Imaginary vibration frequency: 312.18i

SLC-STrain-59

C	1.492557	-1.774568	0.371538
C	0.216964	-1.303942	1.077017
H	1.759872	-2.814799	0.549551
H	0.251169	-0.326241	1.556808
H	-0.274310	-2.032650	1.721950
O	0.734678	-1.723156	-0.929289
C	-0.325074	-1.278582	-0.306105
O	-1.374404	-0.979313	-0.867092
C	2.703125	-0.868985	0.363129
H	3.134990	-0.996024	1.363382
Al	-2.959735	-0.203095	-0.159844
C	-4.179484	0.059753	-1.658618
C	-5.521579	0.683101	-1.272628
H	-4.340555	-0.911009	-2.144413
H	-3.673744	0.686404	-2.404216

H	-6.179048	0.816469	-2.138864
H	-6.062283	0.062411	-0.551470
H	-5.391708	1.667931	-0.813358
Cl	-3.534376	-1.659545	1.343083
Cl	-2.186826	1.572113	0.814501
C	2.338433	0.589112	0.205253
C	2.385737	1.437431	1.309525
C	1.919427	1.111082	-1.018249
C	2.014731	2.770297	1.201666
H	2.716967	1.046752	2.266926
C	1.544109	2.442874	-1.127298
H	1.882811	0.477797	-1.897460
C	1.588369	3.275944	-0.018220
H	2.055933	3.413678	2.073845
H	1.212672	2.829751	-2.084718
H	1.290127	4.314904	-0.104266
C	3.735614	-1.368907	-0.658064
H	3.906699	-2.437960	-0.497794
H	3.321243	-1.258793	-1.666482
C	5.031407	-0.632895	-0.569543
C	6.198772	-1.199568	-0.292837
H	4.987562	0.440413	-0.744879
H	6.284527	-2.268080	-0.111562
H	7.113219	-0.617508	-0.242296

TS-STrain-59

C	-1.425034	0.042211	1.307874
C	-0.132654	-0.291288	0.647050
H	-1.645692	-0.471709	2.235713
H	-0.071470	-0.016333	-0.405439
H	0.141225	-1.342474	0.753180
O	0.140862	1.237042	2.342638
C	0.757106	0.599124	1.482136
O	2.012435	0.670655	1.290039
C	-2.446014	0.907016	0.772767
H	-3.126764	1.266957	1.542709
Al	3.153636	-0.016864	0.036058
C	4.971636	0.616209	0.379562
C	6.024574	0.083202	-0.591961
H	5.237180	0.342108	1.408861
H	4.961515	1.713610	0.359145
H	7.029193	0.458310	-0.364847
H	6.077321	-1.009827	-0.568413
H	5.801429	0.368918	-1.624789

Cl	2.896539	-2.186541	0.169039
Cl	2.294092	0.627307	-1.876767
C	-3.018732	-0.418357	0.207016
C	-3.923380	-1.149239	0.990339
C	-2.679913	-0.881146	-1.071287
C	-4.510552	-2.294244	0.488198
H	-4.171843	-0.797334	1.986222
C	-3.273083	-2.026450	-1.567556
H	-1.971315	-0.337189	-1.683310
C	-4.184973	-2.732603	-0.790631
H	-5.220513	-2.847850	1.091309
H	-3.021238	-2.373880	-2.562593
H	-4.642706	-3.633411	-1.184083
C	-2.085020	1.998067	-0.217627
H	-1.559438	2.780030	0.336590
H	-1.386896	1.621557	-0.970402
C	-3.294111	2.566155	-0.886899
C	-3.671514	3.833678	-0.791219
H	-3.883416	1.875643	-1.487954
H	-4.554331	4.201185	-1.303920
H	-3.106609	4.552305	-0.203367

Imaginary vibration frequency: 311.67i

SLC-STrain-60

C	1.236587	0.179283	-1.035185
C	-0.171397	-0.356375	-1.314837
H	1.628207	0.821081	-1.819693
H	-0.351902	-1.400356	-1.057974
H	-0.602316	-0.117701	-2.286870
O	0.640545	1.071271	0.017292
C	-0.549799	0.594055	-0.236792
O	-1.568457	0.949170	0.347657
C	2.288100	-0.768722	-0.470161
Al	-3.358497	0.322843	0.202632
C	-4.419952	1.332397	1.489311
C	-5.899495	0.946586	1.521407
H	-4.313575	2.400121	1.259327
H	-3.973354	1.195300	2.482341
H	-6.462500	1.532491	2.256309
H	-6.378814	1.103577	0.550169
H	-6.035936	-0.108267	1.779011
Cl	-3.777066	0.642153	-1.901692
Cl	-3.109505	-1.800097	0.573786
C	3.495054	0.039210	0.015363

C	4.073114	-0.203331	1.258153
C	4.077288	1.007159	-0.804303
C	5.192453	0.505693	1.676208
H	3.654742	-0.961539	1.909455
C	5.192813	1.717781	-0.388756
H	3.671518	1.212378	-1.788994
C	5.754888	1.472136	0.857150
H	5.624084	0.297440	2.649306
H	5.625890	2.465870	-1.044018
H	6.627027	2.028141	1.183185
C	2.712623	-1.664383	-1.637114
H	3.480680	-2.365631	-1.307384
H	1.868865	-2.235167	-2.032901
H	3.132912	-1.065958	-2.447269
C	1.672150	-1.551433	0.663863
H	1.350594	-0.955294	1.515246
C	1.481562	-2.862261	0.700214
H	1.009306	-3.326161	1.559693
H	1.784076	-3.522550	-0.105483

TS-STrain-60

C	-1.518632	-0.643849	-0.834429
C	-0.196847	0.017647	-0.639561
H	-1.905683	-0.681677	-1.846293
H	-0.007815	0.384135	0.367454
H	-0.024182	0.830842	-1.346732
O	-0.023851	-2.158699	-1.317027
C	0.653268	-1.184683	-0.961980
O	1.919685	-1.181820	-0.863489
C	-2.387952	-1.140175	0.215874
Al	3.121343	-0.022692	-0.108553
C	4.921545	-0.779860	-0.203451
C	6.010397	0.094324	0.418772
H	5.154561	-0.977579	-1.257728
H	4.903320	-1.762647	0.285019
H	7.003767	-0.363555	0.347673
H	6.071654	1.071298	-0.070977
H	5.818871	0.281703	1.480049
Cl	2.846034	1.859702	-1.186842
Cl	2.356797	0.271792	1.927473
C	-2.965956	0.324343	0.132109
C	-3.945099	0.653058	-0.816851
C	-2.530764	1.308295	1.031681
C	-4.497880	1.920464	-0.840334

H	-4.286222	-0.087825	-1.528174
C	-3.093512	2.569284	1.006060
H	-1.768519	1.085459	1.766478
C	-4.074631	2.879055	0.070296
H	-5.260050	2.160182	-1.572386
H	-2.761796	3.317362	1.716492
H	-4.506980	3.873234	0.050426
C	-1.750503	-1.476898	1.546973
H	-2.495233	-1.449369	2.343287
H	-1.334036	-2.483266	1.489612
H	-0.940177	-0.802743	1.816951
C	-3.377440	-2.159695	-0.269310
H	-3.644973	-2.096192	-1.320070
C	-3.903065	-3.120797	0.474195
H	-3.663058	-3.252701	1.523061
H	-4.603288	-3.825981	0.040183

Imaginary vibration frequency: 351.54i

SLC-STrain-61

C	1.224144	0.534444	-1.149694
C	0.186786	-0.431694	-0.572649
H	1.641039	0.259308	-2.115458
H	0.280625	-0.665644	0.485635
H	-0.016555	-1.330348	-1.154385
O	0.116731	1.521935	-1.378638
C	-0.744390	0.691037	-0.852989
O	-1.939285	0.937086	-0.719362
C	2.283809	1.090402	-0.214292
Al	-3.347919	-0.132664	-0.025685
C	-4.950764	0.978125	-0.009367
C	-6.194776	0.275364	0.536030
H	-5.134626	1.330038	-1.032423
H	-4.736898	1.877691	0.581765
H	-7.073729	0.929485	0.531302
H	-6.450052	-0.609747	-0.054871
H	-6.049165	-0.059538	1.567710
Cl	-3.325120	-1.821985	-1.387522
Cl	-2.557193	-0.750264	1.897489
O	1.597282	1.347041	0.996141
C	2.329767	2.039281	1.987335
H	1.738945	1.981227	2.901763
H	3.307716	1.580653	2.169098
H	2.469443	3.093076	1.727109
C	2.873593	2.360669	-0.814069

H	3.182771	2.200129	-1.847483
H	2.123195	3.152904	-0.805864
H	3.745696	2.692425	-0.249587
C	3.310412	-0.027507	-0.042823
C	4.360869	-0.192180	-0.943081
C	3.168199	-0.942894	0.997802
C	5.252982	-1.246247	-0.801818
H	4.494012	0.503992	-1.763037
C	4.062743	-1.993806	1.141806
H	2.358008	-0.821508	1.707206
C	5.108033	-2.149558	0.241943
H	6.066706	-1.358663	-1.510115
H	3.941309	-2.693064	1.961986
H	5.807572	-2.970644	0.354167

TS-STrain-61

C	-1.453686	-0.563918	-0.975295
C	-0.171507	-0.006769	-0.461771
H	-1.717952	-0.388125	-2.009061
H	-0.109171	0.018031	0.625044
H	0.067726	0.977955	-0.866236
O	0.087907	-1.964026	-1.618431
C	0.722490	-1.085054	-1.019916
O	1.984487	-1.079449	-0.878108
C	-2.426333	-1.250954	-0.161959
Al	3.184703	0.049127	-0.080936
C	4.988377	-0.685754	-0.262650
C	6.086545	0.147875	0.397344
H	5.200064	-0.806745	-1.332975
H	4.985291	-1.701104	0.154626
H	7.080520	-0.297050	0.271798
H	6.132406	1.158192	-0.021467
H	5.917471	0.256787	1.473286
Cl	2.867768	1.972562	-1.078651
Cl	2.477957	0.250706	1.981524
C	-3.057985	0.193938	-0.078348
C	-3.984473	0.642877	-1.029109
C	-2.729897	1.009645	1.011740
C	-4.595303	1.871881	-0.868504
H	-4.230061	0.028905	-1.887199
C	-3.347583	2.236592	1.164510
H	-2.009788	0.665706	1.743380
C	-4.278386	2.668041	0.226791
H	-5.317152	2.214843	-1.600367

H	-3.100791	2.860242	2.015699
H	-4.757347	3.633327	0.347839
C	-3.294131	-2.278152	-0.851892
H	-2.749715	-3.223890	-0.869494
H	-4.239530	-2.412500	-0.325934
H	-3.504802	-1.993049	-1.881421
O	-1.889732	-1.652806	1.046540
C	-2.828626	-2.100557	2.013051
H	-3.264155	-3.063055	1.732031
H	-2.271311	-2.221725	2.940900
H	-3.628473	-1.368851	2.168900

Imaginary vibration frequency: 369.32i

SLC-STrain-62

C	0.667261	-1.364644	-0.255972
C	-0.806594	-1.660935	0.036751
H	1.062144	-1.839254	-1.152255
H	-1.060086	-1.851660	1.080494
H	-1.306623	-2.379561	-0.611980
O	0.259392	0.036629	-0.638612
C	-0.988510	-0.245034	-0.378352
O	-1.911937	0.554598	-0.502644
C	1.630437	-1.366783	0.895403
H	1.726294	-2.412081	1.209056
H	1.185177	-0.822351	1.733715
Al	-3.760531	0.400150	-0.093377
C	-4.629661	2.017390	-0.749922
C	-6.140470	2.055798	-0.515448
H	-4.412448	2.111360	-1.821544
H	-4.151764	2.881748	-0.271689
H	-6.593765	2.977164	-0.897479
H	-6.646637	1.220223	-1.008682
H	-6.385309	1.994941	0.549470
Cl	-4.289544	-1.465624	-1.067454
Cl	-3.700651	0.102976	2.054657
C	2.975328	-0.798399	0.542818
C	3.939170	-1.582055	-0.094570
C	3.285009	0.528053	0.809584
C	5.166183	-1.058143	-0.450343
H	3.728595	-2.625823	-0.308546
C	4.514956	1.073577	0.459722
H	2.554680	1.159912	1.305130
C	5.464091	0.277821	-0.175446
H	5.915147	-1.671428	-0.938604

H	4.719211	2.111749	0.687470
O	6.689169	0.704827	-0.553694
C	7.033136	2.048851	-0.277354
H	6.364938	2.748591	-0.790205
H	7.019183	2.253960	0.798358
H	8.046474	2.184181	-0.652874

TS-STrain-62

C	-1.058815	1.146291	0.318739
C	0.236547	0.422006	0.096358
H	-1.051895	1.765357	1.212988
H	0.143564	-0.432834	-0.578566
H	0.678605	0.053673	1.022099
O	0.665909	2.404104	-1.149892
C	1.159979	1.422218	-0.593819
O	2.420262	1.191287	-0.590988
C	-1.485856	1.848176	-0.858780
H	-2.030940	2.782778	-0.803209
H	-1.387466	1.381896	-1.829334
Al	3.532503	-0.120089	0.002486
C	5.370598	0.287334	-0.535135
C	6.404531	-0.749753	-0.097107
H	5.633918	1.273933	-0.132051
H	5.390167	0.399431	-1.627002
H	7.420391	-0.488837	-0.416383
H	6.428758	-0.858887	0.991818
H	6.182515	-1.738762	-0.510484
Cl	3.239753	-0.209693	2.173635
Cl	2.742132	-1.976901	-0.857455
C	-2.428511	0.493921	0.139414
C	-3.538695	1.068702	0.780712
C	-2.626403	-0.669356	-0.634114
C	-4.790531	0.502254	0.694043
H	-3.399983	1.970783	1.367666
C	-3.865324	-1.243248	-0.721681
H	-1.792116	-1.130538	-1.149730
C	-4.961563	-0.665898	-0.058521
H	-5.624167	0.963209	1.206403
H	-4.023676	-2.146599	-1.298410
O	-6.123454	-1.296053	-0.205588
C	-7.274376	-0.774908	0.450718
H	-7.509702	0.230478	0.091345
H	-8.089055	-1.449890	0.197288
H	-7.134741	-0.763092	1.534954

Imaginary vibration frequency: 407.21i**SLC-STrain-64**

C	2.094119	0.858369	0.515212
C	0.810665	1.107625	-0.282445
H	2.390259	1.677839	1.169806
H	0.818414	0.767017	-1.318307
H	0.363026	2.098770	-0.213485
O	1.324318	-0.128439	1.355007
C	0.241119	0.111776	0.663639
O	-0.842015	-0.420644	0.881622
C	3.253046	0.215417	-0.191355
Al	-2.538734	-0.203107	0.046831
C	-3.703405	-1.593602	0.761632
C	-5.121711	-1.578672	0.189557
H	-3.735899	-1.485134	1.853125
H	-3.231289	-2.566004	0.572201
H	-5.745670	-2.372804	0.614192
H	-5.628291	-0.629765	0.391018
H	-5.120551	-1.716958	-0.896044
Cl	-3.007663	1.852317	0.550150
Cl	-2.025379	-0.334243	-2.058046
C	4.258331	-0.325636	0.835477
H	3.752516	-1.001845	1.531620
H	4.652394	0.506835	1.430319
C	5.364764	-1.035114	0.218110
C	6.271962	-1.624376	-0.306295
H	7.080010	-2.147946	-0.766307
C	3.881438	1.237062	-1.128387
H	3.161277	1.601196	-1.864807
H	4.266554	2.096216	-0.571421
H	4.714372	0.786016	-1.670012
H	2.867717	-0.624749	-0.780373

TS-STrain-64

C	2.643256	-0.559642	0.553985
C	1.187778	-0.291134	0.716505
H	3.122483	-1.153188	1.325654
H	0.824178	0.411715	-0.033854
H	0.965752	0.127265	1.701326
O	1.051042	-2.671216	0.623376
C	0.442998	-1.619278	0.581212
O	-0.837898	-1.525294	0.439512
C	3.300869	-0.467919	-0.667460

Al	-2.040603	-0.246940	0.008484
C	-3.812856	-1.042084	-0.243342
C	-4.906884	-0.055439	-0.649705
H	-4.093421	-1.551886	0.687593
H	-3.722648	-1.834873	-0.997449
H	-5.881011	-0.541048	-0.781628
H	-5.039409	0.730352	0.100812
H	-4.667433	0.444314	-1.593747
Cl	-1.949520	1.257677	1.602924
Cl	-1.236278	0.706490	-1.808249
C	3.554710	0.975158	0.475493
H	3.725806	0.888746	1.554076
H	4.564771	1.015370	0.057686
C	2.747252	2.101532	0.111219
C	2.057980	3.035794	-0.190575
H	2.763970	0.016010	-1.480798
C	4.536242	-1.203632	-1.000834
H	5.185843	-0.634774	-1.667121
H	5.081143	-1.530909	-0.114828
H	4.209170	-2.097849	-1.545547
H	1.433996	3.862082	-0.454059

Imaginary vibration frequency: 155.94i

SLC-STrain-66

C	-2.849196	-1.237354	0.215658
C	-1.565587	-1.159401	-0.620470
H	-3.174369	-2.247555	0.455914
H	-1.544853	-0.445960	-1.443116
H	-1.137284	-2.110908	-0.935859
O	-2.054525	-0.731232	1.390657
C	-0.985600	-0.643441	0.646551
O	0.100409	-0.235620	1.048366
C	-4.000574	-0.319214	-0.097294
H	-4.658050	-0.294708	0.776534
H	-4.562502	-0.797793	-0.907271
Al	1.724097	0.058435	0.106379
C	3.024188	0.729603	1.395055
C	4.392863	1.051692	0.793386
H	3.129700	-0.014166	2.195025
H	2.602559	1.623389	1.872152
H	5.096229	1.425851	1.545475
H	4.850847	0.169099	0.336209
H	4.320646	1.815528	0.013005
Cl	2.102269	-1.895967	-0.758223

Cl	1.082946	1.421483	-1.455728
C	-3.592065	1.066467	-0.490489
C	-3.640967	2.111735	0.323724
H	-3.224263	1.200149	-1.505570
H	-3.321922	3.096484	-0.001188
H	-4.004112	2.021453	1.344010

TS-STrain-66

C	2.947181	-0.104122	-0.476784
C	1.504820	-0.233816	-0.085793
H	3.140176	-0.071133	-1.545540
H	1.391482	-0.650192	0.920349
H	0.956767	-0.888334	-0.764313
O	1.623086	2.144300	-0.013507
C	0.890770	1.164201	-0.060070
O	-0.392979	1.244412	-0.059673
C	3.683152	0.886902	0.276376
Al	-1.814903	0.121806	-0.010165
C	-3.468787	1.162643	0.125636
C	-4.746307	0.328242	0.213197
H	-3.518733	1.836660	-0.739531
H	-3.386441	1.816200	1.003977
H	-5.647289	0.948569	0.287842
H	-4.870026	-0.312464	-0.665723
H	-4.737335	-0.330365	1.087524
Cl	-1.675353	-1.102471	-1.826277
Cl	-1.458479	-1.203001	1.704572
C	3.983726	-0.892184	0.293516
C	5.284644	-0.867905	-0.069439
H	3.673186	-1.355022	1.223343
H	6.044920	-1.341350	0.543262
H	5.604802	-0.392730	-0.991659
H	4.446512	1.496819	-0.189942
H	3.454828	1.079422	1.317159

Imaginary vibration frequency: 133.80i

SLC-STrain-68

C	1.843344	-0.613383	-0.770749
C	0.552659	-1.119231	-0.118145
H	2.163033	-1.174490	-1.647739
H	0.540019	-1.131146	0.972558
H	0.120626	-2.038433	-0.512266
O	1.068913	0.584665	-1.260110
C	-0.018403	0.122649	-0.702190

O	-1.107887	0.684689	-0.753656
C	2.993803	-0.213045	0.119075
Al	-2.783164	0.200041	0.007482
C	-4.068442	1.565160	-0.526189
C	-5.488510	1.324468	-0.011963
H	-4.069405	1.622243	-1.622166
H	-3.700747	2.538311	-0.177040
H	-6.181781	2.109482	-0.333537
H	-5.891855	0.372694	-0.371239
H	-5.522160	1.294315	1.081475
Cl	-3.070462	-1.796617	-0.790947
Cl	-2.280152	0.067856	2.113911
C	3.506087	-1.477244	0.759073
C	4.644106	-2.095354	0.474711
H	2.585117	0.424355	0.914284
C	4.028063	0.594098	-0.668953
H	4.510202	-0.064215	-1.401451
H	3.511729	1.372960	-1.236330
H	2.847478	-1.913626	1.507097
H	4.914936	-3.015220	0.982014
H	5.351971	-1.716345	-0.255151
C	5.057478	1.233471	0.205781
C	5.267170	2.541965	0.272521
H	5.655505	0.567579	0.824140
H	4.689013	3.241976	-0.325414
H	6.025565	2.961786	0.925417

TS-STrain-68

C	-1.943125	0.626607	-0.663494
C	-0.499573	0.563287	-0.339524
H	-2.223543	1.058804	-1.617770
H	-0.321816	0.263881	0.695458
H	0.000809	1.519930	-0.508736
O	-0.539313	-0.994662	-2.146719
C	0.130802	-0.478359	-1.273589
O	1.375019	-0.736817	-1.057818
C	-2.961108	-0.061470	0.069662
Al	2.663415	-0.311606	0.143463
C	4.333532	-1.254102	-0.287485
C	5.550500	-0.374214	-0.571975
H	4.128528	-1.896921	-1.153409
H	4.557231	-1.940011	0.538953
H	6.443156	-0.965769	-0.807501
H	5.376072	0.297020	-1.418248

H	5.800574	0.259639	0.284160
Cl	2.802940	1.879645	0.094341
Cl	1.797170	-0.847819	2.095242
C	-2.836118	1.375938	0.655977
C	-3.443193	2.447430	0.109998
H	-2.593242	-0.749645	0.827863
C	-4.253295	-0.471137	-0.597031
H	-4.494874	0.237965	-1.395418
H	-4.067862	-1.434396	-1.080850
H	-2.253977	1.470536	1.563217
H	-3.388537	3.418047	0.592987
H	-4.003973	2.384959	-0.816668
C	-5.390006	-0.584074	0.365535
C	-6.044938	-1.708884	0.617846
H	-5.678600	0.331006	0.880600
H	-6.867720	-1.738300	1.324475
H	-5.785020	-2.641202	0.123748

Imaginary vibration frequency: 34.66i

SLC-STrain-72

C	-2.455281	0.469218	-0.645463
C	-1.156798	1.060218	-0.088967
H	-2.837948	0.967056	-1.536055
H	-1.094055	1.149847	0.996161
H	-0.777331	1.962925	-0.566816
O	-1.666395	-0.727831	-1.098460
C	-0.568763	-0.199594	-0.619192
O	0.533648	-0.729725	-0.683979
C	-3.532215	0.086238	0.329426
Al	2.225925	-0.153540	-0.015857
C	3.542148	-1.476857	-0.576052
C	4.967809	-1.175221	-0.111436
H	3.509869	-1.550106	-1.670485
H	3.222944	-2.457591	-0.201460
H	5.679365	-1.938592	-0.444750
H	5.323473	-0.214541	-0.496504
H	5.035012	-1.127872	0.979820
Cl	2.381182	1.831438	-0.878394
Cl	1.809225	0.013170	2.105586
C	-4.557592	-0.799178	-0.335434
H	-4.932598	-0.430307	-1.314035
O	-4.987636	-1.812940	0.145736
C	-4.238486	1.351076	0.824055
H	-3.523083	2.038486	1.280763

H	-4.738922	1.872538	0.003764
H	-4.987067	1.092914	1.574272
H	-3.095461	-0.458510	1.171206

TS-STrain-72

C	2.173094	-0.184414	-0.427362
C	1.333220	0.366988	0.648873
H	1.690229	-0.875838	-1.114576
H	1.921507	0.764280	1.478073
H	0.633595	-0.383057	1.015709
O	1.225053	2.574247	-0.242770
C	0.574775	1.597569	0.048195
O	-0.698048	1.478603	-0.077693
C	3.472687	0.191586	-0.715890
Al	-1.944305	0.159906	-0.028893
C	-3.671896	0.827358	-0.658069
C	-4.793843	-0.210896	-0.651985
H	-3.534800	1.227593	-1.670895
H	-3.952047	1.687193	-0.035893
H	-5.744382	0.200350	-1.011079
H	-4.553939	-1.067562	-1.289847
H	-4.973657	-0.603565	0.353757
Cl	-1.082738	-1.435067	-1.277625
Cl	-1.948758	-0.580513	2.033354
C	3.450731	-1.348373	0.456530
O	3.661454	-2.400738	0.002617
H	3.558462	-0.970514	1.483687
C	4.275630	1.214004	-0.015830
H	5.307811	0.880319	0.115375
H	4.307398	2.088280	-0.677878
H	3.848088	1.540772	0.930656
H	3.909066	-0.242001	-1.612856

Imaginary vibration frequency: 211.79i

SLC-STest-2

C	-2.208617	-1.144821	0.123382
C	-0.878523	-1.178744	-0.634769
H	-2.482918	-2.085301	0.599541
H	-0.859888	-0.649584	-1.588272
H	-0.380531	-2.143817	-0.726182
O	-1.527965	-0.302149	1.177901
C	-0.406559	-0.358133	0.511802
O	0.638018	0.169360	0.882735

C	-3.363718	-0.425939	-0.495233
H	-3.694288	-1.038228	-1.342350
H	-3.020515	0.528002	-0.909137
Al	2.367686	0.201700	0.095797
C	3.499506	1.297803	1.244393
C	4.941650	1.435201	0.753996
H	3.484122	0.865733	2.253039
H	3.037111	2.288684	1.337159
H	5.547399	2.056047	1.423289
H	5.437782	0.462421	0.681593
H	4.988441	1.893106	-0.238890
Cl	2.835115	-1.912998	-0.028622
Cl	1.939944	0.962776	-1.890453
C	-4.520452	-0.200328	0.475288
H	-4.186954	0.414131	1.316446
H	-4.829725	-1.170150	0.884853
C	-5.687652	0.450146	-0.191520
H	-6.131070	-0.099665	-1.021406
C	-6.195515	1.626951	0.150436
H	-7.045523	2.052490	-0.373014
H	-5.780503	2.207303	0.970507

TS-STest-2

C	2.329967	-0.655064	0.445798
C	0.888855	-0.325976	0.518412
H	2.687248	-1.554191	0.943614
H	0.683168	0.701505	0.210801
H	0.485518	-0.479433	1.522148
O	0.901622	-2.130621	-1.014236
C	0.210822	-1.300836	-0.448543
O	-1.058044	-1.175158	-0.600451
C	3.258299	0.117453	-0.227857
H	3.072555	0.363914	1.000295
Al	-2.371968	-0.033987	-0.086241
C	-4.077585	-0.560264	-0.888507
C	-5.254858	0.349866	-0.539177
H	-4.295437	-1.591383	-0.581303
H	-3.942626	-0.599041	-1.977280
H	-6.189718	0.022445	-1.008918
H	-5.432586	0.382009	0.540450
H	-5.077204	1.380324	-0.862946
Cl	-2.349073	-0.072634	2.107079
Cl	-1.665046	1.953069	-0.705548
H	2.888422	1.012410	-0.727902

C	4.672766	-0.290508	-0.471589
H	4.681035	-0.631740	-1.516725
H	4.939530	-1.148356	0.149430
C	5.643826	0.835985	-0.300175
C	6.679529	0.794188	0.524944
H	5.464727	1.721906	-0.906116
H	7.366264	1.629579	0.608655
H	6.886371	-0.078340	1.138553

Imaginary vibration frequency: 188.66i

SLC-STest-4

C	1.391303	-0.948230	-0.458690
C	-0.032558	-1.403327	-0.122744
H	1.786373	-1.335800	-1.396400
H	-0.218797	-1.664064	0.919962
H	-0.493680	-2.136030	-0.784361
O	0.836792	0.423602	-0.738335
C	-0.366978	0.007339	-0.451290
O	-1.368376	0.716049	-0.498458
C	2.408241	-0.926773	0.652283
H	1.927672	-0.477327	1.528426
Al	-3.175783	0.312381	-0.067487
C	-4.222858	1.923766	-0.395424
C	-5.713183	1.774840	-0.085720
H	-4.083248	2.215202	-1.444145
H	-3.793546	2.739002	0.200605
H	-6.269238	2.698083	-0.282451
H	-6.174299	0.987303	-0.689727
H	-5.883315	1.514752	0.963603
Cl	-3.568251	-1.400958	-1.340016
Cl	-2.985887	-0.348954	1.991044
C	3.596266	-0.070701	0.280401
C	3.807832	1.144486	0.924209
C	4.486514	-0.463495	-0.717772
C	4.886578	1.950480	0.584983
H	3.118411	1.463249	1.699818
C	5.563627	0.340532	-1.060884
H	4.343683	-1.408300	-1.232495
C	5.767581	1.550628	-0.409656
H	5.036555	2.894130	1.098392
H	6.247746	0.020378	-1.839434
H	6.610492	2.178378	-0.677334
C	2.785898	-2.366814	0.991919
H	1.909515	-2.940691	1.303823

H	3.236100	-2.875812	0.136567
H	3.508202	-2.378511	1.809656

TS-STest-4

C	-1.413346	0.807390	-0.212363
C	0.048142	0.739496	0.020052
H	-1.766145	1.176251	-1.170698
H	0.303479	0.587415	1.070959
H	0.579587	1.617285	-0.354434
O	-0.508428	-1.060814	-1.360512
C	0.418724	-0.490622	-0.796947
O	1.643090	-0.855076	-0.848460
C	-2.374433	0.412361	0.745298
H	-1.978012	-0.182244	1.564142
Al	3.220337	-0.276918	-0.143170
C	4.687174	-1.431998	-0.726396
C	6.064329	-1.018475	-0.207347
H	4.689690	-1.452902	-1.823879
H	4.459189	-2.458556	-0.411600
H	6.859155	-1.689883	-0.552419
H	6.331964	-0.009256	-0.535892
H	6.098749	-1.016520	0.886760
Cl	3.394194	1.811051	-0.793298
Cl	2.883476	-0.256701	2.025346
C	-3.750465	0.019728	0.323194
C	-4.276666	-1.171093	0.810357
C	-4.502479	0.793744	-0.556520
C	-5.540068	-1.589517	0.415648
H	-3.693531	-1.777106	1.495800
C	-5.764035	0.375312	-0.948986
H	-4.107115	1.730348	-0.939050
C	-6.285347	-0.817885	-0.463677
H	-5.941100	-2.521098	0.798877
H	-6.343257	0.983130	-1.635026
H	-7.272873	-1.143576	-0.771027
C	-2.199388	1.977256	1.143498
H	-1.635388	2.028463	2.068999
H	-1.700722	2.644072	0.417460
H	-3.218594	2.353114	1.204318

Imaginary vibration frequency: 178.25i

SLC-STest-8

C	-1.864158	0.510669	-0.859712
C	-0.617835	1.026197	-0.138095

H	-2.187182	1.102177	-1.714767
H	-0.647492	1.005222	0.951918
H	-0.201511	1.970959	-0.486270
O	-1.054068	-0.643577	-1.361509
C	0.009765	-0.177852	-0.747229
O	1.109305	-0.710585	-0.790144
C	-3.013374	0.016894	-0.022173
H	-2.646985	-0.571533	0.819678
Al	2.766817	-0.205248	0.024970
C	4.082331	-1.540209	-0.507821
C	5.487538	-1.287298	0.040621
H	4.106792	-1.576964	-1.604310
H	3.722454	-2.524832	-0.183639
H	6.198811	-2.056007	-0.280704
H	5.883627	-0.323314	-0.293124
H	5.498159	-1.276887	1.134847
Cl	3.010403	1.806439	-0.742760
Cl	2.199785	-0.124647	2.115134
C	-4.021306	-0.777618	-0.837508
H	-4.439153	-0.142676	-1.625017
H	-3.480531	-1.591844	-1.333192
Cl	-3.768524	1.491544	0.689196
C	-5.090183	-1.338488	-0.031921
C	-5.968396	-1.805655	0.640676
H	-6.752097	-2.219319	1.235483

TS-STest-8

C	-2.010670	0.598224	-0.680805
C	-0.598820	0.556866	-0.235505
H	-2.209161	0.804164	-1.729038
H	-0.496415	0.698671	0.844139
H	0.014125	1.303818	-0.739771
O	-0.984229	-1.706183	-0.839195
C	-0.134652	-0.868391	-0.570307
O	1.123539	-1.094905	-0.538031
C	-2.997643	-0.198122	0.013315
Al	2.640951	-0.238859	-0.006181
C	4.171181	-1.447684	-0.163070
C	5.501818	-0.856552	0.302173
H	4.246960	-1.765349	-1.211176
H	3.944960	-2.358644	0.406076
H	6.332529	-1.563899	0.195905
H	5.767588	0.038083	-0.269817
H	5.464747	-0.561329	1.355526

Cl	2.767936	1.551132	-1.265589
Cl	2.195783	0.419431	2.036804
C	-4.165143	-0.790980	-0.680358
H	-4.417361	-0.220741	-1.578751
H	-3.779928	-1.764155	-1.025611
H	-2.731197	-0.577187	0.995725
Cl	-3.166499	1.762509	0.294352
C	-5.321324	-0.983217	0.172880
C	-6.278685	-1.129482	0.880599
H	-7.132795	-1.265738	1.506784

Imaginary vibration frequency: 432.21i

SLC-STest-9

C	1.164181	0.437291	0.849674
C	-0.230750	1.065195	0.802048
H	1.628162	0.424828	1.833254
H	-0.445788	1.758698	-0.008663
H	-0.606868	1.464487	1.743823
O	0.535045	-0.893718	0.605100
C	-0.649993	-0.337932	0.546757
O	-1.685860	-0.958882	0.335396
C	2.190317	0.785068	-0.226625
Al	-3.449934	-0.312514	0.021076
C	-4.617848	-1.867315	-0.114741
C	-6.081877	-1.525931	-0.396737
H	-4.537339	-2.439552	0.818144
H	-4.225321	-2.523071	-0.902183
H	-6.707981	-2.422315	-0.465497
H	-6.508315	-0.895709	0.389802
H	-6.194993	-0.981942	-1.339558
Cl	-3.755229	1.017935	1.705883
Cl	-3.135870	0.859991	-1.776903
O	2.585075	2.079616	0.206121
C	3.505101	2.745961	-0.636763
H	3.829930	3.634727	-0.095365
H	4.380954	2.125511	-0.855137
H	3.041950	3.058372	-1.578072
C	1.577397	0.818369	-1.618759
H	1.018311	-0.093025	-1.837246
H	0.900344	1.668256	-1.716158
H	2.352778	0.913671	-2.379403
C	3.339915	-0.211136	-0.106315
C	3.459201	-1.306575	-0.955552
C	4.271333	-0.050351	0.918520

C	4.490771	-2.221533	-0.786290
H	2.746145	-1.458723	-1.756717
C	5.305222	-0.959040	1.083924
H	4.190937	0.805610	1.579527
C	5.417297	-2.050262	0.231558
H	4.568376	-3.071062	-1.456125
H	6.026507	-0.814610	1.881123
H	6.224356	-2.763187	0.360674

TS-STest-9

C	-1.240901	0.304678	-0.881624
C	0.225297	0.568236	-0.821387
H	-1.681506	0.042692	-1.834689
H	0.555028	1.200843	0.000782
H	0.622852	0.963876	-1.757211
O	-0.380842	-1.605804	-0.634316
C	0.619042	-0.866784	-0.602742
O	1.804012	-1.261778	-0.405210
C	-2.184806	0.550674	0.218180
Al	3.366406	-0.380958	0.002806
C	4.796490	-1.682744	0.283774
C	6.150589	-1.070996	0.643436
H	4.887527	-2.288076	-0.627449
H	4.476559	-2.378223	1.070270
H	6.925477	-1.832408	0.788474
H	6.508035	-0.394514	-0.139253
H	6.096618	-0.488033	1.568252
Cl	3.675873	1.004449	-1.657983
Cl	2.820016	0.811055	1.759822
O	-2.219471	1.818370	-0.531474
C	-1.671137	3.008913	0.053624
H	-2.251283	3.274780	0.937883
H	-0.618406	2.905958	0.314187
H	-1.781203	3.775981	-0.711218
C	-1.676481	0.618440	1.631195
H	-2.416535	1.106563	2.267298
H	-1.558294	-0.406064	1.989180
H	-0.719022	1.127862	1.734495
C	-3.519792	-0.129222	0.109154
C	-3.579244	-1.518267	0.057234
C	-4.692069	0.617185	0.105268
C	-4.810676	-2.154854	0.000399
H	-2.663711	-2.098572	0.053468
C	-5.921227	-0.024939	0.049669

H	-4.647493	1.700001	0.133083
C	-5.983026	-1.410837	-0.002363
H	-4.852347	-3.237481	-0.044738
H	-6.833484	0.561350	0.043581
H	-6.944132	-1.910842	-0.049042

Imaginary vibration frequency: 432.21i

SLC-STest-10

C	-1.305802	-2.796975	0.116618
C	-0.283514	-2.048870	-0.746707
H	-1.218286	-3.881383	0.098994
H	-0.658250	-1.222341	-1.350097
H	0.405664	-2.666048	-1.323193
O	-0.566136	-2.303172	1.332126
C	0.259720	-1.634170	0.572386
O	1.161583	-0.921116	1.001999
C	-2.739499	-2.329930	0.119562
H	-3.209547	-2.779822	-0.760438
H	-3.232614	-2.759424	0.996621
Al	2.369298	0.226184	0.089258
C	3.538324	1.010584	1.439003
C	4.583170	1.976032	0.877699
H	4.032383	0.193961	1.980686
H	2.910851	1.523114	2.179204
H	5.221362	2.396104	1.663004
H	5.243007	1.482486	0.157425
H	4.115904	2.818604	0.358592
Cl	3.284624	-1.129917	-1.337876
Cl	1.020859	1.565860	-0.953291
C	-2.894300	-0.835898	0.085923
C	-2.738031	-0.070654	1.239734
C	-3.146654	-0.173241	-1.112685
C	-2.812017	1.312962	1.189527
H	-2.556000	-0.561786	2.190118
C	-3.222181	1.210642	-1.159698
H	-3.286815	-0.748023	-2.023578
C	-3.045096	1.979358	-0.011680
H	-2.682639	1.887430	2.101564
H	-3.417049	1.703849	-2.106988
C	-3.067100	3.475241	-0.072397
H	-2.058209	3.864718	-0.245845
H	-3.701140	3.833042	-0.886306
H	-3.428394	3.907907	0.862996

TS-STest-10

C	-1.440314	1.137614	0.335436
C	-0.132352	0.435222	0.125326
H	-1.449747	1.784869	1.208990
H	-0.213541	-0.445625	-0.516742
H	0.321641	0.108882	1.061063
O	0.266564	2.382307	-1.189135
C	0.772016	1.424664	-0.607706
O	2.035084	1.199136	-0.607069
C	-1.929274	1.766638	-0.854199
H	-2.511982	2.679227	-0.824070
H	-1.802750	1.282703	-1.812989
Al	3.165029	-0.094596	-0.016051
C	4.991818	0.325773	-0.582401
C	6.045062	-0.693638	-0.149361
H	5.248551	1.319578	-0.192839
H	4.994600	0.427637	-1.675473
H	7.052953	-0.422461	-0.484996
H	6.085653	-0.792444	0.940055
H	5.830581	-1.689250	-0.550692
Cl	2.904730	-0.171982	2.160355
Cl	2.380067	-1.967206	-0.849593
C	-2.800022	0.438243	0.191972
C	-3.914107	0.998303	0.842229
C	-2.969546	-0.747832	-0.545383
C	-5.140231	0.373154	0.788996
H	-3.793800	1.923172	1.396688
C	-4.198489	-1.364302	-0.586369
H	-2.130112	-1.188480	-1.070704
C	-5.303386	-0.820084	0.080072
H	-5.989979	0.811089	1.300845
H	-4.316071	-2.285914	-1.145741
C	-6.621846	-1.514583	0.047229
H	-6.794899	-1.992269	-0.919173
H	-6.644875	-2.303734	0.807219
H	-7.442307	-0.827610	0.258858

Imaginary vibration frequency: 354.80i