Electronic Supplementary Information

Computational investigation into the gas-phase ozonolysis of the conjugated monoterpene α-phellandrene

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S.1 Effect of Chirality

α-phellandrene is a chiral molecule, with **C5** a stereocenter. The effect of chirality was investigated for the transition of **POZ1a** to **CI1a**. Table S.1 shows the two enantiomers of α-phellandrene are energetically identical, lying within the noise resolution of G4(MP2). This is not surprising given the chiral centre's distance from the reactive site, with the respective orientation of the hydrogen atom having little to no influence on chemical kinetics or energetics. As such the effects of chirality are ignored in this study.

	ΔE_e	ΔE_0	ΔH_{298}	ΔG_{298}
POZ1a	0	0	2.63×10^{-3}	5.25×10^{-3}
TS2a	0	0	0	2.63×10^{-3}
CI1a	7.88×10^{-3}	7.88×10^{-3}	1.05×10^{-2}	7.88×10^{-3}

Table S.1. Absolute difference in energies (ΔG_{298}, G4(MP2), in kJ mol^{-1}) for the two enantiomers in going from **POZ1a** to **CI1a**.

S.2 Energies for O_3 addition to α-phellandrene

Addition Pathway		ΔE_e (kJ mol^{-1})	ΔE_0 (kJ mol^{-1})	ΔH_{298} (kJ mol^{-1})	ΔG_{298} (kJ mol^{-1})
	vdW1	–13.6	–10.3	–8.5	28.8
DB1a	**TS1**	–5.0	–0.6	–2.3	46.8
	POZ1a	–239.2	–223.5	–228.4	–171.5
	vdW2	–13.3	–9.6	–8.1	30.3
DB1b	**TS2**	–6.5	–1.7	–2.6	45.7
	POZ1b	–240.2	–224.3	–229.4	–171.1
	vdW3	–12.7	–8.6	–7.5	32.5
DB2a	**TS3**	–11.0	–6.8	–8.2	38.7
	POZ2a	–236.0	–219.4	–224.0	–167.9
	vdW4	–18.8	–14.4	–13.5	27.4
DB2b	**TS4**	–15.0	–10.0	–11.9	37.6
	POZ2b	–234.4	–217.8	–222.6	–166.0

Table S.2. Change in total electronic energy (E_e), total electronic energy including zero-point energy correction (E_0), enthalpy and Gibbs free energy with respect to free reactants for the van der Waals complex (vdW), transition state (TS) and primary ozonide (POZ) for the addition of ozone to α-phellandrene.

S.3 Geometry of O_3 Addition

As an example for all addition reactions in this study, the geometries for ozone addition to **DB1** is shown below in Figure S.3.

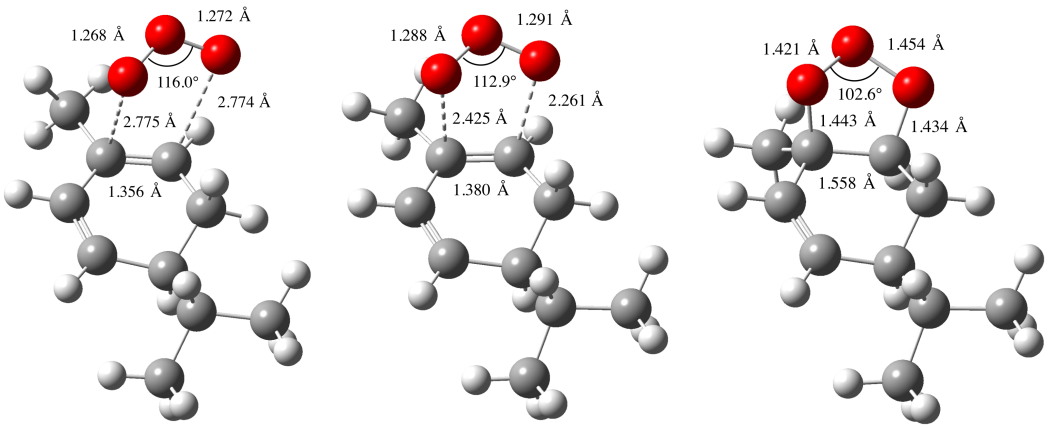


Figure S.3. A set of optimised geometries for a van der Waals complex (**vdW1**), concerted transition state (**TS1**) and POZ (**POZ1**).

S.4 Triplet Surface Analysis

The CIs, being biradicals, can exist as either singlets or triplets. It is therefore important to know on which PES the reaction is occurring. Consequently an analysis of the reaction from POZ's leading to CI formation was undertaken. For computational efficiency, the isopropyl group was replaced by a methyl group, and analysis completed at the B3LYP/6-31+G(d) level of theory. The results from this study were conclusive enough to warrant no further analysis at higher levels of theory. Ozone, α-phellandrene (and its surrogate), and the POZ's all have singlet ground state. Figure S.4 shows that on this singlet surface the POZ can pass through a TS (**TS1-4-s**) and form a singlet Criegee biradical (**CI1-4-s**). Alternatively the POZ can migrate onto the triplet surface, where a stable minima is formed via cleavage of an oxygen-oxygen bond (**POZ1-4-t**). Research by Minaev and Kozlo[68] showed the ISC of Criegee biradicals to be induced by large spin-orbit coupling effects involving the terminal oxygen, with similar effects expected to prompt **POZ1-4-t** formation. **POZ1-4-t** can then pass through **TS-1-4-t**, to form triplet Criegee biradicals **CI1-4-t**. It is evident in Figure S.4 that energetically this is an unlikely pathway, with the singlet surfaces lying at significantly lower energies. Whilst an initial intersystem crossing (ISC) onto the triplet surface may occur, as it is competitive with forming a singlet TS, migration back onto the singlet surface through the singlet TS is more favourable than proceeding through the triplet TS. The triplet surface may therefore act as an alternative pathway to forming the singlet TS's. Nevertheless for the chemically activated POZ's, the energy difference between the singlet TS and the triplet POZ is unlikely to have a large influence on the relative state density of

these two kinetically critical points, resulting in a low probability of transition onto the triplet surface.

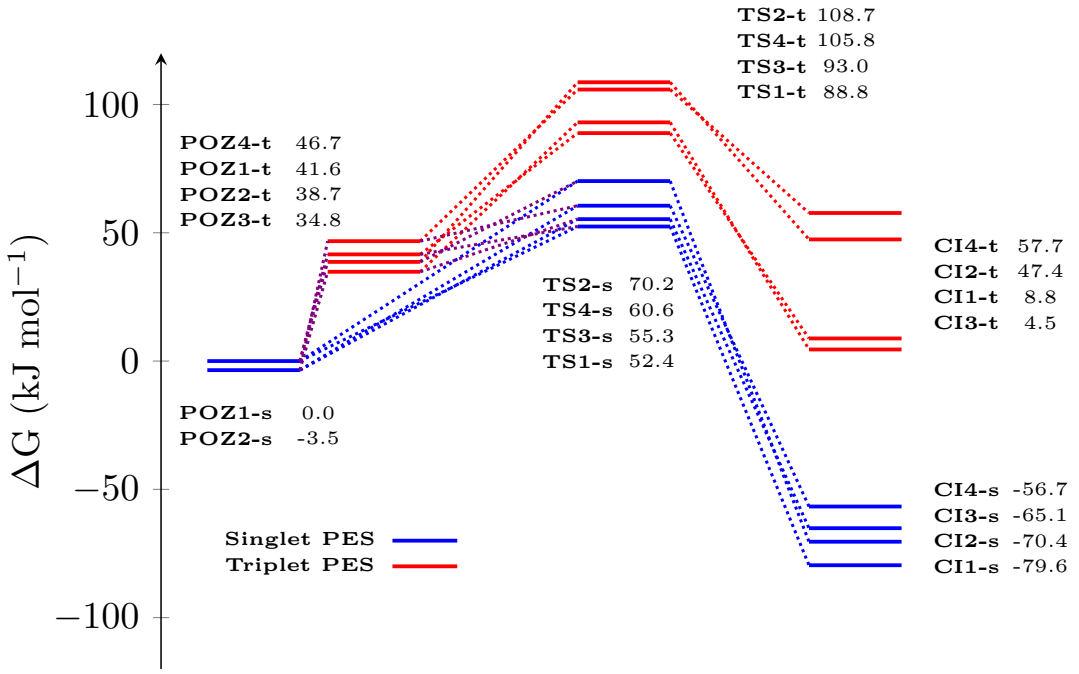


Figure S.4. Comparison of the singlet and triplet PES (ΔG_{298}, G4(MP2), in kJ mol^{-1}) for the transition of POZ's to CIs. ΔG is with respect to **POZ1-s**.

S.5 Uncompetitive Hydroperoxide Channels

The following hydroperoxide channels were found to be uncompetitive with other possible hydroperoxide pathways available for the given Criegee intermediate. Note that in all cases a 1,3-hydrogen migration was uncompetitive.

	Barrier (kJ mol^{-1})	Mechanism
CI1a	106.0	1,8-H acyl migration
CI2a	121.7	1,3-H migrations
CI3a	130.1	1,3-H migrations
CI3b	120.3	1,8-H acyl migration
CI4a	121.3	1,3-H migrations

Table S.5. Barrier heights (ΔG_{298}, G4(MP2)) for hydroperoxide channels not included in the primary analysis.

S.6 Geometry of Epoxidation Reactions

DIO2: Epoxidation proceeds through cleavage of the weak peroxide bond which stretches from 1.496 to 1.843 Å in going from **DIO2** to **TS2i**, followed by breaking of one of the dioxirane C–O and ethylenic π bonds which are both elongated in the **TS2i**. The approach of oxygen to the olefin is close to perpendicular, first bonding with **C6** followed by **C7** in a concerted fashion. Meanwhile a carbonyl π-bond is formed with the residual oxygen from the dioxirane moiety to form **EPOX2**. Labelling the epoxide forming oxygen as **O1**, and the other oxygen in the dioxirane moiety as **O2**, whilst keeping the carbon labels the same as in Figure 1 in the main text, then the C7-O1-C6-C3 and C7-O1-C6-O2 torsion angles in **TS2i** are –127.1° and –163.0° respectively, indicating a spiro transition type.

DIO4: Epoxidation proceeds through cleavage of the weak peroxide bond which stretches from 1.496 to 1.835 Å in going from **DIO4** to **TS4i**, followed by breaking of one of the dioxirane C–O and ethylenic π-bonds which are both elongated in the TS. The approach of oxygen to the olefin is close to perpendicular, first bonding with **C3** followed by **C2** in a concerted fashion. Meanwhile a carbonyl π-bond is formed with the residual oxygen from the dioxirane moiety to form **EPOX4**. Labelling the epoxide forming oxygen as **O1**, and the other oxygen in the dioxirane moiety as **O2**, whilst keeping the carbon labels the same as in Figure 1 in the main text, then the C2-O1-C3-C6 and C2-O1-C3-O2 torsion angles in **TS4i** are 124.5° and 159.3° respectively, indicating a spiro transition type.

S.7 CO_2 Elimination from First Generation Products

Chemically activated products can have sufficient energy to eliminate a CO_2 molecule directly, generating a shorter alkyl chain. The barriers for this channel for some products formed in this study are listed below.

	Barrier (kJ mol^{-1})
ESTER1a	389.4
ESTER1b	308.9
ACID1	290.8
ESTER3a	291.4
ACID3b	289.5

Table S.7. Barrier heights (ΔG_{298}, G4(MP2)) for CO_2 elimination from first generation products.

S.8 α-phellandrene Reaction Equations

The ozonolysis mechanism for α-phellandrene, comprising of all reactions investigated as part of this study, is outlined below. Barrier height for each reaction (ΔG_{298}, kJ mol^{-1}) is given along the line.

α-phellandrene + O_3 $\xrightarrow{46.8}$ **POZ1a**

α-phellandrene + O_3 $\xrightarrow{45.7}$ **POZ1b**

α-phellandrene + O_3 $\xrightarrow{38.7}$ **POZ2a**

α-phellandrene + O_3 $\xrightarrow{37.6}$ **POZ2b**

α-phellandrene + O_3 $\xrightarrow{41.3}$ **POZ1a***

α-phellandrene + O_3 $\xrightarrow{41.3}$ **POZ1b***

α-phellandrene + O_3 $\xrightarrow{43.4}$ **POZ2a***

α-phellandrene + O_3 $\xrightarrow{46.1}$ **POZ2b***

POZ1a $\xrightarrow{50.8}$ **CI1a**

POZ1a $\xrightarrow{70.3}$ **CI2a**

POZ1b $\xrightarrow{67.3}$ **CI1b**

POZ1b $\xrightarrow{62.8}$ **CI2b**

POZ1a $\underset{9.7}{\overset{10.2}{\rightleftharpoons}}$ **POZ1b**

POZ2a $\xrightarrow{58.1}$ **CI3a**

POZ2a $\xrightarrow{55.9}$ **CI4a**

POZ2b $\xrightarrow{68.2}$ **CI3b**

POZ2b $\xrightarrow{68.2}$ **CI4b**

POZ2a $\underset{11.9}{\overset{13.8}{\rightleftharpoons}}$ **POZ2b**

CI1a $\xrightarrow{56.8}$ **SOZ1c**

CI1a $\xrightarrow{76.4}$ **HP1d**

CI1a $\xrightarrow{87.2}$ **DIO1**

CI1b $\xrightarrow{27.0}$ **SOZ1f**

CI1b $\xrightarrow{82.0}$ **HP1g**

CI1b $\xrightarrow{30.3}$ **HP1h**

CI1b $\xrightarrow{74.1}$ **DIO1**

CI1b $\xrightarrow{47.3}$ **CP1j**

CI1a $\underset{170.0}{\overset{175.9}{\rightleftharpoons}}$ **CI1b**

SOZ1c $\underset{16.1}{\overset{9.2}{\rightleftharpoons}}$ **SOZ1f**

SOZ1c $\xrightarrow{165.9}$ **ACID1**

SOZ1c $\xrightarrow{127.5}$ **ESTER1b**

SOZ1f $\xrightarrow{191.1}$ **ESTER1a**

SOZ1f $\xrightarrow{178.0}$ **ESTER1c**

DIO1 $\xrightarrow{149.6}$ **ESTER1a**

DIO1 $\xrightarrow{108.9}$ **ESTER1b**

CI2a $\xrightarrow{17.6}$ **SOZ1f**

CI2a $\xrightarrow{102.2}$ **HP2d**

CI2a $\xrightarrow{66.2}$ **DIO2**

CI2b $\xrightarrow{24.2}$ **SOZ1c**

CI2b $\xrightarrow{71.0}$ **HP2g**

CI2b $\xrightarrow{90.9}$ **DIO2**

CI2a $\underset{172.2}{\overset{160.6}{\rightleftharpoons}}$ **CI2b**

HP2d $\xrightarrow{168.7}$ **RAD2j**

HP2d $\xrightarrow{166.0}$ **RAD2k**

DIO2 $\xrightarrow{75.7}$ **EPOX2**

CI3a $\xrightarrow{60.1}$ **SOZ3c**

CI3a $\xrightarrow{62.3}$ **DIO3**

CI3b $\xrightarrow{39.0}$ **SOZ3e**

CI3b $\xrightarrow{46.7}$ **HP3f**

CI3b $\xrightarrow{70.7}$ **DIO3**

CI3b $\xrightarrow{42.5}$ **CP3h**

CI3a $\underset{151.8}{\overset{156.2}{\rightleftharpoons}}$ **CI3b**

SOZ3c $\xrightarrow{169.5}$ **ACID3b**

SOZ3c $\xrightarrow{127.4}$ **ESTER3a**

SOZ3e $\xrightarrow{169.2}$ **ACID3a**

SOZ3e $\xrightarrow{137.8}$ **ESTER3b**

DIO3 $\xrightarrow{72.1}$ **ESTER3a**

CI4a $\xrightarrow{27.9}$ **SOZ3e**

CI4a $\xrightarrow{95.5}$ **HP4d**

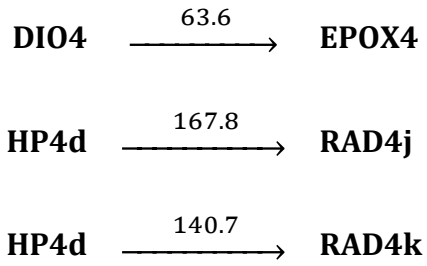
CI4a $\xrightarrow{69.6}$ **DIO4**

CI4b $\xrightarrow{31.3}$ **SOZ3c**

CI4b $\xrightarrow{90.5}$ **HP4g**

CI4b $\xrightarrow{98.3}$ **DIO4**

CI4a $\underset{161.3}{\overset{159.4}{\rightleftharpoons}}$ **CI4b**


DIO4
63.6
EPOX4
HP4d
167.8
RAD4j
HP4d
140.7
RAD4k

S.9 G4(MP2) Cartesian Coordinates and Energies for all Reactants, Transition States and Products on the O_3 addition to α-phellandrene Potential Energy Surface

O3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.431366
2	8	0	0.000000	1.075739	-0.215683
3	8	0	0.000000	-1.075739	-0.215683

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.007358	E(Thermal)=	0.010315
E(CCSD(T))=	-224.87443	E(Empiric)=	-0.085248
DE(MP2)=	-0.252312	DE(HF)=	-0.027476
G4MP2(0 K)=	-225.232107	G4MP2 Energy=	-225.229151
G4MP2 Enthalpy=	-225.228206	G4MP2 Free Energy=	-225.255219

a-phellandrene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.104503	-1.262164	-0.202050
2	6	0	0.636865	0.023683	0.216079
3	6	0	-0.169960	1.231332	-0.218575
4	6	0	-1.505367	1.190139	-0.289619
5	6	0	-2.257985	-0.034235	0.017436
6	6	0	-1.588037	-1.193937	0.070329
7	1	0	0.674749	0.037386	1.321123
8	1	0	0.053048	-1.440148	-1.280677
9	1	0	0.326362	-2.126033	0.311461
10	1	0	-2.068233	2.078527	-0.565738
11	1	0	-2.116833	-2.126242	0.251476
12	1	0	0.353928	2.156527	-0.436350
13	6	0	2.103906	0.077171	-0.283814
14	1	0	2.072977	0.221537	-1.373718
15	6	0	-3.743503	0.076130	0.227284
16	1	0	-4.194216	-0.899592	0.427071
17	1	0	-3.979849	0.739375	1.068832

18	1	0	-4.236159	0.504307	-0.655117
19	6	0	2.868869	1.258134	0.334733
20	1	0	3.887015	1.310195	-0.064510
21	1	0	2.392034	2.222399	0.140095
22	1	0	2.945829	1.140819	1.422487
23	6	0	2.869882	-1.224812	-0.002930
24	1	0	2.859113	-1.462917	1.068014
25	1	0	2.452049	-2.079249	-0.541130
26	1	0	3.917189	-1.125539	-0.306558

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.230482	E(Thermal)=	0.241496
E(CCSD(T))=	-389.414728	E(Empiric)=	-0.265216
DE(MP2)=	-0.497546	DE(HF)=	-0.039176
G4MP2(0 K)=	-389.986184	G4MP2 Energy=	-389.97517
G4MP2 Enthalpy=	-389.974226	G4MP2 Free Energy=	-390.022178

vdW1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.913139	0.048820	1.113889
2	1	0	-1.545521	-0.391638	1.877207
3	6	0	-1.298595	1.182144	0.477289
4	8	0	-2.256204	-0.607359	-1.415806
5	8	0	-3.027432	-1.329636	-0.714039
6	8	0	-2.465218	-2.048318	0.172448
7	6	0	0.372930	-0.643809	0.760013
8	1	0	0.710007	-1.255599	1.600250
9	1	0	0.149510	-1.341509	-0.063553
10	6	0	-2.600834	1.876667	0.760999
11	1	0	-3.203003	1.322452	1.485307
12	1	0	-2.431710	2.885514	1.157768
13	1	0	-3.188243	1.992013	-0.157012
14	6	0	-0.376887	1.786513	-0.484765
15	1	0	-0.753877	2.585679	-1.117186
16	6	0	0.903497	1.401994	-0.571769
17	1	0	1.561280	1.899101	-1.277462
18	6	0	1.487497	0.329635	0.321717
19	1	0	1.871173	0.836193	1.226569
20	6	0	2.697990	-0.391903	-0.329712
21	1	0	2.365304	-0.768184	-1.307728
22	6	0	3.876128	0.568183	-0.558259

23	1	0	4.704824	0.048587	-1.049818
24	1	0	3.613680	1.425384	-1.183961
25	1	0	4.249951	0.956720	0.396819
26	6	0	3.177035	-1.593329	0.499711
27	1	0	2.421122	-2.379007	0.571069
28	1	0	4.069922	-2.036745	0.047359
29	1	0	3.442691	-1.285939	1.518870

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239121	E(Thermal)=	0.254688
E(CCSD(T))=	-614.295245	E(Empiric)=	-0.350464
DE(MP2)=	-0.751082	DE(HF)=	-0.064528
G4MP2(0 K)=	-615.222197	G4MP2 Energy=	-615.20663
G4MP2 Enthalpy=	-615.205686	G4MP2 Free Energy=	-615.266431

vdW2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.868467	-0.009808	-1.212098
2	1	0	1.418281	-0.401442	-2.059785
3	6	0	1.336577	1.068071	-0.530623
4	8	0	2.684968	-0.523917	1.506377
5	8	0	2.346318	-1.599152	0.913582
6	8	0	2.613506	-1.655351	-0.327148
7	6	0	-0.429658	-0.665342	-0.824021
8	1	0	-0.826630	-1.234300	-1.667576
9	1	0	-0.222896	-1.400317	-0.025719
10	6	0	2.650995	1.720907	-0.844331
11	1	0	3.141128	1.241047	-1.694327
12	1	0	2.520585	2.785959	-1.070888
13	1	0	3.323602	1.646908	0.016774
14	6	0	0.491313	1.643279	0.515843
15	1	0	0.937369	2.373725	1.184869
16	6	0	-0.805482	1.323895	0.629008
17	1	0	-1.408616	1.806373	1.391189
18	6	0	-1.477192	0.342156	-0.306543
19	1	0	-1.847937	0.918164	-1.174371
20	6	0	-2.713250	-0.341371	0.336751
21	1	0	-2.382626	-0.787743	1.285701
22	6	0	-3.824336	0.674883	0.644726
23	1	0	-4.670127	0.182104	1.134631
24	1	0	-3.493547	1.483026	1.302390

25	1	0	-4.198059	1.131557	-0.279690
26	6	0	-3.284360	-1.466235	-0.540450
27	1	0	-2.581925	-2.293210	-0.670191
28	1	0	-4.193416	-1.876481	-0.089178
29	1	0	-3.551956	-1.090623	-1.535888

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239222	E(Thermal)=	0.25472
E(CCSD(T))=	-614.295026	E(Empiric)=	-0.350464
DE(MP2)=	-0.751267	DE(HF)=	-0.064423
G4MP2(0 K)=	-615.221958	G4MP2 Energy=	-615.206461
G4MP2 Enthalpy=	-615.205516	G4MP2 Free Energy=	-615.265868

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.918202	-0.289206	1.017422
2	1	0	-1.430115	-0.739301	1.859748
3	6	0	-1.391925	0.889315	0.478788
4	8	0	-2.448882	-0.225307	-1.397476
5	8	0	-3.005325	-1.129464	-0.667665
6	8	0	-2.150292	-1.863738	-0.038077
7	6	0	0.422693	-0.827494	0.598457
8	1	0	0.789630	-1.535550	1.344067
9	1	0	0.261734	-1.394832	-0.330593
10	6	0	-2.680738	1.505536	0.949617
11	1	0	-3.404719	0.737946	1.237436
12	1	0	-2.507642	2.142931	1.826629
13	1	0	-3.129604	2.128636	0.172325
14	6	0	-0.495648	1.663383	-0.374294
15	1	0	-0.919893	2.497333	-0.925750
16	6	0	0.816715	1.401671	-0.443262
17	1	0	1.449960	2.035296	-1.055784
18	6	0	1.465741	0.279075	0.334440
19	1	0	1.786247	0.694986	1.306995
20	6	0	2.746275	-0.257464	-0.361675
21	1	0	2.468624	-0.527037	-1.390629
22	6	0	3.847397	0.812936	-0.423632
23	1	0	4.725980	0.428566	-0.951350
24	1	0	3.530878	1.722902	-0.940269
25	1	0	4.167125	1.098568	0.585841
26	6	0	3.301306	-1.516187	0.322777

27	1	0	2.612689	-2.362338	0.263106
28	1	0	4.239611	-1.823101	-0.150111
29	1	0	3.513803	-1.326328	1.382246

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239544	E(Thermal)=	0.253774
E(CCSD(T))=	-614.291056	E(Empiric)=	-0.350464
DE(MP2)=	-0.753015	DE(HF)=	-0.063511
G4MP2(0 K)=	-615.218502	G4MP2 Energy=	-615.204271
G4MP2 Enthalpy=	-615.203327	G4MP2 Free Energy=	-615.259568

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.940101	-0.223354	1.090745
2	1	0	-1.418108	-0.611515	1.981056
3	6	0	-1.434760	0.912105	0.484623
4	8	0	-2.668270	-0.283383	-1.324880
5	8	0	-2.193572	-1.443914	-1.030183
6	8	0	-2.344825	-1.750054	0.212675
7	6	0	0.391403	-0.781687	0.664073
8	1	0	0.773401	-1.460574	1.428434
9	1	0	0.230370	-1.384232	-0.245570
10	6	0	-2.721780	1.547281	0.924212
11	1	0	-3.371758	0.816226	1.408721
12	1	0	-2.528185	2.365821	1.629950
13	1	0	-3.259144	1.969709	0.071137
14	6	0	-0.564200	1.625367	-0.445673
15	1	0	-1.007358	2.411868	-1.049363
16	6	0	0.751683	1.376609	-0.515062
17	1	0	1.368704	1.973441	-1.178778
18	6	0	1.422458	0.315863	0.328785
19	1	0	1.739095	0.794515	1.273432
20	6	0	2.707030	-0.245006	-0.339007
21	1	0	2.429840	-0.580674	-1.348596
22	6	0	3.791468	0.836018	-0.471713
23	1	0	4.672454	0.434324	-0.982171
24	1	0	3.457635	1.709215	-1.038425
25	1	0	4.112915	1.185195	0.516965
26	6	0	3.283878	-1.451206	0.418215
27	1	0	2.609310	-2.310773	0.412228
28	1	0	4.225730	-1.771124	-0.038651

29	1	0	3.495965	-1.194552	1.463540

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239633	E(Thermal)=	0.253859
E(CCSD(T))=	-614.292036	E(Empiric)=	-0.350464
DE(MP2)=	-0.752621	DE(HF)=	-0.063467
G4MP2(0 K)=	-615.218955	G4MP2 Energy=	-615.204729
G4MP2 Enthalpy=	-615.203785	G4MP2 Free Energy=	-615.260003

vdW3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.291908	-0.121002	1.000357
2	1	0	-1.979795	0.410253	1.649370
3	6	0	0.027763	0.206573	0.992323
4	1	0	0.382314	0.997829	1.641949
5	8	0	-0.143992	2.040823	-0.755437
6	8	0	-1.236989	2.567496	-0.353541
7	8	0	-2.269421	1.825557	-0.457132
8	6	0	1.041113	-0.653271	0.274481
9	1	0	1.278299	-1.482760	0.967727
10	6	0	-1.804994	-1.241985	0.220226
11	6	0	-3.222085	-1.683636	0.459683
12	1	0	-3.376017	-1.989521	1.501749
13	1	0	-3.919761	-0.859751	0.265137
14	1	0	-3.495656	-2.522498	-0.185134
15	6	0	2.378358	0.075959	-0.015742
16	1	0	2.142242	0.979376	-0.591549
17	6	0	3.081942	0.506306	1.281392
18	1	0	4.014238	1.032727	1.053733
19	1	0	2.473953	1.178296	1.892948
20	1	0	3.336646	-0.365998	1.895807
21	6	0	3.337132	-0.786420	-0.851275
22	1	0	4.295501	-0.273357	-0.980183
23	1	0	3.541070	-1.744141	-0.356069
24	1	0	2.944366	-0.999938	-1.848518
25	6	0	0.387857	-1.279794	-0.973801
26	1	0	0.332205	-0.521588	-1.770237
27	1	0	1.012913	-2.089805	-1.358465
28	6	0	-1.002477	-1.793379	-0.706328
29	1	0	-1.375512	-2.596221	-1.337290

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239393	E(Thermal)=	0.254744
E(CCSD(T))=	-614.294733	E(Empiric)=	-0.350464
DE(MP2)=	-0.751442	DE(HF)=	-0.064335
G4MP2(0 K)=	-615.22158	G4MP2 Energy=	-615.206229
G4MP2 Enthalpy=	-615.205285	G4MP2 Free Energy=	-615.265034

vdW4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.169644	-0.217761	1.181561
2	1	0	-1.825117	0.214179	1.929301
3	6	0	0.137088	0.136983	1.133844
4	1	0	0.509655	0.873725	1.835954
5	8	0	-0.366378	1.978127	-0.739638
6	8	0	-1.608492	1.742314	-0.922243
7	8	0	-2.351454	1.907103	0.101155
8	6	0	1.124882	-0.601754	0.261474
9	1	0	1.405662	-1.510024	0.827094
10	6	0	-1.730421	-1.172825	0.236502
11	6	0	-3.158964	-1.599421	0.424657
12	1	0	-3.308825	-2.077108	1.400283
13	1	0	-3.817352	-0.722170	0.394569
14	1	0	-3.478881	-2.298517	-0.351877
15	6	0	2.435696	0.185253	0.006213
16	1	0	2.155491	1.144238	-0.448401
17	6	0	3.193434	0.472017	1.312255
18	1	0	4.104788	1.042634	1.107471
19	1	0	2.604982	1.050742	2.029049
20	1	0	3.492469	-0.462242	1.803165
21	6	0	3.367797	-0.549993	-0.969637
22	1	0	4.309181	-0.002823	-1.081865
23	1	0	3.613124	-1.553688	-0.600208
24	1	0	2.930556	-0.655095	-1.965656
25	6	0	0.427692	-1.064582	-1.033031
26	1	0	0.396187	-0.217364	-1.738651
27	1	0	1.016291	-1.846932	-1.520583
28	6	0	-0.976604	-1.553860	-0.813873
29	1	0	-1.403342	-2.204251	-1.573633

Temperature=	298.15	Pressure=	1

E(ZPE)=	0.239494	E(Thermal)=	0.254749
E(CCSD(T))=	-614.297118	E(Empiric)=	-0.350464
DE(MP2)=	-0.751727	DE(HF)=	-0.063976
G4MP2(0 K)=	-615.223791	G4MP2 Energy=	-615.208536
G4MP2 Enthalpy=	-615.207592	G4MP2 Free Energy=	-615.266973

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.313995	-0.033754	0.973798
2	1	0	-1.985185	0.513483	1.626115
3	6	0	0.017520	0.276301	0.951457
4	1	0	0.385393	1.057942	1.604053
5	8	0	-0.055739	1.970178	-0.738369
6	8	0	-1.167391	2.524898	-0.410610
7	8	0	-2.192233	1.766176	-0.533682
8	6	0	1.016890	-0.639163	0.285120
9	1	0	1.232962	-1.429370	1.029449
10	6	0	-1.842493	-1.178312	0.242674
11	6	0	-3.271037	-1.577212	0.489335
12	1	0	-3.441290	-1.826238	1.543906
13	1	0	-3.948118	-0.749382	0.245635
14	1	0	-3.556498	-2.441975	-0.114758
15	6	0	2.373249	0.036533	-0.043968
16	1	0	2.168986	0.872190	-0.724037
17	6	0	3.052967	0.601650	1.213377
18	1	0	4.019415	1.046134	0.955536
19	1	0	2.462017	1.381463	1.700567
20	1	0	3.240035	-0.189804	1.949626
21	6	0	3.334911	-0.931657	-0.751197
22	1	0	4.305303	-0.452177	-0.914241
23	1	0	3.509326	-1.829152	-0.144411
24	1	0	2.962069	-1.252514	-1.727087
25	6	0	0.359643	-1.326599	-0.928964
26	1	0	0.331729	-0.618873	-1.771426
27	1	0	0.968632	-2.173493	-1.255568
28	6	0	-1.044499	-1.791410	-0.648382
29	1	0	-1.430810	-2.616510	-1.241566

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.23944	E(Thermal)=	0.253838
E(CCSD(T))=	-614.293645	E(Empiric)=	-0.350464

DE(MP2)=	-0.752202	DE(HF)=	-0.064016
G4MP2(0 K)=	-615.220888	G4MP2 Energy=	-615.20649
G4MP2 Enthalpy=	-615.205545	G4MP2 Free Energy=	-615.262653

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.311451	0.060147	1.071685
2	1	0	-1.936417	0.572705	1.792966
3	6	0	0.010640	0.204952	1.069418
4	1	0	0.512270	0.841021	1.788662
5	8	0	0.218316	1.880419	-0.207628
6	8	0	-0.844158	1.886876	-0.926817
7	8	0	-1.920806	2.004211	-0.238971
8	6	0	0.927198	-0.692565	0.202413
9	1	0	1.041562	-1.645278	0.675867
10	6	0	-1.978749	-1.023460	0.152320
11	6	0	-3.380696	-1.533816	0.534002
12	1	0	-3.339487	-2.587500	0.715528
13	1	0	-3.714276	-1.032314	1.418378
14	1	0	-4.062406	-1.336233	-0.266706
15	6	0	2.308373	-0.031187	0.039521
16	1	0	2.187577	0.951824	-0.365446
17	6	0	2.998711	0.060732	1.413051
18	1	0	4.047734	0.220115	1.275038
19	1	0	2.583781	0.876827	1.966875
20	1	0	2.844269	-0.850882	1.951575
21	6	0	3.173066	-0.876529	-0.914053
22	1	0	4.189268	-0.545592	-0.861953
23	1	0	3.118057	-1.905940	-0.627371
24	1	0	2.812666	-0.765403	-1.915384
25	6	0	0.282142	-0.881998	-1.183089
26	1	0	0.388186	0.018027	-1.751955
27	1	0	0.766876	-1.686800	-1.695171
28	6	0	-1.249324	-1.199751	-0.957842
29	1	0	-1.745924	-1.815770	-1.678126

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239735	E(Thermal)=	0.253922
E(CCSD(T))=	-614.295311	E(Empiric)=	-0.350464
DE(MP2)=	-0.752603	DE(HF)=	-0.063466
G4MP2(0 K)=	-615.222109	G4MP2 Energy=	-615.207921

G4MP2 Enthalpy=	-615.206977	G4MP2 Free Energy=	-615.263088

TS1*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.028630	-0.112026	1.211593
2	1	0	1.639420	-0.638865	1.936891
3	6	0	1.579089	0.916355	0.485167
4	8	0	2.019516	-0.585129	-1.543920
5	8	0	2.377864	-1.586423	-0.825989
6	8	0	1.457767	-2.016658	-0.037856
7	6	0	-0.459530	-0.305673	1.275688
8	1	0	-0.681734	-1.355288	1.478336
9	1	0	-0.839111	0.265937	2.141169
10	6	0	3.033349	1.283040	0.603118
11	1	0	3.631578	0.434800	0.946010
12	1	0	3.437949	1.626969	-0.351980
13	1	0	3.165922	2.097646	1.327991
14	6	0	0.673833	1.810955	-0.227511
15	1	0	1.077008	2.750708	-0.594186
16	6	0	-0.608546	1.487157	-0.446298
17	1	0	-1.248067	2.174772	-0.990369
18	6	0	-1.179893	0.158108	-0.006419
19	1	0	-0.928778	-0.571324	-0.792215
20	6	0	-2.723675	0.189658	0.130237
21	1	0	-2.979725	1.031787	0.790277
22	6	0	-3.400764	0.422116	-1.229861
23	1	0	-4.486939	0.492180	-1.113045
24	1	0	-3.065519	1.339540	-1.721202
25	1	0	-3.193013	-0.411787	-1.910774
26	6	0	-3.285163	-1.092735	0.763519
27	1	0	-2.949346	-1.231961	1.794274
28	1	0	-4.379458	-1.063686	0.776703
29	1	0	-2.985338	-1.977492	0.188843

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239369	E(Thermal)=	0.253706
E(CCSD(T))=	-614.293636	E(Empiric)=	-0.350464
DE(MP2)=	-0.752051	DE(HF)=	-0.063692
G4MP2(0 K)=	-615.220475	G4MP2 Energy=	-615.206138
G4MP2 Enthalpy=	-615.205194	G4MP2 Free Energy=	-615.261654

TS2*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.011974	-0.160638	1.280894
2	1	0	-1.576595	0.185057	2.140365
3	6	0	-1.627487	-0.956995	0.350694
4	8	0	-2.744345	1.004992	-0.932809
5	8	0	-1.649653	1.666764	-0.898399
6	8	0	-1.263227	1.980538	0.285576
7	6	0	0.488281	-0.040371	1.339213
8	1	0	0.769628	0.862852	1.883356
9	1	0	0.859467	-0.891284	1.937560
10	6	0	-3.037370	-1.457500	0.517462
11	1	0	-3.611335	-0.806270	1.179765
12	1	0	-3.560342	-1.519334	-0.439876
13	1	0	-3.029862	-2.465515	0.953599
14	6	0	-0.811692	-1.456641	-0.744670
15	1	0	-1.273354	-2.146840	-1.445406
16	6	0	0.451286	-1.041818	-0.950349
17	1	0	0.982806	-1.403665	-1.824641
18	6	0	1.164570	-0.065380	-0.045611
19	1	0	1.045152	0.938178	-0.486504
20	6	0	2.692508	-0.336779	0.036556
21	1	0	2.824890	-1.380008	0.358475
22	6	0	3.379108	-0.163835	-1.327421
23	1	0	4.451553	-0.366462	-1.243594
24	1	0	2.982688	-0.834389	-2.094296
25	1	0	3.264346	0.863901	-1.691998
26	6	0	3.382925	0.568667	1.068752
27	1	0	3.027926	0.389905	2.086724
28	1	0	4.463881	0.396147	1.063817
29	1	0	3.216028	1.627109	0.834596

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.23963	E(Thermal)=	0.253965
E(CCSD(T))=	-614.293622	E(Empiric)=	-0.350464
DE(MP2)=	-0.752386	DE(HF)=	-0.063594
G4MP2(0 K)=	-615.220436	G4MP2 Energy=	-615.206101
G4MP2 Enthalpy=	-615.205157	G4MP2 Free Energy=	-615.261673

TS3*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.296368	-0.107726	0.901356
2	1	0	1.971186	0.337375	1.624601
3	6	0	-0.011018	0.307397	0.842192
4	1	0	-0.377913	1.010343	1.579855
5	8	0	0.223720	2.197255	-0.413368
6	8	0	1.462799	2.491601	-0.224594
7	8	0	2.271208	1.553181	-0.573856
8	6	0	-0.999739	-0.380846	-0.072512
9	1	0	-0.856197	0.075456	-1.065108
10	6	0	1.763003	-1.268971	0.152373
11	6	0	3.244314	-1.498852	0.050738
12	1	0	3.728395	-0.661765	-0.464468
13	1	0	3.702285	-1.565146	1.045565
14	1	0	3.471616	-2.420887	-0.490099
15	6	0	-2.468983	-0.137828	0.355804
16	1	0	-2.557298	-0.444055	1.409119
17	6	0	-2.850961	1.347549	0.253009
18	1	0	-3.863466	1.509584	0.636556
19	1	0	-2.174212	2.001399	0.807829
20	1	0	-2.833072	1.677232	-0.792045
21	6	0	-3.464302	-0.977135	-0.459824
22	1	0	-4.492052	-0.730124	-0.175221
23	1	0	-3.362241	-0.772334	-1.532582
24	1	0	-3.331692	-2.051436	-0.307593
25	6	0	-0.635353	-1.874613	-0.209339
26	1	0	-0.993332	-2.436244	0.670588
27	1	0	-1.162556	-2.301871	-1.066737
28	6	0	0.844116	-2.101835	-0.365384
29	1	0	1.164059	-3.006659	-0.876203

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239742	E(Thermal)=	0.253877
E(CCSD(T))=	-614.292746	E(Empiric)=	-0.350464
DE(MP2)=	-0.75274	DE(HF)=	-0.063899
G4MP2(0 K)=	-615.220107	G4MP2 Energy=	-615.205971
G4MP2 Enthalpy=	-615.205027	G4MP2 Free Energy=	-615.260858

TS4*

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.296159	-0.061362	0.974398
2	1	0	1.939449	0.377286	1.727906
3	6	0	-0.029843	0.302930	0.917128
4	1	0	-0.437600	0.931223	1.698161
5	8	0	0.218881	2.302452	-0.078532
6	8	0	1.153125	2.008822	-0.917222
7	8	0	2.273992	1.735102	-0.340357
8	6	0	-0.973964	-0.388588	-0.045548
9	1	0	-0.823686	0.086024	-1.029209
10	6	0	1.814668	-1.166400	0.176313
11	6	0	3.303549	-1.319505	0.051069
12	1	0	3.723114	-0.457275	-0.479566
13	1	0	3.783407	-1.351178	1.036823
14	1	0	3.571101	-2.231172	-0.488959
15	6	0	-2.461143	-0.205698	0.345766
16	1	0	-2.576639	-0.581224	1.373767
17	6	0	-2.880337	1.272749	0.326071
18	1	0	-3.926975	1.374493	0.630609
19	1	0	-2.278825	1.894337	0.993153
20	1	0	-2.780619	1.690850	-0.681639
21	6	0	-3.403813	-1.016828	-0.556724
22	1	0	-4.447242	-0.817428	-0.293051
23	1	0	-3.272351	-0.739821	-1.609933
24	1	0	-3.244877	-2.094762	-0.469284
25	6	0	-0.554639	-1.864424	-0.211906
26	1	0	-0.889846	-2.457470	0.656243
27	1	0	-1.062721	-2.293756	-1.079535
28	6	0	0.933088	-2.021287	-0.373158
29	1	0	1.293970	-2.890654	-0.917047

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.23988	E(Thermal)=	0.253922
E(CCSD(T))=	-614.292966	E(Empiric)=	-0.350464
DE(MP2)=	-0.752248	DE(HF)=	-0.063529
G4MP2(0 K)=	-615.219327	G4MP2 Energy=	-615.205285
G4MP2 Enthalpy=	-615.204341	G4MP2 Free Energy=	-615.259852

POZ1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.386753	-1.021239	0.062141
2	6	0	1.355477	0.158781	0.250565
3	6	0	0.730310	1.383809	-0.380454
4	6	0	-0.581210	1.557636	-0.530474
5	6	0	-1.610065	0.630730	0.046532
6	6	0	-1.012271	-0.703252	0.586891
7	1	0	1.481292	0.340899	1.331483
8	1	0	0.297431	-1.249557	-1.005454
9	1	0	0.751593	-1.920450	0.563959
10	1	0	-0.970212	2.448366	-1.016454
11	1	0	-1.031046	-0.694020	1.684501
12	1	0	1.399197	2.151308	-0.758865
13	6	0	2.775660	-0.108809	-0.321545
14	1	0	2.693131	-0.094140	-1.417823
15	6	0	-2.466724	1.345477	1.098998
16	1	0	-3.263695	0.685113	1.448090
17	1	0	-1.852048	1.643093	1.953632
18	1	0	-2.917220	2.244534	0.668963
19	8	0	-2.445927	0.147867	-1.025669
20	8	0	-1.903426	-1.715356	0.099863
21	8	0	-3.050148	-0.984610	-0.416428
22	6	0	3.762020	0.991259	0.102636
23	1	0	4.740950	0.829747	-0.359403
24	1	0	3.430048	1.994379	-0.178614
25	1	0	3.904078	0.982858	1.190093
26	6	0	3.336177	-1.478259	0.090807
27	1	0	3.350666	-1.586030	1.182415
28	1	0	2.758749	-2.308674	-0.322417
29	1	0	4.366335	-1.587414	-0.262804

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.243803	E(Thermal)=	0.256859
E(CCSD(T))=	-614.386908	E(Empiric)=	-0.350464
DE(MP2)=	-0.747615	DE(HF)=	-0.062245
G4MP2(0 K)=	-615.303429	G4MP2 Energy=	-615.290373
G4MP2 Enthalpy=	-615.289429	G4MP2 Free Energy=	-615.342735

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.383407	-1.041336	-0.213388
2	6	0	-1.350708	0.140524	-0.388446

3	6	0	-0.712494	1.457192	-0.021087
4	6	0	0.583791	1.701693	0.176315
5	6	0	1.672008	0.701948	0.034225
6	6	0	1.009927	-0.824287	-0.805965
7	1	0	-1.614762	0.211914	-1.458565
8	1	0	-0.258330	-1.282546	0.847502
9	1	0	-0.794443	-1.934158	-0.694170
10	1	0	0.910812	2.719266	0.384129
11	1	0	1.023193	-0.348218	-1.806655
12	1	0	-1.385280	2.306767	0.053228
13	6	0	-2.696761	-0.069973	0.373281
14	1	0	-2.474602	0.000670	1.447471
15	6	0	2.879932	1.105785	-0.783882
16	1	0	3.444565	0.231185	-1.100677
17	1	0	2.556268	1.681312	-1.653701
18	1	0	3.530095	1.738463	-0.167854
19	8	0	1.936653	0.053124	1.200873
20	8	0	1.908219	-1.703339	-0.587656
21	8	0	2.874666	-0.855615	1.038204
22	6	0	-3.738291	1.006363	0.025815
23	1	0	-4.671575	0.818459	0.565705
24	1	0	-3.416879	2.018061	0.285892
25	1	0	-3.970227	0.993203	-1.046060
26	6	0	-3.301779	-1.457368	0.106606
27	1	0	-3.466247	-1.615602	-0.966415
28	1	0	-2.669651	-2.268709	0.473841
29	1	0	-4.272559	-1.546665	0.604114

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240865	E(Thermal)=	0.254201
E(CCSD(T))=	-614.359775	E(Empiric)=	-0.350464
DE(MP2)=	-0.753425	DE(HF)=	-0.061048
G4MP2(0 K)=	-615.283847	G4MP2 Energy=	-615.27051
G4MP2 Enthalpy=	-615.269566	G4MP2 Free Energy=	-615.323418

Cl1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.459439	1.410663	0.626960
2	6	0	1.235956	0.581764	-0.437239
3	6	0	0.359263	0.030210	-1.544998
4	6	0	-0.865007	-0.532414	-1.511697

5	6	0	-1.685876	-0.859080	-0.366936
6	6	0	-0.492485	2.391489	-0.014669
7	1	0	1.924175	1.279552	-0.936108
8	1	0	-0.089131	0.784626	1.330771
9	1	0	1.194906	1.996886	1.191145
10	1	0	-1.346119	-0.741746	-2.464179
11	1	0	-0.002083	3.151952	-0.668200
12	1	0	0.779147	0.147539	-2.541624
13	6	0	2.133184	-0.520268	0.210406
14	6	0	-3.163703	-0.837389	-0.365250
15	1	0	-3.486824	-0.011752	0.281682
16	1	0	-3.565238	-0.701444	-1.369704
17	1	0	-3.537687	-1.750144	0.111027
18	8	0	-1.077717	-1.183313	0.712069
19	8	0	-1.689466	2.390217	0.128826
20	8	0	-1.828786	-1.416275	1.819413
21	6	0	3.099940	0.064191	1.249114
22	1	0	3.753994	-0.723050	1.637110
23	1	0	3.741813	0.835584	0.805304
24	1	0	2.580577	0.503761	2.104254
25	6	0	2.916745	-1.294540	-0.860454
26	1	0	3.587332	-0.629687	-1.419148
27	1	0	3.534132	-2.069302	-0.395642
28	1	0	2.253451	-1.785534	-1.578187
29	1	0	1.460566	-1.220043	0.717614

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240018	E(Thermal)=	0.255353
E(CCSD(T))=	-614.397186	E(Empiric)=	-0.350464
DE(MP2)=	-0.754366	DE(HF)=	-0.06133
G4MP2(0 K)=	-615.323327	G4MP2 Energy=	-615.307993
G4MP2 Enthalpy=	-615.307048	G4MP2 Free Energy=	-615.366126

POZ1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.354079	-1.005762	0.190730
2	6	0	1.308391	0.200013	0.242771
3	6	0	0.652503	1.342126	-0.501633
4	6	0	-0.665900	1.496086	-0.600754
5	6	0	-1.671054	0.634982	0.111798
6	6	0	-1.048091	-0.671852	0.700503

7	1	0	1.443720	0.490898	1.298688
8	1	0	0.260944	-1.342047	-0.847359
9	1	0	0.736187	-1.842127	0.780841
10	1	0	-1.085802	2.319406	-1.172975
11	1	0	-1.080307	-0.649543	1.794259
12	1	0	1.299633	2.052128	-1.008744
13	6	0	2.724725	-0.104834	-0.317125
14	1	0	2.627955	-0.207280	-1.407654
15	6	0	-2.454567	1.436536	1.155871
16	1	0	-3.167406	0.784781	1.668212
17	1	0	-1.774255	1.881440	1.887753
18	1	0	-3.011006	2.245660	0.673814
19	8	0	-2.675494	0.127339	-0.808393
20	8	0	-1.993874	-1.670499	0.316322
21	8	0	-2.306657	-1.245165	-1.015656
22	6	0	3.695880	1.050430	-0.025625
23	1	0	4.671012	0.860376	-0.484923
24	1	0	3.338498	2.012538	-0.402733
25	1	0	3.854121	1.157083	1.054429
26	6	0	3.314418	-1.413673	0.229090
27	1	0	3.345644	-1.404636	1.325673
28	1	0	2.745501	-2.292218	-0.084690
29	1	0	4.341448	-1.544174	-0.126528

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.243901	E(Thermal)=	0.256876
E(CCSD(T))=	-614.387494	E(Empiric)=	-0.350464
DE(MP2)=	-0.747558	DE(HF)=	-0.062093
G4MP2(0 K)=	-615.303708	G4MP2 Energy=	-615.290732
G4MP2 Enthalpy=	-615.289788	G4MP2 Free Energy=	-615.342578

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.442002	1.240555	0.161248
2	6	0	-1.241346	-0.083898	0.066238
3	6	0	-0.505332	-0.972642	-0.906296
4	6	0	0.811056	-1.154188	-0.830371
5	6	0	1.623263	-0.673285	0.310863
6	6	0	1.059729	1.148337	0.508066
7	1	0	-1.253350	-0.548515	1.063933
8	1	0	-0.498801	1.758239	-0.801338

9	1	0	-0.891590	1.893820	0.916279
10	1	0	1.376153	-1.656820	-1.611343
11	1	0	1.269980	1.203886	1.592036
12	1	0	-1.050251	-1.381024	-1.752245
13	6	0	-2.721151	0.116427	-0.346419
14	1	0	-2.723177	0.455347	-1.392833
15	6	0	1.538762	-1.413129	1.628602
16	1	0	2.252402	-0.996451	2.343369
17	1	0	0.534427	-1.335002	2.047250
18	1	0	1.757154	-2.476268	1.485110
19	8	0	2.913573	-0.383785	0.026304
20	8	0	1.868533	1.794039	-0.254925
21	8	0	2.978696	0.382879	-1.048107
22	6	0	-3.490812	-1.211745	-0.268999
23	1	0	-4.514219	-1.090620	-0.637555
24	1	0	-3.018480	-2.004550	-0.856278
25	1	0	-3.552037	-1.561857	0.768647
26	6	0	-3.442216	1.179088	0.495078
27	1	0	-3.387938	0.938296	1.564061
28	1	0	-3.024748	2.178879	0.353231
29	1	0	-4.501643	1.224453	0.223445

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240685	E(Thermal)=	0.254029
E(CCSD(T))=	-614.35319	E(Empiric)=	-0.350464
DE(MP2)=	-0.753682	DE(HF)=	-0.061308
G4MP2(0 K)=	-615.277959	G4MP2 Energy=	-615.264615
G4MP2 Enthalpy=	-615.263671	G4MP2 Free Energy=	-615.31694

Cl1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.977353	1.230119	-0.041866
2	6	0	-1.146807	-0.079582	-0.026257
3	6	0	0.011167	0.086686	-0.973412
4	6	0	1.346396	0.029988	-0.794126
5	6	0	2.116231	-0.218646	0.392306
6	6	0	-1.176708	2.443976	0.380233
7	1	0	-0.793710	-0.245460	0.995617
8	1	0	-2.405829	1.422396	-1.030783
9	1	0	-2.805706	1.139502	0.672294
10	1	0	1.997331	0.184984	-1.648770

11	1	0	-0.589897	2.301954	1.319679
12	1	0	-0.309903	0.299224	-1.994352
13	6	0	-2.006808	-1.316468	-0.433550
14	1	0	-2.330004	-1.155779	-1.472017
15	6	0	1.642097	-0.433086	1.793835
16	1	0	2.508292	-0.571104	2.443539
17	1	0	1.064924	0.424400	2.155794
18	1	0	1.003252	-1.319344	1.867595
19	8	0	3.403923	-0.268017	0.300993
20	8	0	-1.164384	3.496657	-0.200267
21	8	0	4.025665	-0.109415	-0.881272
22	6	0	-1.177175	-2.608357	-0.389533
23	1	0	-1.772396	-3.457770	-0.738024
24	1	0	-0.282720	-2.544686	-1.014096
25	1	0	-0.856943	-2.832868	0.635485
26	6	0	-3.262419	-1.471545	0.436933
27	1	0	-3.000402	-1.538229	1.499891
28	1	0	-3.968834	-0.646944	0.313013
29	1	0	-3.790813	-2.392592	0.172129

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239912	E(Thermal)=	0.255349
E(CCSD(T))=	-614.392912	E(Empiric)=	-0.350464
DE(MP2)=	-0.754441	DE(HF)=	-0.06176
G4MP2(0 K)=	-615.319666	G4MP2 Energy=	-615.304229
G4MP2 Enthalpy=	-615.303285	G4MP2 Free Energy=	-615.363881

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.323546	-0.958791	0.221503
2	6	0	1.335712	0.193847	0.357809
3	6	0	0.717134	1.471005	-0.165318
4	6	0	-0.587008	1.664161	-0.355533
5	6	0	-1.640467	0.655150	0.018324
6	6	0	-1.050324	-0.558451	0.751148
7	1	0	1.557481	0.337741	1.429718
8	1	0	0.217246	-1.231244	-0.833770
9	1	0	0.658812	-1.846711	0.762312
10	1	0	-0.951018	2.607664	-0.752599
11	1	0	-1.038814	-0.399442	1.834997
12	1	0	1.394734	2.283833	-0.410302

13	6	0	2.697050	-0.105688	-0.334488
14	1	0	2.523222	-0.073589	-1.419457
15	6	0	-2.811893	1.292082	0.769915
16	1	0	-3.541244	0.529393	1.050948
17	1	0	-2.461812	1.800571	1.674063
18	1	0	-3.305316	2.028782	0.129959
19	8	0	-2.101937	0.029956	-1.195003
20	8	0	-2.050486	-1.540906	0.538307
21	8	0	-2.499458	-1.330489	-0.829355
22	6	0	3.757828	0.950095	0.015601
23	1	0	4.696038	0.737198	-0.506332
24	1	0	3.458912	1.965414	-0.257740
25	1	0	3.970264	0.943923	1.091567
26	6	0	3.237290	-1.500533	0.016314
27	1	0	3.351736	-1.617433	1.101108
28	1	0	2.588361	-2.302887	-0.342409
29	1	0	4.223242	-1.648971	-0.435304

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.243251	E(Thermal)=	0.255795
E(CCSD(T))=	-614.384644	E(Empiric)=	-0.350464
DE(MP2)=	-0.746383	DE(HF)=	-0.062277
G4MP2(0 K)=	-615.300518	G4MP2 Energy=	-615.287974
G4MP2 Enthalpy=	-615.28703	G4MP2 Free Energy=	-615.338874

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.703345	1.520640	-0.046496
2	6	0	1.315631	0.196259	-0.427786
3	6	0	0.288238	-0.921866	-0.213450
4	6	0	-1.052148	-0.592583	-0.819832
5	6	0	-1.755263	0.763104	0.239571
6	6	0	-0.575367	1.734758	0.244715
7	1	0	0.621159	-1.855230	-0.682904
8	1	0	1.578266	0.238677	-1.498996
9	1	0	1.375818	2.372946	-0.009089
10	1	0	-1.068996	-0.255638	-1.856949
11	1	0	-0.895528	2.743524	0.502416
12	1	0	0.146822	-1.113485	0.850628
13	6	0	2.644394	-0.075017	0.338033
14	1	0	2.418217	-0.005380	1.411031

15	6	0	-2.960322	1.324035	-0.533951
16	1	0	-3.737841	0.562449	-0.614520
17	1	0	-3.372505	2.170898	0.025575
18	1	0	-2.688135	1.680086	-1.532671
19	8	0	-2.018669	0.133374	1.326753
20	8	0	-2.067136	-1.453357	-0.627014
21	8	0	-2.115832	-1.845237	0.630234
22	6	0	3.721862	0.968606	0.004420
23	1	0	3.426829	1.986044	0.272494
24	1	0	4.646033	0.746712	0.547052
25	1	0	3.958495	0.958049	-1.066535
26	6	0	3.195628	-1.481885	0.057648
27	1	0	2.530234	-2.272161	0.413918
28	1	0	3.358825	-1.634368	-1.016556
29	1	0	4.159414	-1.617679	0.558079

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240929	E(Thermal)=	0.25429
E(CCSD(T))=	-614.354692	E(Empiric)=	-0.350464
DE(MP2)=	-0.754161	DE(HF)=	-0.060944
G4MP2(0 K)=	-615.279332	G4MP2 Energy=	-615.265972
G4MP2 Enthalpy=	-615.265027	G4MP2 Free Energy=	-615.31863

Cl2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.846704	0.011992	1.383199
2	6	0	-0.042682	0.990772	0.636972
3	6	0	-1.240286	0.301761	-0.048100
4	6	0	-2.047126	-0.535721	0.855509
5	6	0	1.569740	-1.686009	-0.386033
6	6	0	1.495528	-1.092930	0.975351
7	1	0	-1.940695	1.020051	-0.494980
8	1	0	-0.455660	1.663705	1.401842
9	1	0	0.979034	0.249962	2.438040
10	1	0	-1.789562	-0.785451	1.881292
11	1	0	2.058176	-1.637719	1.730639
12	1	0	-0.920882	-0.318278	-0.896978
13	6	0	0.771147	1.894954	-0.339443
14	1	0	1.202001	1.236227	-1.099224
15	6	0	2.297802	-3.015339	-0.471301
16	1	0	2.296213	-3.372242	-1.501095

17	1	0	3.330116	-2.906353	-0.118710
18	1	0	1.817767	-3.755757	0.179053
19	8	0	1.101824	-1.161677	-1.380196
20	8	0	-3.150603	-1.034837	0.486610
21	8	0	-3.555431	-0.784914	-0.781832
22	6	0	-0.120852	2.929395	-1.040794
23	1	0	0.493301	3.595620	-1.655097
24	1	0	-0.859522	2.469486	-1.701551
25	1	0	-0.655700	3.553472	-0.313885
26	6	0	1.913295	2.608002	0.400370
27	1	0	2.493293	3.223682	-0.293992
28	1	0	1.523735	3.272445	1.182012
29	1	0	2.602442	1.901322	0.871588

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239953	E(Thermal)=	0.255343
E(CCSD(T))=	-614.392637	E(Empiric)=	-0.350464
DE(MP2)=	-0.753293	DE(HF)=	-0.061636
G4MP2(0 K)=	-615.318078	G4MP2 Energy=	-615.302688
G4MP2 Enthalpy=	-615.301743	G4MP2 Free Energy=	-615.361804

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.606081	-1.049299	-0.911741
2	6	0	1.252540	-0.099302	0.069350
3	6	0	0.383112	1.189771	0.152783
4	6	0	-1.085786	0.947462	0.390498
5	6	0	-1.670000	-0.867841	0.146281
6	6	0	-0.692240	-1.349964	-0.896439
7	1	0	0.759391	1.842344	0.945387
8	1	0	1.268416	-0.552749	1.070874
9	1	0	1.228297	-1.439071	-1.712882
10	1	0	-1.491700	1.048616	1.394799
11	1	0	-1.132000	-1.960259	-1.680323
12	1	0	0.474217	1.729066	-0.796324
13	6	0	2.725425	0.203755	-0.304520
14	1	0	2.734826	0.522900	-1.357166
15	6	0	-1.499706	-1.437664	1.569393
16	1	0	-2.259444	-1.000445	2.222104
17	1	0	-1.662697	-2.519361	1.532992
18	1	0	-0.508192	-1.263786	1.995052

19	8	0	-2.889120	-0.725282	-0.239269
20	8	0	-1.863207	1.495454	-0.553460
21	8	0	-3.134988	1.243107	-0.320915
22	6	0	3.584467	-1.064511	-0.178248
23	1	0	3.186290	-1.899618	-0.760830
24	1	0	4.606362	-0.875937	-0.521565
25	1	0	3.640678	-1.388753	0.867897
26	6	0	3.346141	1.328885	0.536565
27	1	0	2.869363	2.297127	0.362754
28	1	0	3.276936	1.104377	1.608195
29	1	0	4.407581	1.441561	0.294653

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241221	E(Thermal)=	0.254455
E(CCSD(T))=	-614.35261	E(Empiric)=	-0.350464
DE(MP2)=	-0.75399	DE(HF)=	-0.061351
G4MP2(0 K)=	-615.277194	G4MP2 Energy=	-615.26396
G4MP2 Enthalpy=	-615.263016	G4MP2 Free Energy=	-615.315979

Cl2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.212327	0.285371	-1.044593
2	6	0	-0.523469	-0.746233	0.008901
3	6	0	0.697347	-1.709198	0.129061
4	6	0	1.960674	-1.010672	0.477978
5	6	0	-0.329516	2.619148	0.083607
6	6	0	-0.130209	1.622667	-1.007407
7	1	0	0.488168	-2.447940	0.911946
8	1	0	-0.679774	-0.278974	0.983982
9	1	0	-0.017308	-0.166901	-2.019206
10	1	0	2.111162	-0.430511	1.387847
11	1	0	0.113581	2.134038	-1.935459
12	1	0	0.848430	-2.252674	-0.809554
13	6	0	-1.822287	-1.526443	-0.358036
14	1	0	-1.662806	-1.968636	-1.352235
15	6	0	-0.599912	2.206003	1.520307
16	1	0	-0.660643	3.108761	2.129214
17	1	0	-1.541920	1.654227	1.601123
18	1	0	0.197669	1.563182	1.906428
19	8	0	-0.266991	3.797917	-0.206863
20	8	0	2.945922	-1.084172	-0.308169

21	8	0	4.095101	-0.462834	0.018314
22	6	0	-3.027969	-0.578889	-0.448729
23	1	0	-2.856077	0.238517	-1.152942
24	1	0	-3.918794	-1.124745	-0.773871
25	1	0	-3.253162	-0.138152	0.530060
26	6	0	-2.128092	-2.665358	0.626530
27	1	0	-1.378677	-3.460847	0.604640
28	1	0	-2.196839	-2.290725	1.654970
29	1	0	-3.090704	-3.124289	0.381080

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.24008	E(Thermal)=	0.255619
E(CCSD(T))=	-614.385348	E(Empiric)=	-0.350464
DE(MP2)=	-0.75536	DE(HF)=	-0.061811
G4MP2(0 K)=	-615.312903	G4MP2 Energy=	-615.297365
G4MP2 Enthalpy=	-615.29642	G4MP2 Free Energy=	-615.357386

POZ2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.416118	-1.826591	0.205786
2	6	0	-0.922720	-0.402877	-0.103688
3	6	0	1.951045	-1.005191	0.043768
4	6	0	1.060727	-1.995820	-0.010238
5	1	0	-0.801448	-0.232527	-1.181442
6	1	0	-0.680692	-2.106478	1.238011
7	1	0	-0.944864	-2.541631	-0.430650
8	1	0	1.411358	-3.003376	-0.224986
9	6	0	-2.420290	-0.230941	0.265944
10	1	0	-2.495929	-0.365390	1.356247
11	6	0	3.423886	-1.187102	-0.201968
12	1	0	3.660220	-2.229321	-0.430770
13	1	0	3.761817	-0.564260	-1.037707
14	1	0	4.012793	-0.883488	0.672855
15	6	0	1.515885	0.369674	0.453763
16	1	0	2.002561	0.647905	1.400197
17	6	0	-0.017276	0.623581	0.595770
18	1	0	-0.268326	0.695100	1.663093
19	8	0	-0.187340	1.906481	-0.029351
20	8	0	1.907534	1.326768	-0.536075
21	8	0	1.152117	2.454808	-0.119315
22	6	0	-2.975019	1.162083	-0.073760

23	1	0	-2.443364	1.963338	0.442000
24	1	0	-2.903408	1.360829	-1.148887
25	1	0	-4.031801	1.221253	0.206771
26	6	0	-3.304785	-1.300640	-0.397284
27	1	0	-3.072840	-2.313783	-0.059542
28	1	0	-4.358509	-1.114651	-0.167244
29	1	0	-3.198077	-1.275034	-1.488577

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.244136	E(Thermal)=	0.257316
E(CCSD(T))=	-614.386232	E(Empiric)=	-0.350464
DE(MP2)=	-0.746645	DE(HF)=	-0.062665
G4MP2(0 K)=	-615.301869	G4MP2 Energy=	-615.28869
G4MP2 Enthalpy=	-615.287746	G4MP2 Free Energy=	-615.341338

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.360058	-1.755443	0.101607
2	6	0	-0.926516	-0.336207	-0.082115
3	6	0	2.050273	-0.942149	0.051753
4	6	0	1.129576	-1.906374	-0.013439
5	1	0	-0.782225	-0.026721	-1.124999
6	1	0	-0.667492	-2.149659	1.084384
7	1	0	-0.821536	-2.431541	-0.625281
8	1	0	1.482290	-2.930150	-0.130985
9	6	0	-2.450720	-0.270719	0.236847
10	1	0	-2.556827	-0.369664	1.328363
11	6	0	3.535267	-1.198196	-0.034697
12	1	0	3.742585	-2.264934	-0.150927
13	1	0	3.977451	-0.665320	-0.884756
14	1	0	4.053833	-0.843816	0.864820
15	6	0	1.661263	0.470889	0.279813
16	1	0	2.099782	1.006892	1.122093
17	6	0	-0.155413	0.661942	0.799593
18	1	0	0.045724	0.283304	1.825215
19	8	0	-0.329346	1.912958	0.677802
20	8	0	1.582118	1.235881	-0.817111
21	8	0	1.307491	2.484163	-0.500622
22	6	0	-3.070914	1.069830	-0.184844
23	1	0	-2.547617	1.920509	0.252048
24	1	0	-3.033172	1.183447	-1.274968

25	1	0	-4.123014	1.109538	0.116636
26	6	0	-3.242063	-1.420636	-0.410862
27	1	0	-2.965030	-2.403781	-0.021521
28	1	0	-4.312320	-1.286800	-0.224376
29	1	0	-3.098715	-1.432942	-1.498236

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241	E(Thermal)=	0.254408
E(CCSD(T))=	-614.356484	E(Empiric)=	-0.350464
DE(MP2)=	-0.752515	DE(HF)=	-0.061303
G4MP2(0 K)=	-615.279767	G4MP2 Energy=	-615.266359
G4MP2 Enthalpy=	-615.265415	G4MP2 Free Energy=	-615.319211

Cl3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.042398	-0.463783	1.231992
2	6	0	1.100107	-0.485932	0.081422
3	6	0	-2.291597	-0.477871	0.173154
4	6	0	-1.271860	-1.071736	0.838800
5	1	0	0.628519	-0.109584	-0.830980
6	1	0	0.446588	-1.006141	2.095735
7	1	0	-0.101256	0.573902	1.535750
8	1	0	-1.422323	-2.112753	1.114172
9	6	0	2.367286	0.347805	0.389415
10	1	0	2.869570	-0.116222	1.252048
11	6	0	-3.572408	-1.225434	-0.134004
12	1	0	-3.536558	-2.238680	0.270235
13	1	0	-4.443194	-0.718792	0.297597
14	1	0	-3.742813	-1.298779	-1.213815
15	6	0	-2.276513	0.880704	-0.303036
16	1	0	-3.148712	1.354285	-0.751280
17	6	0	1.461411	-1.941048	-0.155115
18	1	0	2.183990	-2.353017	0.592042
19	8	0	1.004594	-2.642754	-1.020353
20	8	0	-1.229831	1.605970	-0.248887
21	8	0	-1.286895	2.870762	-0.718158
22	6	0	2.056060	1.809688	0.747044
23	1	0	1.413546	2.284640	-0.002039
24	1	0	1.558260	1.904145	1.716153
25	1	0	2.986520	2.383300	0.808730
26	6	0	3.330365	0.286192	-0.808202

27	1	0	4.261684	0.814871	-0.583636
28	1	0	3.589616	-0.742682	-1.080535
29	1	0	2.882102	0.758181	-1.689813

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239771	E(Thermal)=	0.255409
E(CCSD(T))=	-614.38963	E(Empiric)=	-0.350464
DE(MP2)=	-0.753967	DE(HF)=	-0.061654
G4MP2(0 K)=	-615.315944	G4MP2 Energy=	-615.300306
G4MP2 Enthalpy=	-615.299362	G4MP2 Free Energy=	-615.359592

POZ2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.369922	1.818547	0.153249
2	6	0	0.903551	0.391803	-0.080677
3	6	0	-1.966990	0.925623	0.065661
4	6	0	-1.107288	1.931120	-0.093511
5	1	0	0.780818	0.166276	-1.148228
6	1	0	0.614008	2.147831	1.176045
7	1	0	0.892307	2.515408	-0.507540
8	1	0	-1.481068	2.897655	-0.425191
9	6	0	2.405900	0.266892	0.290124
10	1	0	2.489063	0.494216	1.364679
11	6	0	-3.442135	1.041061	-0.202868
12	1	0	-3.700521	2.035629	-0.574710
13	1	0	-3.760476	0.296813	-0.940163
14	1	0	-4.028282	0.851308	0.706020
15	6	0	-1.508514	-0.393751	0.627381
16	1	0	-1.934697	-0.528729	1.630356
17	6	0	0.039437	-0.634923	0.670063
18	1	0	0.373628	-0.737803	1.708206
19	8	0	0.152289	-1.949210	0.110213
20	8	0	-2.010881	-1.522780	-0.115449
21	8	0	-0.870433	-1.931322	-0.887860
22	6	0	2.979994	-1.141725	0.064634
23	1	0	2.481373	-1.905781	0.663582
24	1	0	2.886441	-1.440956	-0.985025
25	1	0	4.044003	-1.154386	0.323147
26	6	0	3.270452	1.288504	-0.468369
27	1	0	3.021941	2.323120	-0.219494
28	1	0	4.328155	1.141329	-0.228489

29	1	0	3.159538	1.165669	-1.552551

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.244163	E(Thermal)=	0.257277
E(CCSD(T))=	-614.386202	E(Empiric)=	-0.350464
DE(MP2)=	-0.746478	DE(HF)=	-0.062281
G4MP2(0 K)=	-615.301262	G4MP2 Energy=	-615.288148
G4MP2 Enthalpy=	-615.287204	G4MP2 Free Energy=	-615.340621

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.624348	1.660708	0.352247
2	6	0	1.089209	0.265809	-0.134512
3	6	0	-1.748564	1.070363	-0.032163
4	6	0	-0.750616	1.946481	-0.181569
5	1	0	1.013989	0.253773	-1.227878
6	1	0	0.643939	1.687330	1.453122
7	1	0	1.318921	2.432413	0.016650
8	1	0	-0.907019	2.843966	-0.773250
9	6	0	2.546937	-0.090098	0.263496
10	1	0	2.564767	-0.233910	1.354609
11	6	0	-3.111641	1.209995	-0.654863
12	1	0	-3.165698	2.137311	-1.230156
13	1	0	-3.324931	0.368553	-1.319509
14	1	0	-3.900171	1.227386	0.106685
15	6	0	-1.507699	-0.079063	0.875453
16	1	0	-1.396712	0.158056	1.935244
17	6	0	0.160208	-0.873173	0.354173
18	1	0	0.421757	-1.228687	1.371229
19	8	0	-0.195236	-1.766920	-0.489066
20	8	0	-2.239565	-1.196261	0.762805
21	8	0	-2.211177	-1.638081	-0.484248
22	6	0	2.999963	-1.400981	-0.399277
23	1	0	2.320684	-2.230737	-0.190501
24	1	0	3.046420	-1.284581	-1.488326
25	1	0	3.999269	-1.681060	-0.051094
26	6	0	3.546392	1.028966	-0.073285
27	1	0	3.372601	1.939266	0.506373
28	1	0	4.567449	0.697074	0.140097
29	1	0	3.501333	1.289892	-1.137424

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241067	E(Thermal)=	0.254434
E(CCSD(T))=	-614.352027	E(Empiric)=	-0.350464
DE(MP2)=	-0.752783	DE(HF)=	-0.061202
G4MP2(0 K)=	-615.275409	G4MP2 Energy=	-615.262042
G4MP2 Enthalpy=	-615.261098	G4MP2 Free Energy=	-615.314642

Cl3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.473081	-0.759364	0.419324
2	6	0	1.716724	0.152484	0.249238
3	6	0	-1.991523	0.047353	0.579508
4	6	0	-0.698755	-0.015496	0.991198
5	1	0	1.981637	0.591046	1.219063
6	1	0	0.246667	-1.241268	-0.536816
7	1	0	0.735897	-1.567523	1.113003
8	1	0	-0.455549	0.555093	1.886600
9	6	0	2.949789	-0.595695	-0.328133
10	1	0	2.685470	-0.928760	-1.343098
11	6	0	-2.993647	0.873258	1.354881
12	1	0	-2.490137	1.376795	2.185110
13	1	0	-3.468541	1.618111	0.714246
14	1	0	-3.802842	0.250820	1.739762
15	6	0	-2.373548	-0.679263	-0.602438
16	1	0	-1.635494	-1.220872	-1.182953
17	6	0	1.347072	1.301774	-0.673849
18	1	0	1.003013	0.969727	-1.684368
19	8	0	1.406162	2.470196	-0.395227
20	8	0	-3.525850	-0.809594	-1.138401
21	8	0	-4.628360	-0.249726	-0.606145
22	6	0	4.157525	0.349192	-0.436578
23	1	0	3.939173	1.235961	-1.038192
24	1	0	4.470582	0.694674	0.555300
25	1	0	5.007300	-0.166337	-0.894096
26	6	0	3.324174	-1.838100	0.492957
27	1	0	2.545597	-2.605290	0.478314
28	1	0	4.235153	-2.292636	0.091219
29	1	0	3.521097	-1.573406	1.538451

Temperature=	298.15	Pressure=	1

E(ZPE)=	0.239793	E(Thermal)=	0.255482
E(CCSD(T))=	-614.385819	E(Empiric)=	-0.350464
DE(MP2)=	-0.753946	DE(HF)=	-0.061905
G4MP2(0 K)=	-615.31234	G4MP2 Energy=	-615.296652
G4MP2 Enthalpy=	-615.295708	G4MP2 Free Energy=	-615.357906

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.524171	-1.730351	0.281594
2	6	0	-1.049324	-0.334953	-0.170385
3	6	0	1.858556	-1.086057	-0.022535
4	6	0	0.877636	-1.973611	-0.215858
5	1	0	-1.044545	-0.335921	-1.267827
6	1	0	-0.582841	-1.792117	1.378290
7	1	0	-1.192887	-2.501754	-0.103683
8	1	0	1.059796	-2.868854	-0.804395
9	6	0	-2.487238	-0.011342	0.317510
10	1	0	-2.448662	0.079609	1.413300
11	6	0	3.237408	-1.188678	-0.604905
12	1	0	3.459484	-0.301599	-1.207048
13	1	0	3.999265	-1.220544	0.182900
14	1	0	3.340154	-2.079339	-1.230023
15	6	0	1.573825	0.114330	0.839059
16	1	0	1.172022	-0.141965	1.839489
17	6	0	-0.086746	0.752909	0.254925
18	1	0	-0.316885	1.348415	1.137271
19	8	0	0.398561	1.495592	-0.755503
20	8	0	2.329604	1.147530	0.789660
21	8	0	1.215874	2.425235	-0.298189
22	6	0	-2.978102	1.326877	-0.257995
23	1	0	-3.974371	1.567568	0.125208
24	1	0	-2.316745	2.161182	-0.007358
25	1	0	-3.045156	1.277231	-1.351120
26	6	0	-3.487867	-1.124194	-0.027355
27	1	0	-3.265111	-2.062957	0.485477
28	1	0	-4.499433	-0.824322	0.263512
29	1	0	-3.500265	-1.321066	-1.106072

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241313	E(Thermal)=	0.254647
E(CCSD(T))=	-614.357524	E(Empiric)=	-0.350464

DE(MP2)=	-0.752819	DE(HF)=	-0.061395
G4MP2(0 K)=	-615.280889	G4MP2 Energy=	-615.267555
G4MP2 Enthalpy=	-615.266611	G4MP2 Free Energy=	-615.320073

Cl4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.032625	-1.138091	0.250989
2	6	0	1.239849	-0.244440	0.295168
3	6	0	-2.463460	-0.288687	0.401107
4	6	0	-1.219031	-0.462045	0.881500
5	1	0	1.477012	-0.018216	1.342525
6	1	0	-0.223175	-1.444474	-0.780729
7	1	0	0.181891	-2.054122	0.813812
8	1	0	-1.017060	-0.068616	1.878760
9	6	0	2.482853	-0.925864	-0.356351
10	1	0	2.240929	-1.101728	-1.414450
11	6	0	-3.541488	0.408907	1.187326
12	1	0	-3.913951	1.280747	0.640234
13	1	0	-4.402032	-0.251958	1.332176
14	1	0	-3.175194	0.735515	2.163038
15	6	0	-2.872954	-0.778475	-0.933843
16	1	0	-2.088666	-1.270879	-1.544095
17	6	0	0.950800	1.055307	-0.376429
18	1	0	0.644049	1.143897	-1.419184
19	8	0	1.069575	2.134345	0.267215
20	8	0	-3.998399	-0.664109	-1.366709
21	8	0	0.822731	3.303928	-0.357753
22	6	0	2.802616	-2.280676	0.291276
23	1	0	2.010425	-3.018673	0.142671
24	1	0	3.718038	-2.694937	-0.142098
25	1	0	2.968706	-2.171197	1.369487
26	6	0	3.709625	-0.003368	-0.292098
27	1	0	3.535759	0.955796	-0.788346
28	1	0	3.985987	0.207971	0.747368
29	1	0	4.568916	-0.477852	-0.775063

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239557	E(Thermal)=	0.255361
E(CCSD(T))=	-614.386	E(Empiric)=	-0.350464
DE(MP2)=	-0.754507	DE(HF)=	-0.061856
G4MP2(0 K)=	-615.31327	G4MP2 Energy=	-615.297465

G4MP2		G4MP2 Free	
Enthalpy=	-615.296521	Energy=	-615.358114

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.041768	-1.803505	0.110554
2	6	0	-0.750752	-0.448745	-0.062735
3	6	0	2.214604	-0.663528	0.063085
4	6	0	1.454808	-1.753865	0.050683
5	1	0	-0.646765	-0.116744	-1.098303
6	1	0	-0.352013	-2.264775	1.062113
7	1	0	-0.395255	-2.489085	-0.666274
8	1	0	1.947855	-2.722918	-0.011765
9	6	0	-2.271146	-0.569705	0.286890
10	1	0	-2.336988	-0.888754	1.338236
11	6	0	3.719750	-0.712728	-0.010997
12	1	0	4.075171	-0.197876	-0.911461
13	1	0	4.178420	-0.201942	0.844879
14	1	0	4.082538	-1.743759	-0.029514
15	6	0	1.704083	0.769133	0.152409
16	1	0	2.143406	1.299311	1.023480
17	6	0	-0.073280	0.588539	0.808503
18	1	0	-0.006403	0.375108	1.876796
19	8	0	-0.346925	1.890984	0.648288
20	8	0	1.556172	1.442634	-0.918828
21	8	0	-0.364452	2.236631	-0.621440
22	6	0	-3.058174	0.742326	0.141216
23	1	0	-2.717721	1.518689	0.828220
24	1	0	-2.978021	1.141180	-0.874669
25	1	0	-4.116839	0.558716	0.351134
26	6	0	-2.941119	-1.656131	-0.574157
27	1	0	-2.537358	-2.654264	-0.390979
28	1	0	-4.013106	-1.692677	-0.357371
29	1	0	-2.827327	-1.432953	-1.641389

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241276	E(Thermal)=	0.254681
E(CCSD(T))=	-614.351541	E(Empiric)=	-0.350464
DE(MP2)=	-0.753508	DE(HF)=	-0.060979
G4MP2(0 K)=	-615.275216	G4MP2 Energy=	-615.261812
G4MP2 Enthalpy=	-615.260868	G4MP2 Free Energy=	-615.314647

Cl4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.156020	-1.046889	-1.050041
2	6	0	0.972431	0.000244	-0.226674
3	6	0	-2.213932	-0.474575	-0.286999
4	6	0	-1.284161	-0.625098	-1.243250
5	1	0	0.671680	-0.081906	0.820443
6	1	0	0.626722	-1.173806	-2.031406
7	1	0	0.211262	-1.998901	-0.520206
8	1	0	-1.567926	-0.359662	-2.260541
9	6	0	2.506808	-0.181584	-0.354249
10	1	0	2.778595	-0.023841	-1.409464
11	6	0	-3.579593	0.096340	-0.567350
12	1	0	-4.378915	-0.581920	-0.245575
13	1	0	-3.710256	1.034579	-0.015235
14	1	0	-3.717760	0.303404	-1.631099
15	6	0	-1.965302	-0.830562	1.138464
16	1	0	-2.723149	-0.421358	1.840137
17	6	0	0.570262	1.362915	-0.670016
18	1	0	0.954186	1.820599	-1.581414
19	8	0	-0.219180	2.136222	-0.054815
20	8	0	-1.073326	-1.541890	1.547509
21	8	0	-0.803292	1.735526	1.105055
22	6	0	3.252453	0.859151	0.495481
23	1	0	2.987341	1.885734	0.219626
24	1	0	3.017419	0.733113	1.557983
25	1	0	4.335077	0.753578	0.375482
26	6	0	2.937668	-1.600618	0.040957
27	1	0	2.516477	-2.361908	-0.620396
28	1	0	4.027708	-1.690638	-0.002538
29	1	0	2.621996	-1.831876	1.064266

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240151	E(Thermal)=	0.25543
E(CCSD(T))=	-614.392501	E(Empiric)=	-0.350464
DE(MP2)=	-0.752959	DE(HF)=	-0.061052
G4MP2(0 K)=	-615.316824	G4MP2 Energy=	-615.301545
G4MP2 Enthalpy=	-615.300601	G4MP2 Free Energy=	-615.358833

TS34

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.226985	-1.823020	0.098452
2	6	0	-0.827711	-0.409904	-0.082221
3	6	0	2.085719	-0.828994	0.070671
4	6	0	1.270117	-1.879039	-0.028682
5	1	0	-0.701184	-0.122499	-1.133705
6	1	0	-0.527143	-2.233561	1.076415
7	1	0	-0.662408	-2.501938	-0.641054
8	1	0	1.700706	-2.860826	-0.217660
9	6	0	-2.339543	-0.369177	0.266678
10	1	0	-2.425350	-0.509441	1.355814
11	6	0	3.577495	-0.900882	-0.100631
12	1	0	3.905251	-1.922695	-0.307911
13	1	0	3.907309	-0.259932	-0.926739
14	1	0	4.098811	-0.548011	0.798153
15	6	0	1.511686	0.521345	0.401197
16	1	0	2.086295	1.007864	1.203637
17	6	0	0.021161	0.555242	0.758923
18	1	0	-0.126693	0.373838	1.830625
19	8	0	-0.243153	1.942268	0.596223
20	8	0	1.547425	1.338752	-0.771419
21	8	0	0.521840	2.356779	-0.570024
22	6	0	-3.004528	0.969665	-0.095761
23	1	0	-2.554207	1.815265	0.422556
24	1	0	-2.921632	1.161915	-1.172060
25	1	0	-4.070515	0.937774	0.153162
26	6	0	-3.120416	-1.510485	-0.408693
27	1	0	-2.810896	-2.500810	-0.065460
28	1	0	-4.189226	-1.410841	-0.195179
29	1	0	-2.999970	-1.476999	-1.498424

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.243493	E(Thermal)=	0.256189
E(CCSD(T))=	-614.382043	E(Empiric)=	-0.350464
DE(MP2)=	-0.745548	DE(HF)=	-0.062526
G4MP2(0 K)=	-615.297088	G4MP2 Energy=	-615.284392
G4MP2 Enthalpy=	-615.283448	G4MP2 Free Energy=	-615.336092

TS1c

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.316782	-1.428557	-0.198980
2	6	0	-1.141413	-0.156484	-0.536640
3	6	0	-0.639194	1.240669	-0.220854
4	6	0	0.577372	1.733647	0.064793
5	6	0	1.719857	0.860681	0.273850
6	6	0	1.104770	-1.485674	-0.760821
7	1	0	-1.215924	-0.135224	-1.636669
8	1	0	-0.296841	-1.633700	0.872151
9	1	0	-0.854505	-2.270774	-0.657019
10	1	0	0.744345	2.806983	0.060144
11	1	0	1.534843	-2.492664	-0.875478
12	1	0	-1.410111	1.992305	-0.383223
13	6	0	-2.603712	-0.335663	-0.009655
14	6	0	3.114717	1.176638	-0.141191
15	1	0	3.753773	0.318484	0.055483
16	1	0	3.155787	1.440081	-1.197660
17	1	0	3.455118	2.040749	0.447305
18	8	0	1.454419	-0.059077	1.151740
19	8	0	1.538497	-0.533317	-1.430187
20	8	0	2.145547	-1.261345	0.956606
21	6	0	-3.627440	0.525987	-0.764314
22	1	0	-4.644547	0.262050	-0.456826
23	1	0	-3.504288	1.595858	-0.563308
24	1	0	-3.556784	0.377339	-1.847035
25	6	0	-2.714793	-0.117461	1.506776
26	1	0	-2.495187	0.922411	1.774107
27	1	0	-3.728048	-0.341253	1.855439
28	1	0	-2.022004	-0.753473	2.064784
29	1	0	-2.863626	-1.381959	-0.215247

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240725	E(Thermal)=	0.254199
E(CCSD(T))=	-614.38275	E(Empiric)=	-0.350464
DE(MP2)=	-0.752397	DE(HF)=	-0.060524
G4MP2(0 K)=	-615.305409	G4MP2 Energy=	-615.291935
G4MP2 Enthalpy=	-615.290991	G4MP2 Free Energy=	-615.344489

SOZ1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.384149	-1.331695	-0.159596
2	6	0	-1.171969	-0.028370	-0.436865
3	6	0	-0.634220	1.146257	0.359859
4	6	0	0.644979	1.441567	0.592772
5	6	0	1.811247	0.634706	0.072127
6	6	0	1.061039	-1.321165	-0.706847
7	1	0	-1.033756	0.208841	-1.501353
8	1	0	-0.326823	-1.517080	0.915484
9	1	0	-0.919215	-2.176433	-0.607596
10	1	0	0.898021	2.313194	1.189769
11	1	0	1.209364	-2.015023	-1.539204
12	1	0	-1.377840	1.817534	0.782132
13	6	0	-2.698152	-0.236693	-0.231927
14	6	0	3.080486	1.439314	-0.141340
15	1	0	3.877022	0.774401	-0.479950
16	1	0	2.913435	2.215354	-0.894012
17	1	0	3.383769	1.917615	0.793660
18	8	0	2.057367	-0.440628	1.048007
19	8	0	1.480301	-0.043090	-1.126702
20	8	0	2.022330	-1.665967	0.268703
21	6	0	-3.515623	0.934888	-0.795477
22	1	0	-4.587431	0.718036	-0.741147
23	1	0	-3.345383	1.862160	-0.237540
24	1	0	-3.264512	1.127735	-1.843948
25	6	0	-3.087291	-0.530692	1.224956
26	1	0	-2.840918	0.308237	1.884983
27	1	0	-4.165038	-0.705392	1.305619
28	1	0	-2.578890	-1.417686	1.613761
29	1	0	-2.959873	-1.122722	-0.826697

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.244811	E(Thermal)=	0.257591
E(CCSD(T))=	-614.459999	E(Empiric)=	-0.350464
DE(MP2)=	-0.749097	DE(HF)=	-0.06057
G4MP2(0 K)=	-615.37532	G4MP2 Energy=	-615.362539
G4MP2 Enthalpy=	-615.361595	G4MP2 Free Energy=	-615.413393

TS1f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.701642	-1.413101	-0.150178
2	6	0	1.183112	0.033386	0.054785

3	6	0	0.321320	1.061364	-0.647612
4	6	0	-0.990818	1.320030	-0.619784
5	6	0	-2.177175	0.664533	-0.063936
6	6	0	-0.623315	-1.654815	0.542697
7	1	0	1.067515	0.223378	1.131625
8	1	0	0.626090	-1.687125	-1.206175
9	1	0	1.418439	-2.104825	0.309598
10	1	0	-1.302392	2.246606	-1.108630
11	1	0	-1.004417	-2.687420	0.487574
12	1	0	0.888704	1.785644	-1.229603
13	6	0	2.677126	0.274472	-0.309366
14	6	0	-3.112541	1.432853	0.808551
15	1	0	-4.084512	0.939222	0.855904
16	1	0	-2.685160	1.473777	1.815613
17	1	0	-3.227453	2.460787	0.450768
18	8	0	-2.677925	-0.420598	-0.525853
19	8	0	-1.074847	-0.864668	1.376076
20	8	0	-1.811962	-1.264368	-1.165579
21	6	0	3.616863	-0.844539	0.162601
22	1	0	4.658642	-0.562064	-0.020502
23	1	0	3.510703	-1.023882	1.239445
24	1	0	3.439733	-1.789364	-0.356894
25	6	0	3.165691	1.613912	0.269069
26	1	0	3.174378	1.574675	1.364982
27	1	0	4.184780	1.834091	-0.064083
28	1	0	2.534123	2.458286	-0.021890
29	1	0	2.747276	0.326720	-1.405849

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240697	E(Thermal)=	0.254367
E(CCSD(T))=	-614.389805	E(Empiric)=	-0.350464
DE(MP2)=	-0.753597	DE(HF)=	-0.060951
G4MP2(0 K)=	-615.314121	G4MP2 Energy=	-615.300451
G4MP2 Enthalpy=	-615.299507	G4MP2 Free Energy=	-615.353592

SOZ1f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.620751	-1.379185	0.018685
2	6	0	1.172419	0.063763	0.100967
3	6	0	0.355868	1.051484	-0.721035
4	6	0	-0.956859	1.274926	-0.675793

5	6	0	-1.961785	0.502622	0.143535
6	6	0	-0.877434	-1.453147	0.336031
7	1	0	1.085551	0.359454	1.155353
8	1	0	0.775729	-1.807416	-0.978364
9	1	0	1.156134	-2.012214	0.731790
10	1	0	-1.394295	2.021170	-1.334327
11	1	0	-1.145566	-2.363045	0.887037
12	1	0	0.925408	1.650854	-1.428117
13	6	0	2.674919	0.159459	-0.278654
14	6	0	-3.010998	1.354854	0.830183
15	1	0	-3.719527	0.711660	1.355090
16	1	0	-2.526215	2.021873	1.546494
17	1	0	-3.545300	1.960420	0.094404
18	8	0	-2.644149	-0.435016	-0.695522
19	8	0	-1.336319	-0.351912	1.088156
20	8	0	-1.602791	-1.410710	-0.913946
21	6	0	3.537242	-0.942834	0.354126
22	1	0	4.594402	-0.773828	0.125311
23	1	0	3.435337	-0.945851	1.446409
24	1	0	3.279678	-1.940105	-0.011347
25	6	0	3.246335	1.533372	0.108921
26	1	0	3.248299	1.652972	1.199122
27	1	0	4.279330	1.637292	-0.238010
28	1	0	2.670112	2.362579	-0.310604
29	1	0	2.744251	0.053403	-1.371543

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.245069	E(Thermal)=	0.257769
E(CCSD(T))=	-614.462775	E(Empiric)=	-0.350464
DE(MP2)=	-0.749181	DE(HF)=	-0.06074
G4MP2(0 K)=	-615.378091	G4MP2 Energy=	-615.365392
G4MP2 Enthalpy=	-615.364448	G4MP2 Free Energy=	-615.416035

TS1k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.457939	-1.359623	-0.266714
2	6	0	-1.182419	-0.003669	-0.412607
3	6	0	-0.612222	1.020741	0.546850
4	6	0	0.677937	1.276780	0.756321
5	6	0	1.847054	0.612088	0.065057
6	6	0	1.029916	-1.327755	-0.693710

7	1	0	-0.989479	0.349377	-1.434609
8	1	0	-0.494249	-1.707230	0.768925
9	1	0	-0.975088	-2.109178	-0.877306
10	1	0	0.961091	2.021039	1.496223
11	1	0	1.224634	-2.036072	-1.505757
12	1	0	-1.329023	1.589849	1.133382
13	6	0	-2.722012	-0.158937	-0.288211
14	6	0	2.979484	1.578404	-0.241901
15	1	0	3.783195	1.043748	-0.750453
16	1	0	2.615864	2.389372	-0.878689
17	1	0	3.363690	2.009479	0.685915
18	8	0	2.379058	-0.431678	0.924775
19	8	0	1.479240	-0.067126	-1.116907
20	8	0	1.919174	-1.693129	0.359191
21	6	0	-3.452447	1.124469	-0.709824
22	1	0	-4.536343	0.970170	-0.712128
23	1	0	-3.244324	1.956163	-0.027702
24	1	0	-3.155277	1.438991	-1.715913
25	6	0	-3.188783	-0.628493	1.098243
26	1	0	-2.934295	0.096471	1.879052
27	1	0	-4.276252	-0.753969	1.111997
28	1	0	-2.742987	-1.587170	1.378534
29	1	0	-3.002349	-0.939605	-1.008969

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.24451	E(Thermal)=	0.256715
E(CCSD(T))=	-614.456536	E(Empiric)=	-0.350464
DE(MP2)=	-0.749054	DE(HF)=	-0.060896
G4MP2(0 K)=	-615.37244	G4MP2 Energy=	-615.360235
G4MP2 Enthalpy=	-615.359291	G4MP2 Free Energy=	-615.409891

TS1l

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.359873	1.392675	-0.031991
2	6	0	1.103746	0.065056	-0.375625
3	6	0	0.609431	-1.139094	0.373861
4	6	0	-0.685987	-1.468305	0.625112
5	6	0	-1.854525	-0.634698	-0.046909
6	6	0	-1.115536	1.484323	-0.545686
7	1	0	0.861631	-0.136980	-1.434726
8	1	0	0.324573	1.558111	1.046565

9	1	0	0.935780	2.214714	-0.473451
10	1	0	-0.973572	-2.344632	1.190759
11	1	0	-1.159843	2.098808	-1.466067
12	1	0	1.353304	-1.867603	0.687111
13	6	0	2.647058	0.220548	-0.279512
14	6	0	-3.181797	-1.335230	-0.253967
15	1	0	-3.957983	-0.565347	-0.271370
16	1	0	-3.186592	-1.862862	-1.210386
17	1	0	-3.391155	-2.036319	0.556782
18	8	0	-1.611801	-0.053216	1.142898
19	8	0	-1.471635	0.124783	-1.107846
20	8	0	-2.014143	1.864184	0.327964
21	6	0	3.394558	-0.946303	-0.941692
22	1	0	4.470518	-0.746599	-0.967831
23	1	0	3.259048	-1.889137	-0.399352
24	1	0	3.057246	-1.103449	-1.971724
25	6	0	3.138241	0.452283	1.157148
26	1	0	2.918794	-0.408424	1.800021
27	1	0	4.222043	0.604344	1.173825
28	1	0	2.670509	1.330505	1.610647
29	1	0	2.885950	1.121334	-0.859365

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240024	E(Thermal)=	0.25301
E(CCSD(T))=	-614.40423	E(Empiric)=	-0.350464
DE(MP2)=	-0.752753	DE(HF)=	-0.059391
G4MP2(0 K)=	-615.326813	G4MP2 Energy=	-615.313828
G4MP2 Enthalpy=	-615.312884	G4MP2 Free Energy=	-615.364835

ESTER1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.225135	1.040845	-0.393543
2	6	0	1.211967	-0.122842	-0.299348
3	6	0	0.400656	-0.000495	0.965764
4	6	0	-0.924709	0.050173	1.052553
5	6	0	-3.074367	0.019043	0.085404
6	6	0	1.543310	2.385287	-0.531403
7	1	0	0.524671	-0.025891	-1.148395
8	1	0	2.895734	1.084639	0.469018
9	1	0	2.843981	0.900719	-1.292727
10	1	0	-1.480973	0.151586	1.975015

11	1	0	0.727389	2.405589	-1.293002
12	1	0	0.942374	0.074033	1.904411
13	6	0	1.904712	-1.509623	-0.454116
14	6	0	-3.753018	-0.046096	-1.257311
15	1	0	-3.445495	-0.950312	-1.790022
16	1	0	-4.832995	-0.042229	-1.117463
17	1	0	-3.452586	0.809862	-1.868609
18	8	0	-1.714544	-0.017882	-0.078740
19	8	0	-3.615575	0.092830	1.153959
20	8	0	1.830621	3.373988	0.091293
21	6	0	0.868452	-2.625228	-0.641655
22	1	0	1.361315	-3.585417	-0.825039
23	1	0	0.242775	-2.735110	0.250276
24	1	0	0.207127	-2.418643	-1.489627
25	6	0	2.867516	-1.851510	0.692306
26	1	0	2.332999	-1.960901	1.641958
27	1	0	3.373363	-2.801267	0.491801
28	1	0	3.641526	-1.090004	0.826605
29	1	0	2.496843	-1.445451	-1.378196

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240906	E(Thermal)=	0.256723
E(CCSD(T))=	-614.555921	E(Empiric)=	-0.350464
DE(MP2)=	-0.752914	DE(HF)=	-0.060619
G4MP2(0 K)=	-615.479012	G4MP2 Energy=	-615.463195
G4MP2 Enthalpy=	-615.462251	G4MP2 Free Energy=	-615.524811

TS1m

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.497150	1.224646	-0.210719
2	6	0	-1.184991	-0.113788	0.139983
3	6	0	-0.436178	-1.321235	-0.404101
4	6	0	0.873948	-1.556031	-0.493511
5	6	0	2.036490	-0.645635	-0.200938
6	6	0	0.889943	1.338604	0.447721
7	1	0	-1.173390	-0.186749	1.237015
8	1	0	-0.337100	1.326245	-1.288785
9	1	0	-1.118335	2.064430	0.107424
10	1	0	1.193326	-2.516754	-0.896264
11	1	0	1.084043	2.437968	0.906575
12	1	0	-1.077566	-2.124565	-0.759115

13	6	0	-2.676669	-0.177978	-0.307706
14	6	0	3.194111	-1.223934	0.582913
15	1	0	3.890399	-0.424632	0.839065
16	1	0	2.852265	-1.727203	1.489085
17	1	0	3.715632	-1.952665	-0.049144
18	8	0	2.286814	0.230877	-1.112584
19	8	0	1.275885	0.379095	1.216112
20	8	0	1.866503	1.909388	-0.270874
21	6	0	-3.458730	1.121011	-0.060131
22	1	0	-4.519534	0.968478	-0.283041
23	1	0	-3.387887	1.433906	0.989013
24	1	0	-3.113161	1.948323	-0.685289
25	6	0	-3.401814	-1.336198	0.399336
26	1	0	-3.472297	-1.140816	1.476146
27	1	0	-4.420416	-1.447964	0.014707
28	1	0	-2.894895	-2.296496	0.273850
29	1	0	-2.688455	-0.373159	-1.389557

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.237417	E(Thermal)=	0.251103
E(CCSD(T))=	-614.381532	E(Empiric)=	-0.350464
DE(MP2)=	-0.75362	DE(HF)=	-0.060602
G4MP2(0 K)=	-615.3088	G4MP2 Energy=	-615.295115
G4MP2 Enthalpy=	-615.29417	G4MP2 Free Energy=	-615.348102

ACID1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.295901	-0.138567	-0.585583
2	6	0	0.570396	0.766853	0.426849
3	6	0	-0.378332	-0.030735	1.303572
4	6	0	-1.470216	-0.756181	1.000770
5	6	0	-2.092164	-1.009399	-0.319727
6	6	0	2.104427	-1.222685	0.085190
7	1	0	1.340734	1.158966	1.102721
8	1	0	0.584840	-0.597823	-1.277432
9	1	0	1.990699	0.440554	-1.201692
10	1	0	-1.982901	-1.235190	1.832179
11	1	0	3.245009	-2.649758	-0.316706
12	1	0	-0.126075	-0.005179	2.360691
13	6	0	-0.118162	2.001016	-0.228697
14	6	0	-3.345197	-1.869245	-0.285478

15	1	0	-3.733823	-1.997268	-1.295864
16	1	0	-3.122378	-2.848998	0.152751
17	1	0	-4.108802	-1.405441	0.349603
18	8	0	-1.663160	-0.579766	-1.377735
19	8	0	2.200198	-1.413840	1.273150
20	8	0	2.750986	-1.988611	-0.824272
21	6	0	0.866954	2.838035	-1.058453
22	1	0	0.374882	3.746663	-1.420421
23	1	0	1.730344	3.149860	-0.457240
24	1	0	1.240150	2.303763	-1.936042
25	6	0	-0.771549	2.888131	0.842925
26	1	0	-0.019799	3.287402	1.535453
27	1	0	-1.278188	3.740915	0.379995
28	1	0	-1.512510	2.340050	1.431365
29	1	0	-0.898732	1.625883	-0.896711

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.242674	E(Thermal)=	0.257933
E(CCSD(T))=	-614.573153	E(Empiric)=	-0.350464
DE(MP2)=	-0.756741	DE(HF)=	-0.060723
G4MP2(0 K)=	-615.498407	G4MP2 Energy=	-615.483148
G4MP2 Enthalpy=	-615.482204	G4MP2 Free Energy=	-615.541807

TS1o

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.643475	1.465160	-0.444326
2	6	0	1.167406	0.006259	-0.384488
3	6	0	0.531267	-0.815566	0.723016
4	6	0	-0.764269	-1.091240	0.879178
5	6	0	-1.819521	-0.480428	-0.001694
6	6	0	-0.881697	1.665226	-0.500643
7	1	0	0.871072	-0.453113	-1.332237
8	1	0	0.980340	2.024354	0.433561
9	1	0	1.079735	1.941676	-1.329964
10	1	0	-1.112702	-1.663279	1.733537
11	1	0	-1.267148	2.156882	-1.404556
12	1	0	1.206175	-1.213986	1.477115
13	6	0	2.719313	-0.031448	-0.338167
14	6	0	-3.164159	-1.588766	-0.239184
15	1	0	-2.562506	-2.404520	-0.641072
16	1	0	-3.654085	-1.859270	0.689099

17	1	0	-3.818430	-1.142622	-0.978726
18	8	0	-2.751825	0.219731	0.618930
19	8	0	-1.439644	-0.021755	-1.153426
20	8	0	-1.496097	1.813939	0.600875
21	6	0	3.243350	-1.449550	-0.611464
22	1	0	4.336906	-1.457691	-0.663724
23	1	0	2.948992	-2.149286	0.178871
24	1	0	2.857672	-1.839713	-1.559231
25	6	0	3.334924	0.538877	0.949196
26	1	0	3.061366	-0.050695	1.831080
27	1	0	4.427674	0.529101	0.881968
28	1	0	3.027167	1.571988	1.133127
29	1	0	3.057768	0.603713	-1.168420

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239594	E(Thermal)=	0.253522
E(CCSD(T))=	-614.378168	E(Empiric)=	-0.350464
DE(MP2)=	-0.754291	DE(HF)=	-0.060365
G4MP2(0 K)=	-615.303694	G4MP2 Energy=	-615.289766
G4MP2 Enthalpy=	-615.288822	G4MP2 Free Energy=	-615.343239

TS1n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.791456	-1.451401	-0.113928
2	6	0	1.135658	0.014143	0.031630
3	6	0	0.295544	0.929489	-0.862501
4	6	0	-1.016815	1.145033	-0.831568
5	6	0	-2.108310	0.489657	0.011324
6	6	0	-1.025094	-1.527270	0.455825
7	1	0	0.961552	0.281734	1.079216
8	1	0	0.937766	-1.884725	-1.098372
9	1	0	1.135838	-2.118502	0.676485
10	1	0	-1.443768	1.827568	-1.564442
11	1	0	-1.098299	-2.424014	1.093448
12	1	0	0.865521	1.454014	-1.626214
13	6	0	2.657366	0.232204	-0.259000
14	6	0	-2.829011	1.485155	0.929717
15	1	0	-3.572641	0.951113	1.523995
16	1	0	-2.115800	1.988681	1.587374
17	1	0	-3.336423	2.229084	0.310835
18	8	0	-2.907756	-0.299096	-0.638535

19	8	0	-1.306626	-0.404429	1.072918
20	8	0	-1.192864	-1.609664	-0.815043
21	6	0	3.565705	-0.784654	0.448584
22	1	0	4.617403	-0.532147	0.281365
23	1	0	3.395575	-0.779565	1.531943
24	1	0	3.415896	-1.806765	0.087904
25	6	0	3.062865	1.657562	0.145838
26	1	0	2.980566	1.786137	1.231373
27	1	0	4.102489	1.853106	-0.135601
28	1	0	2.436513	2.418050	-0.326485
29	1	0	2.799589	0.122243	-1.343071

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.2394	E(Thermal)=	0.252894
E(CCSD(T))=	-614.382951	E(Empiric)=	-0.350464
DE(MP2)=	-0.756064	DE(HF)=	-0.059612
G4MP2(0 K)=	-615.309691	G4MP2 Energy=	-615.296196
G4MP2 Enthalpy=	-615.295252	G4MP2 Free Energy=	-615.348258

ESTER1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.412676	1.233713	-0.602693
2	6	0	-0.828438	-0.144557	-0.228448
3	6	0	0.223099	-0.522048	-1.236226
4	6	0	1.532662	-0.778798	-1.112406
5	6	0	2.454325	-0.798389	0.060437
6	6	0	0.247236	2.767575	0.104105
7	1	0	-0.406599	-0.063522	0.772830
8	1	0	-2.013948	1.165535	-1.513280
9	1	0	-2.023761	1.623159	0.212547
10	1	0	2.084560	-1.015116	-2.019312
11	1	0	0.961881	3.508717	-0.284234
12	1	0	-0.171558	-0.579582	-2.253092
13	6	0	-1.963421	-1.213556	-0.194039
14	6	0	1.966316	-0.588033	1.481896
15	1	0	1.534620	0.409170	1.614313
16	1	0	1.195827	-1.319657	1.745172
17	1	0	2.818227	-0.703386	2.153373
18	8	0	3.634973	-1.000662	-0.156172
19	8	0	0.084230	2.510995	1.267996
20	8	0	-0.401098	2.213710	-0.924709

21	6	0	-3.131391	-0.801925	0.716877
22	1	0	-3.865567	-1.611549	0.775709
23	1	0	-2.782368	-0.597599	1.735754
24	1	0	-3.657836	0.086266	0.357117
25	6	0	-1.421485	-2.583666	0.237356
26	1	0	-1.063658	-2.552575	1.273384
27	1	0	-2.210052	-3.340862	0.185758
28	1	0	-0.592706	-2.912972	-0.394310
29	1	0	-2.349268	-1.310282	-1.219802

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.2431	E(Thermal)=	0.258124
E(CCSD(T))=	-614.555255	E(Empiric)=	-0.350464
DE(MP2)=	-0.753224	DE(HF)=	-0.060248
G4MP2(0 K)=	-615.476092	G4MP2 Energy=	-615.461068
G4MP2 Enthalpy=	-615.460123	G4MP2 Free Energy=	-615.518953

ESTER1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.611211	1.479316	-0.478925
2	6	0	-1.259316	0.467903	0.507660
3	6	0	-0.234620	-0.317946	1.305665
4	6	0	0.891233	-0.922099	0.908523
5	6	0	1.383286	-1.062137	-0.490433
6	6	0	0.381440	2.366895	0.228829
7	1	0	-1.827140	1.057519	1.242290
8	1	0	-0.121919	0.966887	-1.307457
9	1	0	-1.402728	2.123943	-0.877857
10	1	0	1.512705	-1.385737	1.669597
11	1	0	-0.070383	3.060663	0.977481
12	1	0	-0.444338	-0.374930	2.372125
13	6	0	-2.285238	-0.475834	-0.194200
14	6	0	3.579354	-0.473710	0.323822
15	1	0	3.194203	0.477005	0.699040
16	1	0	3.726324	-1.179625	1.148826
17	1	0	4.537297	-0.306566	-0.170850
18	8	0	2.718245	-1.015156	-0.683250
19	8	0	1.575135	2.355629	0.053477
20	8	0	0.667743	-1.272838	-1.440969
21	6	0	-3.371390	0.305448	-0.945569
22	1	0	-4.109535	-0.386880	-1.362890

23	1	0	-3.906687	0.990932	-0.276155
24	1	0	-2.970151	0.888391	-1.778628
25	6	0	-2.934548	-1.429992	0.820208
26	1	0	-3.491554	-0.876700	1.587054
27	1	0	-3.641869	-2.096805	0.317463
28	1	0	-2.193379	-2.055250	1.325630
29	1	0	-1.713772	-1.070989	-0.913207

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.242299	E(Thermal)=	0.257616
E(CCSD(T))=	-614.537075	E(Empiric)=	-0.350464
DE(MP2)=	-0.754137	DE(HF)=	-0.060216
G4MP2(0 K)=	-615.459594	G4MP2 Energy=	-615.444276
G4MP2 Enthalpy=	-615.443332	G4MP2 Free Energy=	-615.502505

TS1j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.003052	-0.872769	-0.015942
2	6	0	-0.929494	0.239848	-0.105151
3	6	0	0.189598	-0.072742	0.857190
4	6	0	1.492528	0.432915	0.947874
5	6	0	2.491508	0.119354	0.046363
6	6	0	-1.495527	-2.289536	-0.219352
7	1	0	-0.531756	0.291331	-1.120588
8	1	0	-2.509673	-0.844624	0.955790
9	1	0	-2.757280	-0.698710	-0.792690
10	1	0	1.837135	0.816952	1.904897
11	1	0	-0.992745	-2.478991	-1.188206
12	1	0	-0.220057	-0.392950	1.825043
13	6	0	-1.536403	1.645602	0.249017
14	1	0	-1.710695	1.672903	1.334360
15	6	0	3.890100	0.641980	0.040202
16	1	0	4.157142	1.035414	1.023467
17	1	0	4.591670	-0.147151	-0.241244
18	1	0	3.990136	1.458109	-0.684542
19	8	0	2.296943	-0.891363	-0.769244
20	8	0	-1.655997	-3.170140	0.588559
21	8	0	0.986377	-1.308089	-0.810109
22	6	0	-0.573712	2.784706	-0.116471
23	1	0	-0.991582	3.748944	0.190326
24	1	0	0.403593	2.674009	0.357586

25	1	0	-0.415701	2.821791	-1.200824
26	6	0	-2.887731	1.887902	-0.444357
27	1	0	-2.798670	1.776305	-1.531533
28	1	0	-3.669922	1.210243	-0.095503
29	1	0	-3.227075	2.909597	-0.246226

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239126	E(Thermal)=	0.253763
E(CCSD(T))=	-614.37812	E(Empiric)=	-0.350464
DE(MP2)=	-0.752888	DE(HF)=	-0.061484
G4MP2(0 K)=	-615.30383	G4MP2 Energy=	-615.289193
G4MP2 Enthalpy=	-615.288249	G4MP2 Free Energy=	-615.345869

CP1j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836989	0.967685	-0.018084
2	6	0	-0.872015	-0.226415	0.104031
3	6	0	0.363094	0.027812	-0.801193
4	6	0	1.521601	-0.920929	-0.660349
5	6	0	2.512328	-0.273590	-0.052855
6	6	0	-1.323935	2.265299	0.582591
7	1	0	-0.508647	-0.252126	1.140581
8	1	0	-2.137171	1.162788	-1.053194
9	1	0	-2.754022	0.746824	0.544183
10	1	0	1.533215	-1.949927	-0.977494
11	1	0	-0.783734	2.141637	1.548675
12	1	0	0.015096	0.122184	-1.841536
13	6	0	-1.500946	-1.621516	-0.223774
14	1	0	-1.214237	-1.872124	-1.255997
15	6	0	3.863108	-0.698276	0.410053
16	1	0	4.017097	-1.757329	0.197895
17	1	0	4.644490	-0.116285	-0.088974
18	1	0	3.969827	-0.535978	1.487719
19	8	0	2.232635	1.037390	0.204101
20	8	0	-1.535187	3.355606	0.119925
21	8	0	0.969366	1.304302	-0.484962
22	6	0	-0.930513	-2.708421	0.704246
23	1	0	-1.260013	-3.704624	0.390918
24	1	0	0.161514	-2.701803	0.726790
25	1	0	-1.280700	-2.551532	1.731450
26	6	0	-3.035809	-1.676620	-0.175071

27	1	0	-3.416567	-1.449365	0.827426
28	1	0	-3.504038	-0.984921	-0.880091
29	1	0	-3.376168	-2.685975	-0.428426

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241621	E(Thermal)=	0.256174
E(CCSD(T))=	-614.444754	E(Empiric)=	-0.350464
DE(MP2)=	-0.750812	DE(HF)=	-0.061431
G4MP2(0 K)=	-615.36584	G4MP2 Energy=	-615.351288
G4MP2 Enthalpy=	-615.350344	G4MP2 Free Energy=	-615.407716

TS1e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.821256	1.254741	0.396009
2	6	0	1.142024	0.026572	-0.503139
3	6	0	0.033884	-0.297690	-1.479524
4	6	0	-1.295142	-0.516786	-1.319700
5	6	0	-2.061165	-0.550121	-0.101184
6	6	0	0.592196	2.507738	-0.415779
7	1	0	2.003675	0.305823	-1.125970
8	1	0	-0.081426	1.076020	0.998582
9	1	0	1.655396	1.455704	1.070239
10	1	0	-1.886457	-0.633483	-2.224660
11	1	0	-0.153699	2.403514	-1.239522
12	1	0	0.360443	-0.336321	-2.517893
13	6	0	1.606307	-1.232250	0.304448
14	6	0	-3.556170	-0.468143	-0.179265
15	1	0	-3.878981	0.524221	-0.508932
16	1	0	-3.914048	-1.188688	-0.927646
17	1	0	-3.989291	-0.663516	0.799066
18	8	0	-1.452659	-0.809821	1.016493
19	8	0	1.142460	3.561503	-0.222646
20	8	0	-2.004048	0.378272	1.690823
21	6	0	2.845141	-0.933370	1.159282
22	1	0	3.190532	-1.851804	1.644718
23	1	0	3.671470	-0.554807	0.545297
24	1	0	2.646537	-0.204543	1.947945
25	6	0	1.899084	-2.409360	-0.639547
26	1	0	2.704630	-2.163110	-1.342494
27	1	0	2.218912	-3.285884	-0.067976
28	1	0	1.019840	-2.698709	-1.223415

29	1	0	0.781956	-1.512032	0.965696

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.23872	E(Thermal)=	0.253652
E(CCSD(T))=	-614.365508	E(Empiric)=	-0.350464
DE(MP2)=	-0.751959	DE(HF)=	-0.061259
G4MP2(0 K)=	-615.29047	G4MP2 Energy=	-615.275538
G4MP2 Enthalpy=	-615.274593	G4MP2 Free Energy=	-615.332931

DIO1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.416243	1.497326	-0.552615
2	6	0	-1.136083	0.565985	0.455287
3	6	0	-0.179825	-0.091446	1.438702
4	6	0	0.980353	-0.720402	1.241569
5	6	0	1.722675	-1.003392	-0.023654
6	6	0	0.392228	2.560556	0.150404
7	1	0	-1.788166	1.213400	1.060640
8	1	0	0.224277	0.951102	-1.247348
9	1	0	-1.176451	2.025357	-1.142360
10	1	0	1.512320	-1.090126	2.116856
11	1	0	-0.198492	3.189099	0.858129
12	1	0	-0.504890	-0.037106	2.475815
13	6	0	-2.075039	-0.472173	-0.231866
14	6	0	3.060470	-0.328690	-0.190849
15	1	0	2.919732	0.754224	-0.256246
16	1	0	3.700222	-0.539466	0.671920
17	1	0	3.541600	-0.699975	-1.097487
18	8	0	1.643140	-2.337042	-0.468621
19	8	0	1.570738	2.763499	-0.004144
20	8	0	0.989616	-1.210560	-1.194129
21	6	0	-3.102051	0.193881	-1.158305
22	1	0	-3.790383	-0.557506	-1.558136
23	1	0	-3.704573	0.935482	-0.618489
24	1	0	-2.638467	0.692051	-2.014079
25	6	0	-2.798775	-1.331116	0.816792
26	1	0	-3.434708	-0.713937	1.464113
27	1	0	-3.443875	-2.067519	0.327650
28	1	0	-2.095660	-1.875767	1.452205
29	1	0	-1.436689	-1.129670	-0.830823

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240463	E(Thermal)=	0.255442
E(CCSD(T))=	-614.430514	E(Empiric)=	-0.350464
DE(MP2)=	-0.749519	DE(HF)=	-0.060878
G4MP2(0 K)=	-615.350912	G4MP2 Energy=	-615.335934
G4MP2 Enthalpy=	-615.33499	G4MP2 Free Energy=	-615.392741

TS1i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.355923	-0.526468	-0.032264
2	6	0	1.022273	0.258771	0.016228
3	6	0	0.061900	-0.356605	-0.968076
4	6	0	-1.250212	-0.647430	-0.880780
5	6	0	-2.135865	-0.629016	0.261254
6	6	0	2.171449	-1.989084	0.307101
7	1	0	0.632562	0.204081	1.037646
8	1	0	2.828799	-0.453845	-1.017100
9	1	0	3.049945	-0.112996	0.709973
10	1	0	-1.776269	-0.922620	-1.789260
11	1	0	1.628921	-2.168854	1.267431
12	1	0	0.505317	-0.506748	-1.952508
13	6	0	1.204746	1.777560	-0.316243
14	1	0	1.413699	1.847721	-1.392822
15	6	0	-1.723386	-0.696655	1.693739
16	1	0	-2.503445	-1.222088	2.251359
17	1	0	-0.755930	-1.176451	1.839682
18	1	0	-1.676144	0.324076	2.094240
19	8	0	-3.422437	-0.717071	0.069914
20	8	0	2.567689	-2.910980	-0.355872
21	8	0	-3.415490	0.515411	-0.726557
22	6	0	-0.086005	2.558300	-0.022906
23	1	0	0.000627	3.587527	-0.384596
24	1	0	-0.968791	2.111106	-0.485944
25	1	0	-0.264131	2.609876	1.058811
26	6	0	2.381294	2.416489	0.436398
27	1	0	2.277692	2.283564	1.520368
28	1	0	3.349429	2.008473	0.134762
29	1	0	2.406920	3.493127	0.241376

Temperature=	298.15	Pressure=	1

E(ZPE)=	0.238219	E(Thermal)=	0.25322
E(CCSD(T))=	-614.36486	E(Empiric)=	-0.350464
DE(MP2)=	-0.753878	DE(HF)=	-0.061835
G4MP2(0 K)=	-615.292818	G4MP2 Energy=	-615.277816
G4MP2 Enthalpy=	-615.276872	G4MP2 Free Energy=	-615.335681

TS1q

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.556514	1.529337	-0.520436
2	6	0	-1.180669	0.524502	0.480994
3	6	0	-0.142520	-0.078847	1.417835
4	6	0	1.007031	-0.693897	1.155937
5	6	0	1.682269	-1.084999	-0.176173
6	6	0	0.204535	2.620763	0.189120
7	1	0	-1.873645	1.093859	1.116251
8	1	0	0.101747	1.022835	-1.232071
9	1	0	-1.364937	2.014413	-1.081367
10	1	0	1.644322	-1.038332	1.969594
11	1	0	-0.412276	3.241448	0.881166
12	1	0	-0.393046	-0.014649	2.476073
13	6	0	-2.021289	-0.589454	-0.213490
14	6	0	3.008231	-0.151789	-0.260322
15	1	0	2.631343	0.871402	-0.334520
16	1	0	3.633070	-0.280733	0.622920
17	1	0	3.536873	-0.461204	-1.160834
18	8	0	2.103696	-2.337746	-0.263138
19	8	0	1.382688	2.847032	0.059515
20	8	0	0.909241	-1.008506	-1.258627
21	6	0	-3.055479	-0.018695	-1.194625
22	1	0	-3.681701	-0.825549	-1.588090
23	1	0	-3.719602	0.701355	-0.699561
24	1	0	-2.592669	0.477512	-2.051386
25	6	0	-2.719029	-1.472393	0.832768
26	1	0	-3.432171	-0.889364	1.429212
27	1	0	-3.278075	-2.275601	0.343132
28	1	0	-2.004110	-1.936369	1.517265
29	1	0	-1.319517	-1.214430	-0.779433

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.235723	E(Thermal)=	0.250884
E(CCSD(T))=	-614.370098	E(Empiric)=	-0.350464

DE(MP2)=	-0.75105	DE(HF)=	-0.060057
G4MP2(0 K)=	-615.295947	G4MP2 Energy=	-615.280785
G4MP2 Enthalpy=	-615.279841	G4MP2 Free Energy=	-615.337734

TS1p

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.115820	1.247690	-0.828966
2	6	0	-1.204779	0.239502	0.345801
3	6	0	-0.006375	0.362292	1.252631
4	6	0	1.315628	0.106683	1.050473
5	6	0	2.018259	-0.407473	-0.219669
6	6	0	-0.909596	2.667193	-0.386583
7	1	0	-2.066183	0.549408	0.952076
8	1	0	-0.283471	0.977100	-1.492635
9	1	0	-2.026280	1.219708	-1.439285
10	1	0	1.980381	0.218928	1.902133
11	1	0	-1.002123	3.420716	-1.201114
12	1	0	-0.231323	0.769799	2.234817
13	6	0	-1.487367	-1.218763	-0.132483
14	6	0	3.518162	-0.043820	-0.201334
15	1	0	3.653841	1.035261	-0.309060
16	1	0	3.960370	-0.371251	0.744564
17	1	0	4.009193	-0.555013	-1.030859
18	8	0	1.706345	-1.706934	-0.036833
19	8	0	-0.650488	3.016083	0.740268
20	8	0	1.482485	-0.236397	-1.440990
21	6	0	-2.757487	-1.301798	-0.990662
22	1	0	-2.982454	-2.347866	-1.221703
23	1	0	-3.626474	-0.889860	-0.461750
24	1	0	-2.659872	-0.776872	-1.944622
25	6	0	-1.612783	-2.162637	1.072401
26	1	0	-2.450289	-1.871059	1.718845
27	1	0	-1.796269	-3.187864	0.736772
28	1	0	-0.701515	-2.169795	1.675435
29	1	0	-0.631320	-1.536586	-0.732815

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.236707	E(Thermal)=	0.251745
E(CCSD(T))=	-614.386755	E(Empiric)=	-0.350464
DE(MP2)=	-0.750899	DE(HF)=	-0.059905
G4MP2(0 K)=	-615.311316	G4MP2 Energy=	-615.296279

G4MP2		G4MP2 Free	
Enthalpy=	-615.295334	Energy=	-615.353223

TS1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.134462	0.949813	-1.015866
2	6	0	-1.288016	0.099862	0.260956
3	6	0	-0.288190	0.494973	1.329992
4	6	0	1.060700	0.485936	1.356016
5	6	0	2.041159	0.119619	0.358015
6	6	0	-1.299392	2.429628	-0.776444
7	1	0	-2.271446	0.356666	0.674077
8	1	0	-0.170790	0.788036	-1.512565
9	1	0	-1.888589	0.670919	-1.763418
10	1	0	1.531575	0.851288	2.263927
11	1	0	-1.234637	3.052843	-1.697146
12	1	0	-0.745244	0.860734	2.245043
13	6	0	-1.309878	-1.438606	0.003262
14	6	0	3.446943	0.117362	0.519020
15	1	0	4.011294	0.697013	-0.215163
16	1	0	3.814710	0.236471	1.533182
17	1	0	3.479215	-0.862867	-0.400908
18	8	0	1.625344	-0.434183	-0.762642
19	8	0	-1.495347	2.939241	0.299098
20	8	0	2.725484	-0.908940	-1.499417
21	6	0	-2.371775	-1.833456	-1.033683
22	1	0	-2.430642	-2.923659	-1.112140
23	1	0	-3.365955	-1.470727	-0.744120
24	1	0	-2.148122	-1.451718	-2.033350
25	6	0	-1.559095	-2.199155	1.315577
26	1	0	-2.536658	-1.940236	1.741010
27	1	0	-1.550928	-3.279387	1.140613
28	1	0	-0.795991	-1.978249	2.067081
29	1	0	-0.329611	-1.731927	-0.383507

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.236343	E(Thermal)=	0.250882
E(CCSD(T))=	-614.361024	E(Empiric)=	-0.350464
DE(MP2)=	-0.757495	DE(HF)=	-0.062214
G4MP2(0 K)=	-615.294853	G4MP2 Energy=	-615.280314
G4MP2 Enthalpy=	-615.27937	G4MP2 Free Energy=	-615.337031

HP1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.122899	0.901647	-1.016397
2	6	0	-1.244351	0.066028	0.272108
3	6	0	-0.246201	0.516117	1.328184
4	6	0	1.096240	0.541379	1.367049
5	6	0	2.146696	0.155228	0.424534
6	6	0	-1.424211	2.366842	-0.819737
7	1	0	-2.230656	0.307656	0.688371
8	1	0	-0.130574	0.813445	-1.472497
9	1	0	-1.825206	0.553997	-1.786944
10	1	0	1.536240	0.940037	2.277544
11	1	0	-1.308105	2.982184	-1.742070
12	1	0	-0.717426	0.905972	2.226064
13	6	0	-1.241553	-1.474536	0.041764
14	6	0	3.447749	0.343389	0.671998
15	1	0	4.213131	0.076417	-0.039444
16	1	0	3.744517	0.799892	1.605902
17	1	0	2.854762	-1.674268	-1.450856
18	8	0	1.653255	-0.422759	-0.728532
19	8	0	-1.778777	2.873791	0.215243
20	8	0	2.697325	-0.740306	-1.659976
21	6	0	-2.306596	-1.914958	-0.974087
22	1	0	-2.347285	-3.007803	-1.029864
23	1	0	-3.303912	-1.564856	-0.679986
24	1	0	-2.104899	-1.548840	-1.984528
25	6	0	-1.460018	-2.215596	1.370558
26	1	0	-2.440515	-1.972115	1.798346
27	1	0	-1.426796	-3.299464	1.219334
28	1	0	-0.697950	-1.954668	2.109548
29	1	0	-0.258887	-1.756625	-0.348649

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240283	E(Thermal)=	0.255828
E(CCSD(T))=	-614.414089	E(Empiric)=	-0.350464
DE(MP2)=	-0.758632	DE(HF)=	-0.062249
G4MP2(0 K)=	-615.34515	G4MP2 Energy=	-615.329605
G4MP2 Enthalpy=	-615.328661	G4MP2 Free Energy=	-615.388402

RAD1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.844721	1.160309	-0.858584
2	6	0	-0.955144	0.180488	0.324744
3	6	0	0.266371	0.257488	1.221547
4	6	0	1.562318	-0.010749	0.979968
5	6	0	2.210156	-0.462819	-0.272257
6	6	0	-0.693566	2.599551	-0.444072
7	1	0	-1.796218	0.529413	0.937690
8	1	0	-0.004083	0.894395	-1.511502
9	1	0	-1.736647	1.114076	-1.497580
10	1	0	2.248810	0.121933	1.812904
11	1	0	-0.661551	3.318745	-1.294960
12	1	0	0.049285	0.583677	2.235393
13	6	0	-1.290621	-1.279676	-0.103050
14	6	0	3.630759	-0.693411	-0.212469
15	1	0	4.135881	-1.026902	-1.111178
16	1	0	4.207658	-0.546019	0.693394
17	8	0	1.610081	-0.648005	-1.344535
18	8	0	-0.616820	2.993570	0.694027
19	6	0	-2.562881	-1.352855	-0.960528
20	1	0	-2.823435	-2.397894	-1.157574
21	1	0	-3.416896	-0.893190	-0.447127
22	1	0	-2.446839	-0.862804	-1.930841
23	6	0	-1.449437	-2.181871	1.131088
24	1	0	-2.285549	-1.847349	1.758136
25	1	0	-1.656416	-3.213773	0.829969
26	1	0	-0.547893	-2.189530	1.749709
27	1	0	-0.451602	-1.648017	-0.700697

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.223687	E(Thermal)=	0.237722
E(CCSD(T))=	-538.847889	E(Empiric)=	-0.325479
DE(MP2)=	-0.65526	DE(HF)=	-0.052841
G4MP2(0 K)=	-539.657782	G4MP2 Energy=	-539.643747
G4MP2 Enthalpy=	-539.642803	G4MP2 Free Energy=	-539.699314

TS1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.727508	1.373522	-0.066583
2	6	0	1.327027	0.021648	-0.483123
3	6	0	0.332866	-1.121243	-0.473369
4	6	0	-0.951114	-1.158614	-0.110218
5	6	0	-1.916954	-0.481349	0.620500
6	6	0	-0.476297	1.822525	-0.867269
7	1	0	1.674281	0.112681	-1.526426
8	1	0	0.475524	1.402957	0.997409
9	1	0	1.480157	2.156033	-0.229641
10	1	0	-1.890300	-1.734492	-0.834253
11	1	0	-0.438643	1.578169	-1.952696
12	1	0	0.736587	-2.037950	-0.901575
13	6	0	2.597310	-0.331730	0.361239
14	6	0	-1.874325	0.131963	1.978525
15	1	0	-2.807268	-0.056687	2.515912
16	1	0	-1.032230	-0.260157	2.551034
17	1	0	-1.753591	1.216058	1.865905
18	8	0	-3.129828	-0.603235	0.123022
19	8	0	-1.396990	2.450397	-0.406012
20	8	0	-3.055433	-1.218284	-1.136977
21	6	0	3.674404	0.760710	0.260164
22	1	0	4.569619	0.458487	0.812387
23	1	0	3.970956	0.924814	-0.782969
24	1	0	3.348984	1.718302	0.673803
25	6	0	3.210409	-1.686742	-0.029219
26	1	0	3.460299	-1.715490	-1.096794
27	1	0	4.136919	-1.853648	0.528546
28	1	0	2.546051	-2.526723	0.185147
29	1	0	2.275660	-0.397511	1.410063

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.235516	E(Thermal)=	0.25048
E(CCSD(T))=	-614.354653	E(Empiric)=	-0.350464
DE(MP2)=	-0.758422	DE(HF)=	-0.062204
G4MP2(0 K)=	-615.290226	G4MP2 Energy=	-615.275262
G4MP2 Enthalpy=	-615.274318	G4MP2 Free Energy=	-615.332677

HP1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.156978	1.140764	0.068658
2	6	0	1.244104	-0.099178	-0.083271

3	6	0	0.024240	0.088405	0.804087
4	6	0	-1.210609	0.187424	0.396595
5	6	0	-2.432835	0.341225	-0.039225
6	6	0	1.452710	2.413677	-0.346821
7	1	0	0.904708	-0.148224	-1.126194
8	1	0	2.517557	1.256819	1.096013
9	1	0	3.030722	1.036736	-0.587795
10	1	0	-2.896415	-2.033475	1.022730
11	1	0	0.965982	2.352965	-1.349311
12	1	0	0.245985	0.158697	1.872952
13	6	0	1.964364	-1.435472	0.249101
14	6	0	-3.078955	1.645122	-0.412856
15	1	0	-3.969097	1.824376	0.199725
16	1	0	-2.376072	2.465425	-0.264359
17	1	0	-3.395187	1.628475	-1.461363
18	8	0	-3.351695	-0.683557	-0.210394
19	8	0	1.407279	3.427526	0.300475
20	8	0	-2.758084	-1.959697	0.065343
21	6	0	3.313595	-1.588559	-0.468222
22	1	0	3.732319	-2.581561	-0.275868
23	1	0	3.196419	-1.488033	-1.554213
24	1	0	4.053684	-0.854682	-0.137931
25	6	0	1.059316	-2.632340	-0.081487
26	1	0	0.923348	-2.723147	-1.165866
27	1	0	1.506482	-3.565712	0.275020
28	1	0	0.065960	-2.531068	0.361377
29	1	0	2.156155	-1.438170	1.332341

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238499	E(Thermal)=	0.255015
E(CCSD(T))=	-614.398154	E(Empiric)=	-0.350464
DE(MP2)=	-0.757769	DE(HF)=	-0.062461
G4MP2(0 K)=	-615.330348	G4MP2 Energy=	-615.313832
G4MP2 Enthalpy=	-615.312888	G4MP2 Free Energy=	-615.375963

RAD1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.170499	1.632875	0.106569
2	6	0	1.054848	0.095567	-0.058189
3	6	0	-0.097277	-0.393821	0.819159
4	6	0	-1.290695	-0.685355	0.408391

5	6	0	-2.572779	-0.992908	-0.078598
6	6	0	-0.066126	2.326943	-0.418740
7	1	0	0.802247	-0.116746	-1.105233
8	1	0	1.319634	1.911543	1.154200
9	1	0	2.022452	1.999068	-0.479156
10	1	0	-0.261782	2.138825	-1.501238
11	1	0	0.125275	-0.446676	1.889998
12	6	0	2.363907	-0.663593	0.281585
13	6	0	-3.593798	0.135683	-0.110155
14	1	0	-4.288135	0.013887	0.728765
15	1	0	-3.129189	1.121244	-0.032038
16	1	0	-4.174960	0.064270	-1.033203
17	8	0	-2.855810	-2.139133	-0.452485
18	8	0	-0.808016	3.017866	0.230502
19	6	0	3.562113	-0.172971	-0.543901
20	1	0	4.442722	-0.786752	-0.330692
21	1	0	3.359168	-0.253151	-1.618664
22	1	0	3.830823	0.864137	-0.326286
23	6	0	2.180431	-2.176988	0.090671
24	1	0	1.976359	-2.413953	-0.960185
25	1	0	3.088213	-2.713863	0.382416
26	1	0	1.349410	-2.568049	0.682895
27	1	0	2.581636	-0.476241	1.343529

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.222153	E(Thermal)=	0.237279
E(CCSD(T))=	-538.829338	E(Empiric)=	-0.325479
DE(MP2)=	-0.656768	DE(HF)=	-0.053059
G4MP2(0 K)=	-539.642492	G4MP2 Energy=	-539.627365
G4MP2 Enthalpy=	-539.626421	G4MP2 Free Energy=	-539.687589

TS1h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.393016	0.831756	-1.192720
2	6	0	0.724971	-0.108325	-0.022591
3	6	0	-0.043127	0.089629	1.171522
4	6	0	-1.430619	0.117567	1.241822
5	6	0	-2.348721	-0.252310	0.262287
6	6	0	0.634586	2.298550	-0.896228
7	1	0	0.070242	-1.109876	-0.418865
8	1	0	0.989071	0.573567	-2.077962

9	1	0	-0.644447	0.745531	-1.538245
10	1	0	-1.873715	0.518224	2.149787
11	1	0	0.505155	2.963300	-1.782293
12	1	0	0.475372	0.181511	2.121624
13	6	0	2.247332	-0.350505	0.102548
14	1	0	2.759030	0.593137	-0.133786
15	6	0	-3.783622	0.192270	0.281250
16	1	0	-3.889489	1.176790	0.739708
17	1	0	-4.175749	0.219922	-0.738448
18	1	0	-4.397228	-0.520962	0.845243
19	8	0	-2.123705	-1.056966	-0.756952
20	8	0	0.929622	2.757022	0.177252
21	8	0	-1.012586	-1.891519	-0.704737
22	6	0	2.712950	-0.774122	1.501839
23	1	0	3.777575	-1.027526	1.480199
24	1	0	2.585996	0.022643	2.240238
25	1	0	2.170164	-1.658763	1.855586
26	6	0	2.700740	-1.399008	-0.931086
27	1	0	2.279866	-2.382493	-0.694273
28	1	0	2.384656	-1.144846	-1.947623
29	1	0	3.791818	-1.491465	-0.937268

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.235093	E(Thermal)=	0.249824
E(CCSD(T))=	-614.37628	E(Empiric)=	-0.350464
DE(MP2)=	-0.757028	DE(HF)=	-0.061733
G4MP2(0 K)=	-615.310412	G4MP2 Energy=	-615.295681
G4MP2 Enthalpy=	-615.294736	G4MP2 Free Energy=	-615.352329

HP1h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.468886	0.882158	-1.063208
2	6	0	0.856774	-0.029288	0.078562
3	6	0	-0.000093	-0.365233	1.062000
4	6	0	-1.410538	0.013776	1.217995
5	6	0	-2.430441	-0.086522	0.353943
6	6	0	0.841549	2.337656	-0.827872
7	1	0	-0.672462	-1.524825	-0.715807
8	1	0	0.971793	0.593181	-1.998507
9	1	0	-0.599678	0.854125	-1.300682
10	1	0	-1.673268	0.393931	2.202503

11	1	0	0.519473	3.015631	-1.651569
12	1	0	0.403547	-0.923752	1.903870
13	6	0	2.320114	-0.456136	0.077037
14	1	0	2.888290	0.418356	-0.266845
15	6	0	-3.819231	0.424628	0.593745
16	1	0	-3.873557	0.981321	1.530964
17	1	0	-4.126130	1.090217	-0.221279
18	1	0	-4.537038	-0.402462	0.618636
19	8	0	-2.352925	-0.633988	-0.910851
20	8	0	1.432252	2.762718	0.130086
21	8	0	-1.562691	-1.841463	-0.959539
22	6	0	2.879389	-0.843870	1.450462
23	1	0	3.956681	-1.022257	1.377032
24	1	0	2.714833	-0.049911	2.184038
25	1	0	2.425790	-1.765414	1.831548
26	6	0	2.559413	-1.592618	-0.940223
27	1	0	2.054675	-2.510284	-0.617643
28	1	0	2.190604	-1.341689	-1.939882
29	1	0	3.628431	-1.811615	-1.028589

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239412	E(Thermal)=	0.255208
E(CCSD(T))=	-614.421832	E(Empiric)=	-0.350464
DE(MP2)=	-0.757295	DE(HF)=	-0.062126
G4MP2(0 K)=	-615.352304	G4MP2 Energy=	-615.336509
G4MP2 Enthalpy=	-615.335565	G4MP2 Free Energy=	-615.395979

RAD1h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.396812	1.132038	-0.910530
2	6	0	0.717155	-0.177208	-0.260557
3	6	0	-0.208502	-1.054718	0.280197
4	6	0	-1.604700	-1.083181	0.409250
5	6	0	-2.681917	-0.202255	-0.037101
6	6	0	0.831554	2.349399	-0.115149
7	1	0	0.906216	1.214541	-1.885066
8	1	0	-0.676109	1.243665	-1.106389
9	1	0	-1.973260	-1.950670	0.952263
10	1	0	0.601953	3.309724	-0.629833
11	1	0	0.249304	-1.936490	0.727141
12	6	0	2.194874	-0.546165	-0.201755

13	1	0	2.751775	0.308561	-0.601558
14	6	0	-4.074710	-0.624836	0.416499
15	1	0	-4.130579	-0.664805	1.510149
16	1	0	-4.809158	0.087171	0.039549
17	1	0	-4.315045	-1.628032	0.046694
18	8	0	-2.550308	0.801709	-0.730321
19	8	0	1.362426	2.339403	0.966393
20	6	0	2.697272	-0.772878	1.236450
21	1	0	3.779455	-0.940960	1.232533
22	1	0	2.480611	0.100309	1.855099
23	1	0	2.230521	-1.650260	1.696122
24	6	0	2.505640	-1.757187	-1.105209
25	1	0	1.998888	-2.659469	-0.747572
26	1	0	2.185641	-1.581761	-2.137229
27	1	0	3.581974	-1.958475	-1.113059

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.223807	E(Thermal)=	0.238263
E(CCSD(T))=	-538.868718	E(Empiric)=	-0.325479
DE(MP2)=	-0.654316	DE(HF)=	-0.053122
G4MP2(0 K)=	-539.677829	G4MP2 Energy=	-539.663373
G4MP2 Enthalpy=	-539.662429	G4MP2 Free Energy=	-539.720837

TS2e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.564329	-0.057550	-1.127138
2	6	0	-0.052090	0.831713	-0.076907
3	6	0	-1.589949	0.692679	-0.179846
4	6	0	-2.087299	-0.692966	0.006521
5	6	0	2.047950	-1.805803	0.092128
6	6	0	1.388388	-1.112590	-1.052461
7	1	0	-2.081919	1.290187	0.602539
8	1	0	0.248052	0.519950	0.926391
9	1	0	0.256161	0.223182	-2.136685
10	1	0	-1.563575	-1.414395	0.630945
11	1	0	1.673025	-1.590998	-1.986586
12	1	0	-1.978404	1.073501	-1.133115
13	6	0	0.402417	2.308919	-0.271800
14	1	0	0.112832	2.604233	-1.290956
15	6	0	1.839896	-1.373902	1.533174
16	1	0	2.434308	-2.026289	2.173815

17	1	0	2.151441	-0.335660	1.684372
18	1	0	0.787095	-1.450822	1.824500
19	8	0	2.777671	-2.744349	-0.161807
20	8	0	-3.154951	-1.072742	-0.577781
21	8	0	-3.700091	-1.669742	0.647690
22	6	0	1.928247	2.439571	-0.156634
23	1	0	2.451002	1.781328	-0.854923
24	1	0	2.240450	3.467735	-0.362628
25	1	0	2.266340	2.191782	0.856874
26	6	0	-0.281328	3.267784	0.714392
27	1	0	-1.362559	3.331705	0.565781
28	1	0	-0.098519	2.963364	1.751899
29	1	0	0.119868	4.278725	0.594384

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238266	E(Thermal)=	0.253484
E(CCSD(T))=	-614.358755	E(Empiric)=	-0.350464
DE(MP2)=	-0.755277	DE(HF)=	-0.06198
G4MP2(0 K)=	-615.28821	G4MP2 Energy=	-615.272992
G4MP2 Enthalpy=	-615.272047	G4MP2 Free Energy=	-615.332151

DIO2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.359817	0.025312	-1.032927
2	6	0	-0.564070	0.600267	0.010298
3	6	0	-1.802897	-0.321822	0.139253
4	6	0	-1.451729	-1.748397	0.469378
5	6	0	2.632889	-0.473441	0.114285
6	6	0	1.628607	-0.406155	-0.983522
7	1	0	-2.456516	0.048209	0.936066
8	1	0	-0.071605	0.646638	0.985075
9	1	0	-0.121401	-0.055247	-2.009315
10	1	0	-0.849614	-1.905503	1.370964
11	1	0	2.062015	-0.788905	-1.904417
12	1	0	-2.381040	-0.331223	-0.790921
13	6	0	-0.972726	2.054558	-0.378406
14	1	0	-1.431269	2.003457	-1.376635
15	6	0	2.316896	-0.030982	1.533360
16	1	0	3.207435	-0.184292	2.144134
17	1	0	2.034105	1.025827	1.564548
18	1	0	1.487918	-0.608670	1.954998

19	8	0	3.740861	-0.898454	-0.153100
20	8	0	-1.167727	-2.622404	-0.573452
21	8	0	-2.418129	-2.721716	0.240937
22	6	0	0.254735	2.973276	-0.467200
23	1	0	1.009100	2.585100	-1.155888
24	1	0	-0.036741	3.970421	-0.811053
25	1	0	0.726234	3.091608	0.516146
26	6	0	-2.004850	2.655782	0.587481
27	1	0	-2.963812	2.132264	0.563063
28	1	0	-1.635236	2.639979	1.620029
29	1	0	-2.199652	3.700542	0.326140

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241238	E(Thermal)=	0.256331
E(CCSD(T))=	-614.431912	E(Empiric)=	-0.350464
DE(MP2)=	-0.751151	DE(HF)=	-0.061409
G4MP2(0 K)=	-615.353697	G4MP2 Energy=	-615.338604
G4MP2 Enthalpy=	-615.33766	G4MP2 Free Energy=	-615.397264

TS2h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.385753	-0.116915	1.279415
2	6	0	-0.597335	0.593409	0.366886
3	6	0	-1.172000	-0.330884	-0.748129
4	6	0	-1.555088	-1.690267	-0.289072
5	6	0	2.321782	-0.806872	-0.238394
6	6	0	1.580478	-0.688103	1.042707
7	1	0	-2.063667	0.138363	-1.162915
8	1	0	-1.464475	0.837619	0.988305
9	1	0	0.062438	-0.155178	2.318654
10	1	0	-0.752464	-2.426998	-0.147277
11	1	0	2.098805	-1.113667	1.899421
12	1	0	-0.393435	-0.467390	-1.509455
13	6	0	-0.026989	1.925888	-0.198917
14	1	0	0.856965	1.681291	-0.795915
15	6	0	3.722191	-1.382508	-0.120829
16	1	0	4.189192	-1.425061	-1.104795
17	1	0	4.330981	-0.768816	0.553130
18	1	0	3.685136	-2.387601	0.315343
19	8	0	1.869426	-0.479820	-1.321777
20	8	0	-2.741385	-2.164215	-0.211664

21	8	0	-3.162994	-1.076209	0.699997
22	6	0	-1.038119	2.641755	-1.105924
23	1	0	-0.639688	3.612564	-1.417875
24	1	0	-1.259904	2.075455	-2.014161
25	1	0	-1.983413	2.825177	-0.581006
26	6	0	0.396819	2.858273	0.947411
27	1	0	0.822760	3.784877	0.549923
28	1	0	-0.463478	3.130834	1.570783
29	1	0	1.148916	2.397830	1.594476

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238861	E(Thermal)=	0.253974
E(CCSD(T))=	-614.358834	E(Empiric)=	-0.350464
DE(MP2)=	-0.751416	DE(HF)=	-0.061749
G4MP2(0 K)=	-615.283602	G4MP2 Energy=	-615.268489
G4MP2 Enthalpy=	-615.267545	G4MP2 Free Energy=	-615.327185

TS2i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.131600	-0.058315	-0.970744
2	6	0	0.936265	-0.008060	0.114145
3	6	0	1.147993	1.488254	0.439378
4	6	0	-0.244191	2.122995	0.451579
5	6	0	-2.253773	-1.139665	0.150805
6	6	0	-1.410031	-0.589647	-0.938714
7	1	0	1.671409	1.628818	1.388083
8	1	0	0.573888	-0.511386	1.013842
9	1	0	0.257085	0.140828	-1.966839
10	1	0	-0.791469	1.949866	1.396080
11	1	0	-1.950821	-0.612465	-1.880536
12	1	0	1.721842	1.978371	-0.354734
13	6	0	2.221074	-0.739494	-0.349295
14	1	0	2.558719	-0.246537	-1.272693
15	6	0	-1.805036	-1.185477	1.599411
16	1	0	-2.639826	-1.549826	2.199183
17	1	0	-0.957509	-1.868416	1.721499
18	1	0	-1.496460	-0.201536	1.962327
19	8	0	-3.342657	-1.585318	-0.165458
20	8	0	-0.948714	1.609703	-0.687366
21	8	0	-0.453972	3.298441	-0.139503
22	6	0	1.940834	-2.215649	-0.668085

23	1	0	1.157752	-2.334813	-1.423212
24	1	0	2.842877	-2.708690	-1.042971
25	1	0	1.619672	-2.755417	0.231003
26	6	0	3.345513	-0.622594	0.688643
27	1	0	3.643116	0.414980	0.860563
28	1	0	3.038364	-1.050245	1.650669
29	1	0	4.231814	-1.170224	0.353601

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240277	E(Thermal)=	0.254434
E(CCSD(T))=	-614.403513	E(Empiric)=	-0.350464
DE(MP2)=	-0.753149	DE(HF)=	-0.060642
G4MP2(0 K)=	-615.327491	G4MP2 Energy=	-615.313334
G4MP2 Enthalpy=	-615.31239	G4MP2 Free Energy=	-615.368427

EPOX2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.081331	-0.222591	-1.097714
2	6	0	-0.704041	0.480613	-0.003579
3	6	0	-2.114901	-0.145052	0.063251
4	6	0	-2.140475	-1.599524	0.491432
5	6	0	2.333899	-0.579884	0.238000
6	6	0	1.463989	-0.734968	-0.989493
7	1	0	-2.708180	0.390934	0.815457
8	1	0	-0.207381	0.311718	0.960776
9	1	0	-0.244826	0.041515	-2.107212
10	1	0	-1.502261	-1.829504	1.376409
11	1	0	2.049680	-0.772572	-1.909125
12	1	0	-2.641959	-0.056297	-0.892687
13	6	0	-0.741594	2.012498	-0.256846
14	1	0	-1.264350	2.169820	-1.212040
15	6	0	2.083179	-1.506983	1.404941
16	1	0	2.763910	-1.260322	2.220269
17	1	0	1.044737	-1.456734	1.742974
18	1	0	2.244259	-2.542499	1.082752
19	8	0	3.227452	0.236166	0.216502
20	8	0	0.343763	-1.620276	-0.943774
21	8	0	-2.823199	-2.448384	-0.017389
22	6	0	0.671914	2.603485	-0.387170
23	1	0	1.245797	2.148697	-1.197841
24	1	0	0.615218	3.678882	-0.581864

25	1	0	1.246111	2.462548	0.534998
26	6	0	-1.516611	2.767606	0.833550
27	1	0	-2.573936	2.493188	0.872610
28	1	0	-1.081510	2.583972	1.823328
29	1	0	-1.469578	3.845401	0.650257

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240589	E(Thermal)=	0.255928
E(CCSD(T))=	-614.521191	E(Empiric)=	-0.350464
DE(MP2)=	-0.752369	DE(HF)=	-0.059853
G4MP2(0 K)=	-615.443287	G4MP2 Energy=	-615.427948
G4MP2 Enthalpy=	-615.427004	G4MP2 Free Energy=	-615.486992

TS2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.302586	0.830452	-0.885162
2	6	0	-1.156127	0.013558	0.073471
3	6	0	-0.702363	-1.487770	0.145506
4	6	0	0.784212	-1.594227	0.256574
5	6	0	1.819730	0.803162	0.393986
6	6	0	0.978279	1.214099	-0.741639
7	1	0	-1.181044	-1.978656	0.994126
8	1	0	-1.003104	0.412578	1.081472
9	1	0	-0.807193	1.142077	-1.798336
10	1	0	1.331892	-2.036684	1.080011
11	1	0	1.447085	1.805876	-1.521515
12	1	0	-1.009773	-2.005306	-0.771551
13	6	0	-2.657953	0.148359	-0.282302
14	1	0	-2.775604	-0.142105	-1.337352
15	6	0	3.143223	1.478957	0.636889
16	1	0	3.765344	0.840010	1.263869
17	1	0	3.658163	1.692894	-0.301056
18	1	0	2.974968	2.428305	1.161790
19	8	0	1.304129	0.080749	1.280555
20	8	0	1.393185	-1.412553	-0.856928
21	8	0	2.719970	-1.000549	-0.686605
22	6	0	-3.114530	1.608532	-0.131876
23	1	0	-2.501996	2.298032	-0.719576
24	1	0	-4.153878	1.725857	-0.454124
25	1	0	-3.052640	1.924444	0.916289
26	6	0	-3.561623	-0.762022	0.562021

27	1	0	-3.379678	-1.824166	0.377674
28	1	0	-3.417934	-0.574786	1.633153
29	1	0	-4.614449	-0.568149	0.334136

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241344	E(Thermal)=	0.254781
E(CCSD(T))=	-614.389287	E(Empiric)=	-0.350464
DE(MP2)=	-0.752896	DE(HF)=	-0.060677
G4MP2(0 K)=	-615.31198	G4MP2 Energy=	-615.298544
G4MP2 Enthalpy=	-615.297599	G4MP2 Free Energy=	-615.35067

TS2f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.402037	-1.165647	1.209987
2	6	0	1.222592	0.054791	0.837965
3	6	0	-1.475143	-0.915687	-0.428505
4	6	0	-0.775608	-1.553114	0.709462
5	1	0	1.909139	0.216497	1.681412
6	1	0	0.815585	-1.766709	2.016701
7	1	0	-1.272455	-2.415262	1.147034
8	6	0	2.133227	-0.165136	-0.405465
9	1	0	1.478173	-0.348058	-1.260727
10	6	0	-2.847646	-1.440029	-0.786353
11	1	0	-3.349763	-0.732795	-1.446151
12	1	0	-2.734056	-2.394547	-1.318425
13	1	0	-3.456998	-1.616602	0.101394
14	8	0	-0.856299	-0.194072	-1.236351
15	6	0	3.023594	-1.401334	-0.206371
16	1	0	3.655352	-1.565654	-1.084979
17	1	0	3.687558	-1.278213	0.658777
18	1	0	2.429842	-2.306073	-0.049553
19	6	0	3.004167	1.063308	-0.705008
20	1	0	2.414662	1.942817	-0.981917
21	1	0	3.624924	1.334320	0.158392
22	1	0	3.679436	0.854113	-1.540855
23	6	0	-0.588217	1.672844	-0.286016
24	1	0	-0.267810	2.248663	-1.151617
25	8	0	-1.850280	1.749513	-0.105876
26	8	0	-2.321102	0.851225	0.834187
27	6	0	0.366172	1.351437	0.820517
28	1	0	-0.243688	1.364518	1.728461

29	1	0	1.060500	2.201050	0.845100

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241442	E(Thermal)=	0.254997
E(CCSD(T))=	-614.392218	E(Empiric)=	-0.350464
DE(MP2)=	-0.751826	DE(HF)=	-0.060578
G4MP2(0 K)=	-615.313644	G4MP2 Energy=	-615.300089
G4MP2 Enthalpy=	-615.299145	G4MP2 Free Energy=	-615.352604

TS2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.585474	-1.353860	-0.653982
2	6	0	1.145871	-0.069768	-0.083471
3	6	0	0.535818	1.168797	-0.826566
4	6	0	-0.936210	1.239447	-0.677834
5	6	0	-1.876030	-1.472155	0.184706
6	6	0	-0.623954	-1.914313	-0.518326
7	1	0	0.958032	2.089240	-0.418199
8	1	0	0.866988	0.032450	0.969807
9	1	0	1.279252	-1.876321	-1.312584
10	1	0	-1.628382	0.652517	-1.268539
11	1	0	-0.811589	-2.833696	-1.068417
12	1	0	0.790665	1.100881	-1.891334
13	6	0	2.695954	-0.073694	-0.150188
14	1	0	2.978716	-0.264116	-1.196176
15	6	0	-1.868023	-0.364459	1.148189
16	1	0	-2.730112	-0.450536	1.817980
17	1	0	-0.950906	-0.216616	1.713829
18	1	0	-2.491622	0.900873	0.720827
19	8	0	-2.910641	-2.044473	-0.141726
20	8	0	-1.411379	2.245546	-0.023871
21	8	0	-2.733113	1.976085	0.341409
22	6	0	3.251734	-1.217680	0.713892
23	1	0	2.826321	-2.187029	0.441115
24	1	0	4.338946	-1.285156	0.610788
25	1	0	3.027870	-1.044289	1.773086
26	6	0	3.332589	1.255078	0.281106
27	1	0	3.113094	2.075424	-0.407664
28	1	0	2.993074	1.550720	1.281125
29	1	0	4.421382	1.154026	0.322697

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.237218	E(Thermal)=	0.2509
E(CCSD(T))=	-614.340441	E(Empiric)=	-0.350464
DE(MP2)=	-0.762462	DE(HF)=	-0.062034
G4MP2(0 K)=	-615.278182	G4MP2 Energy=	-615.264501
G4MP2 Enthalpy=	-615.263556	G4MP2 Free Energy=	-615.318449

HP2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843949	1.308351	-0.749572
2	6	0	-1.188912	0.038421	0.001844
3	6	0	-0.219939	-1.116878	-0.340293
4	6	0	1.271872	-0.749555	-0.288477
5	6	0	1.436045	1.755814	0.234804
6	6	0	0.265890	2.048631	-0.627214
7	1	0	-0.373659	-1.925530	0.380969
8	1	0	-1.076374	0.245405	1.075176
9	1	0	-1.598979	1.663226	-1.448912
10	1	0	1.621740	-0.428097	-1.275766
11	1	0	0.361501	2.976457	-1.184498
12	1	0	-0.451860	-1.525865	-1.329368
13	6	0	-2.675816	-0.345129	-0.219465
14	1	0	-2.834134	-0.416221	-1.306095
15	6	0	1.638962	0.329596	0.744241
16	1	0	2.698628	0.246146	0.992628
17	1	0	1.069157	0.182925	1.670821
18	1	0	3.690344	-1.990458	0.606538
19	8	0	2.248976	2.625696	0.480069
20	8	0	1.903531	-1.997839	0.011405
21	8	0	3.314415	-1.856911	-0.274768
22	6	0	-3.608768	0.744254	0.333412
23	1	0	-3.390429	1.733681	-0.078491
24	1	0	-4.653705	0.512512	0.105326
25	1	0	-3.514715	0.813958	1.423794
26	6	0	-3.046150	-1.699985	0.400503
27	1	0	-2.514093	-2.533921	-0.063432
28	1	0	-2.826224	-1.714308	1.475075
29	1	0	-4.117983	-1.888614	0.283894

Temperature=	298.15	Pressure=	1

E(ZPE)=	0.244171	E(Thermal)=	0.258182
E(CCSD(T))=	-614.453588	E(Empiric)=	-0.350464
DE(MP2)=	-0.75673	DE(HF)=	-0.061813
G4MP2(0 K)=	-615.378425	G4MP2 Energy=	-615.364413
G4MP2 Enthalpy=	-615.363469	G4MP2 Free Energy=	-615.418799

RAD2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160911	-1.218531	0.754539
2	6	0	-0.860690	-0.105578	0.004205
3	6	0	-0.302473	1.291034	0.368827
4	6	0	1.266270	1.371258	0.347143
5	6	0	2.149883	-0.970841	-0.231463
6	6	0	1.116729	-1.601244	0.628152
7	1	0	-0.674698	2.017878	-0.357460
8	1	0	-0.674860	-0.252897	-1.067879
9	1	0	-0.779853	-1.779306	1.452587
10	1	0	1.607664	1.069650	1.353728
11	1	0	1.480308	-2.463679	1.180102
12	1	0	-0.645037	1.608670	1.357548
13	6	0	-2.399101	-0.186167	0.202577
14	1	0	-2.587029	-0.177864	1.286520
15	6	0	1.928209	0.460578	-0.713531
16	1	0	2.909920	0.865429	-0.969485
17	1	0	1.335625	0.455699	-1.636977
18	8	0	3.178102	-1.566304	-0.485985
19	8	0	1.516528	2.695650	0.150571
20	6	0	-2.949029	-1.501412	-0.373161
21	1	0	-2.449500	-2.382289	0.039806
22	1	0	-4.018972	-1.596590	-0.164158
23	1	0	-2.819360	-1.528910	-1.461617
24	6	0	-3.151371	0.999853	-0.417638
25	1	0	-2.906196	1.951183	0.060660
26	1	0	-2.928648	1.091584	-1.487680
27	1	0	-4.231496	0.852971	-0.320271

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.227471	E(Thermal)=	0.239909
E(CCSD(T))=	-538.845758	E(Empiric)=	-0.325479
DE(MP2)=	-0.654197	DE(HF)=	-0.052876
G4MP2(0 K)=	-539.65084	G4MP2 Energy=	-539.638402

G4MP2		G4MP2 Free	
Enthalpy=	-539.637458	Energy=	-539.689748

TS2j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246359	-1.237796	0.706414
2	6	0	-0.929854	-0.044159	0.070140
3	6	0	-0.424462	1.247559	0.653538
4	6	0	1.656470	1.472053	0.253202
5	6	0	2.127700	-1.019577	-0.195667
6	6	0	1.026366	-1.635733	0.585612
7	1	0	-0.727808	2.164609	0.162590
8	1	0	-0.720774	-0.035745	-1.007713
9	1	0	-0.883737	-1.839709	1.352363
10	1	0	1.876549	1.185495	1.301109
11	1	0	1.346691	-2.536367	1.102935
12	1	0	-0.370133	1.318423	1.736984
13	6	0	-2.486747	-0.179064	0.194812
14	1	0	-2.713074	-0.317767	1.261394
15	6	0	1.972202	0.375812	-0.781407
16	1	0	2.932981	0.637369	-1.235099
17	1	0	1.226409	0.391448	-1.582501
18	8	0	3.174970	-1.626325	-0.320217
19	8	0	1.662888	2.666266	-0.077412
20	6	0	-2.970830	-1.418793	-0.572819
21	1	0	-2.460530	-2.333140	-0.257117
22	1	0	-4.044748	-1.567246	-0.423239
23	1	0	-2.797950	-1.297536	-1.648661
24	6	0	-3.234411	1.067037	-0.296498
25	1	0	-3.028008	1.947379	0.317225
26	1	0	-2.964650	1.306540	-1.332074
27	1	0	-4.314531	0.892694	-0.271120

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.224108	E(Thermal)=	0.236852
E(CCSD(T))=	-538.816625	E(Empiric)=	-0.325479
DE(MP2)=	-0.65939	DE(HF)=	-0.052777
G4MP2(0 K)=	-539.630162	G4MP2 Energy=	-539.617418
G4MP2 Enthalpy=	-539.616474	G4MP2 Free Energy=	-539.670378

RAD2j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.231063	-1.177025	0.849517
2	6	0	-1.071002	0.031759	0.501420
3	6	0	-1.212973	0.755437	1.808022
4	6	0	2.065908	1.651123	-0.307703
5	6	0	2.150697	-0.834255	-0.101922
6	6	0	1.058651	-1.501030	0.634754
7	1	0	-0.513534	1.537197	2.076141
8	1	0	-0.559407	0.696150	-0.196173
9	1	0	-0.785357	-1.886746	1.465901
10	1	0	3.092286	1.809011	0.086401
11	1	0	1.428630	-2.408278	1.106961
12	1	0	-1.882011	0.374019	2.573179
13	6	0	-2.433662	-0.388082	-0.112287
14	1	0	-2.936214	-1.032197	0.625043
15	6	0	1.889811	0.343436	-1.057146
16	1	0	2.677355	0.282376	-1.814822
17	1	0	0.909718	0.308972	-1.530581
18	8	0	3.296580	-1.215534	0.046565
19	8	0	1.189763	2.456859	-0.120636
20	6	0	-2.242732	-1.196571	-1.402005
21	1	0	-1.623660	-2.084267	-1.240557
22	1	0	-3.207173	-1.526369	-1.801092
23	1	0	-1.758805	-0.587627	-2.175501
24	6	0	-3.321767	0.837269	-0.361214
25	1	0	-3.483724	1.409709	0.556595
26	1	0	-2.861558	1.509539	-1.094772
27	1	0	-4.298514	0.535540	-0.752774

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.222565	E(Thermal)=	0.237177
E(CCSD(T))=	-538.83387	E(Empiric)=	-0.325479
DE(MP2)=	-0.658913	DE(HF)=	-0.052946
G4MP2(0 K)=	-539.648643	G4MP2 Energy=	-539.634031
G4MP2 Enthalpy=	-539.633087	G4MP2 Free Energy=	-539.691498

TS2k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.167904	-1.245306	-0.655673
2	6	0	0.887311	-0.082174	-0.005344
3	6	0	0.349157	1.289283	-0.482752
4	6	0	-1.162148	1.564318	-0.465540
5	6	0	-2.193657	-0.972194	0.225326
6	6	0	-1.106616	-1.638258	-0.520590
7	1	0	0.794498	2.084102	0.119446
8	1	0	0.723424	-0.135559	1.078897
9	1	0	0.780882	-1.842581	-1.328884
10	1	0	-1.737728	1.052468	-1.260035
11	1	0	-1.452184	-2.513408	-1.063967
12	1	0	0.667754	1.447593	-1.523373
13	6	0	2.420827	-0.219331	-0.215120
14	1	0	2.593324	-0.306767	-1.298376
15	6	0	-1.947300	0.282761	0.970344
16	1	0	-2.849043	0.806130	1.266570
17	1	0	-1.125746	0.341343	1.675815
18	8	0	-3.333287	-1.419195	0.186036
19	8	0	-1.590862	2.639224	-0.001545
20	6	0	2.947388	-1.495104	0.462044
21	1	0	2.416726	-2.394418	0.136260
22	1	0	4.010022	-1.639018	0.244253
23	1	0	2.838695	-1.425242	1.551067
24	6	0	3.212561	0.993716	0.293370
25	1	0	2.990851	1.906048	-0.265124
26	1	0	3.002058	1.186133	1.352498
27	1	0	4.287104	0.806690	0.202621

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.224701	E(Thermal)=	0.237252
E(CCSD(T))=	-538.817474	E(Empiric)=	-0.325479
DE(MP2)=	-0.661172	DE(HF)=	-0.052878
G4MP2(0 K)=	-539.632301	G4MP2 Energy=	-539.619751
G4MP2 Enthalpy=	-539.618807	G4MP2 Free Energy=	-539.671414

RAD2k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.288083	-0.339305	1.197097
2	6	0	-0.749645	0.033808	0.167376
3	6	0	-1.166187	1.516401	0.382889
4	6	0	-0.037396	2.501893	0.158470

5	6	0	2.435384	-0.676272	-0.166321
6	6	0	1.585119	-0.638805	1.060967
7	1	0	-1.975981	1.799718	-0.290912
8	1	0	-0.333347	-0.047925	-0.842926
9	1	0	-0.096125	-0.309195	2.218740
10	1	0	0.862984	2.348056	0.791555
11	1	0	2.175206	-0.786348	1.962372
12	1	0	-1.520714	1.637039	1.417632
13	6	0	-1.976471	-0.922577	0.264429
14	1	0	-2.375385	-0.826487	1.285288
15	6	0	1.945234	-1.189850	-1.412950
16	1	0	2.607264	-1.149571	-2.270326
17	1	0	0.990432	-1.690948	-1.505988
18	8	0	3.615431	-0.308426	-0.076108
19	8	0	-0.084840	3.400835	-0.642491
20	6	0	-1.562272	-2.387656	0.057509
21	1	0	-0.757789	-2.688288	0.733596
22	1	0	-2.413602	-3.054286	0.226215
23	1	0	-1.219707	-2.555235	-0.971180
24	6	0	-3.097842	-0.560300	-0.720937
25	1	0	-3.554550	0.408940	-0.508373
26	1	0	-2.723840	-0.538243	-1.751513
27	1	0	-3.893614	-1.310527	-0.676565

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.223152	E(Thermal)=	0.237535
E(CCSD(T))=	-538.842173	E(Empiric)=	-0.325479
DE(MP2)=	-0.657543	DE(HF)=	-0.05308
G4MP2(0 K)=	-539.655123	G4MP2 Energy=	-539.64074
G4MP2 Enthalpy=	-539.639796	G4MP2 Free Energy=	-539.698517

TS2g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.800110	0.094079	1.573285
2	6	0	-0.373303	0.782530	0.896268
3	6	0	-1.521516	-0.229137	0.748013
4	6	0	-1.475426	-1.207556	-0.267722
5	6	0	2.255935	-0.937433	-0.266522
6	6	0	1.862411	-0.594878	1.120506
7	1	0	-1.899060	-0.613227	1.702038
8	1	0	-0.734674	1.510383	1.635937

9	1	0	0.748875	0.165503	2.660058
10	1	0	-0.645069	-1.456451	-0.922535
11	1	0	2.565042	-0.948801	1.872593
12	1	0	-2.824409	-0.114769	0.454491
13	6	0	-0.077747	1.610713	-0.382957
14	1	0	0.242717	0.930971	-1.176385
15	6	0	3.721410	-1.287275	-0.454474
16	1	0	4.360896	-0.467023	-0.109641
17	1	0	3.978520	-2.164591	0.150668
18	1	0	3.919844	-1.498250	-1.505368
19	8	0	1.482245	-0.979682	-1.208924
20	8	0	-2.611554	-1.721701	-0.622152
21	8	0	-3.640424	-1.163242	0.148863
22	6	0	-1.338984	2.350820	-0.855879
23	1	0	-1.112768	2.951544	-1.742539
24	1	0	-2.152846	1.669514	-1.113708
25	1	0	-1.708609	3.033502	-0.080570
26	6	0	1.049741	2.624365	-0.134950
27	1	0	1.246783	3.206636	-1.040449
28	1	0	0.772423	3.331911	0.656841
29	1	0	1.984424	2.142779	0.162876

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.2362	E(Thermal)=	0.251034
E(CCSD(T))=	-614.360115	E(Empiric)=	-0.350464
DE(MP2)=	-0.755868	DE(HF)=	-0.062142
G4MP2(0 K)=	-615.292389	G4MP2 Energy=	-615.277556
G4MP2 Enthalpy=	-615.276612	G4MP2 Free Energy=	-615.334763

HP2g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.704704	-0.054068	1.545111
2	6	0	-0.248824	0.906508	0.855440
3	6	0	-1.569944	0.182351	0.594285
4	6	0	-1.667195	-0.872426	-0.212265
5	6	0	2.095656	-1.202970	-0.270575
6	6	0	1.663537	-0.890133	1.110485
7	1	0	-2.457547	0.546247	1.094845
8	1	0	-0.478518	1.657879	1.623553
9	1	0	0.563473	-0.060722	2.625806
10	1	0	-0.823975	-1.299697	-0.748743

11	1	0	2.221922	-1.426403	1.875742
12	1	0	-4.401163	-0.653208	-0.556859
13	6	0	0.289349	1.717153	-0.356257
14	1	0	0.505597	1.017374	-1.166353
15	6	0	3.498208	-1.773772	-0.398582
16	1	0	4.234924	-1.089443	0.036925
17	1	0	3.573232	-2.715413	0.157857
18	1	0	3.730369	-1.951970	-1.448786
19	8	0	1.389308	-1.064680	-1.255385
20	8	0	-2.779030	-1.594962	-0.533367
21	8	0	-3.940876	-1.105620	0.165711
22	6	0	-0.777246	2.707979	-0.845304
23	1	0	-0.409926	3.271056	-1.709310
24	1	0	-1.696538	2.196337	-1.141264
25	1	0	-1.031720	3.434268	-0.062545
26	6	0	1.577571	2.473302	-0.000038
27	1	0	1.940324	3.042004	-0.862426
28	1	0	1.400689	3.188539	0.813632
29	1	0	2.378744	1.801705	0.318451

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240006	E(Thermal)=	0.256021
E(CCSD(T))=	-614.41838	E(Empiric)=	-0.350464
DE(MP2)=	-0.75588	DE(HF)=	-0.062222
G4MP2(0 K)=	-615.346941	G4MP2 Energy=	-615.330925
G4MP2 Enthalpy=	-615.329981	G4MP2 Free Energy=	-615.390794

RAD2g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.322522	-1.035650	1.337684
2	6	0	0.921752	-0.280709	0.869553
3	6	0	0.646438	1.196202	0.935901
4	6	0	0.574042	2.150909	-0.127683
5	6	0	-2.096374	-0.325845	-0.337849
6	6	0	-1.574174	-1.043880	0.851865
7	1	0	0.438234	1.606857	1.922323
8	1	0	1.670476	-0.475188	1.654218
9	1	0	-0.163791	-1.640436	2.228629
10	1	0	0.746642	1.787308	-1.153446
11	1	0	-2.310635	-1.638139	1.388413
12	6	0	1.545592	-0.816383	-0.450933

13	1	0	0.881182	-0.536618	-1.272078
14	6	0	-3.604135	-0.351754	-0.506476
15	1	0	-3.960582	-1.385698	-0.582515
16	1	0	-4.092505	0.088453	0.370623
17	1	0	-3.885960	0.202101	-1.401932
18	8	0	-1.381172	0.245460	-1.140099
19	8	0	0.329285	3.340108	0.084536
20	6	0	2.933175	-0.198458	-0.680105
21	1	0	3.351015	-0.542996	-1.631349
22	1	0	2.909568	0.893900	-0.704437
23	1	0	3.628741	-0.497916	0.113551
24	6	0	1.660583	-2.347937	-0.427211
25	1	0	2.130005	-2.708095	-1.347931
26	1	0	2.282439	-2.685681	0.411696
27	1	0	0.684008	-2.831359	-0.339747

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.223805	E(Thermal)=	0.238144
E(CCSD(T))=	-538.85247	E(Empiric)=	-0.325479
DE(MP2)=	-0.655169	DE(HF)=	-0.052745
G4MP2(0 K)=	-539.662058	G4MP2 Energy=	-539.647719
G4MP2 Enthalpy=	-539.646775	G4MP2 Free Energy=	-539.704057

TS3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.157461	1.423938	0.123539
2	6	0	0.992216	0.127560	-0.058811
3	6	0	-2.330793	0.626762	-0.121297
4	6	0	-1.338936	1.534375	-0.093081
5	1	0	0.922850	-0.195006	-1.100693
6	1	0	0.317700	1.795864	1.148449
7	1	0	0.598881	2.191542	-0.520808
8	1	0	-1.657947	2.577746	-0.114670
9	6	0	2.509002	0.350524	0.246951
10	1	0	2.632290	0.370128	1.340122
11	6	0	-3.795627	0.981873	-0.122646
12	1	0	-4.304947	0.543839	0.744510
13	1	0	-3.934621	2.064840	-0.083643
14	1	0	-4.304261	0.603474	-1.016808
15	6	0	-1.957163	-0.778901	-0.057589
16	1	0	-2.409278	-1.530280	0.580786

17	6	0	0.486365	-1.006186	0.848632
18	1	0	1.192456	-1.812977	1.086862
19	8	0	-0.509083	-0.828942	1.563516
20	8	0	-1.152066	-1.163413	-0.980754
21	8	0	-0.372226	-2.258169	-0.614270
22	6	0	3.344391	-0.814730	-0.311266
23	1	0	2.995674	-1.792569	0.029079
24	1	0	3.306254	-0.819762	-1.406807
25	1	0	4.393077	-0.713021	-0.013742
26	6	0	3.071013	1.671696	-0.301606
27	1	0	2.639203	2.550938	0.182701
28	1	0	4.153075	1.710165	-0.138879
29	1	0	2.899017	1.757795	-1.381354

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240954	E(Thermal)=	0.254542
E(CCSD(T))=	-614.373451	E(Empiric)=	-0.350464
DE(MP2)=	-0.753812	DE(HF)=	-0.060776
G4MP2(0 K)=	-615.297549	G4MP2 Energy=	-615.283961
G4MP2 Enthalpy=	-615.283017	G4MP2 Free Energy=	-615.336715

SOZ3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.198662	1.501971	0.508687
2	6	0	0.931467	0.243160	-0.017237
3	6	0	-2.160055	0.699017	-0.078447
4	6	0	-1.232902	1.653784	0.036698
5	1	0	0.743229	0.179318	-1.095301
6	1	0	0.235374	1.514946	1.606489
7	1	0	0.742804	2.388852	0.176850
8	1	0	-1.519395	2.663129	-0.253995
9	6	0	2.468835	0.263745	0.192403
10	1	0	2.659508	0.180713	1.273587
11	6	0	-3.544616	0.943230	-0.611999
12	1	0	-4.311140	0.657269	0.119761
13	1	0	-3.693582	1.994850	-0.868580
14	1	0	-3.732314	0.344861	-1.512720
15	6	0	-1.848409	-0.724450	0.322893
16	1	0	-2.736374	-1.265310	0.673206
17	6	0	0.331262	-1.046424	0.607853
18	1	0	1.024226	-1.550940	1.287063

19	8	0	-0.864503	-0.817209	1.321109
20	8	0	-1.293715	-1.417120	-0.838272
21	8	0	-0.056942	-2.007459	-0.353225
22	6	0	3.127913	-0.939972	-0.504659
23	1	0	2.709141	-1.899773	-0.190210
24	1	0	2.997880	-0.871613	-1.590869
25	1	0	4.202393	-0.963612	-0.297161
26	6	0	3.135348	1.557077	-0.300586
27	1	0	2.844647	2.432597	0.285142
28	1	0	4.224586	1.469119	-0.233604
29	1	0	2.885266	1.753066	-1.350199

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.245386	E(Thermal)=	0.258254
E(CCSD(T))=	-614.454275	E(Empiric)=	-0.350464
DE(MP2)=	-0.749621	DE(HF)=	-0.060777
G4MP2(0 K)=	-615.369752	G4MP2 Energy=	-615.356883
G4MP2 Enthalpy=	-615.355939	G4MP2 Free Energy=	-615.408258

TS3e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.325182	1.300377	0.440015
2	6	0	1.106996	0.223074	-0.344494
3	6	0	-2.159354	0.692115	-0.154515
4	6	0	-1.118910	1.518453	0.065997
5	1	0	1.157719	0.553884	-1.391768
6	1	0	0.384862	1.078103	1.508772
7	1	0	0.833145	2.257072	0.288588
8	1	0	-1.358829	2.569269	-0.094060
9	6	0	2.552463	0.029955	0.179324
10	1	0	2.478097	-0.529243	1.123615
11	6	0	-3.472479	1.252276	-0.678062
12	1	0	-4.312486	1.019982	-0.012991
13	1	0	-3.417427	2.337062	-0.786417
14	1	0	-3.712839	0.828458	-1.660911
15	6	0	-2.254910	-0.752838	0.036873
16	1	0	-3.094932	-1.259037	-0.435063
17	6	0	0.383549	-1.128788	-0.395927
18	1	0	0.935015	-1.986194	0.019837
19	8	0	-0.564947	-1.335588	-1.171837
20	8	0	-1.779104	-1.480798	0.979850

21	8	0	-0.572977	-1.042721	1.465205
22	6	0	3.375841	-0.808605	-0.813188
23	1	0	2.896159	-1.760765	-1.057381
24	1	0	3.518677	-0.261010	-1.752590
25	1	0	4.366721	-1.032262	-0.405197
26	6	0	3.291584	1.344034	0.471018
27	1	0	2.829721	1.915278	1.280214
28	1	0	4.325470	1.137245	0.766174
29	1	0	3.327381	1.984690	-0.418811

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241629	E(Thermal)=	0.255124
E(CCSD(T))=	-614.380916	E(Empiric)=	-0.350464
DE(MP2)=	-0.753212	DE(HF)=	-0.060922
G4MP2(0 K)=	-615.303885	G4MP2 Energy=	-615.290389
G4MP2 Enthalpy=	-615.289445	G4MP2 Free Energy=	-615.343043

SOZ3e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.373556	1.472705	0.132596
2	6	0	1.085394	0.158242	-0.271945
3	6	0	-2.096961	0.767153	0.016411
4	6	0	-1.091414	1.608961	-0.235911
5	1	0	1.116560	0.100543	-1.367881
6	1	0	0.482543	1.599018	1.217271
7	1	0	0.908787	2.305447	-0.328866
8	1	0	-1.347576	2.534761	-0.748402
9	6	0	2.541346	0.063606	0.258088
10	1	0	2.484995	-0.141071	1.337646
11	6	0	-3.519084	1.035222	-0.396516
12	1	0	-3.612968	1.997760	-0.904712
13	1	0	-3.881038	0.251749	-1.072833
14	1	0	-4.193012	1.041019	0.470510
15	6	0	-1.883352	-0.574655	0.676919
16	1	0	-2.656085	-0.817371	1.414699
17	6	0	0.246698	-1.045222	0.203752
18	1	0	0.853439	-1.895016	0.534199
19	8	0	-0.610133	-1.446915	-0.886417
20	8	0	-0.617686	-0.719927	1.275658
21	8	0	-1.909552	-1.634115	-0.274537
22	6	0	3.341077	1.362178	0.072526

23	1	0	2.933093	2.192656	0.653495
24	1	0	4.377415	1.215271	0.393335
25	1	0	3.363521	1.664540	-0.981550
26	6	0	3.297311	-1.094470	-0.414809
27	1	0	2.783282	-2.054912	-0.316506
28	1	0	3.424083	-0.898400	-1.486107
29	1	0	4.294516	-1.210660	0.021404

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.245664	E(Thermal)=	0.258415
E(CCSD(T))=	-614.457587	E(Empiric)=	-0.350464
DE(MP2)=	-0.749364	DE(HF)=	-0.060828
G4MP2(0 K)=	-615.372579	G4MP2 Energy=	-615.359828
G4MP2 Enthalpy=	-615.358884	G4MP2 Free Energy=	-615.41085

TS3j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.193751	1.499068	0.365033
2	6	0	0.963846	0.240324	-0.091926
3	6	0	-2.225050	0.674962	-0.064063
4	6	0	-1.274191	1.609486	0.006127
5	1	0	0.827896	0.113201	-1.173441
6	1	0	0.299610	1.598681	1.454426
7	1	0	0.688799	2.372059	-0.067273
8	1	0	-1.594972	2.632657	-0.186577
9	6	0	2.490602	0.301064	0.201652
10	1	0	2.620952	0.224326	1.291587
11	6	0	-3.658163	1.004116	-0.401626
12	1	0	-4.340212	0.657614	0.385299
13	1	0	-3.798416	2.080945	-0.523426
14	1	0	-3.970197	0.508616	-1.329297
15	6	0	-1.998476	-0.809216	0.108031
16	1	0	-2.720958	-1.321860	0.759454
17	6	0	0.296670	-1.006480	0.531343
18	1	0	1.088875	-1.850616	0.899349
19	8	0	-0.674559	-0.826001	1.364954
20	8	0	-1.538597	-1.445420	-0.910976
21	8	0	0.169393	-2.102185	-0.223492
22	6	0	3.241205	-0.868226	-0.459147
23	1	0	2.862980	-1.852113	-0.168016
24	1	0	3.163181	-0.807486	-1.550571

25	1	0	4.302932	-0.835277	-0.195976
26	6	0	3.134023	1.621788	-0.250134
27	1	0	2.776104	2.481936	0.320037
28	1	0	4.219591	1.572818	-0.118999
29	1	0	2.938632	1.812033	-1.312204

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.237649	E(Thermal)=	0.251446
E(CCSD(T))=	-614.376193	E(Empiric)=	-0.350464
DE(MP2)=	-0.754211	DE(HF)=	-0.060577
G4MP2(0 K)=	-615.303795	G4MP2 Energy=	-615.289999
G4MP2 Enthalpy=	-615.289054	G4MP2 Free Energy=	-615.343717

TS3k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.133492	1.367256	0.578496
2	6	0	0.948116	0.192355	-0.040840
3	6	0	-2.227929	0.613162	-0.094930
4	6	0	-1.276641	1.564894	0.106005
5	1	0	0.785414	0.189998	-1.123205
6	1	0	0.090597	1.205302	1.669236
7	1	0	0.657458	2.312932	0.424842
8	1	0	-1.604748	2.597168	-0.004559
9	6	0	2.473749	0.314003	0.205989
10	1	0	2.651172	0.196124	1.285998
11	6	0	-3.630097	0.849927	-0.566580
12	1	0	-4.362392	0.452853	0.144189
13	1	0	-3.817226	1.920390	-0.689552
14	1	0	-3.800508	0.359195	-1.528544
15	6	0	-1.836109	-0.862289	0.390540
16	1	0	-2.721749	-1.463229	0.648696
17	6	0	0.433324	-1.211726	0.456471
18	1	0	1.094392	-1.591445	1.260058
19	8	0	-0.834815	-0.970254	1.278382
20	8	0	-1.460491	-0.807584	-0.888687
21	8	0	0.202957	-2.105617	-0.464946
22	6	0	3.225224	-0.810729	-0.529787
23	1	0	2.831668	-1.802936	-0.301016
24	1	0	3.141381	-0.676903	-1.614532
25	1	0	4.288923	-0.792380	-0.271050
26	6	0	3.061196	1.669362	-0.220305

27	1	0	2.718428	2.500798	0.401691
28	1	0	4.153454	1.644866	-0.148225
29	1	0	2.806572	1.897601	-1.262370

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240041	E(Thermal)=	0.253353
E(CCSD(T))=	-614.396854	E(Empiric)=	-0.350464
DE(MP2)=	-0.75399	DE(HF)=	-0.059488
G4MP2(0 K)=	-615.320754	G4MP2 Energy=	-615.307442
G4MP2 Enthalpy=	-615.306498	G4MP2 Free Energy=	-615.359723

TS3I

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.388052	1.450351	0.150545
2	6	0	1.115691	0.163490	-0.322785
3	6	0	-2.095163	0.809978	-0.021681
4	6	0	-1.057986	1.614852	-0.276125
5	1	0	1.191516	0.208963	-1.416521
6	1	0	0.451235	1.501594	1.241638
7	1	0	0.943595	2.305256	-0.242530
8	1	0	-1.267857	2.501007	-0.873169
9	6	0	2.547896	0.034939	0.260710
10	1	0	2.441907	-0.245940	1.318719
11	6	0	-3.492700	1.049248	-0.516522
12	1	0	-3.558226	1.983795	-1.078372
13	1	0	-3.817992	0.229290	-1.165811
14	1	0	-4.208927	1.104079	0.313995
15	6	0	-1.823798	-0.496876	0.676266
16	1	0	-2.810234	-0.959576	1.209030
17	6	0	0.332384	-1.144361	-0.038225
18	1	0	0.835598	-1.881080	0.600252
19	8	0	-0.466451	-1.554178	-0.946526
20	8	0	-0.744281	-0.606514	1.376734
21	8	0	-2.177970	-1.612209	0.016025
22	6	0	3.352132	1.342238	0.201815
23	1	0	2.920209	2.129727	0.823924
24	1	0	4.374114	1.169480	0.554384
25	1	0	3.419450	1.719536	-0.825850
26	6	0	3.330002	-1.076003	-0.460205
27	1	0	2.806390	-2.036261	-0.451867
28	1	0	3.502306	-0.805269	-1.508676

29	1	0	4.307485	-1.228531	0.008236

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238194	E(Thermal)=	0.251784
E(CCSD(T))=	-614.38068	E(Empiric)=	-0.350464
DE(MP2)=	-0.753819	DE(HF)=	-0.060489
G4MP2(0 K)=	-615.307258	G4MP2 Energy=	-615.293668
G4MP2 Enthalpy=	-615.292723	G4MP2 Free Energy=	-615.346391

TS3m

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.389969	1.444649	0.317487
2	6	0	1.202859	0.339200	-0.312908
3	6	0	-2.080577	0.783728	-0.019641
4	6	0	-1.046994	1.614503	-0.164322
5	1	0	1.159805	0.335495	-1.399388
6	1	0	0.439509	1.353262	1.406462
7	1	0	0.927626	2.366965	0.053142
8	1	0	-1.230925	2.545995	-0.694845
9	6	0	2.577722	-0.008293	0.224985
10	1	0	2.483064	-0.319105	1.272704
11	6	0	-3.443270	1.098273	-0.573610
12	1	0	-3.460764	2.064694	-1.083380
13	1	0	-3.743939	0.313146	-1.274506
14	1	0	-4.199022	1.114856	0.222968
15	6	0	-2.039805	-0.600792	0.637737
16	1	0	-2.651949	-0.599725	1.563784
17	6	0	0.126521	-1.233082	0.252095
18	1	0	0.873579	-1.958145	0.612570
19	8	0	-0.314639	-1.251093	-0.934623
20	8	0	-0.652160	-0.779703	1.233414
21	8	0	-2.326911	-1.614362	-0.136341
22	6	0	3.466258	1.261414	0.201872
23	1	0	3.085234	2.039473	0.866875
24	1	0	4.476286	0.997629	0.530461
25	1	0	3.540301	1.674385	-0.809830
26	6	0	3.244829	-1.125053	-0.589891
27	1	0	2.630198	-2.027135	-0.641617
28	1	0	3.426557	-0.792244	-1.617763
29	1	0	4.209041	-1.395565	-0.150069

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239714	E(Thermal)=	0.253326
E(CCSD(T))=	-614.394493	E(Empiric)=	-0.350464
DE(MP2)=	-0.754418	DE(HF)=	-0.059671
G4MP2(0 K)=	-615.319333	G4MP2 Energy=	-615.305721
G4MP2 Enthalpy=	-615.304777	G4MP2 Free Energy=	-615.358366

TS3i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.307780	1.515482	0.451306
2	6	0	0.981704	0.228944	-0.075862
3	6	0	-2.080126	0.787710	-0.073780
4	6	0	-1.105872	1.699470	-0.054223
5	1	0	0.831393	0.196678	-1.161631
6	1	0	0.329905	1.517542	1.548431
7	1	0	0.890574	2.380184	0.128178
8	1	0	-1.330629	2.676654	-0.478046
9	6	0	2.508684	0.143618	0.189542
10	1	0	2.649924	-0.030829	1.267219
11	6	0	-3.437834	1.042555	-0.670494
12	1	0	-3.512217	2.053735	-1.077332
13	1	0	-3.645175	0.331872	-1.480015
14	1	0	-4.234004	0.913489	0.074459
15	6	0	-1.903034	-0.604429	0.489721
16	1	0	-2.802807	-0.932344	1.025399
17	6	0	0.277462	-1.034959	0.501798
18	1	0	0.975908	-1.649784	1.078200
19	8	0	-0.262691	-1.884616	-0.509997
20	8	0	-0.808875	-0.756678	1.350115
21	8	0	-1.686961	-1.565503	-0.565036
22	6	0	3.268193	1.427154	-0.176915
23	1	0	3.000328	2.271871	0.462507
24	1	0	4.346671	1.269583	-0.073402
25	1	0	3.076792	1.715290	-1.217629
26	6	0	3.122052	-1.043332	-0.574306
27	1	0	2.621949	-1.993026	-0.362903
28	1	0	3.055916	-0.876444	-1.655747
29	1	0	4.179626	-1.163374	-0.319065

Temperature=	298.15	Pressure=	1

E(ZPE)=	0.245194	E(Thermal)=	0.257394
E(CCSD(T))=	-614.450851	E(Empiric)=	-0.350464
DE(MP2)=	-0.749705	DE(HF)=	-0.06112
G4MP2(0 K)=	-615.366946	G4MP2 Energy=	-615.354746
G4MP2 Enthalpy=	-615.353802	G4MP2 Free Energy=	-615.404602

ACID3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.385281	1.058875	-0.354593
2	6	0	-1.433525	0.124763	0.325266
3	6	0	2.064267	0.665196	0.340527
4	6	0	0.852914	1.230184	0.475396
5	1	0	-1.614445	0.477194	1.348839
6	1	0	-0.146615	0.669781	-1.344334
7	1	0	-0.844680	2.045785	-0.471353
8	1	0	0.737417	1.911889	1.317918
9	6	0	-2.775531	0.055971	-0.444681
10	1	0	-2.561020	-0.361461	-1.439387
11	6	0	3.194929	0.988032	1.286767
12	1	0	2.864864	1.694550	2.051946
13	1	0	3.564303	0.086283	1.785597
14	1	0	4.047557	1.423287	0.755842
15	6	0	2.344934	-0.309506	-0.747155
16	1	0	3.741053	-1.273786	-1.525711
17	6	0	-0.825126	-1.264656	0.438744
18	1	0	-0.811777	-1.836178	-0.515660
19	8	0	-0.364171	-1.729354	1.450257
20	8	0	1.545567	-0.805461	-1.512938
21	8	0	3.660902	-0.628123	-0.808165
22	6	0	-3.429084	1.431107	-0.639467
23	1	0	-2.832130	2.096059	-1.268836
24	1	0	-4.406605	1.320358	-1.119866
25	1	0	-3.590305	1.929915	0.323734
26	6	0	-3.752286	-0.893231	0.269416
27	1	0	-3.336072	-1.897952	0.393956
28	1	0	-4.001918	-0.515356	1.267784
29	1	0	-4.685278	-0.987277	-0.295016

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.242518	E(Thermal)=	0.257782
E(CCSD(T))=	-614.567707	E(Empiric)=	-0.350464

DE(MP2)=	-0.757773	DE(HF)=	-0.060761
G4MP2(0 K)=	-615.494187	G4MP2 Energy=	-615.478924
G4MP2 Enthalpy=	-615.477979	G4MP2 Free Energy=	-615.537713

ACID3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.235248	0.298355	-1.100198
2	6	0	-0.845455	0.007105	-0.026914
3	6	0	2.568463	-0.038499	-0.101623
4	6	0	1.520111	-0.438260	-0.845488
5	1	0	-0.480982	0.363564	0.940088
6	1	0	-0.159597	-0.010359	-2.073665
7	1	0	0.417186	1.371790	-1.107952
8	1	0	1.596659	-1.414201	-1.322774
9	6	0	-2.202971	0.702435	-0.338531
10	1	0	-2.573540	0.269782	-1.277444
11	6	0	3.814541	-0.878386	0.049112
12	1	0	3.731120	-1.814973	-0.506496
13	1	0	4.701318	-0.346504	-0.316944
14	1	0	4.008040	-1.125774	1.100048
15	6	0	2.601884	1.266733	0.600351
16	1	0	3.607973	1.533955	0.997598
17	6	0	-1.066387	-1.492859	0.057770
18	1	0	-1.249682	-2.900258	1.276417
19	8	0	-1.079813	-1.946924	1.332738
20	8	0	-1.227438	-2.225825	-0.887846
21	8	0	1.668051	2.022177	0.771615
22	6	0	-2.041117	2.217402	-0.529333
23	1	0	-1.449503	2.465789	-1.413764
24	1	0	-3.022803	2.686634	-0.650380
25	1	0	-1.553481	2.674261	0.338917
26	6	0	-3.239699	0.419911	0.760382
27	1	0	-3.421661	-0.649438	0.897844
28	1	0	-2.909512	0.826341	1.723251
29	1	0	-4.195641	0.890342	0.510030

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.242449	E(Thermal)=	0.257934
E(CCSD(T))=	-614.570135	E(Empiric)=	-0.350464
DE(MP2)=	-0.756898	DE(HF)=	-0.060726
G4MP2(0 K)=	-615.495775	G4MP2 Energy=	-615.48029

G4MP2		G4MP2 Free	
Enthalpy=	-615.479346	Energy=	-615.539756

ESTER3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.100877	-0.970078	-0.384374
2	6	0	1.286482	-0.417454	0.430598
3	6	0	-2.370058	-0.603154	0.233718
4	6	0	-1.142105	-1.107606	0.447570
5	1	0	1.500273	-1.115482	1.249176
6	1	0	-0.048717	-0.363350	-1.275266
7	1	0	0.393060	-1.974019	-0.717845
8	1	0	-1.006895	-1.714595	1.344391
9	6	0	2.583406	-0.198717	-0.372732
10	1	0	2.365266	0.532225	-1.157959
11	6	0	-3.523493	-0.870875	1.164928
12	1	0	-3.220139	-1.498928	2.005879
13	1	0	-3.934471	0.066818	1.552731
14	1	0	-4.343262	-1.363165	0.631941
15	6	0	-2.690867	0.245483	-0.937413
16	1	0	-1.853116	0.503442	-1.611429
17	6	0	0.473669	1.863744	0.508394
18	1	0	0.227495	2.642027	1.248228
19	8	0	0.905795	0.784432	1.167058
20	8	0	0.360835	1.997702	-0.681475
21	8	0	-3.808989	0.659480	-1.159268
22	6	0	3.045446	-1.505557	-1.036438
23	1	0	2.344723	-1.860947	-1.796333
24	1	0	4.010750	-1.353169	-1.528271
25	1	0	3.177908	-2.303403	-0.295159
26	6	0	3.696959	0.360376	0.525682
27	1	0	3.405148	1.296161	1.007353
28	1	0	3.959537	-0.354004	1.315430
29	1	0	4.599405	0.550511	-0.062981

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.242221	E(Thermal)=	0.25756
E(CCSD(T))=	-614.556374	E(Empiric)=	-0.350464
DE(MP2)=	-0.751628	DE(HF)=	-0.060257
G4MP2(0 K)=	-615.476502	G4MP2 Energy=	-615.461162
G4MP2		G4MP2 Free	
Enthalpy=	-615.460218	Energy=	-615.519701

ESTER3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.419512	-0.991733	-0.561335
2	6	0	1.455672	-0.182766	0.278890
3	6	0	-2.011975	-1.052137	0.139957
4	6	0	-0.752160	-1.467917	0.245995
5	1	0	1.660064	-0.727322	1.208946
6	1	0	0.077737	-0.386649	-1.407653
7	1	0	0.930188	-1.863684	-0.982158
8	1	0	-0.552298	-2.232336	0.992141
9	6	0	2.782518	0.093845	-0.468139
10	1	0	2.537386	0.663058	-1.377071
11	6	0	-3.182320	-1.558651	0.922959
12	1	0	-3.943985	-1.967156	0.249171
13	1	0	-2.876449	-2.336928	1.624728
14	1	0	-3.658335	-0.750111	1.491204
15	6	0	-2.560235	1.174699	-0.444079
16	1	0	-2.324513	1.334428	0.622006
17	6	0	0.775633	1.119342	0.653413
18	1	0	0.766447	1.875405	-0.168744
19	8	0	0.222171	1.342624	1.700434
20	8	0	-2.926426	2.017115	-1.204688
21	8	0	-2.357339	-0.111081	-0.840759
22	6	0	3.712381	0.958745	0.399163
23	1	0	3.245787	1.905747	0.689749
24	1	0	3.987063	0.431199	1.320028
25	1	0	4.635928	1.196055	-0.137730
26	6	0	3.508333	-1.190031	-0.893607
27	1	0	2.939722	-1.777637	-1.618871
28	1	0	4.468756	-0.944412	-1.357831
29	1	0	3.715089	-1.829282	-0.027119

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240744	E(Thermal)=	0.256451
E(CCSD(T))=	-614.544655	E(Empiric)=	-0.350464
DE(MP2)=	-0.754134	DE(HF)=	-0.060449
G4MP2(0 K)=	-615.468959	G4MP2 Energy=	-615.453252
G4MP2 Enthalpy=	-615.452308	G4MP2 Free Energy=	-615.513458

TS3d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.021464	-0.281640	0.992069
2	6	0	1.237312	-0.380741	0.017123
3	6	0	-2.317356	-0.665628	0.008290
4	6	0	-1.155054	-1.101692	0.555633
5	1	0	0.878140	-0.271958	-1.011302
6	1	0	0.344352	-0.651047	1.976309
7	1	0	-0.263112	0.761880	1.110135
8	1	0	-1.084054	-2.170892	0.752198
9	6	0	2.310671	0.695742	0.315188
10	1	0	2.547134	0.638873	1.388225
11	6	0	-3.498966	-1.581908	-0.219223
12	1	0	-3.293721	-2.587117	0.154301
13	1	0	-4.390201	-1.204354	0.295080
14	1	0	-3.749118	-1.659504	-1.282678
15	6	0	-2.506101	0.718845	-0.330539
16	1	0	-3.500129	1.161279	-0.376621
17	6	0	1.794790	-1.782552	0.169984
18	1	0	2.395079	-1.929888	1.101199
19	8	0	1.587315	-2.702097	-0.580038
20	8	0	-1.514544	1.471482	-0.665583
21	8	0	-1.896374	2.548856	0.247906
22	6	0	1.814742	2.114977	-0.000695
23	1	0	1.633943	2.224753	-1.075848
24	1	0	0.886682	2.382249	0.509736
25	1	0	2.576908	2.847988	0.283105
26	6	0	3.599982	0.410691	-0.474092
27	1	0	4.355503	1.173819	-0.263584
28	1	0	4.037165	-0.562691	-0.228349
29	1	0	3.405339	0.424115	-1.552621

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238437	E(Thermal)=	0.253718
E(CCSD(T))=	-614.365225	E(Empiric)=	-0.350464
DE(MP2)=	-0.753342	DE(HF)=	-0.061689
G4MP2(0 K)=	-615.292283	G4MP2 Energy=	-615.277002
G4MP2 Enthalpy=	-615.276058	G4MP2 Free Energy=	-615.335866

TS3g

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.392075	-0.723470	0.336380
2	6	0	1.683611	0.132707	0.259395
3	6	0	-2.035168	0.163936	0.498595
4	6	0	-0.759527	0.024478	0.939893
5	1	0	1.931449	0.505423	1.260838
6	1	0	0.159499	-1.132828	-0.651700
7	1	0	0.595595	-1.590489	0.977214
8	1	0	-0.526792	0.489321	1.897359
9	6	0	2.898123	-0.644308	-0.316385
10	1	0	2.647767	-0.924482	-1.350601
11	6	0	-3.065264	0.888712	1.331175
12	1	0	-2.566119	1.541264	2.052787
13	1	0	-3.719504	1.493523	0.698810
14	1	0	-3.704404	0.179716	1.858838
15	6	0	-2.394385	-0.308841	-0.809041
16	1	0	-1.596263	-0.597335	-1.499266
17	6	0	1.397669	1.346131	-0.609276
18	1	0	1.136005	1.086989	-1.665235
19	8	0	1.430626	2.491907	-0.245611
20	8	0	-3.574380	-0.258314	-1.336293
21	8	0	-4.156606	-1.094629	-0.281689
22	6	0	4.145966	0.252745	-0.355246
23	1	0	3.981724	1.168704	-0.930396
24	1	0	4.442904	0.549767	0.657066
25	1	0	4.987793	-0.280058	-0.807518
26	6	0	3.198068	-1.933188	0.462246
27	1	0	2.388519	-2.664885	0.397333
28	1	0	4.099007	-2.410747	0.064655
29	1	0	3.378698	-1.719007	1.522142

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238044	E(Thermal)=	0.253436
E(CCSD(T))=	-614.358082	E(Empiric)=	-0.350464
DE(MP2)=	-0.753837	DE(HF)=	-0.062076
G4MP2(0 K)=	-615.286415	G4MP2 Energy=	-615.271023
G4MP2 Enthalpy=	-615.270079	G4MP2 Free Energy=	-615.330978

DIO3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.396063	-0.796297	0.431627
2	6	0	1.628762	0.132538	0.288019
3	6	0	-2.034919	0.037798	0.641721
4	6	0	-0.771788	-0.093131	1.070131
5	1	0	1.914379	0.516534	1.275121
6	1	0	0.145962	-1.217125	-0.547423
7	1	0	0.677402	-1.644093	1.066657
8	1	0	-0.529825	0.374013	2.024837
9	6	0	2.855668	-0.568024	-0.360234
10	1	0	2.574838	-0.832985	-1.390771
11	6	0	-3.081684	0.783017	1.429060
12	1	0	-2.669790	1.156363	2.368729
13	1	0	-3.470398	1.628952	0.853941
14	1	0	-3.935177	0.134014	1.648044
15	6	0	-2.496797	-0.553195	-0.640854
16	1	0	-1.755219	-1.064304	-1.254811
17	6	0	1.233590	1.329825	-0.559408
18	1	0	0.835338	1.050482	-1.566159
19	8	0	1.329299	2.483671	-0.233227
20	8	0	-3.465505	0.137125	-1.375937
21	8	0	-3.765488	-1.143450	-0.676064
22	6	0	4.059018	0.386324	-0.424863
23	1	0	3.826505	1.313427	-0.955933
24	1	0	4.391209	0.660408	0.583029
25	1	0	4.900723	-0.092067	-0.934906
26	6	0	3.248583	-1.862224	0.367074
27	1	0	2.472907	-2.630242	0.311157
28	1	0	4.155575	-2.282649	-0.078717
29	1	0	3.460141	-1.669287	1.425392

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240235	E(Thermal)=	0.255773
E(CCSD(T))=	-614.426532	E(Empiric)=	-0.350464
DE(MP2)=	-0.750935	DE(HF)=	-0.061453
G4MP2(0 K)=	-615.349149	G4MP2 Energy=	-615.333611
G4MP2 Enthalpy=	-615.332667	G4MP2 Free Energy=	-615.394076

TS3n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.292700	-0.638513	0.407464
2	6	0	1.595600	0.192439	0.285550

3	6	0	-2.109305	0.218513	0.540352
4	6	0	-0.844151	0.130378	1.002702
5	1	0	1.874894	0.575187	1.275046
6	1	0	0.012280	-1.067064	-0.562662
7	1	0	0.494826	-1.501447	1.054354
8	1	0	-0.604480	0.690762	1.907399
9	6	0	2.779584	-0.615522	-0.308590
10	1	0	2.492873	-0.916343	-1.327265
11	6	0	-3.242782	0.843425	1.295884
12	1	0	-3.934151	0.069722	1.643972
13	1	0	-2.873411	1.394635	2.164584
14	1	0	-3.813308	1.509003	0.643687
15	6	0	-2.525120	-0.438228	-0.817783
16	1	0	-1.664898	-0.398714	-1.524884
17	6	0	1.303772	1.399734	-0.590264
18	1	0	1.051397	1.136471	-1.646916
19	8	0	1.316081	2.545798	-0.225353
20	8	0	-3.655471	-0.055619	-1.411981
21	8	0	-2.898802	-1.627124	-0.340340
22	6	0	4.036984	0.263454	-0.407960
23	1	0	3.866743	1.166090	-1.002515
24	1	0	4.367766	0.583144	0.586842
25	1	0	4.858350	-0.291525	-0.871080
26	6	0	3.086256	-1.889310	0.491568
27	1	0	2.263717	-2.609103	0.472048
28	1	0	3.965552	-2.391420	0.076138
29	1	0	3.306159	-1.652055	1.539110

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.235622	E(Thermal)=	0.251385
E(CCSD(T))=	-614.391866	E(Empiric)=	-0.350464
DE(MP2)=	-0.753961	DE(HF)=	-0.060689
G4MP2(0 K)=	-615.321358	G4MP2 Energy=	-615.305595
G4MP2 Enthalpy=	-615.304651	G4MP2 Free Energy=	-615.366622

TS3f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.073251	-0.509035	1.166329
2	6	0	1.067821	0.491999	0.494839
3	6	0	-2.252869	-0.006706	0.343390
4	6	0	-1.316541	-0.247647	1.351622

5	1	0	1.386802	1.183470	1.287382
6	1	0	-0.075729	-1.406636	0.267825
7	1	0	0.537220	-0.882386	2.079408
8	1	0	-1.716295	-0.294651	2.365935
9	6	0	2.315053	-0.211353	-0.097183
10	1	0	1.967243	-0.829333	-0.935830
11	6	0	-3.569486	0.659309	0.708177
12	1	0	-4.041955	0.131024	1.543469
13	1	0	-3.423391	1.699398	1.016158
14	1	0	-4.275799	0.650407	-0.125144
15	6	0	-2.047041	-0.307438	-0.997712
16	1	0	-2.662583	0.145727	-1.771734
17	6	0	0.417390	1.367729	-0.563105
18	1	0	0.399287	0.931470	-1.586313
19	8	0	-0.038696	2.462716	-0.349075
20	8	0	-1.208684	-1.146009	-1.566958
21	8	0	-0.561737	-2.072815	-0.766053
22	6	0	3.314019	0.827446	-0.631784
23	1	0	2.868641	1.486647	-1.384284
24	1	0	3.689309	1.462356	0.179601
25	1	0	4.174607	0.334094	-1.093961
26	6	0	3.007822	-1.137583	0.911306
27	1	0	2.368682	-1.970711	1.213457
28	1	0	3.915548	-1.562919	0.471537
29	1	0	3.304844	-0.589417	1.813912

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.235541	E(Thermal)=	0.250233
E(CCSD(T))=	-614.363876	E(Empiric)=	-0.350464
DE(MP2)=	-0.757468	DE(HF)=	-0.061714
G4MP2(0 K)=	-615.297981	G4MP2 Energy=	-615.283289
G4MP2 Enthalpy=	-615.282345	G4MP2 Free Energy=	-615.340131

HP3f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.141429	-0.116491	1.489612
2	6	0	-1.092187	-0.752018	0.491810
3	6	0	2.012778	-0.081077	0.166942
4	6	0	1.159595	0.169102	1.353013
5	1	0	-1.685896	-1.479386	1.064182
6	1	0	0.370615	2.089530	0.429491

7	1	0	-0.595964	0.103725	2.453373
8	1	0	1.676450	0.564113	2.228581
9	6	0	-2.073675	0.257273	-0.169329
10	1	0	-1.478622	0.886147	-0.846091
11	6	0	3.027051	-1.189868	0.310017
12	1	0	3.687567	-1.009638	1.167141
13	1	0	2.520521	-2.146380	0.481235
14	1	0	3.651215	-1.281591	-0.582801
15	6	0	1.949106	0.628937	-0.965308
16	1	0	2.564326	0.388583	-1.829197
17	6	0	-0.367725	-1.579828	-0.572759
18	1	0	-0.273540	-1.095945	-1.568137
19	8	0	0.046817	-2.695300	-0.381512
20	8	0	1.130489	1.687182	-1.267932
21	8	0	0.964520	2.594279	-0.152888
22	6	0	-3.127154	-0.488132	-1.003100
23	1	0	-2.677016	-1.135704	-1.762238
24	1	0	-3.754623	-1.117985	-0.361335
25	1	0	-3.782627	0.219267	-1.520330
26	6	0	-2.763678	1.170226	0.853175
27	1	0	-2.053926	1.793775	1.404461
28	1	0	-3.467927	1.840096	0.350275
29	1	0	-3.331254	0.583363	1.585608

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239756	E(Thermal)=	0.25541
E(CCSD(T))=	-614.412196	E(Empiric)=	-0.350464
DE(MP2)=	-0.758011	DE(HF)=	-0.061836
G4MP2(0 K)=	-615.342751	G4MP2 Energy=	-615.327098
G4MP2 Enthalpy=	-615.326154	G4MP2 Free Energy=	-615.385661

RAD3f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003347	-0.899338	-1.086662
2	6	0	-1.063281	0.103812	-0.738162
3	6	0	2.197155	-0.372298	0.159033
4	6	0	1.321940	-1.033859	-0.740778
5	1	0	-1.696852	0.170283	-1.639796
6	1	0	-0.336752	-1.650862	-1.795949
7	1	0	1.826766	-1.821388	-1.301589
8	6	0	-2.018360	-0.339029	0.415265

9	1	0	-1.479589	-0.165877	1.350636
10	6	0	3.670653	-0.640609	0.008597
11	1	0	3.873520	-1.712152	-0.100040
12	1	0	4.067316	-0.151877	-0.891179
13	1	0	4.241619	-0.269362	0.863648
14	6	0	1.800607	0.475856	1.263384
15	1	0	2.649920	0.850350	1.871078
16	6	0	-0.524771	1.527994	-0.572489
17	1	0	-1.035355	2.142017	0.195181
18	8	0	0.343472	1.993385	-1.266218
19	8	0	0.656180	0.773989	1.584527
20	6	0	-3.303769	0.502515	0.412810
21	1	0	-3.108403	1.575935	0.485964
22	1	0	-3.882232	0.330615	-0.503457
23	1	0	-3.938898	0.228201	1.261281
24	6	0	-2.375391	-1.829731	0.331579
25	1	0	-1.490660	-2.466960	0.415758
26	1	0	-3.060432	-2.100324	1.141535
27	1	0	-2.875965	-2.069477	-0.615014

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.223839	E(Thermal)=	0.238083
E(CCSD(T))=	-538.856509	E(Empiric)=	-0.325479
DE(MP2)=	-0.655817	DE(HF)=	-0.052853
G4MP2(0 K)=	-539.666819	G4MP2 Energy=	-539.652575
G4MP2 Enthalpy=	-539.65163	G4MP2 Free Energy=	-539.708593

TS3h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005078	0.168337	0.823050
2	6	0	-1.306681	0.313084	-0.011737
3	6	0	2.540042	0.278255	0.304213
4	6	0	1.211027	0.682084	0.119378
5	1	0	-1.089065	-0.008602	-1.034346
6	1	0	-0.105717	0.769449	1.746885
7	1	0	0.145261	-0.863597	1.129697
8	1	0	1.090521	1.707546	-0.247292
9	6	0	-2.499100	-0.498370	0.547668
10	1	0	-2.723501	-0.117151	1.555802
11	6	0	3.620754	1.311139	0.563403
12	1	0	3.491387	2.166919	-0.109882

13	1	0	3.579398	1.698712	1.587167
14	1	0	4.622468	0.906829	0.397232
15	6	0	2.925544	-1.007409	-0.029990
16	1	0	3.930311	-1.400702	0.089157
17	6	0	-1.642406	1.792370	-0.042906
18	1	0	-2.173187	2.154169	0.872703
19	8	0	-1.338820	2.563638	-0.917864
20	8	0	2.202508	-1.752980	-0.823661
21	8	0	0.928322	-1.281393	-1.004451
22	6	0	-3.741224	-0.275518	-0.331196
23	1	0	-4.004790	0.784260	-0.416850
24	1	0	-3.570081	-0.654822	-1.345129
25	1	0	-4.608843	-0.800214	0.080487
26	6	0	-2.194577	-1.999496	0.658911
27	1	0	-1.449893	-2.220407	1.427686
28	1	0	-3.104215	-2.550172	0.919698
29	1	0	-1.815938	-2.393187	-0.289973

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238992	E(Thermal)=	0.253815
E(CCSD(T))=	-614.372909	E(Empiric)=	-0.350464
DE(MP2)=	-0.752899	DE(HF)=	-0.061664
G4MP2(0 K)=	-615.298943	G4MP2 Energy=	-615.28412
G4MP2 Enthalpy=	-615.283176	G4MP2 Free Energy=	-615.341705

CP3h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.036389	-0.031894	0.627572
2	6	0	-1.328057	0.169228	-0.076418
3	6	0	2.574106	0.204385	0.433709
4	6	0	1.233639	0.391872	-0.243146
5	1	0	-1.237623	-0.171017	-1.114240
6	1	0	0.057542	0.536142	1.568523
7	1	0	0.175729	-1.083587	0.890177
8	1	0	1.089756	1.414255	-0.620034
9	6	0	-2.504443	-0.568996	0.610106
10	1	0	-2.571816	-0.199107	1.644485
11	6	0	3.068645	1.017502	1.582629
12	1	0	3.141776	2.080425	1.319300
13	1	0	2.401587	0.951782	2.451267
14	1	0	4.059719	0.684085	1.901668

15	6	0	3.155870	-0.817756	-0.182884
16	1	0	4.097805	-1.316454	0.003566
17	6	0	-1.593965	1.663059	-0.095933
18	1	0	-1.937624	2.067667	0.888781
19	8	0	-1.420691	2.398937	-1.033518
20	8	0	2.465496	-1.351391	-1.224844
21	8	0	1.323782	-0.446447	-1.414957
22	6	0	-3.828984	-0.242143	-0.099628
23	1	0	-4.035819	0.832959	-0.118755
24	1	0	-3.808075	-0.590986	-1.138496
25	1	0	-4.669821	-0.732215	0.400834
26	6	0	-2.301489	-2.089852	0.660230
27	1	0	-1.438550	-2.382885	1.263357
28	1	0	-3.181823	-2.573589	1.095608
29	1	0	-2.161726	-2.498699	-0.346921

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241186	E(Thermal)=	0.256116
E(CCSD(T))=	-614.445172	E(Empiric)=	-0.350464
DE(MP2)=	-0.750544	DE(HF)=	-0.061674
G4MP2(0 K)=	-615.366668	G4MP2 Energy=	-615.351738
G4MP2 Enthalpy=	-615.350794	G4MP2 Free Energy=	-615.409929

TS4e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.305219	-1.129304	-0.355745
2	6	0	1.370844	-0.127236	0.220998
3	6	0	-2.164227	-0.777291	0.253344
4	6	0	-0.923308	-1.220685	0.506057
5	1	0	1.439994	-0.313303	1.301956
6	1	0	0.079633	-0.860568	-1.389785
7	1	0	0.781820	-2.114144	-0.383201
8	1	0	-0.749543	-1.704372	1.467614
9	6	0	2.773139	-0.242395	-0.427332
10	1	0	2.662596	-0.009656	-1.496375
11	6	0	-3.292358	-0.939916	1.234185
12	1	0	-3.671780	0.041519	1.537246
13	1	0	-4.134307	-1.464939	0.772647
14	1	0	-2.973738	-1.486770	2.124785
15	6	0	-2.525444	-0.085296	-1.010197
16	1	0	-1.703750	0.110905	-1.722374

17	6	0	0.818868	1.241590	0.038801
18	1	0	1.057609	1.827220	-0.848751
19	8	0	0.061569	1.775666	0.916831
20	8	0	-3.660902	0.242044	-1.273752
21	8	0	-0.916008	2.193013	-0.108212
22	6	0	3.371399	-1.650101	-0.303530
23	1	0	2.807310	-2.401667	-0.861172
24	1	0	4.393762	-1.657727	-0.693509
25	1	0	3.416945	-1.967394	0.744969
26	6	0	3.728915	0.790245	0.193311
27	1	0	3.347697	1.813425	0.107349
28	1	0	3.884610	0.584393	1.258721
29	1	0	4.705604	0.759630	-0.298401

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238403	E(Thermal)=	0.253602
E(CCSD(T))=	-614.361638	E(Empiric)=	-0.350464
DE(MP2)=	-0.753307	DE(HF)=	-0.061619
G4MP2(0 K)=	-615.288625	G4MP2 Energy=	-615.273425
G4MP2 Enthalpy=	-615.272481	G4MP2 Free Energy=	-615.331577

DIO4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002494	-1.044947	-0.235678
2	6	0	-1.244400	-0.115970	-0.260403
3	6	0	2.451598	-0.265930	-0.393533
4	6	0	1.207865	-0.428537	-0.881125
5	1	0	-1.449896	0.180340	-1.297183
6	1	0	0.190203	-1.365494	0.792032
7	1	0	-0.250595	-1.952895	-0.797785
8	1	0	1.027874	-0.077956	-1.897532
9	6	0	-2.508603	-0.791498	0.333309
10	1	0	-2.268196	-1.090006	1.364858
11	6	0	3.558250	0.357875	-1.202778
12	1	0	3.951577	1.246185	-0.698339
13	1	0	4.400540	-0.334009	-1.304595
14	1	0	3.210683	0.643302	-2.198162
15	6	0	2.830798	-0.689356	0.970311
16	1	0	2.026461	-1.129093	1.594643
17	6	0	-0.916947	1.160293	0.482253
18	1	0	-0.746333	1.055692	1.560184

19	8	0	-1.552670	2.339294	0.108117
20	8	0	3.952260	-0.575312	1.416019
21	8	0	-0.098825	2.094702	-0.143942
22	6	0	-2.906948	-2.056698	-0.441552
23	1	0	-2.144824	-2.838949	-0.397583
24	1	0	-3.828004	-2.478214	-0.027403
25	1	0	-3.095092	-1.825845	-1.496755
26	6	0	-3.700651	0.179441	0.389176
27	1	0	-3.502028	1.054016	1.014593
28	1	0	-3.959084	0.541585	-0.611920
29	1	0	-4.580212	-0.326169	0.799503

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240757	E(Thermal)=	0.256059
E(CCSD(T))=	-614.432044	E(Empiric)=	-0.350464
DE(MP2)=	-0.750115	DE(HF)=	-0.061443
G4MP2(0 K)=	-615.353308	G4MP2 Energy=	-615.338006
G4MP2 Enthalpy=	-615.337062	G4MP2 Free Energy=	-615.397031

TS4h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.264982	-0.487258	1.196861
2	6	0	-0.868490	0.033254	0.240901
3	6	0	2.537291	-0.048726	0.110832
4	6	0	1.570993	0.230944	1.004507
5	1	0	-0.524012	-0.042532	-0.788816
6	1	0	-0.061006	-0.381267	2.239407
7	1	0	0.387289	-1.546997	0.978835
8	1	0	1.747211	1.081548	1.662401
9	6	0	-2.194189	-0.763125	0.420845
10	1	0	-2.558150	-0.567924	1.441869
11	6	0	3.810257	0.757224	0.024792
12	1	0	4.693202	0.127003	0.186529
13	1	0	3.925113	1.214242	-0.965370
14	1	0	3.825973	1.557961	0.767185
15	6	0	2.444484	-1.181607	-0.843351
16	1	0	3.386623	-1.369137	-1.405957
17	6	0	-1.055868	1.471240	0.592768
18	1	0	-1.418054	1.670847	1.615758
19	8	0	-0.639395	2.501255	-0.036111
20	8	0	1.473101	-1.879405	-1.045363

21	8	0	-1.397042	2.135028	-1.254779
22	6	0	-3.267540	-0.281885	-0.568488
23	1	0	-3.436896	0.794676	-0.506280
24	1	0	-2.962567	-0.492723	-1.599071
25	1	0	-4.210503	-0.805098	-0.379999
26	6	0	-1.985055	-2.278192	0.276646
27	1	0	-1.401320	-2.705675	1.095928
28	1	0	-2.955028	-2.785125	0.270721
29	1	0	-1.472372	-2.516032	-0.661003

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.238169	E(Thermal)=	0.253446
E(CCSD(T))=	-614.353484	E(Empiric)=	-0.350464
DE(MP2)=	-0.75059	DE(HF)=	-0.061749
G4MP2(0 K)=	-615.278118	G4MP2 Energy=	-615.262841
G4MP2 Enthalpy=	-615.261897	G4MP2 Free Energy=	-615.3214

TS4i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.224065	-1.088104	-0.605494
2	6	0	-1.320597	-0.025293	-0.358682
3	6	0	2.252959	-0.307626	-0.368315
4	6	0	1.041960	-0.377001	-1.041180
5	1	0	-1.614057	0.413238	-1.321431
6	1	0	-0.065451	-1.681191	0.299123
7	1	0	-0.522075	-1.785547	-1.394110
8	1	0	1.055741	-0.078123	-2.085734
9	6	0	-2.569987	-0.536295	0.375806
10	1	0	-2.246759	-0.889001	1.367391
11	6	0	3.473919	0.275621	-1.008938
12	1	0	4.271481	-0.475126	-1.052928
13	1	0	3.267125	0.636984	-2.017869
14	1	0	3.866122	1.099866	-0.405439
15	6	0	2.411876	-0.774167	1.021792
16	1	0	1.501876	-1.147242	1.529142
17	6	0	-0.580627	1.088585	0.396551
18	1	0	-0.445653	0.848987	1.468593
19	8	0	-0.801697	2.375189	0.105026
20	8	0	3.478604	-0.759182	1.598812
21	8	0	0.653575	1.323469	-0.271744
22	6	0	-3.235179	-1.714854	-0.348694

23	1	0	-2.572676	-2.582461	-0.425312
24	1	0	-4.135944	-2.035596	0.184122
25	1	0	-3.536107	-1.429938	-1.363921
26	6	0	-3.575800	0.607568	0.582528
27	1	0	-3.124342	1.467050	1.086833
28	1	0	-3.962984	0.961360	-0.379779
29	1	0	-4.426912	0.270316	1.182322

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239741	E(Thermal)=	0.254217
E(CCSD(T))=	-614.407996	E(Empiric)=	-0.350464
DE(MP2)=	-0.752129	DE(HF)=	-0.060606
G4MP2(0 K)=	-615.331454	G4MP2 Energy=	-615.316978
G4MP2 Enthalpy=	-615.316034	G4MP2 Free Energy=	-615.372791

EPOX4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.132585	-0.616468	0.171806
2	6	0	1.489169	0.119622	0.239519
3	6	0	-2.426285	0.172605	0.202370
4	6	0	-1.010311	0.250134	0.654233
5	1	0	1.672663	0.462462	1.265676
6	1	0	-0.048212	-0.956684	-0.852803
7	1	0	0.170662	-1.509254	0.803608
8	1	0	-0.884172	0.621171	1.674730
9	6	0	2.686477	-0.764640	-0.216773
10	1	0	2.542402	-0.983159	-1.285584
11	6	0	-3.550177	0.568262	1.127730
12	1	0	-3.981858	-0.321469	1.593080
13	1	0	-3.188446	1.245495	1.904128
14	1	0	-4.346015	1.069120	0.568879
15	6	0	-2.785978	-0.791415	-0.890912
16	1	0	-2.077841	-0.797519	-1.746184
17	6	0	1.438651	1.360387	-0.640477
18	1	0	1.154542	1.149895	-1.698861
19	8	0	1.700026	2.477321	-0.278521
20	8	0	-3.771139	-1.484447	-0.870224
21	8	0	-1.541157	1.222986	-0.237636
22	6	0	2.752061	-2.104163	0.531960
23	1	0	1.893850	-2.748280	0.324085
24	1	0	3.650342	-2.654837	0.235587

25	1	0	2.804836	-1.946515	1.615702
26	6	0	4.016091	-0.009839	-0.058781
27	1	0	4.019210	0.944301	-0.592115
28	1	0	4.216846	0.204459	0.997239
29	1	0	4.845659	-0.612971	-0.440161

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.240492	E(Thermal)=	0.25591
E(CCSD(T))=	-614.518871	E(Empiric)=	-0.350464
DE(MP2)=	-0.751671	DE(HF)=	-0.06004
G4MP2(0 K)=	-615.440554	G4MP2 Energy=	-615.425136
G4MP2 Enthalpy=	-615.424192	G4MP2 Free Energy=	-615.484519

TS4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.337869	-1.543388	0.039402
2	6	0	-1.120310	-0.220841	-0.301755
3	6	0	2.064798	-0.853455	-0.184099
4	6	0	1.040794	-1.624644	-0.567327
5	1	0	-1.226450	-0.181690	-1.393343
6	1	0	-0.287845	-1.624993	1.130918
7	1	0	-0.937250	-2.383254	-0.315445
8	1	0	1.196239	-2.356211	-1.357211
9	6	0	-2.528026	-0.162196	0.351503
10	1	0	-2.380246	-0.125148	1.440494
11	6	0	3.446603	-0.890851	-0.771863
12	1	0	3.713574	0.080091	-1.206383
13	1	0	4.190977	-1.109128	0.003026
14	1	0	3.522574	-1.650750	-1.554249
15	6	0	1.786418	0.210523	0.832736
16	1	0	1.661951	1.434981	0.307163
17	6	0	-0.294702	0.958690	0.089621
18	1	0	-0.368849	1.439958	1.061618
19	8	0	0.228199	1.653361	-0.888016
20	8	0	1.983587	0.127076	2.021588
21	8	0	1.252227	2.436755	-0.388425
22	6	0	-3.381517	-1.397183	0.030293
23	1	0	-2.970245	-2.315651	0.455600
24	1	0	-4.389705	-1.272275	0.437351
25	1	0	-3.479144	-1.537221	-1.052969
26	6	0	-3.269527	1.114132	-0.076413

27	1	0	-2.705201	2.021155	0.161229
28	1	0	-3.453311	1.113660	-1.157252
29	1	0	-4.239144	1.184229	0.425688

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.236086	E(Thermal)=	0.250445
E(CCSD(T))=	-614.34579	E(Empiric)=	-0.350464
DE(MP2)=	-0.758981	DE(HF)=	-0.06171
G4MP2(0 K)=	-615.280859	G4MP2 Energy=	-615.2665
G4MP2 Enthalpy=	-615.265556	G4MP2 Free Energy=	-615.321755

HP4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.305675	-1.806179	-0.376769
2	6	0	0.852657	-0.473772	0.176865
3	6	0	-2.041347	-0.995743	0.059941
4	6	0	-1.169633	-1.989252	-0.173467
5	1	0	0.746398	-0.507836	1.270540
6	1	0	0.526898	-1.879926	-1.453769
7	1	0	0.829760	-2.648572	0.084351
8	1	0	-1.538475	-3.012708	-0.220422
9	6	0	2.352326	-0.223643	-0.158016
10	1	0	2.391457	0.222794	-1.161518
11	6	0	-3.510257	-1.196243	0.307000
12	1	0	-3.794570	-0.802022	1.287798
13	1	0	-4.108940	-0.648555	-0.428228
14	1	0	-3.777350	-2.254770	0.261849
15	6	0	-1.540048	0.393954	0.076554
16	1	0	-1.209165	2.855695	-0.250889
17	6	0	-0.082820	0.630526	-0.356817
18	1	0	-0.060598	0.609088	-1.459704
19	8	0	0.357680	1.898914	0.082649
20	8	0	-2.261192	1.331333	0.381265
21	8	0	-0.336725	2.904791	-0.686716
22	6	0	3.188639	-1.514809	-0.190220
23	1	0	2.871831	-2.212047	-0.970429
24	1	0	4.237978	-1.268773	-0.379948
25	1	0	3.148467	-2.040776	0.771516
26	6	0	3.000851	0.760261	0.831050
27	1	0	2.465699	1.707887	0.871414
28	1	0	3.017901	0.330537	1.840423

29	1	0	4.038337	0.959082	0.542706

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.243971	E(Thermal)=	0.257922
E(CCSD(T))=	-614.470961	E(Empiric)=	-0.350464
DE(MP2)=	-0.753367	DE(HF)=	-0.061454
G4MP2(0 K)=	-615.392275	G4MP2 Energy=	-615.378325
G4MP2 Enthalpy=	-615.37738	G4MP2 Free Energy=	-615.43229

RAD4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.210200	-1.580186	0.291536
2	6	0	-0.832374	-0.252470	-0.168194
3	6	0	2.092937	-0.628254	-0.076960
4	6	0	1.261153	-1.672160	0.038241
5	1	0	-0.786231	-0.210475	-1.265457
6	1	0	-0.396372	-1.727072	1.368359
7	1	0	-0.701981	-2.423642	-0.201172
8	1	0	1.680024	-2.674023	-0.042012
9	6	0	-2.319641	-0.132546	0.267247
10	1	0	-2.325629	-0.070435	1.366936
11	6	0	3.572050	-0.756478	-0.329784
12	1	0	3.858621	-0.229462	-1.245500
13	1	0	4.146593	-0.299896	0.481927
14	1	0	3.859765	-1.806298	-0.423900
15	6	0	1.604980	0.756289	0.116286
16	6	0	-0.000343	0.942449	0.353620
17	1	0	-0.003766	0.951621	1.470529
18	8	0	-0.306745	2.124547	-0.166781
19	8	0	2.338273	1.703075	0.165153
20	6	0	-3.142620	-1.371072	-0.130972
21	1	0	-2.810563	-2.283671	0.370751
22	1	0	-4.195009	-1.222490	0.129905
23	1	0	-3.094566	-1.542388	-1.213282
24	6	0	-3.009534	1.126032	-0.279339
25	1	0	-2.506998	2.045347	0.026916
26	1	0	-3.029104	1.116064	-1.375105
27	1	0	-4.045451	1.166231	0.074048

Temperature=	298.15	Pressure=	1

E(ZPE)=	0.225642	E(Thermal)=	0.238724
E(CCSD(T))=	-538.853345	E(Empiric)=	-0.325479
DE(MP2)=	-0.652585	DE(HF)=	-0.05287
G4MP2(0 K)=	-539.658636	G4MP2 Energy=	-539.645554
G4MP2 Enthalpy=	-539.64461	G4MP2 Free Energy=	-539.69902

TS4j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.228225	-1.656864	0.311827
2	6	0	-0.896645	-0.432126	-0.240635
3	6	0	2.070978	-0.621986	-0.011425
4	6	0	1.272680	-1.681259	0.177069
5	1	0	-0.594630	-0.163582	-1.253276
6	1	0	-0.517975	-1.810282	1.362959
7	1	0	-0.627094	-2.541405	-0.214521
8	1	0	1.724907	-2.670846	0.210209
9	6	0	-2.319887	-0.097838	0.123832
10	1	0	-2.359724	0.098076	1.204616
11	6	0	3.553616	-0.740326	-0.241293
12	1	0	3.822639	-0.260644	-1.187172
13	1	0	4.117488	-0.218707	0.540510
14	1	0	3.873148	-1.784801	-0.263274
15	6	0	1.522860	0.768892	-0.073742
16	6	0	0.314942	1.094884	0.830063
17	1	0	0.238099	0.452995	1.733038
18	8	0	-0.252567	2.180256	0.777196
19	8	0	2.048491	1.639479	-0.730386
20	6	0	-3.247265	-1.308711	-0.151736
21	1	0	-2.964831	-2.188488	0.433219
22	1	0	-4.277318	-1.048007	0.110139
23	1	0	-3.231413	-1.582872	-1.212357
24	6	0	-2.825604	1.143087	-0.623172
25	1	0	-2.183699	2.004496	-0.431524
26	1	0	-2.847849	0.959017	-1.703916
27	1	0	-3.843852	1.390650	-0.307859

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.223352	E(Thermal)=	0.236559
E(CCSD(T))=	-538.830996	E(Empiric)=	-0.325479
DE(MP2)=	-0.658484	DE(HF)=	-0.05275
G4MP2(0 K)=	-539.644358	G4MP2 Energy=	-539.631151

G4MP2		G4MP2 Free	
Enthalpy=	-539.630207	Energy=	-539.684189

TS4k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.182655	-1.475907	0.370064
2	6	0	-0.853006	-0.173511	-0.092011
3	6	0	2.188310	-0.620092	-0.068243
4	6	0	1.293115	-1.597453	0.140920
5	1	0	-0.703398	-0.059955	-1.173955
6	1	0	-0.369089	-1.622072	1.447753
7	1	0	-0.655044	-2.336669	-0.112438
8	1	0	1.675719	-2.617602	0.151234
9	6	0	-2.392114	-0.160291	0.179023
10	1	0	-2.529072	0.021519	1.255609
11	6	0	3.659502	-0.854859	-0.318748
12	1	0	3.956829	-0.449411	-1.291220
13	1	0	4.270052	-0.347553	0.435171
14	1	0	3.891006	-1.922569	-0.298558
15	6	0	1.763902	0.784628	-0.048124
16	6	0	-0.208883	1.030368	0.622934
17	1	0	0.153379	0.770176	1.650012
18	8	0	-0.480378	2.204229	0.355086
19	8	0	2.386180	1.766258	-0.250903
20	6	0	-3.082388	-1.492921	-0.157251
21	1	0	-2.764692	-2.316533	0.488148
22	1	0	-4.165420	-1.387722	-0.037486
23	1	0	-2.896664	-1.784256	-1.198377
24	6	0	-3.077140	0.979151	-0.590491
25	1	0	-2.592171	1.937087	-0.402167
26	1	0	-3.037533	0.786933	-1.669958
27	1	0	-4.132168	1.050050	-0.305661

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.224387	E(Thermal)=	0.237438
E(CCSD(T))=	-538.842229	E(Empiric)=	-0.325479
DE(MP2)=	-0.658359	DE(HF)=	-0.052867
G4MP2(0 K)=	-539.654547	G4MP2 Energy=	-539.641496
G4MP2 Enthalpy=	-539.640552	G4MP2 Free Energy=	-539.694539

RAD4j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.287749	-1.681000	0.385139
2	6	0	-0.972992	-0.538381	-0.294103
3	6	0	2.027859	-0.671607	-0.008103
4	6	0	1.214582	-1.709201	0.233806
5	1	0	-0.644387	-0.315263	-1.308163
6	1	0	-0.564058	-1.713834	1.451070
7	1	0	-0.676538	-2.632682	-0.021315
8	1	0	1.663506	-2.699185	0.295808
9	6	0	-2.346735	-0.083376	0.097766
10	1	0	-2.343080	0.129143	1.177326
11	6	0	3.503485	-0.841556	-0.264236
12	1	0	3.762617	-0.411025	-1.236234
13	1	0	4.100957	-0.304962	0.481927
14	1	0	3.792786	-1.894823	-0.249022
15	6	0	1.538436	0.741254	-0.113313
16	6	0	0.481327	1.215982	0.906998
17	1	0	0.331365	0.539626	1.774901
18	8	0	-0.022301	2.313018	0.856927
19	8	0	2.028012	1.536689	-0.884518
20	6	0	-3.383398	-1.213913	-0.131491
21	1	0	-3.138249	-2.115035	0.438453
22	1	0	-4.377205	-0.877424	0.180829
23	1	0	-3.436792	-1.484785	-1.191497
24	6	0	-2.759650	1.190719	-0.652232
25	1	0	-2.053818	2.003370	-0.468270
26	1	0	-2.799881	1.006313	-1.732226
27	1	0	-3.753900	1.519376	-0.334239

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.222951	E(Thermal)=	0.237268
E(CCSD(T))=	-538.833361	E(Empiric)=	-0.325479
DE(MP2)=	-0.657357	DE(HF)=	-0.052822
G4MP2(0 K)=	-539.646069	G4MP2 Energy=	-539.631752
G4MP2 Enthalpy=	-539.630807	G4MP2 Free Energy=	-539.687728

RAD4k

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.141392	-1.369707	0.416994
2	6	0	-0.901767	-0.100046	0.003330
3	6	0	2.290724	-0.548519	-0.028590
4	6	0	1.356753	-1.447708	0.322943
5	1	0	-0.667054	0.155759	-1.036117
6	1	0	-0.408377	-1.624854	1.456263
7	1	0	-0.514305	-2.218939	-0.166880
8	1	0	1.729659	-2.441325	0.575406
9	6	0	-2.457118	-0.275955	0.106393
10	1	0	-2.721731	-0.235591	1.173712
11	6	0	3.767478	-0.868920	-0.092942
12	1	0	4.154034	-0.699359	-1.103287
13	1	0	4.336429	-0.213807	0.574914
14	1	0	3.960102	-1.907653	0.187148
15	6	0	1.911722	0.833262	-0.367406
16	6	0	-0.486592	1.078714	0.888528
17	1	0	0.073631	0.781094	1.806649
18	8	0	-0.807944	2.228937	0.719313
19	8	0	2.595216	1.712894	-0.776037
20	6	0	-2.957485	-1.621922	-0.443045
21	1	0	-2.624700	-2.479005	0.148402
22	1	0	-4.052064	-1.634420	-0.441473
23	1	0	-2.630520	-1.773239	-1.478918
24	6	0	-3.185098	0.870754	-0.611753
25	1	0	-2.837276	1.846829	-0.273578
26	1	0	-3.014958	0.809986	-1.693692
27	1	0	-4.264383	0.800155	-0.441470

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.22427	E(Thermal)=	0.238656
E(CCSD(T))=	-538.849107	E(Empiric)=	-0.325479
DE(MP2)=	-0.656062	DE(HF)=	-0.052924
G4MP2(0 K)=	-539.659303	G4MP2 Energy=	-539.644916
G4MP2 Enthalpy=	-539.643972	G4MP2 Free Energy=	-539.701659

TS4g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.008447	0.831923	-0.465081
2	6	0	-1.217395	-0.053869	-0.033845
3	6	0	2.419164	-0.006215	-0.641583
4	6	0	1.139140	0.035733	-1.044430

5	1	0	-0.832591	0.005872	1.258319
6	1	0	-0.373804	1.495459	-1.252525
7	1	0	0.369661	1.465976	0.340644
8	1	0	0.858252	-0.612592	-1.876690
9	6	0	-2.554435	0.405885	-0.634159
10	1	0	-2.407547	0.589704	-1.709061
11	6	0	3.433571	-0.913819	-1.295034
12	1	0	4.278365	-0.346691	-1.704910
13	1	0	3.852600	-1.623437	-0.571126
14	1	0	2.987683	-1.487673	-2.110743
15	6	0	2.942445	0.780988	0.507223
16	1	0	3.895369	0.373971	0.917002
17	6	0	-1.013043	-1.442596	0.140366
18	1	0	-1.568979	-2.275825	-0.280773
19	8	0	-0.249257	-1.819571	1.123851
20	8	0	2.458316	1.780256	0.988398
21	8	0	0.188062	-0.689895	1.827468
22	6	0	-3.695432	-0.612656	-0.492132
23	1	0	-3.518210	-1.526319	-1.068474
24	1	0	-3.849889	-0.895662	0.555491
25	1	0	-4.631272	-0.180467	-0.859654
26	6	0	-2.964881	1.742730	0.010639
27	1	0	-2.182369	2.500748	-0.084581
28	1	0	-3.871651	2.135547	-0.460936
29	1	0	-3.168082	1.606439	1.078502

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.235786	E(Thermal)=	0.250739
E(CCSD(T))=	-614.348428	E(Empiric)=	-0.350464
DE(MP2)=	-0.756405	DE(HF)=	-0.062023
G4MP2(0 K)=	-615.281533	G4MP2 Energy=	-615.26658
G4MP2 Enthalpy=	-615.265636	G4MP2 Free Energy=	-615.32435

HP4g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.096890	-0.507952	-0.874759
2	6	0	0.955987	0.229232	-0.059086
3	6	0	-2.391153	-0.897574	0.229057
4	6	0	-1.090850	-1.183700	0.029630
5	1	0	4.056435	-2.460089	-0.022257
6	1	0	-0.603469	0.179669	-1.548539

7	1	0	0.406954	-1.284494	-1.460510
8	1	0	-0.674000	-2.013411	0.601389
9	6	0	0.595695	1.613152	0.454989
10	1	0	-0.417429	1.536227	0.874432
11	6	0	-3.243859	-1.705189	1.181258
12	1	0	-3.668845	-1.076526	1.973420
13	1	0	-4.090407	-2.172108	0.662921
14	1	0	-2.663774	-2.498370	1.657909
15	6	0	-3.117330	0.191112	-0.471285
16	1	0	-4.215531	0.173170	-0.280891
17	6	0	2.121833	-0.359298	0.224618
18	1	0	2.931027	0.098694	0.781021
19	8	0	2.354890	-1.663747	-0.126918
20	8	0	-2.651544	1.053451	-1.185774
21	8	0	3.735921	-1.750829	-0.597844
22	6	0	1.516519	2.135652	1.565707
23	1	0	1.578728	1.435983	2.404816
24	1	0	2.532563	2.315223	1.196534
25	1	0	1.139041	3.089633	1.946435
26	6	0	0.525146	2.631168	-0.702998
27	1	0	-0.214594	2.342263	-1.452301
28	1	0	0.237822	3.616366	-0.321073
29	1	0	1.500748	2.727144	-1.191807

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.239842	E(Thermal)=	0.255975
E(CCSD(T))=	-614.421435	E(Empiric)=	-0.350464
DE(MP2)=	-0.755131	DE(HF)=	-0.062691
G4MP2(0 K)=	-615.349879	G4MP2 Energy=	-615.333746
G4MP2 Enthalpy=	-615.332802	G4MP2 Free Energy=	-615.394997

RAD4g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.062850	0.458402	-1.121276
2	6	0	-1.147071	0.412126	-0.217744
3	6	0	2.300316	0.190237	0.125171
4	6	0	1.256573	0.914917	-0.317533
5	1	0	0.244107	-0.518533	-1.566214
6	1	0	-0.115025	1.208302	-1.899619
7	1	0	1.235507	1.976758	-0.079784
8	6	0	-1.589666	-0.918485	0.327199

9	1	0	-0.675156	-1.500563	0.494860
10	6	0	3.438910	0.825506	0.889741
11	1	0	3.558544	0.373623	1.882070
12	1	0	4.393502	0.692707	0.366114
13	1	0	3.275732	1.896589	1.025764
14	6	0	2.460809	-1.260870	-0.133514
15	1	0	3.493197	-1.631673	0.059837
16	6	0	-1.800473	1.653575	0.067890
17	1	0	-2.694084	1.612262	0.716876
18	8	0	-1.409244	2.740587	-0.372439
19	8	0	1.607093	-2.038468	-0.507014
20	6	0	-2.372520	-0.851064	1.647860
21	1	0	-1.833756	-0.278911	2.409233
22	1	0	-3.360801	-0.398163	1.519353
23	1	0	-2.528280	-1.862834	2.034966
24	6	0	-2.401894	-1.682658	-0.749017
25	1	0	-1.837027	-1.790632	-1.678749
26	1	0	-2.648663	-2.685574	-0.386666
27	1	0	-3.337585	-1.160423	-0.975074

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.224189	E(Thermal)=	0.238666
E(CCSD(T))=	-538.859838	E(Empiric)=	-0.325479
DE(MP2)=	-0.653242	DE(HF)=	-0.053078
G4MP2(0 K)=	-539.667447	G4MP2 Energy=	-539.652971
G4MP2 Enthalpy=	-539.652026	G4MP2 Free Energy=	-539.710338

TS4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.355650	-1.450453	0.017767
2	6	0	-1.153424	-0.156123	-0.394633
3	6	0	2.128784	-0.770435	0.054298
4	6	0	1.096660	-1.503253	-0.408474
5	1	0	-1.274656	-0.184101	-1.486817
6	1	0	-0.426770	-1.537057	1.104950
7	1	0	-0.874736	-2.304567	-0.424310
8	1	0	1.322662	-2.227291	-1.189193
9	6	0	-2.544014	-0.050897	0.269904
10	1	0	-2.375113	0.095199	1.346074
11	6	0	3.525671	-0.889216	-0.487995
12	1	0	3.609526	-1.695745	-1.220145

13	1	0	3.808518	0.053686	-0.969598
14	1	0	4.253038	-1.076379	0.311258
15	6	0	1.908348	0.273841	1.075602
16	1	0	2.791847	0.763533	1.506957
17	6	0	-0.299534	1.038339	-0.094076
18	1	0	-0.516331	1.816619	0.627518
19	8	0	0.657315	1.222850	-0.922212
20	8	0	0.789276	0.433611	1.597419
21	8	0	1.727330	1.944538	-0.375520
22	6	0	-3.381990	-1.324020	0.088479
23	1	0	-2.930032	-2.192886	0.572892
24	1	0	-4.377109	-1.186114	0.522489
25	1	0	-3.516058	-1.559277	-0.974363
26	6	0	-3.313420	1.165328	-0.269500
27	1	0	-2.757703	2.100198	-0.144805
28	1	0	-3.527258	1.047905	-1.338471
29	1	0	-4.269776	1.279620	0.249838

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241347	E(Thermal)=	0.254803
E(CCSD(T))=	-614.386029	E(Empiric)=	-0.350464
DE(MP2)=	-0.752911	DE(HF)=	-0.060572
G4MP2(0 K)=	-615.308629	G4MP2 Energy=	-615.295173
G4MP2 Enthalpy=	-615.294229	G4MP2 Free Energy=	-615.347485

TS4f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.054608	0.993434	1.445322
2	6	0	-1.067668	-0.037572	0.856350
3	6	0	1.913110	0.781141	-0.134500
4	6	0	0.974713	1.516237	0.474265
5	1	0	-1.820211	-0.160931	1.650218
6	1	0	-0.643174	1.830370	1.828648
7	1	0	0.436862	0.525600	2.300776
8	1	0	0.913634	2.574215	0.227187
9	6	0	-1.833831	0.458808	-0.407077
10	1	0	-1.113280	0.526278	-1.224209
11	6	0	2.859130	1.332081	-1.165476
12	1	0	2.698742	2.400691	-1.326764
13	1	0	3.906048	1.184169	-0.873209
14	1	0	2.722476	0.816764	-2.124196

15	6	0	2.051371	-0.666685	0.163906
16	1	0	2.775378	-1.216477	-0.458845
17	6	0	-0.544144	-1.452929	0.696035
18	1	0	-0.810044	-2.184941	1.457454
19	8	0	-0.165921	-2.045223	-0.366307
20	8	0	1.588798	-1.208767	1.177869
21	8	0	0.454043	-1.248333	-1.306363
22	6	0	-2.936445	-0.529084	-0.822509
23	1	0	-2.536011	-1.507076	-1.098176
24	1	0	-3.668267	-0.670277	-0.016664
25	1	0	-3.478673	-0.144082	-1.691574
26	6	0	-2.450926	1.844722	-0.165151
27	1	0	-1.696548	2.620355	-0.011059
28	1	0	-3.047848	2.139867	-1.033791
29	1	0	-3.118652	1.843129	0.705629

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.241502	E(Thermal)=	0.255051
E(CCSD(T))=	-614.386509	E(Empiric)=	-0.350464
DE(MP2)=	-0.751916	DE(HF)=	-0.060524
G4MP2(0 K)=	-615.307911	G4MP2 Energy=	-615.294362
G4MP2 Enthalpy=	-615.293418	G4MP2 Free Energy=	-615.346924

ESTER1b - CO2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.746100	1.316544	-0.833239
2	6	0	-1.107737	0.374683	0.328455
3	6	0	0.041473	0.215594	1.307084
4	6	0	1.286073	-0.150103	1.309721
5	6	0	1.912697	-1.052651	-0.556063
6	6	0	-0.340981	2.699943	-0.400148
7	1	0	-1.900858	0.868188	0.902394
8	1	0	0.045343	0.884980	-1.460223
9	1	0	-1.607892	1.443069	-1.501434
10	1	0	2.078839	-0.369459	1.993152
11	1	0	-0.119415	3.396534	-1.240378
12	1	0	-0.192867	0.462631	2.352552
13	6	0	-1.664727	-1.005445	-0.134609
14	8	0	2.137051	-1.968522	0.247767
15	8	0	-0.254130	3.071208	0.745522
16	8	0	1.289456	-0.930997	-1.594179

17	6	0	-2.919998	-0.835209	-1.004083
18	1	0	-3.337019	-1.816579	-1.250001
19	1	0	-3.698627	-0.269862	-0.476526
20	1	0	-2.713316	-0.329068	-1.950574
21	6	0	-1.983210	-1.907402	1.067133
22	1	0	-2.736807	-1.449207	1.720415
23	1	0	-2.383616	-2.866248	0.724868
24	1	0	-1.093112	-2.118218	1.665218
25	1	0	-0.888525	-1.486308	-0.737880
26	6	0	2.839397	0.395131	-0.253632
27	1	0	3.459659	0.216871	-1.139131
28	1	0	3.492878	0.415684	0.616006
29	1	0	2.314998	1.336967	-0.395060

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.23502	E(Thermal)=	0.250846
E(CCSD(T))=	-614.383958	E(Empiric)=	-0.350464
DE(MP2)=	-0.761244	DE(HF)=	-0.060435
G4MP2(0 K)=	-615.321081	G4MP2 Energy=	-615.305255
G4MP2 Enthalpy=	-615.30431	G4MP2 Free Energy=	-615.36407

ESTER1a - CO2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.506236	1.180207	0.402407
2	6	0	0.741122	-0.019902	-0.543013
3	6	0	-0.516773	-0.564055	-1.158398
4	6	0	-1.705380	-0.803420	-0.528280
5	6	0	-2.032669	-0.369038	0.886124
6	6	0	1.530284	2.282995	0.266557
7	1	0	1.388158	0.333569	-1.353544
8	1	0	-0.466999	1.658912	0.228352
9	1	0	0.454208	0.871301	1.452555
10	1	0	-2.404149	-1.522572	-0.953763
11	1	0	1.411803	3.097304	1.016302
12	1	0	-0.461407	-0.810905	-2.218318
13	6	0	1.502055	-1.191159	0.179483
14	6	0	-2.999934	0.685229	-1.387498
15	1	0	-2.744455	0.252388	-2.347665
16	1	0	-4.020956	0.518510	-1.078564
17	1	0	-2.621481	1.684119	-1.226815
18	8	0	-2.854819	0.611167	0.798643

19	8	0	2.396176	2.338703	-0.570412
20	8	0	-1.551901	-0.884391	1.884063
21	6	0	2.824793	-0.714004	0.793095
22	1	0	3.334284	-1.556916	1.271292
23	1	0	3.492625	-0.301365	0.029891
24	1	0	2.680508	0.051022	1.560609
25	6	0	1.764241	-2.363454	-0.777508
26	1	0	2.379847	-2.048878	-1.629266
27	1	0	2.302258	-3.163876	-0.260488
28	1	0	0.837145	-2.792673	-1.169679
29	1	0	0.839101	-1.534169	0.982934

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.237863	E(Thermal)=	0.253088
E(CCSD(T))=	-614.410905	E(Empiric)=	-0.350464
DE(MP2)=	-0.758782	DE(HF)=	-0.060028
G4MP2(0 K)=	-615.342316	G4MP2 Energy=	-615.327092
G4MP2 Enthalpy=	-615.326148	G4MP2 Free Energy=	-615.384843

ACID1 - CO2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.010596	0.641533	-0.815644
2	6	0	-0.890474	-0.399606	0.304495
3	6	0	0.239646	-0.075148	1.264947
4	6	0	1.558987	0.086518	1.062086
5	6	0	2.333048	-0.027733	-0.199458
6	6	0	-1.379995	2.279102	0.034561
7	1	0	-1.815963	-0.309939	0.886477
8	1	0	-0.156505	0.504187	-1.515356
9	1	0	-1.920621	0.546460	-1.407205
10	1	0	2.163877	0.321272	1.934979
11	1	0	-0.368834	1.820717	-0.900710
12	1	0	-0.081874	0.046350	2.297741
13	6	0	-0.820577	-1.872505	-0.205643
14	6	0	3.832260	0.154143	-0.053072
15	1	0	4.053332	1.147007	0.355703
16	1	0	4.238209	-0.577033	0.655409
17	1	0	4.316564	0.038669	-1.022636
18	8	0	1.835746	-0.252612	-1.290662
19	8	0	-2.255986	2.228536	0.827470
20	8	0	-0.539939	3.065305	-0.476291

21	6	0	-1.987117	-2.204372	-1.146472
22	1	0	-1.951663	-3.260807	-1.431271
23	1	0	-2.953657	-2.026583	-0.659004
24	1	0	-1.960072	-1.618197	-2.068607
25	6	0	-0.804937	-2.855461	0.975331
26	1	0	-1.723709	-2.771981	1.568878
27	1	0	-0.737746	-3.887111	0.615967
28	1	0	0.043823	-2.680718	1.642734
29	1	0	0.114795	-1.980955	-0.764029

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.234628	E(Thermal)=	0.250002
E(CCSD(T))=	-614.444709	E(Empiric)=	-0.350464
DE(MP2)=	-0.765771	DE(HF)=	-0.060998
G4MP2(0 K)=	-615.387314	G4MP2 Energy=	-615.371941
G4MP2 Enthalpy=	-615.370996	G4MP2 Free Energy=	-615.431043

ESTER3a - CO2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.154518	0.259641	-0.382873
2	6	0	1.592847	-0.289804	-0.230637
3	6	0	-2.148076	-0.786776	-0.394722
4	6	0	-0.859207	-0.813505	-0.665034
5	1	0	1.878227	-0.798411	-1.160208
6	1	0	-0.138438	0.806217	0.524804
7	1	0	0.133512	0.996536	-1.192505
8	1	0	-0.519787	-1.741999	-1.124855
9	6	0	2.634502	0.807179	0.101499
10	1	0	2.354752	1.241015	1.073069
11	6	0	-3.322741	-1.640809	-0.655573
12	1	0	-3.922966	-1.237667	-1.473451
13	1	0	-2.951268	-2.635266	-0.931897
14	1	0	-3.960412	-1.749033	0.224963
15	6	0	-2.822006	1.070244	0.621037
16	1	0	-2.413495	-0.072763	0.935004
17	6	0	1.575497	-1.344270	0.862164
18	1	0	1.463157	-0.926576	1.891905
19	8	0	1.640804	-2.533196	0.681728
20	8	0	-2.936182	1.843138	1.524004
21	8	0	-2.967078	1.056464	-0.625915
22	6	0	4.036571	0.192628	0.240891

23	1	0	4.069789	-0.596459	0.999100
24	1	0	4.364043	-0.249094	-0.707366
25	1	0	4.767410	0.956277	0.523595
26	6	0	2.652459	1.940733	-0.933639
27	1	0	1.711844	2.496261	-0.966021
28	1	0	3.445143	2.656550	-0.694283
29	1	0	2.851946	1.551601	-1.939070

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.234136	E(Thermal)=	0.250133
E(CCSD(T))=	-614.418927	E(Empiric)=	-0.350464
DE(MP2)=	-0.760761	DE(HF)=	-0.060906
G4MP2(0 K)=	-615.356922	G4MP2 Energy=	-615.340926
G4MP2 Enthalpy=	-615.339982	G4MP2 Free Energy=	-615.402452

ACID3b - CO2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.212595	-0.241661	-1.113081
2	6	0	0.821360	-0.086556	0.016811
3	6	0	-2.558867	0.005406	-0.116875
4	6	0	-1.512025	0.462404	-0.828936
5	1	0	0.392788	-0.637739	0.890020
6	1	0	0.226726	0.179355	-2.023374
7	1	0	-0.393180	-1.306965	-1.271850
8	1	0	-1.604694	1.459059	-1.258279
9	6	0	2.224607	-0.656551	-0.252487
10	1	0	2.639488	-0.079097	-1.088601
11	6	0	-3.824577	0.807526	0.064516
12	1	0	-3.759968	1.771294	-0.444757
13	1	0	-4.694999	0.271349	-0.332835
14	1	0	-4.028853	0.999794	1.124590
15	6	0	-2.564862	-1.338079	0.508887
16	1	0	-3.572943	-1.681709	0.831883
17	6	0	1.075577	1.778186	0.119793
18	1	0	0.612576	0.775312	1.034762
19	8	0	0.744012	2.076391	1.298310
20	8	0	1.460924	2.261847	-0.890929
21	8	0	-1.598643	-2.050498	0.691267
22	6	0	2.185245	-2.137248	-0.663718
23	1	0	1.630565	-2.293038	-1.592894
24	1	0	3.201723	-2.511628	-0.822055

25	1	0	1.717324	-2.751971	0.113453
26	6	0	3.140367	-0.464439	0.966574
27	1	0	3.221516	0.585555	1.263419
28	1	0	2.766903	-1.028491	1.829873
29	1	0	4.149308	-0.826930	0.748558

Temperature=	298.15	Pressure=	1
E(ZPE)=	0.234368	E(Thermal)=	0.249885
E(CCSD(T))=	-614.443968	E(Empiric)=	-0.350464
DE(MP2)=	-0.765012	DE(HF)=	-0.060991
G4MP2(0 K)=	-615.386068	G4MP2 Energy=	-615.37055
G4MP2 Enthalpy=	-615.369606	G4MP2 Free Energy=	-615.429485