Theoretical Investigation on Donor-acceptor Interaction between Carbonyl Compound and *N*, *N*'-dioxide-Sc(III) Complex

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Supporting Information

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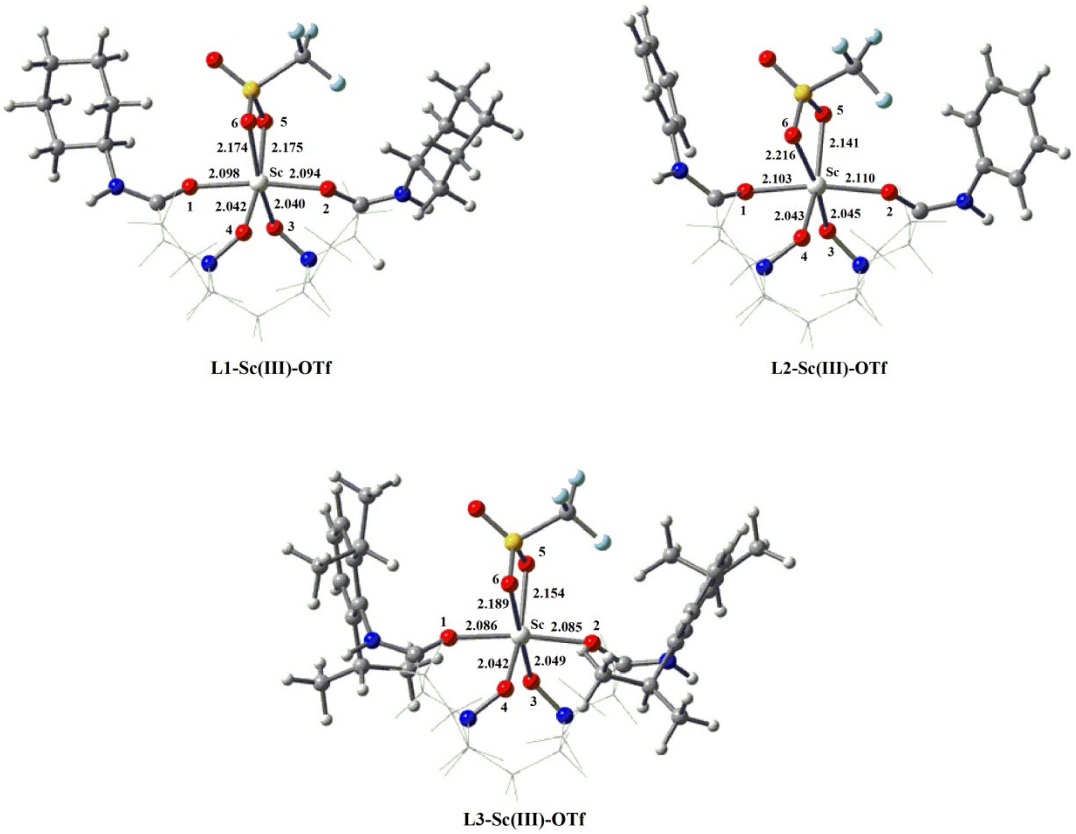


Figure S1 Optimized geometries of hexacoordinate complexes L1-Sc(III)-OTf, L2-Sc(III)-OTf and L3-Sc(III)-OTf, respectively.

Table S1 Variation of selected parameters for L1-CH_2O-OTf as increasing distance between CH_2O and catalyst.

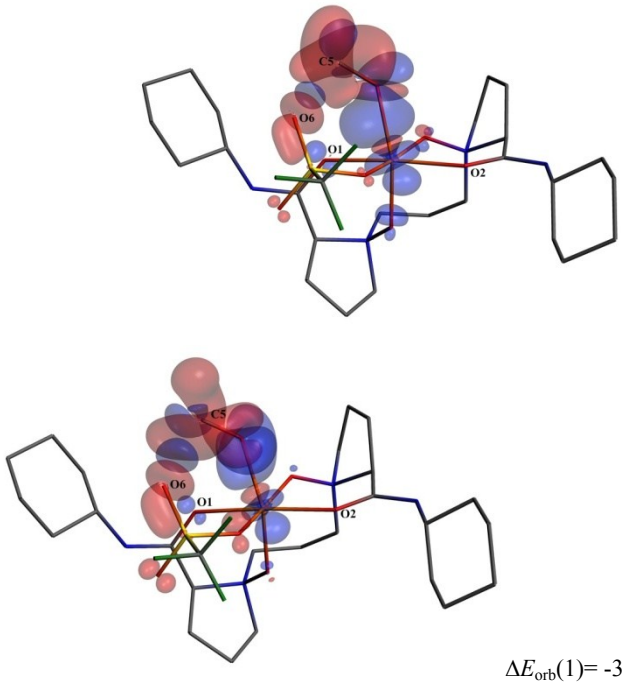
No.	$R_{O8\cdots Sc}$ (Å)	WIB O8···Sc	WIB C5=O8	$\nu_{C=O}$ (cm^{-1})	Charge			ΔE_{int} (kcal mol^{-1})	ΔE_{strain} (kcal mol^{-1})			ΔE_r (kcal mol^{-1})
					Sc	CH_2O	ligand		CAT	CH_2O	Sum	
1	2.176	0.311	1.654	1765.2	1.600	0.147	0.906	-39.2	16.3	0.7	17.0	-22.3
2	2.226	0.300	1.668	1766.9	1.612	0.144	0.902	-39.0	16.3	0.7	17.0	-22.0
3	2.276	0.287	1.687	1775.8	1.621	0.143	0.899	-38.1	15.8	0.6	16.4	-21.7
4	2.326	0.275	1.703	1782.0	1.631	0.142	0.894	-37.0	15.4	0.5	15.9	-21.1
5	2.376	0.264	1.716	1785.9	1.640	0.138	0.891	-35.9	15.1	0.4	15.5	-20.4
6	2.426	0.252	1.729	1788.3	1.649	0.135	0.887	-34.8	14.8	0.4	15.2	-19.6
7	2.476	0.242	1.740	1791.5	1.660	0.131	0.882	-33.6	14.6	0.4	15.0	-18.6
8	2.526	0.231	1.756	1795.4	1.669	0.130	0.877	-32.3	14.3	0.3	14.6	-17.1
9	2.576	0.221	1.764	1797.3	1.679	0.126	0.873	-31.0	14.1	0.3	14.4	-16.6
10	2.626	0.212	1.772	1799.0	1.689	0.121	0.869	-29.8	13.9	0.3	14.2	-15.6
11	2.676	0.203	1.779	1801.1	1.699	0.117	0865	-28.6	13.8	0.3	14.1	-14.5
12	2.726	0.194	1.785	1803.1	1.707	0.112	0.862	27.4	13.6	0.2	13.8	-13.6

Table S2 Variation of selected parameters for L2-CH_2O-OTf as increasing distance between CH_2O and catalyst.

No.	$R_{O8\cdots Sc}$ (Å)	WIB O8···Sc	WIB C5=O8	$\nu_{C=O}$ (cm^{-1})	Charge			ΔE_{int} (kcal mol^{-1})	ΔE_{strain} (kcal mol^{-1})			ΔE_r (kcal mol^{-1})
					Sc	CH_2O	ligand		CAT	CH_2O	Sum	
1	2.167	0.317	1.640	1750.2	1.598	0.148	0.909	-42.4	15.0	0.8	15.8	-26.6
2	2.217	0.303	1.660	1756.8	1.606	0.146	0.907	-41.7	14.5	0.7	15.2	-26.5
3	2.267	0.291	1.675	1765.4	1.615	0.143	0.905	-40.9	14.2	0.6	14.8	-26.1
4	2.317	0.280	1.690	1770.4	1.625	0.140	0.901	-39.9	13.9	0.6	14.4	-25.5
5	2.367	0.269	1.704	1774.4	1.635	0.137	0.898	-38.8	13.6	0.5	14.1	-24.7
6	2.416	0.258	1.716	1779.0	1.644	0.134	0.894	-37.6	13.3	0.5	13.8	-23.8
7	2.467	0.248	1.728	1783.6	1.654	0.131	0.889	-36.3	13.1	0.4	13.5	-22.9
8	2.516	0.237	1.741	1788.4	1.664	0.129	0.885	-35.0	12.8	0.4	13.2	-21.8
9	2.567	0.227	1.755	1793.6	1.674	0.127	0.880	-33.6	12.5	0.3	12.9	-20.7
10	2.617	0.218	1.765	1795.9	1.684	0.124	0.875	-32.3	12.3	0.3	12.6	-19.7
11	2.667	0.208	1.773	1798.0	1.694	0.119	0.871	-31.0	12.1	0.3	12.4	-18.6
12	2.717	0.200	1.781	1799.9	1.704	0.116	0.866	-29.7	11.9	0.3	12.2	-17.6
13	2.767	0.191	1.787	1802.1	1.713	0.111	0.863	-28.5	11.8	0.3	12.1	-16.5

Table S3 Variation of selected parameters for L3-CH_2O-OTf as increasing distance between CH_2O and catalyst.

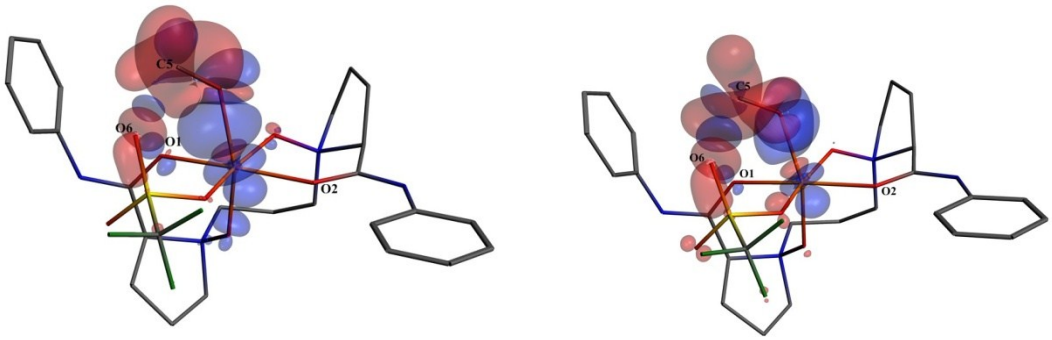
No.	$R_{O8\cdots Sc}$ (Å)	WIB O8···Sc	WIB C5=O8	$\nu_{C=O}$ (cm^{-1})	Charge			ΔE_{int} (kcal mol^{-1})	ΔE_{strain} (kcal mol^{-1})			ΔE_r (kcal mol^{-1})
					Sc	CH_2O	ligand		CAT	CH_2O	Sum	
1	2.166	0.280	1.635	1747.0	1.647	0.132	0.863	-43.6	19.1	0.8	20.0	-23.6
2	2.216	0.268	1.654	1753.0	1.656	0.132	0.860	-42.9	18.7	0.7	19.4	-23.5
3	2.266	0.257	1.672	1758.1	1.666	0.131	0.855	-42.1	18.3	0.7	19.0	-23.1
4	2.316	0.246	1.691	1765.4	1.675	0.132	0.850	-41.0	17.9	0.6	18.5	-22.5
5	2.366	0.236	1.705	1768.2	1.687	0.130	0.844	-39.8	17.5	0.5	18.1	-21.8
6	2.416	0.227	1.717	1771.5	1.698	0.128	0.838	-38.7	17.2	0.5	17.7	-20.9
7	2.466	0.219	1.729	1774.3	1.708	0.126	0.833	-37.5	17.0	0.5	17.5	-20.0



$\Delta E_{orb}(1)$= -31.5 kcal mol^{-1}

$\Delta E_{orb}(2)$= -15.6 kcal mol^{-1}

(a) L1-CH_2O-OTf



$\Delta E_{orb}(1)$= -34.5 kcal mol^{-1}

$\Delta E_{orb}(2)$= -16.8 kcal mol^{-1}

(b) L2-CH_2O-OTf

Figure S2 Dominating contributions to the deformation density Δρ describing the coordination interaction between CH_2O and scandium-based fragments for L1-CH_2O-OTf (a) and L2-CH_2O-OTf (b) complexes according to EST-NOCV analysis. The contour value is |Δρ|=0.001 a. u. The blue/red contours corresponds to accumulation/depletion of electron density.

Table S4 Molecule Orbitals (MO) composition and the corresponding contribution of fragments orbitals (FO) involving donor-acceptor interaction between CH_2O (Frag. 1) and L-Sc(III)(counterion) (Frag. 2), as well as electronic density transfer from CH_2O to L-Sc(III)(counterion) fragment (1->2) by CDA calculations in hexacoordinate complexes.

Ligand	Counter - ion	CDA (1→2)	MO	FO			
				CH_2O (Frag. 1)	Ligand-Sc(III)(counterion) (Frag. 2)		
L1	OTf	0.635	HOMO-117	HOFO-5 (75.7%)	LUFO-2 (2.6%)	LUFO-3 (4.4%)	LUFO-6 (2.4%)
L2	OTf	1.223	HOMO-110	HOFO-5 (70.8%)	LUFO-2 (3.6%)	LUFO-3 (4.1%)	LUFO-6 (3.2%)
L3	OTf	1.379	HOMO-146	HOFO-5 (66.4%)	LUFO-2 (3.3%)	LUFO-3 (5.8%)	LUFO-26 (4.1%)

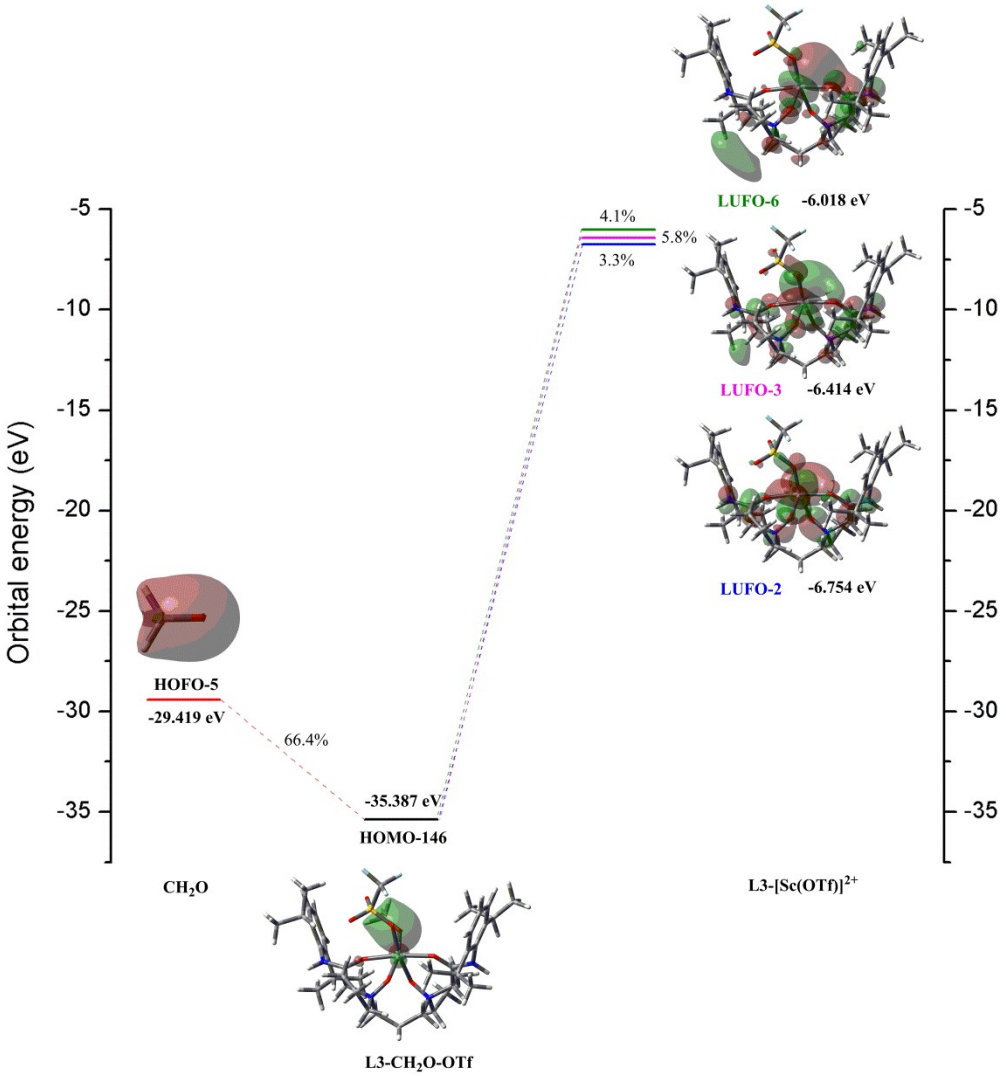
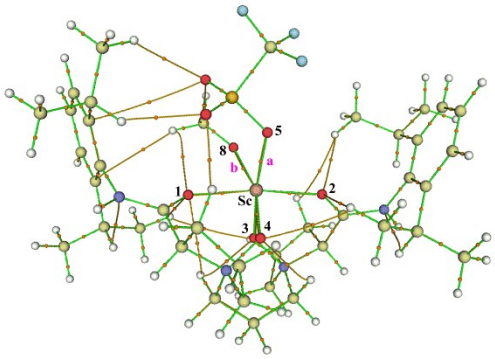


Figure S3 Results of CDA analysis and the corresponding molecule orbitals interaction between CH_2O and L3-$[ScOTf)]^{2+}$ in L3-CH_2O-OTf complex.



L3-CH_2O-OTf

$\rho_a = 0.727$ $\nabla^2\rho_a = 0.388$
$\rho_b = 0.054$ $\nabla^2\rho_b = 0.285$

Figure S4 Charge density (ρ) and Laplacian ($\nabla^2\rho$) of selected bond critical ponits for L3-CH_2O-OTf obtained by AIM theory and visualized by Multiwfn program package.

Table S5 Comparison of selected parameters for hexacoordinate complexes with different substituent in ligand(Cy, Ph or 2,6-*i*Pr), carbonyl substrates(CH_2O, PhCHO or Chalcone) and counterion(OTf or O*i*Pr), respectively.

Ligand	Substi-tuent	Counter-ion	Carbonyl substrate	R (Å)	$R_{O8...Sc}$ (Å)	WIB (O8-Sc)	$\Delta\nu_{C=O}$ (cm^{-1})	Charge		
								Sc	CH_2O	ligand
L1	Cy	OTf	CH_2O	2.052	2.176	0.311	99.6	1.600	0.147	0.906
L2	Ph	OTf	CH_2O	2.052	2.167	0.317	114.6	1.598	0.148	0.909
L3	2,6-iPr	OTf	CH_2O	2.058	2.166	0.280	117.8	1.647	0.132	0.863
L3	2,6-iPr	O*i*Pr	CH_2O	1.862	2.259	0.192	69.3	1.731	0.137	0.726
L3	2,6-iPr	OTf	PhCHO	2.047	2.114	0.296	149.3	1.663	0.173	0.829
L3	2,6-iPr	OTf	Chalcone	2.058	2.058	0.280	200.5	1.710	0.201	0.771

Cartesian coordinates of all stationary points

$[Sc(OTf)]^{2+}$

Zero-point correction= 0.02838 (a.u.)
Thermal correction to Gibbs Free Energy= -0.00925 (a.u.)
Sum of electronic and zero-point Energies= -1721.16036 (a.u.)
Sum of electronic and thermal Free Energies= -1721.19799 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-2.338280	-0.538611	-0.000024
2	16	0	-0.018491	0.705373	0.000026
3	8	0	0.129481	2.120605	-0.000345
4	8	0	-0.985518	0.104446	-1.154412
5	8	0	-0.986171	0.105255	1.154530
6	6	0	1.759654	-0.435383	0.000096

7	9	0	2.321420	-0.069051	-1.081735
8	9	0	2.323192	-0.066837	1.080222
9	9	0	1.308663	-1.642478	0.001658

L1

Zero-point correction= 0.68921 (a.u.)

Thermal correction to Gibbs Free Energy= 0.62458 (a.u.)

Sum of electronic and zero-point Energies= -1497.38179 (a.u.)

Sum of electronic and thermal Free Energies= -1497.44641 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.735216	-2.245508	-1.730724
2	8	0	-2.708782	-0.669604	2.014462
3	7	0	-4.307304	-0.671746	-0.170742
4	1	0	-4.011180	-0.335518	0.757739
5	7	0	-1.945510	-1.555845	1.324015
6	6	0	-5.097098	0.160623	-1.062622
7	6	0	-3.650999	-1.762951	-0.604656
8	6	0	-2.780674	-2.469050	0.428157
9	1	0	-2.065268	-3.070844	-0.148409
10	6	0	-0.897329	-0.848486	0.514199
11	1	0	-1.458001	-0.232550	-0.202205
12	1	0	-0.328341	-1.604421	-0.045982
13	1	0	-0.641375	0.621455	2.022662
14	8	0	3.735553	2.242675	-1.736513
15	8	0	2.710644	0.674726	2.012313
16	7	0	4.308121	0.671746	-0.173817
17	1	0	4.012801	0.337791	0.755683
18	7	0	1.947899	1.560481	1.320728
19	6	0	3.652338	1.762662	-0.609275
20	6	0	0.898622	0.852950	0.512430
21	1	0	1.458339	0.235421	-0.203317
22	1	0	0.330203	1.608669	-0.048591
23	1	0	0.642328	-0.613381	2.024085
24	6	0	0.000467	0.003290	1.382149
25	6	0	5.095973	-0.163801	-1.064543
26	6	0	-1.362523	-2.560118	2.284897
27	1	0	-0.962541	-1.997057	3.129828
28	1	0	-0.551171	-3.095443	1.772420
29	6	0	-2.538758	-3.467526	2.626245

30	1	0	-3.016014	-3.136791	3.552306
31	1	0	-2.197526	-4.497111	2.773528
32	6	0	-3.516441	-3.337182	1.439366
33	1	0	-3.781231	-4.297606	0.987726
34	1	0	-4.441418	-2.842825	1.750752
35	6	0	2.543834	3.473215	2.619922
36	1	0	3.021176	3.142723	3.546034
37	1	0	2.203969	4.503362	2.766389
38	6	0	3.520709	3.340382	1.432668
39	1	0	3.786107	4.299934	0.979540
40	1	0	4.445430	2.845715	1.744284
41	6	0	1.366308	2.566933	2.280157
42	1	0	0.965607	2.005835	3.126054
43	1	0	0.555646	3.102689	1.767019
44	6	0	2.783598	2.471469	0.423068
45	1	0	2.068555	3.073202	-0.153995
46	6	0	-4.220656	1.178449	-1.792770
47	1	0	-3.451829	0.646929	-2.370297
48	1	0	-3.697156	1.786610	-1.033903
49	6	0	-6.200614	0.856514	-0.276583
50	1	0	-5.737248	1.460603	0.522697
51	1	0	-6.828736	0.105243	0.219903
52	6	0	-7.034258	1.761291	-1.176859
53	1	0	-7.809751	2.268612	-0.588819
54	1	0	-7.562147	1.143137	-1.920993
55	6	0	-6.158932	2.777341	-1.903507
56	1	0	-5.701397	3.455089	-1.164106
57	1	0	-6.769544	3.404702	-2.565935
58	6	0	-5.055404	2.081607	-2.693396
59	1	0	-4.413561	2.817954	-3.193947
60	1	0	-5.508982	1.471813	-3.491362
61	6	0	6.198229	-0.860133	-0.277204
62	1	0	5.733788	-1.461247	0.523697
63	1	0	6.828073	-0.108980	0.217283
64	6	0	7.029780	-1.768934	-1.175386
65	1	0	7.804238	-2.276392	-0.586107
66	1	0	7.558969	-1.153819	-1.921130
67	6	0	6.152119	-2.784865	-1.899418
68	1	0	5.693225	-3.459689	-1.158193
69	1	0	6.761232	-3.415270	-2.560344
70	6	0	5.049763	-2.088819	-2.690754
71	1	0	5.504374	-1.482241	-3.490587
72	1	0	4.406023	-2.825020	-3.189083
73	6	0	4.217286	-1.181532	-1.792135

74	1	0	3.449390	-0.649806	-2.370633
75	1	0	3.692839	-1.786680	-1.031502
76	1	0	-5.546810	-0.511653	-1.809681
77	1	0	5.546845	0.506094	-1.813003

L2

Zero-point correction= 0.55010 (a.u.)

Thermal correction to Gibbs Free Energy= 0.48627 (a.u.)

Sum of electronic and zero-point Energies= -1490.26963 (a.u.)

Sum of electronic and thermal Free Energies= -1490.33346 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.168441	2.018457	1.835284
2	8	0	-2.733311	0.619179	-1.858920
3	7	0	-4.292259	0.319596	0.278453
4	1	0	-3.896304	0.107848	-0.657239
5	7	0	-2.055880	1.528509	-1.105486
6	6	0	-5.143550	-0.616647	0.887417
7	6	0	-5.715271	-0.440170	2.151966
8	6	0	-3.870571	1.510471	0.761782
9	6	0	-2.983322	2.315240	-0.182900
10	1	0	-2.334062	2.923483	0.461351
11	6	0	-0.958137	0.867154	-0.320830
12	1	0	-1.468966	0.181408	0.367259
13	1	0	-0.447406	1.639875	0.271009
14	1	0	-0.603478	-0.498187	-1.901627
15	8	0	4.114149	-2.158280	1.647042
16	8	0	2.716314	-0.423017	-1.920388
17	7	0	4.299129	-0.347198	0.226424
18	1	0	3.903102	-0.045407	-0.684132
19	7	0	2.007229	-1.359434	-1.232220
20	6	0	3.830642	-1.554013	0.620491
21	6	0	0.939886	-0.716955	-0.391967
22	1	0	1.479542	-0.101788	0.339512
23	1	0	0.406864	-1.512783	0.147747
24	1	0	0.601523	0.809618	-1.831012
25	6	0	-0.001812	0.122163	-1.225391
26	6	0	5.453616	1.743242	0.306914
27	6	0	6.340594	2.631518	0.899583
28	1	0	6.527791	3.594253	0.429307

29	6	0	6.985855	2.292516	2.087199
30	1	0	7.681310	2.986883	2.551914
31	6	0	6.731343	1.054341	2.668864
32	1	0	7.230888	0.777226	3.594560
33	6	0	5.844923	0.152035	2.087325
34	6	0	5.199987	0.497813	0.895208
35	6	0	-6.546717	-1.431548	2.666544
36	1	0	-6.988152	-1.287770	3.650347
37	6	0	-6.819292	-2.591125	1.947087
38	1	0	-7.472278	-3.355093	2.361468
39	6	0	-6.248011	-2.759977	0.687378
40	1	0	-6.452711	-3.657922	0.108811
41	6	0	-5.415885	-1.782438	0.160245
42	6	0	-1.544181	2.626639	-2.002002
43	1	0	-1.072734	2.145648	-2.861024
44	1	0	-0.797811	3.205258	-1.440417
45	6	0	-2.788050	3.440153	-2.331628
46	1	0	-3.230654	3.087007	-3.266390
47	1	0	-2.534391	4.497249	-2.457156
48	6	0	-3.756006	3.201764	-1.155215
49	1	0	-4.066216	4.121426	-0.651075
50	1	0	-4.659521	2.684834	-1.493700
51	6	0	2.651086	-3.219407	-2.588569
52	1	0	3.100272	-2.843027	-3.511138
53	1	0	2.347119	-4.256299	-2.762406
54	6	0	3.640650	-3.086285	-1.413886
55	1	0	3.933415	-4.045096	-0.976808
56	1	0	4.552290	-2.569921	-1.730828
57	6	0	1.448341	-2.368554	-2.202988
58	1	0	1.006354	-1.807069	-3.027712
59	1	0	0.671345	-2.946596	-1.684100
60	6	0	2.905294	-2.245845	-0.374900
61	1	0	2.235479	-2.874922	0.226665
62	1	0	-5.505961	0.463971	2.713080
63	1	0	-4.971054	-1.910104	-0.825770
64	1	0	5.648649	-0.811921	2.541763
65	1	0	4.950053	2.004375	-0.622966

L3

Zero-point correction= 0.88605 (a.u.)

Thermal correction to Gibbs Free Energy= 0.80756 (a.u.)

Sum of electronic and zero-point Energies= -1961.35781 (a.u.)

Sum of electronic and thermal Free Energies= -1961.43629 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.156545	1.393235	1.862673
2	8	0	-2.529371	0.925161	-1.921671
3	7	0	-4.500565	0.404575	-0.182422
4	1	0	-4.031851	0.377415	-1.101977
5	7	0	-1.953040	1.661257	-0.936079
6	6	0	-5.362733	-0.652893	0.227018
7	6	0	-6.660426	-0.366403	0.678874
8	6	0	-7.208179	1.042634	0.756341
9	1	0	-6.465157	1.721143	0.316327
10	6	0	-7.426889	1.470846	2.207424
11	1	0	-8.185892	0.841485	2.691686
12	1	0	-7.780827	2.508708	2.251218
13	1	0	-6.495456	1.397035	2.779150
14	6	0	-8.492808	1.192652	-0.058317
15	1	0	-8.352122	0.873147	-1.097705
16	1	0	-9.312100	0.598014	0.365931
17	6	0	-3.462511	-2.267387	-0.291148
18	1	0	-3.102544	-1.438158	-0.917111
19	6	0	-2.576971	-2.332582	0.955415
20	1	0	-2.873757	-3.176681	1.592659
21	1	0	-2.663915	-1.422072	1.563351
22	1	0	-1.520748	-2.479309	0.680024
23	6	0	-3.310814	-3.540598	-1.117236
24	1	0	-2.284108	-3.619336	-1.498918
25	1	0	-3.989835	-3.549389	-1.977283
26	1	0	-3.502625	-4.444485	-0.524328
27	6	0	-3.936988	1.298250	0.661863
28	6	0	-2.989188	2.292089	-0.004951
29	1	0	-2.423977	2.758930	0.812705
30	6	0	-0.977261	0.843864	-0.139785
31	1	0	-1.583111	0.145619	0.451619
32	1	0	-0.460553	1.519006	0.558323
33	1	0	-0.591003	-0.563553	-1.687492
34	8	0	4.110162	-1.421081	1.827545
35	8	0	2.492178	-0.801426	-1.944906
36	7	0	4.489125	-0.400529	-0.195560
37	1	0	4.021122	-0.332310	-1.112979
38	7	0	1.887031	-1.530078	-0.971131
39	6	0	7.164925	-1.192766	0.715688

40	1	0	6.382985	-1.824393	0.273307
41	6	0	7.380833	-1.662808	2.153800
42	1	0	8.177229	-1.084047	2.641107
43	1	0	7.681066	-2.718224	2.171034
44	1	0	6.461644	-1.553311	2.739144
45	6	0	8.429510	-1.386827	-0.120625
46	1	0	8.290707	-1.037261	-1.150556
47	1	0	8.705439	-2.448236	-0.152225
48	1	0	9.282266	-0.842123	0.304808
49	6	0	3.584209	2.317314	-0.242358
50	1	0	3.192895	1.526970	-0.898858
51	6	0	2.698550	2.372571	1.005143
52	1	0	3.013390	3.195641	1.661031
53	1	0	2.765400	1.448004	1.593623
54	1	0	1.645670	2.546786	0.733251
55	6	0	3.485696	3.625223	-1.020408
56	1	0	2.463910	3.760401	-1.398317
57	1	0	4.165508	3.638354	-1.879850
58	1	0	3.713275	4.497416	-0.393740
59	6	0	3.888990	-1.287222	0.630646
60	6	0	0.950285	-0.685769	-0.158850
61	1	0	1.585421	-0.008489	0.425591
62	1	0	0.424839	-1.347938	0.544703
63	1	0	0.566412	0.768759	-1.670604
64	6	0	-0.011109	0.093207	-1.027013
65	1	0	-8.819995	2.239848	-0.062379
66	6	0	4.996760	1.950121	0.166098
67	6	0	5.899519	2.934816	0.563946
68	1	0	5.607220	3.982291	0.524025
69	6	0	7.166163	2.596867	1.025982
70	1	0	7.856596	3.375938	1.341466
71	6	0	7.549384	1.264918	1.079573
72	1	0	8.546952	1.009531	1.433994
73	6	0	6.686533	0.242731	0.675395
74	6	0	5.404522	0.603572	0.233367
75	6	0	-7.471091	-1.439077	1.059437
76	1	0	-8.479240	-1.242104	1.420880
77	6	0	-7.022759	-2.749023	0.975739
78	1	0	-7.672909	-3.568668	1.273319
79	6	0	-5.741364	-3.012358	0.505956
80	1	0	-5.394826	-4.042075	0.442328
81	6	0	-4.889822	-1.975343	0.128475
82	6	0	-1.329329	2.891067	-1.544330
83	1	0	-0.749771	2.562773	-2.409597

84	1	0	-0.664570	3.345041	-0.795914
85	6	0	-2.523199	3.777481	-1.874641
86	1	0	-2.840704	3.612996	-2.907417
87	1	0	-2.259005	4.834019	-1.767416
88	6	0	-3.635956	3.346551	-0.894667
89	1	0	-4.015906	4.171110	-0.284089
90	1	0	-4.482010	2.911863	-1.436039
91	6	0	2.358048	-3.659780	-1.938688
92	1	0	2.679656	-3.501791	-2.971250
93	1	0	2.044866	-4.703673	-1.839704
94	6	0	3.493202	-3.290208	-0.959810
95	1	0	3.841062	-4.138305	-0.362406
96	1	0	4.354307	-2.884264	-1.499935
97	6	0	1.207631	-2.721153	-1.597504
98	1	0	0.649265	-2.355231	-2.461232
99	1	0	0.516318	-3.151198	-0.858046
100	6	0	2.895215	-2.222486	-0.052475
101	1	0	2.310380	-2.677856	0.757714

OTf^-

Zero-point correction= 0.02781 (a.u.)

Thermal correction to Gibbs Free Energy= -0.00436 (a.u.)

Sum of electronic and zero-point Energies= -961.30640 (a.u.)

Sum of electronic and thermal Free Energies= -961.33857 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.938457	-0.000454	-0.000344
2	9	0	-1.436816	0.436816	1.165526
3	9	0	-1.432104	-1.230320	-0.204111
4	9	0	-1.435341	0.789970	-0.963240
5	16	0	0.923616	0.000787	0.000320
6	8	0	1.233503	-0.913143	1.109238
7	8	0	1.235261	-0.502962	-1.345157
8	8	0	1.230141	1.418845	0.237590

L1-Sc(III)-OTf

Zero-point correction= 0.72500 (a.u.)

Thermal correction to Gibbs Free Energy= 0.65399 (a.u.)

Sum of electronic and zero-point Energies= -3219.03680 (a.u.)

Sum of electronic and thermal Free Energies= -3219.10781 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.596543	-0.489973	-0.462600
2	6	0	5.352660	-1.583016	0.280897
3	6	0	5.462323	0.185582	-1.519486
4	6	0	5.895292	-2.611612	-0.708144
5	6	0	6.003121	-0.851558	-2.499915
6	6	0	6.766072	-1.951402	-1.771443
7	1	0	7.126429	-2.700204	-2.485313
8	1	0	7.661655	-1.521662	-1.295728
9	1	0	5.049364	-3.127041	-1.190486
10	1	0	6.456036	-3.380770	-0.165798
11	1	0	4.694806	-2.055283	1.022818
12	1	0	6.192986	-1.125715	0.831446
13	1	0	4.880846	0.958701	-2.040287
14	1	0	6.305121	0.693562	-1.020200
15	1	0	5.163441	-1.294421	-3.058317
16	1	0	6.641616	-0.358118	-3.241022
17	6	0	-4.815235	-0.532666	0.243519
18	6	0	-4.582366	-1.780823	-0.601677
19	6	0	-6.280919	-0.355555	0.606435
20	6	0	-5.094851	-3.014536	0.133638
21	6	0	-6.798859	-1.599258	1.325664
22	6	0	-6.566873	-2.859298	0.498679
23	1	0	-6.915977	-3.739831	1.049413
24	1	0	-7.170578	-2.810646	-0.421354
25	1	0	-4.498107	-3.162990	1.046789
26	1	0	-4.933194	-3.903966	-0.485487
27	1	0	-3.513196	-1.878587	-0.839341
28	1	0	-5.123681	-1.663804	-1.556095
29	1	0	-6.415268	0.541735	1.224841
30	1	0	-6.862724	-0.205377	-0.320260
31	1	0	-6.284575	-1.695302	2.294624
32	1	0	-7.862798	-1.471577	1.553641
33	1	0	-4.202224	-0.581600	1.154690
34	8	0	1.933449	0.450928	-0.075333
35	8	0	0.213102	1.771549	1.566766
36	8	0	-0.391876	1.797605	-1.326166
37	8	0	-2.230658	0.600319	0.262568
38	7	0	1.264981	2.656096	1.590569

39	7	0	-1.377528	2.758296	-1.357005
40	7	0	-4.343892	0.658579	-0.506520
41	1	0	-5.003139	1.070215	-1.162380
42	7	0	4.110480	0.522893	0.503160
43	1	0	4.817044	0.944582	1.101248
44	6	0	2.857788	0.906929	0.642007
45	6	0	2.589424	1.918508	1.742281
46	1	0	3.357268	2.705056	1.700963
47	6	0	2.492704	1.332252	3.150616
48	1	0	3.491210	1.187323	3.573204
49	1	0	2.001751	0.353410	3.115232
50	6	0	1.645999	2.352793	3.938594
51	1	0	0.788176	1.858824	4.399874
52	1	0	2.215950	2.836955	4.735598
53	6	0	1.187636	3.386725	2.915553
54	1	0	0.156557	3.723839	3.038785
55	1	0	1.858012	4.252159	2.848736
56	6	0	1.261242	3.564924	0.383456
57	1	0	1.501887	2.937608	-0.478284
58	1	0	2.083364	4.273123	0.542343
59	6	0	-0.021175	4.352191	0.144184
60	1	0	0.210531	5.040503	-0.679958
61	1	0	-0.221260	5.010995	1.000145
62	6	0	-1.340624	3.640832	-0.130975
63	1	0	-1.633365	3.011860	0.712524
64	1	0	-2.118893	4.397514	-0.287794
65	6	0	-1.211878	3.509000	-2.661685
66	1	0	-0.158567	3.783432	-2.746585
67	6	0	-1.701282	2.527541	-3.719494
68	1	0	-0.863559	1.971908	-4.146218
69	6	0	-2.661867	1.571272	-2.984480
70	1	0	-3.657175	1.536582	-3.436907
71	1	0	-2.273191	0.545913	-2.967499
72	6	0	-2.744896	2.120075	-1.557776
73	1	0	-3.463293	2.950836	-1.497759
74	6	0	-3.094329	1.072658	-0.517228
75	1	0	-2.192803	3.063233	-4.535456
76	1	0	-1.829022	4.413360	-2.596172
77	21	0	-0.149599	0.377889	0.121636
78	16	0	-0.514614	-2.348179	0.281819
79	8	0	-0.205693	-1.380408	1.401090
80	8	0	-1.673246	-3.187712	0.419710
81	8	0	-0.422919	-1.487647	-0.960744
82	6	0	0.977675	-3.449138	0.207808

83	9	0	1.042974	-4.142895	1.322401
84	9	0	2.065575	-2.691961	0.087924
85	9	0	0.871749	-4.243160	-0.833297
86	1	0	3.699746	-0.911776	-0.934027

L2-Sc(III)-OTf

Zero-point correction= 0.58538 (a.u.)

Thermal correction to Gibbs Free Energy= 0.51644 (a.u.)

Sum of electronic and zero-point Energies= -3211.90199 (a.u.)

Sum of electronic and thermal Free Energies= -3211.97093 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.118645	-0.942951	-0.488710
2	8	0	-0.373586	-1.639059	1.492644
3	8	0	0.381234	-2.016860	-1.357166
4	8	0	1.993778	-0.343484	0.049164
5	7	0	-1.355453	-2.598900	1.601970
6	7	0	1.441683	-2.874318	-1.184837
7	7	0	4.191162	-0.470721	-0.475803
8	1	0	4.910318	-1.026800	-0.930707
9	7	0	-4.084401	-0.325532	0.447971
10	1	0	-4.696725	-0.429654	1.252078
11	6	0	-2.961286	-1.021777	0.439672
12	6	0	-2.729929	-1.937829	1.631556
13	1	0	-3.453495	-2.766551	1.593616
14	6	0	-2.757903	-1.241920	2.997306
15	1	0	-3.779570	-1.213151	3.388557
16	1	0	-2.404916	-0.210042	2.894247
17	6	0	-1.812562	-2.064129	3.893883
18	1	0	-1.002157	-1.434158	4.266811
19	1	0	-2.323458	-2.493312	4.759269
20	6	0	-1.265268	-3.167732	3.002633
21	1	0	-0.219491	-3.425574	3.183181
22	1	0	-1.881368	-4.075199	3.018954
23	6	0	-1.232171	-3.656100	0.525902
24	1	0	-1.483775	-3.170833	-0.417979
25	1	0	-2.002441	-4.402950	0.752152
26	6	0	0.119595	-4.355953	0.450972
27	1	0	-0.006105	-5.154689	-0.292657
28	1	0	0.318589	-4.887706	1.391208

29	6	0	1.393520	-3.572968	0.155332
30	1	0	1.569787	-2.807162	0.914265
31	1	0	2.241501	-4.268282	0.155848
32	6	0	1.433371	-3.825932	-2.363881
33	1	0	0.415848	-4.209391	-2.463038
34	6	0	1.912466	-2.974918	-3.532213
35	1	0	1.063307	-2.566562	-4.084350
36	6	0	2.741426	-1.837332	-2.902897
37	1	0	3.763842	-1.788907	-3.288714
38	1	0	2.277013	-0.860904	-3.081890
39	6	0	2.755301	-2.145543	-1.402093
40	1	0	3.536910	-2.882469	-1.165369
41	6	0	2.944070	-0.916893	-0.528221
42	1	0	2.499226	-3.580194	-4.227529
43	1	0	2.119340	-4.646616	-2.120659
44	21	0	-0.105458	-0.444656	-0.143035
45	6	0	4.620111	0.781309	0.099161
46	6	0	4.129448	1.977761	-0.413707
47	6	0	4.620665	3.173635	0.097720
48	6	0	5.588957	0.752718	1.097168
49	6	0	6.071635	1.956413	1.599289
50	1	0	5.961589	-0.197410	1.474339
51	1	0	6.829107	1.950366	2.377661
52	1	0	4.254629	4.117299	-0.297637
53	1	0	3.378589	1.975830	-1.203202
54	6	0	-4.481726	0.681919	-0.499188
55	6	0	-4.276956	0.519917	-1.866568
56	6	0	-4.699599	1.528620	-2.725287
57	6	0	-5.110812	1.813116	0.015193
58	6	0	-5.533547	2.808368	-0.856231
59	1	0	-5.257500	1.921672	1.088615
60	1	0	-6.021693	3.695423	-0.463438
61	1	0	-4.550595	1.415224	-3.795398
62	1	0	-3.807912	-0.377405	-2.256769
63	16	0	-0.812413	2.235062	-0.091529
64	8	0	-0.976926	1.227191	1.022293
65	8	0	-0.143235	1.424342	-1.187194
66	8	0	-1.942788	3.044108	-0.450099
67	6	0	0.539488	3.346788	0.529462
68	9	0	1.498515	2.585039	1.036571
69	9	0	0.049904	4.134771	1.459421
70	9	0	1.017498	4.053916	-0.476020
71	6	0	-5.323240	2.668937	-2.225562
72	1	0	-5.653766	3.448070	-2.906494

73	6	0	5.588550	3.163393	1.099474
74	1	0	5.974120	4.102061	1.487693

L3-Sc(III)-OTf

Zero-point correction= 0.92403 (a.u.)

Thermal correction to Gibbs Free Energy= 0.84173 (a.u.)

Sum of electronic and zero-point Energies= -3683.00884 (a.u.)

Sum of electronic and thermal Free Energies= -3683.09114 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.171809	-0.358784	0.014633
2	8	0	-0.254650	-1.373307	1.667455
3	8	0	-0.056802	-2.007648	-1.180115
4	8	0	1.978212	-0.544589	-0.166800
5	7	0	-1.320316	-2.161007	2.028916
6	7	0	0.885009	-3.007012	-1.125152
7	7	0	4.071083	-1.201347	-0.654395
8	1	0	4.655172	-1.872422	-1.146203
9	7	0	-4.243659	-0.198872	0.872327
10	1	0	-4.853582	-0.406466	1.659268
11	6	0	-2.985041	-0.586880	0.938590
12	6	0	-2.581166	-1.324305	2.198332
13	1	0	-3.368615	-2.049172	2.453991
14	6	0	-2.249234	-0.442835	3.399799
15	1	0	-3.167518	-0.139017	3.912368
16	1	0	-1.735211	0.466584	3.068562
17	6	0	-1.326930	-1.321914	4.272284
18	1	0	-0.389799	-0.798370	4.476065
19	1	0	-1.781844	-1.575515	5.233132
20	6	0	-1.067795	-2.588178	3.459662
21	1	0	-0.040715	-2.958143	3.509217
22	1	0	-1.769869	-3.399601	3.686974
23	6	0	-1.538614	-3.296566	1.056241
24	1	0	-1.888106	-2.842197	0.124943
25	1	0	-2.352955	-3.898461	1.477745
26	6	0	-0.340406	-4.202842	0.803493
27	1	0	-0.713272	-5.003331	0.149814
28	1	0	-0.057740	-4.718063	1.731869
29	6	0	0.960399	-3.641742	0.245004
30	1	0	1.377285	-2.884278	0.914693

31	1	0	1.684842	-4.459706	0.150196
32	6	0	0.557813	-3.971078	-2.246080
33	1	0	-0.515122	-4.169433	-2.193337
34	6	0	1.009988	-3.243241	-3.510477
35	1	0	0.162781	-2.763896	-4.006191
36	6	0	2.030693	-2.182712	-3.045585
37	1	0	2.978888	-2.225223	-3.590583
38	1	0	1.629199	-1.169428	-3.159369
39	6	0	2.250425	-2.496771	-1.568255
40	1	0	2.925320	-3.357357	-1.453511
41	6	0	2.759012	-1.341056	-0.731906
42	1	0	1.446160	-3.953049	-4.218024
43	1	0	1.118725	-4.894252	-2.056135
44	21	0	-0.088387	-0.293868	-0.058334
45	6	0	4.719347	-0.080585	-0.003878
46	6	0	4.733220	-0.017072	1.395233
47	6	0	5.372027	1.086246	1.966697
48	6	0	5.317801	0.879482	-0.836665
49	6	0	5.943776	1.955408	-0.211042
50	6	0	5.232648	0.770584	-2.345997
51	1	0	6.425169	2.722800	-0.811193
52	1	0	5.412309	1.181330	3.049928
53	6	0	-4.790317	0.542168	-0.246602
54	6	0	-5.209225	-0.177807	-1.372214
55	6	0	-5.739513	0.563382	-2.430184
56	6	0	-4.864595	1.940525	-0.132885
57	6	0	-5.407327	2.625470	-1.218592
58	6	0	-4.401728	2.655044	1.122300
59	1	0	-5.487284	3.707947	-1.184990
60	1	0	-6.081212	0.049542	-3.326070
61	6	0	-5.079031	-1.683304	-1.486931
62	16	0	-0.176348	2.456183	-0.172419
63	8	0	-1.232523	3.428304	-0.242109
64	8	0	-0.107111	1.585925	1.062596
65	8	0	-0.060067	1.460329	-1.308070
66	6	0	1.440095	3.372143	-0.179809
67	9	0	1.464116	4.173550	0.863681
68	9	0	1.528347	4.061573	-1.298011
69	9	0	2.435319	2.501945	-0.105401
70	6	0	-5.839849	1.944955	-2.352503
71	1	0	-6.260070	2.502510	-3.185449
72	6	0	5.966472	2.059387	1.176080
73	1	0	6.461617	2.906055	1.644422
74	6	0	-5.397083	2.446243	2.268696

75	6	0	-4.177245	4.149395	0.926065
76	1	0	-6.370398	2.878172	2.004661
77	1	0	-5.047487	2.945618	3.179703
78	1	0	-5.574398	1.391211	2.518432
79	1	0	-3.718934	4.575105	1.825145
80	1	0	-3.512302	4.358955	0.082907
81	1	0	-5.125830	4.678068	0.768958
82	1	0	-3.426825	2.219368	1.411668
83	6	0	-6.365942	-2.345693	-1.974279
84	1	0	-4.869992	-2.090418	-0.483684
85	6	0	-3.904004	-2.055386	-2.397062
86	1	0	-7.228432	-2.058856	-1.363325
87	1	0	-6.589978	-2.077029	-3.013305
88	1	0	-3.783975	-3.146524	-2.442336
89	1	0	-2.962507	-1.605749	-2.055295
90	1	0	-6.270071	-3.436919	-1.939371
91	1	0	-4.084757	-1.702609	-3.420316
92	6	0	3.885468	1.307845	-2.839896
93	6	0	6.374771	1.465444	-3.077009
94	6	0	4.103117	-1.066374	2.286679
95	6	0	2.903171	-0.495498	3.046996
96	6	0	5.119880	-1.673106	3.252818
97	1	0	3.739995	-1.888774	1.649985
98	1	0	5.289028	-0.297939	-2.616718
99	1	0	6.329789	1.234361	-4.146519
100	1	0	7.354335	1.148623	-2.703365
101	1	0	3.781017	1.162917	-3.921888
102	1	0	3.029257	0.834169	-2.338737
103	1	0	3.817319	2.384418	-2.638480
104	1	0	5.501161	-0.923699	3.956043
105	1	0	5.980258	-2.097396	2.724057
106	1	0	2.364179	-1.296770	3.571929
107	1	0	3.229209	0.229320	3.802988
108	1	0	6.309890	2.556320	-2.986431
109	1	0	4.656640	-2.469415	3.847250
110	1	0	2.199612	0.017971	2.379907

L1-CH_2O-OTf

Zero-point correction= 0.75551 (a.u.)

Thermal correction to Gibbs Free Energy= 0.68096 (a.u.)

Sum of electronic and zero-point Energies= -3333.48598 (a.u.)

Sum of electronic and thermal Free Energies= -3333.56053 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.820750	-1.085870	-0.115115
2	8	0	0.278081	-1.173719	1.595041
3	8	0	0.854074	-2.376648	-1.017748
4	8	0	2.263031	-0.125621	-0.422771
5	7	0	-0.520435	-2.140234	2.161233
6	7	0	2.037351	-2.995449	-0.705400
7	7	0	4.490267	-0.223948	-0.702834
8	1	0	5.298254	-0.793295	-0.939799
9	7	0	-3.818472	-0.914316	0.909755
10	1	0	-4.344906	-1.022460	1.772562
11	6	0	-2.535529	-1.205024	0.914910
12	6	0	-1.962432	-1.656928	2.245365
13	1	0	-2.536294	-2.523053	2.607271
14	6	0	-1.903733	-0.553865	3.308576
15	1	0	-2.857088	-0.497072	3.842595
16	1	0	-1.739976	0.417196	2.829162
17	6	0	-0.729673	-0.944193	4.226291
18	1	0	0.020617	-0.150576	4.237389
19	1	0	-1.043373	-1.118727	5.258519
20	6	0	-0.150466	-2.216763	3.628059
21	1	0	0.936903	-2.295206	3.687372
22	1	0	-0.612211	-3.128530	4.027341
23	6	0	-0.390908	-3.461587	1.442775
24	1	0	-0.794393	-3.309279	0.439557
25	1	0	-1.042778	-4.160830	1.980014
26	6	0	1.017293	-4.043053	1.401768
27	1	0	0.920991	-5.022081	0.913008
28	1	0	1.347038	-4.279176	2.422624
29	6	0	2.163910	-3.260022	0.775631
30	1	0	2.281031	-2.284871	1.256267
31	1	0	3.092736	-3.829428	0.900466
32	6	0	2.120251	-4.244529	-1.558601
33	1	0	1.163882	-4.762352	-1.463000
34	6	0	2.425169	-3.721578	-2.957692
35	1	0	1.507890	-3.629056	-3.543033
36	6	0	3.075207	-2.337578	-2.753105
37	1	0	4.051111	-2.245581	-3.238577
38	1	0	2.435914	-1.537073	-3.141052
39	6	0	3.224157	-2.202427	-1.238171
40	1	0	4.110742	-2.751026	-0.888582

41	6	0	3.290658	-0.772038	-0.736600
42	1	0	3.084859	-4.414771	-3.485604
43	1	0	2.924410	-4.867529	-1.148812
44	21	0	0.203304	-0.525905	-0.345680
45	6	0	4.756812	1.183400	-0.322511
46	6	0	4.942272	1.295455	1.187466
47	6	0	5.262590	2.736757	1.573210
48	6	0	5.979285	1.679843	-1.080732
49	6	0	6.302816	3.117711	-0.683010
50	1	0	6.840136	1.033832	-0.832933
51	1	0	5.812297	1.600487	-2.163199
52	1	0	7.198625	3.451400	-1.217895
53	1	0	5.483464	3.775971	-1.011122
54	1	0	5.412127	2.803060	2.656802
55	1	0	4.395914	3.375014	1.339582
56	1	0	5.774561	0.638050	1.489413
57	1	0	4.038617	0.938912	1.700868
58	1	0	3.868286	1.755012	-0.626035
59	6	0	-4.516812	-0.247935	-0.214282
60	6	0	-5.124771	-1.263377	-1.172665
61	6	0	-5.836633	-0.534496	-2.310443
62	6	0	-5.556520	0.708850	0.347789
63	6	0	-6.260990	1.429767	-0.797858
64	1	0	-6.296923	0.136673	0.933802
65	1	0	-5.070303	1.425348	1.022347
66	1	0	-7.020065	2.109168	-0.395259
67	1	0	-5.526091	2.060557	-1.323534
68	1	0	-6.291188	-1.262709	-2.991719
69	1	0	-5.095169	0.027100	-2.904088
70	1	0	-5.846057	-1.889718	-0.623579
71	1	0	-4.341809	-1.934426	-1.555261
72	1	0	-3.749989	0.341389	-0.736376
73	16	0	-1.540802	2.233785	-0.031557
74	8	0	-2.374762	1.970500	1.132857
75	8	0	-0.236737	1.444229	0.023662
76	8	0	-2.165467	2.140601	-1.354334
77	6	0	-0.910150	3.969886	0.128406
78	9	0	-0.265340	4.089914	1.276224
79	9	0	-1.936751	4.793480	0.096324
80	9	0	-0.088056	4.227122	-0.874854
81	6	0	-6.881881	0.438004	-1.774824
82	1	0	-7.364109	0.969361	-2.602957
83	1	0	-7.677283	-0.128363	-1.265568
84	6	0	6.488968	3.246402	0.824350

85	1	0	6.692005	4.289017	1.092748
86	1	0	7.373735	2.668650	1.134884
87	6	0	-1.418466	0.292441	-2.909669
88	1	0	-1.409213	0.947499	-3.793291
89	1	0	-2.391281	-0.070281	-2.538716
90	8	0	-0.368019	-0.072040	-2.396035

L2-CH_2O-OTf

Zero-point correction= 0.61557 (a.u.)

Thermal correction to Gibbs Free Energy= 0.54183 (a.u.)

Sum of electronic and zero-point Energies= -3326.35846 (a.u.)

Sum of electronic and thermal Free Energies= -3326.43220 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.916256	-1.016612	-0.130585
2	8	0	0.102952	-1.109369	1.675138
3	8	0	0.755483	-2.382996	-0.885312
4	8	0	2.203678	-0.168206	-0.303226
5	7	0	-0.744061	-2.036481	2.231162
6	7	0	1.910529	-3.021885	-0.508939
7	7	0	4.444635	-0.317223	-0.577540
8	1	0	5.206608	-0.950294	-0.802895
9	7	0	-3.971133	-0.844320	0.767613
10	1	0	-4.542665	-0.890473	1.606495
11	6	0	-2.676566	-1.105053	0.860701
12	6	0	-2.178128	-1.519563	2.232331
13	1	0	-2.786151	-2.365065	2.587303
14	6	0	-2.152192	-0.389853	3.268296
15	1	0	-3.127369	-0.310560	3.758676
16	1	0	-1.956224	0.567079	2.772753
17	6	0	-1.023986	-0.771133	4.246408
18	1	0	-0.258380	0.007705	4.260602
19	1	0	-1.383516	-0.902447	5.269991
20	6	0	-0.447409	-2.074747	3.717334
21	1	0	0.633918	-2.176989	3.830170
22	1	0	-0.949946	-2.962539	4.121413
23	6	0	-0.604663	-3.382351	1.560383
24	1	0	-0.958920	-3.257613	0.535274
25	1	0	-1.288354	-4.056788	2.089843
26	6	0	0.796827	-3.980997	1.595522

27	1	0	0.705110	-4.976196	1.139765
28	1	0	1.084892	-4.183155	2.635966
29	6	0	1.977929	-3.236088	0.984871
30	1	0	2.092751	-2.248770	1.439720
31	1	0	2.891563	-3.815717	1.163331
32	6	0	1.983917	-4.306598	-1.309564
33	1	0	1.008227	-4.789761	-1.229379
34	6	0	2.358174	-3.854355	-2.716763
35	1	0	1.470985	-3.780480	-3.349219
36	6	0	3.016559	-2.470316	-2.548472
37	1	0	4.000719	-2.401799	-3.021140
38	1	0	2.388473	-1.679239	-2.971985
39	6	0	3.136357	-2.282361	-1.036345
40	1	0	3.996238	-2.845225	-0.644329
41	6	0	3.223625	-0.835328	-0.588050
42	1	0	3.033156	-4.579083	-3.179093
43	1	0	2.750527	-4.937308	-0.843430
44	21	0	0.135200	-0.503437	-0.277681
45	6	0	4.874519	1.023630	-0.323720
46	6	0	4.000070	2.086655	-0.089331
47	6	0	4.539172	3.350003	0.132902
48	6	0	6.257398	1.219948	-0.335064
49	6	0	6.775385	2.486751	-0.109181
50	1	0	6.931262	0.384098	-0.521877
51	1	0	7.850928	2.637039	-0.119082
52	1	0	3.866491	4.183837	0.313413
53	1	0	2.926277	1.946503	-0.079218
54	6	0	-4.596115	-0.404179	-0.460732
55	6	0	-4.912745	-1.354588	-1.427875
56	6	0	-5.516824	-0.936560	-2.608999
57	6	0	-4.870994	0.946825	-0.639993
58	6	0	-5.479116	1.351343	-1.826124
59	1	0	-4.589650	1.668138	0.123534
60	1	0	-5.699142	2.403697	-1.982208
61	1	0	-5.780163	-1.666987	-3.369031
62	1	0	-4.697226	-2.406209	-1.250007
63	16	0	-1.379852	2.383217	0.048603
64	8	0	-2.372168	2.049302	1.064060
65	8	0	-0.154914	1.480457	0.157330
66	8	0	-1.827520	2.512840	-1.336641
67	6	0	-0.653007	4.020561	0.528910
68	9	0	-0.179998	3.934165	1.761353
69	9	0	-1.599237	4.933896	0.468141
70	9	0	0.329402	4.326217	-0.301908

71	6	0	-1.463515	0.466545	-2.761811
72	1	0	-1.443070	1.077786	-3.675616
73	1	0	-2.438357	0.246440	-2.295132
74	8	0	-0.423421	-0.004798	-2.310794
75	6	0	-5.798688	0.414982	-2.806293
76	1	0	-6.279440	0.737953	-3.725850
77	6	0	5.915113	3.556664	0.125747
78	1	0	6.318325	4.550026	0.300263

L3-CH_2O-OTf

Zero-point correction= 0.95279 (a.u.)

Thermal correction to Gibbs Free Energy= 0.86310 (a.u.)

Sum of electronic and zero-point Energies= -3797.46192 (a.u.)

Sum of electronic and thermal Free Energies= -3797.55161 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.908114	-0.681489	0.111073
2	8	0	0.129201	-0.957977	1.838408
3	8	0	0.455050	-2.486149	-0.638352
4	8	0	2.251554	-0.500306	-0.247818
5	7	0	-0.817580	-1.710914	2.489435
6	7	0	1.514046	-3.277165	-0.272513
7	7	0	4.423175	-1.007676	-0.484913
8	1	0	5.114030	-1.721437	-0.700125
9	7	0	-3.964509	-0.439745	0.970750
10	1	0	-4.547380	-0.407913	1.802993
11	6	0	-2.671199	-0.681778	1.104328
12	6	0	-2.169052	-1.001484	2.497672
13	1	0	-2.861274	-1.720686	2.961129
14	6	0	-1.934215	0.197673	3.418287
15	1	0	-2.869327	0.472751	3.916516
16	1	0	-1.608386	1.061863	2.831757
17	6	0	-0.840589	-0.269727	4.400951
18	1	0	0.027422	0.391895	4.338593
19	1	0	-1.182178	-0.274209	5.439052
20	6	0	-0.465373	-1.677907	3.961489
21	1	0	0.598545	-1.911939	4.045295
22	1	0	-1.060326	-2.457170	4.454006
23	6	0	-0.914563	-3.103979	1.917377
24	1	0	-1.301646	-2.997392	0.901024

25	1	0	-1.666182	-3.625341	2.522823
26	6	0	0.373655	-3.917351	1.938499
27	1	0	0.100142	-4.912125	1.561095
28	1	0	0.681126	-4.094484	2.978258
29	6	0	1.624426	-3.419591	1.226541
30	1	0	1.932588	-2.442384	1.610206
31	1	0	2.437401	-4.135246	1.399543
32	6	0	1.353429	-4.589800	-1.009754
33	1	0	0.322002	-4.917957	-0.863269
34	6	0	1.716061	-4.251485	-2.451880
35	1	0	0.816885	-4.036150	-3.034003
36	6	0	2.617131	-3.000497	-2.373251
37	1	0	3.584369	-3.132353	-2.868048
38	1	0	2.130138	-2.129521	-2.825635
39	6	0	2.817320	-2.767797	-0.877082
40	1	0	3.594510	-3.436915	-0.479913
41	6	0	3.143052	-1.338482	-0.499809
42	1	0	2.221524	-5.097303	-2.924789
43	1	0	2.042956	-5.309831	-0.552240
44	21	0	0.167047	-0.487761	-0.156871
45	6	0	4.877239	0.342205	-0.213912
46	6	0	4.917018	0.783571	1.115207
47	6	0	5.336624	2.098576	1.326542
48	6	0	5.237280	1.137558	-1.312823
49	6	0	5.652734	2.439607	-1.041387
50	6	0	5.108516	0.624958	-2.732264
51	1	0	5.945163	3.092779	-1.859392
52	1	0	5.389504	2.488706	2.340907
53	6	0	-4.559460	-0.161091	-0.319889
54	6	0	-4.660257	-1.211192	-1.246979
55	6	0	-5.180107	-0.894190	-2.503919
56	6	0	-4.985564	1.151545	-0.580348
57	6	0	-5.505630	1.405302	-1.850430
58	6	0	-4.959728	2.220310	0.490151
59	1	0	-5.845796	2.408217	-2.095143
60	1	0	-5.285221	-1.676190	-3.253717
61	6	0	-4.278533	-2.646668	-0.938110
62	16	0	-1.012603	2.528817	-0.041604
63	8	0	-1.840299	2.459278	1.155453
64	8	0	0.162070	1.561534	0.036620
65	8	0	-1.682361	2.457742	-1.341774
66	6	0	-0.156425	4.172072	0.008379
67	9	0	0.538814	4.270192	1.128075
68	9	0	-1.082059	5.111477	-0.033581

69	9	0	0.650894	4.283505	-1.031060
70	6	0	-5.590300	0.399088	-2.805338
71	1	0	-5.998061	0.620535	-3.788455
72	6	0	5.696814	2.916038	0.264291
73	1	0	6.021908	3.935453	0.454822
74	6	0	-6.245513	2.143564	1.320530
75	6	0	-4.766017	3.628383	-0.060452
76	1	0	-7.121365	2.348400	0.691827
77	1	0	-6.229677	2.887855	2.124619
78	1	0	-6.404787	1.156006	1.776536
79	1	0	-4.583184	4.324488	0.765403
80	1	0	-3.909263	3.678588	-0.742260
81	1	0	-5.655736	3.988855	-0.591581
82	1	0	-4.099581	2.023174	1.145235
83	6	0	-5.479318	-3.579473	-1.101977
84	1	0	-3.970412	-2.705977	0.118087
85	6	0	-3.103386	-3.128275	-1.792125
86	1	0	-6.337351	-3.242874	-0.510302
87	1	0	-5.801631	-3.636001	-2.148389
88	1	0	-2.858500	-4.170699	-1.547164
89	1	0	-2.202959	-2.518791	-1.639504
90	1	0	-5.222646	-4.597078	-0.785416
91	1	0	-3.356445	-3.101125	-2.859584
92	6	0	3.688595	0.878357	-3.251992
93	6	0	6.135273	1.215837	-3.691318
94	6	0	4.534968	-0.086340	2.294416
95	6	0	3.266620	0.427324	2.980950
96	6	0	5.680894	-0.209105	3.298960
97	1	0	4.325859	-1.102791	1.922890
98	1	0	5.273086	-0.465244	-2.718421
99	1	0	6.076543	0.710715	-4.661413
100	1	0	7.157946	1.109101	-3.314078
101	1	0	3.555347	0.440019	-4.248800
102	1	0	2.913898	0.477239	-2.583528
103	1	0	3.508400	1.957845	-3.334422
104	1	0	5.903988	0.755714	3.769216
105	1	0	6.601512	-0.566092	2.824633
106	1	0	2.973050	-0.253950	3.792075
107	1	0	3.436819	1.413138	3.431015
108	1	0	5.950491	2.280484	-3.877571
109	1	0	5.416557	-0.907491	4.101530
110	1	0	2.424647	0.522917	2.283225
111	6	0	-1.397695	0.403816	-2.697675
112	1	0	-1.325872	0.965312	-3.640684

113	1	0	-2.391302	0.278840	-2.235858
114	8	0	-0.396016	-0.120106	-2.216358

L3-CH_2O-O*i*Pr

Zero-point correction= 1.01868 (a.u.)

Thermal correction to Gibbs Free Energy= 0.93372 (a.u.)

Sum of electronic and zero-point Energies= -3029.79182 (a.u.)

Sum of electronic and thermal Free Energies= -3029.87678 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.197921	-0.422993	0.006976
2	8	0	-0.102858	-1.044349	1.660544
3	8	0	0.083676	-2.040369	-1.103235
4	8	0	2.020394	-0.242923	-0.428047
5	7	0	-1.080030	-1.874954	2.140871
6	7	0	1.102417	-2.936017	-0.943955
7	7	0	4.147172	-0.857991	-0.766350
8	1	0	4.791440	-1.564072	-1.109894
9	7	0	-4.098679	0.064907	1.089166
10	1	0	-4.632112	0.012588	1.952164
11	6	0	-2.881558	-0.464827	1.045976
12	6	0	-2.380238	-1.105363	2.323964
13	1	0	-3.120179	-1.843840	2.669779
14	6	0	-2.030026	-0.119775	3.438828
15	1	0	-2.930464	0.192739	3.977355
16	1	0	-1.567346	0.772897	3.001758
17	6	0	-1.026812	-0.884351	4.325831
18	1	0	-0.116618	-0.295114	4.463891
19	1	0	-1.433440	-1.103859	5.316512
20	6	0	-0.722302	-2.179793	3.579465
21	1	0	0.329750	-2.473288	3.591168
22	1	0	-1.348447	-3.020165	3.904085
23	6	0	-1.261975	-3.110045	1.288555
24	1	0	-1.642910	-2.764836	0.324762
25	1	0	-2.036065	-3.707000	1.786964
26	6	0	-0.015117	-3.968037	1.117032
27	1	0	-0.338008	-4.851169	0.548777
28	1	0	0.297477	-4.366733	2.091833
29	6	0	1.244146	-3.384437	0.490225
30	1	0	1.591099	-2.516828	1.058234

31	1	0	2.030537	-4.149579	0.495782
32	6	0	0.857482	-4.068769	-1.917019
33	1	0	-0.185616	-4.369873	-1.801649
34	6	0	1.198140	-3.468287	-3.277514
35	1	0	0.294548	-3.113138	-3.777659
36	6	0	2.147770	-2.287267	-2.985121
37	1	0	3.086773	-2.338107	-3.544806
38	1	0	1.668102	-1.329008	-3.215992
39	6	0	2.415915	-2.384213	-1.485282
40	1	0	3.166200	-3.160993	-1.275513
41	6	0	2.839625	-1.084285	-0.838470
42	1	0	1.659994	-4.221852	-3.920663
43	1	0	1.519751	-4.897557	-1.637144
44	21	0	-0.093171	-0.086122	-0.203489
45	6	0	4.662964	0.387442	-0.237036
46	6	0	4.841832	0.497219	1.149377
47	6	0	5.254951	1.738838	1.636067
48	6	0	4.905247	1.434969	-1.137944
49	6	0	5.313745	2.653726	-0.595910
50	6	0	4.707236	1.267140	-2.631486
51	1	0	5.514608	3.494449	-1.255872
52	1	0	5.404216	1.873640	2.705686
53	6	0	-4.639577	0.797841	-0.035907
54	6	0	-5.305676	0.089964	-1.043844
55	6	0	-5.789191	0.831117	-2.126840
56	6	0	-4.415413	2.185624	-0.078428
57	6	0	-4.930322	2.876041	-1.175813
58	6	0	-3.671726	2.897237	1.034301
59	1	0	-4.798212	3.952311	-1.246064
60	1	0	-6.320581	0.321847	-2.928051
61	6	0	-5.470700	-1.414797	-1.018802
62	6	0	-5.611812	2.206125	-2.188347
63	1	0	-6.010176	2.765496	-3.031177
64	6	0	5.476373	2.806966	0.776347
65	1	0	5.796776	3.765199	1.177425
66	6	0	-4.600614	3.146516	2.225717
67	6	0	-3.026399	4.205393	0.593523
68	1	0	-5.429753	3.801803	1.930690
69	1	0	-4.061535	3.636618	3.044832
70	1	0	-5.046004	2.224198	2.621518
71	1	0	-2.419481	4.613331	1.409578
72	1	0	-2.371369	4.064260	-0.276443
73	1	0	-3.772458	4.969691	0.344378
74	1	0	-2.850616	2.236455	1.361679

75	6	0	-6.900762	-1.850593	-1.328949
76	1	0	-5.235486	-1.769602	-0.003851
77	6	0	-4.481543	-2.073780	-1.985548
78	1	0	-7.628175	-1.355222	-0.677031
79	1	0	-7.175959	-1.628804	-2.366927
80	1	0	-4.565984	-3.166281	-1.936699
81	1	0	-3.442965	-1.791785	-1.762944
82	1	0	-7.005202	-2.932906	-1.195024
83	1	0	-4.697813	-1.775662	-3.019845
84	6	0	3.306543	1.721828	-3.052827
85	6	0	5.767597	1.988314	-3.458520
86	6	0	4.597681	-0.657196	2.100808
87	6	0	3.308383	-0.457960	2.903294
88	6	0	5.782294	-0.891069	3.036763
89	1	0	4.477318	-1.573239	1.500886
90	1	0	4.795698	0.194095	-2.864532
91	1	0	5.664133	1.722419	-4.516187
92	1	0	6.782526	1.727151	-3.140293
93	1	0	3.141131	1.521129	-4.118532
94	1	0	2.510954	1.228989	-2.475824
95	1	0	3.198113	2.803884	-2.898989
96	1	0	5.908379	-0.063466	3.744696
97	1	0	6.721420	-1.001976	2.484182
98	1	0	3.125846	-1.328710	3.548365
99	1	0	3.389763	0.421578	3.555823
100	1	0	5.662915	3.077802	-3.394184
101	1	0	5.625877	-1.799899	3.629095
102	1	0	2.431705	-0.305494	2.258287
103	6	0	-1.659520	1.196465	-2.604146
104	1	0	-1.834094	1.462318	-3.659986
105	1	0	-2.373411	1.576592	-1.846256
106	8	0	-0.706252	0.502812	-2.296289
107	8	0	-0.064251	1.688323	0.361358
108	6	0	0.513936	2.897584	0.786418
109	1	0	-0.292983	3.534691	1.191691
110	6	0	1.522808	2.620007	1.885765
111	1	0	2.328614	1.980474	1.497459
112	1	0	1.973222	3.547926	2.258617
113	1	0	1.048496	2.103579	2.730703
114	6	0	1.153537	3.602203	-0.395254
115	1	0	0.423392	3.761398	-1.199288
116	1	0	1.559948	4.578170	-0.105261
117	1	0	1.979323	2.990991	-0.786876

L3-PhCHO-OTf

Zero-point correction= 1.03459 (a.u.)

Thermal correction to Gibbs Free Energy= 0.93960 (a.u.)

Sum of electronic and zero-point Energies= -4028.30050 (a.u.)

Sum of electronic and thermal Free Energies= -4028.39549 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.757156	-1.008768	-0.334593
2	8	0	0.389249	-2.465870	0.351083
3	8	0	0.634370	-1.241613	-2.292154
4	8	0	2.381445	-0.306513	-0.419975
5	7	0	-0.479573	-3.491200	0.067891
6	7	0	1.747957	-1.898164	-2.744649
7	7	0	4.549913	-0.239783	-1.007370
8	1	0	5.234862	-0.412306	-1.737751
9	7	0	-3.759561	-1.756212	0.342915
10	1	0	-4.280449	-2.485988	0.822006
11	6	0	-2.452107	-1.903452	0.192965
12	6	0	-1.864593	-3.223925	0.648915
13	1	0	-2.494196	-4.034550	0.252124
14	6	0	-1.671996	-3.382111	2.160806
15	1	0	-2.585131	-3.790404	2.606376
16	1	0	-1.483590	-2.408947	2.623517
17	6	0	-0.461419	-4.325176	2.311081
18	1	0	0.352280	-3.810930	2.829435
19	1	0	-0.699579	-5.228561	2.878186
20	6	0	-0.043582	-4.682844	0.894442
21	1	0	1.033439	-4.799553	0.752040
22	1	0	-0.571800	-5.560215	0.500065
23	6	0	-0.546077	-3.777522	-1.413156
24	1	0	-0.972959	-2.886206	-1.882035
25	1	0	-1.249496	-4.610921	-1.529813
26	6	0	0.775272	-4.163077	-2.065738
27	1	0	0.530638	-4.411975	-3.107430
28	1	0	1.140902	-5.106773	-1.638587
29	6	0	1.959750	-3.207922	-2.026302
30	1	0	2.224845	-2.958081	-0.993707
31	1	0	2.821557	-3.684413	-2.509687
32	6	0	1.593724	-2.028319	-4.245102
33	1	0	0.592345	-2.422269	-4.431330

34	6	0	1.825967	-0.611929	-4.760945
35	1	0	0.872857	-0.098099	-4.907582
36	6	0	2.654205	0.098480	-3.669804
37	1	0	3.575933	0.551536	-4.048288
38	1	0	2.067892	0.884621	-3.179762
39	6	0	2.975831	-1.003512	-2.662132
40	1	0	3.809647	-1.626494	-3.017364
41	6	0	3.277598	-0.502217	-1.265916
42	1	0	2.342890	-0.638047	-5.723633
43	1	0	2.348393	-2.744257	-4.593379
44	21	0	0.289484	-0.522846	-0.362363
45	6	0	5.009654	0.346180	0.233900
46	6	0	5.051494	-0.447590	1.386764
47	6	0	5.498178	0.169717	2.557564
48	6	0	5.402483	1.694171	0.199035
49	6	0	5.846248	2.255386	1.394182
50	6	0	5.288183	2.511596	-1.072050
51	1	0	6.164960	3.294079	1.417018
52	1	0	5.548328	-0.404455	3.480503
53	6	0	-4.461687	-0.560371	-0.070712
54	6	0	-4.635122	-0.322314	-1.443438
55	6	0	-5.299261	0.854203	-1.799722
56	6	0	-4.939811	0.296804	0.933849
57	6	0	-5.606589	1.449738	0.518378
58	6	0	-4.807044	-0.057688	2.398159
59	1	0	-5.997776	2.137172	1.264078
60	1	0	-5.463435	1.080510	-2.851558
61	6	0	-4.178630	-1.279550	-2.527760
62	16	0	-0.926871	0.849126	2.332088
63	8	0	-1.605608	-0.303574	2.914620
64	8	0	0.242419	0.416575	1.455839
65	8	0	-1.740181	1.873788	1.690042
66	6	0	-0.020342	1.674441	3.718467
67	9	0	0.793601	0.802281	4.292295
68	9	0	-0.903737	2.109912	4.597398
69	9	0	0.681301	2.690238	3.244315
70	6	0	-5.779538	1.728120	-0.832708
71	1	0	-6.310241	2.628107	-1.135589
72	6	0	5.887228	1.501600	2.562440
73	1	0	6.234432	1.957986	3.485755
74	6	0	-5.964659	-0.974002	2.809464
75	6	0	-4.734945	1.155680	3.317383
76	1	0	-6.925183	-0.454861	2.697547
77	1	0	-5.866240	-1.274726	3.858633

78	1	0	-6.026011	-1.888028	2.200718
79	1	0	-4.473739	0.832481	4.331148
80	1	0	-3.972186	1.868965	2.982443
81	1	0	-5.697881	1.677638	3.386778
82	1	0	-3.860962	-0.602103	2.527601
83	6	0	-5.343569	-1.702008	-3.423409
84	1	0	-3.800682	-2.195318	-2.046403
85	6	0	-3.042404	-0.687834	-3.365328
86	1	0	-6.179636	-2.103083	-2.840547
87	1	0	-5.723702	-0.858961	-4.011919
88	1	0	-2.719039	-1.403285	-4.133409
89	1	0	-2.173099	-0.428012	-2.749080
90	1	0	-5.020892	-2.472476	-4.133223
91	1	0	-3.372494	0.220420	-3.886458
92	6	0	3.857910	3.037383	-1.234563
93	6	0	6.283479	3.662809	-1.152722
94	6	0	4.643494	-1.905767	1.408878
95	6	0	3.380386	-2.113445	2.247479
96	6	0	5.778986	-2.802459	1.900734
97	1	0	4.413887	-2.214810	0.376297
98	1	0	5.500847	1.846497	-1.926347
99	1	0	6.241968	4.124726	-2.145000
100	1	0	7.311886	3.329533	-0.977279
101	1	0	3.748288	3.570143	-2.187938
102	1	0	3.106285	2.237092	-1.192721
103	1	0	3.620914	3.740080	-0.425436
104	1	0	6.026400	-2.594627	2.948375
105	1	0	6.692263	-2.664022	1.311760
106	1	0	3.023965	-3.148675	2.153294
107	1	0	3.581059	-1.929042	3.310096
108	1	0	6.052117	4.450989	-0.426099
109	1	0	5.489190	-3.858184	1.840723
110	1	0	2.571019	-1.440226	1.941333
111	6	0	-1.424660	1.941532	-1.113585
112	1	0	-2.323805	1.455183	-0.693765
113	8	0	-0.388649	1.259747	-1.273651
114	6	0	-1.526502	3.331054	-1.450506
115	6	0	-2.727260	3.993905	-1.147924
116	6	0	-0.456526	4.028292	-2.040530
117	6	0	-2.860236	5.343265	-1.438554
118	1	0	-3.534543	3.439185	-0.669731
119	6	0	-0.599329	5.371094	-2.335388
120	1	0	0.470012	3.499796	-2.254252
121	6	0	-1.799876	6.024923	-2.033848

122	1	0	-3.780204	5.869118	-1.200589
123	1	0	0.215321	5.922810	-2.795896
124	1	0	-1.904470	7.082396	-2.263579

L3- chalcone-OTf

Zero-point correction= 1.15083 (a.u.)

Thermal correction to Gibbs Free Energy= 1.05254 (a.u.)

Sum of electronic and zero-point Energies= -4336.44024 (a.u.)

Sum of electronic and thermal Free Energies= -4336.53852 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.378625	-0.873608	0.010301
2	8	0	0.656375	-2.670028	-1.061011
3	8	0	0.396658	-2.333850	1.811393
4	8	0	-1.765979	-1.465918	0.384235
5	7	0	1.813618	-3.407588	-1.111192
6	7	0	-0.416646	-3.397113	2.089143
7	7	0	-3.757261	-2.342390	0.954292
8	1	0	-4.258976	-2.941742	1.602601
9	7	0	4.446274	-0.802066	-0.858474
10	1	0	5.096514	-1.191408	-1.535522
11	6	0	3.240123	-1.339752	-0.765617
12	6	0	2.984625	-2.569764	-1.614320
13	1	0	3.858707	-3.233820	-1.534978
14	6	0	2.636632	-2.318295	-3.080687
15	1	0	3.552413	-2.178300	-3.664292
16	1	0	2.046923	-1.401887	-3.173958
17	6	0	1.831595	-3.561762	-3.506953
18	1	0	0.859211	-3.259259	-3.903682
19	1	0	2.337707	-4.144175	-4.281304
20	6	0	1.661934	-4.398908	-2.245329
21	1	0	0.680369	-4.865987	-2.134000
22	1	0	2.448832	-5.154296	-2.124800
23	6	0	2.135155	-4.056013	0.213119
24	1	0	2.335636	-3.243283	0.915152
25	1	0	3.059364	-4.625430	0.056221
26	6	0	1.067969	-4.996691	0.753448
27	1	0	1.490668	-5.441157	1.664722
28	1	0	0.937067	-5.843685	0.066516
29	6	0	-0.332009	-4.473514	1.034378

30	1	0	-0.776702	-4.055617	0.126541
31	1	0	-0.958898	-5.299271	1.392524
32	6	0	-0.057677	-3.867304	3.482621
33	1	0	1.029232	-3.969190	3.518438
34	6	0	-0.623894	-2.781443	4.389942
35	1	0	0.143953	-2.039078	4.619821
36	6	0	-1.772475	-2.128417	3.590857
37	1	0	-2.732302	-2.154973	4.116817
38	1	0	-1.545749	-1.081712	3.359749
39	6	0	-1.854460	-2.946259	2.302406
40	1	0	-2.421000	-3.873460	2.471270
41	6	0	-2.446996	-2.200651	1.124022
42	1	0	-0.966736	-3.212709	5.333872
43	1	0	-0.529982	-4.846253	3.633055
44	21	0	0.301957	-1.016918	0.192754
45	6	0	-4.542640	-1.601472	-0.005954
46	6	0	-4.371822	-1.845733	-1.374906
47	6	0	-5.181482	-1.117862	-2.251587
48	6	0	-5.484616	-0.690527	0.508530
49	6	0	-6.284066	-0.016498	-0.411351
50	6	0	-5.579160	-0.416760	1.996927
51	1	0	-7.037595	0.682737	-0.058271
52	1	0	-5.079938	-1.274160	-3.323476
53	6	0	4.850505	0.383078	-0.133526
54	6	0	5.015904	0.307519	1.258057
55	6	0	5.436888	1.470750	1.905445
56	6	0	5.079230	1.550283	-0.879383
57	6	0	5.499757	2.680508	-0.178696
58	6	0	4.950443	1.570711	-2.386160
59	1	0	5.691199	3.602724	-0.721726
60	1	0	5.587664	1.455881	2.983765
61	6	0	4.784457	-0.952109	2.069020
62	16	0	0.868633	1.323103	-1.999184
63	8	0	1.880944	0.709769	-2.852635
64	8	0	-0.043981	0.268621	-1.376409
65	8	0	1.288139	2.330245	-1.038163
66	6	0	-0.328683	2.140270	-3.149237
67	9	0	-0.816357	1.246348	-3.996860
68	9	0	0.302721	3.090519	-3.813802
69	9	0	-1.326614	2.670736	-2.453849
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71	1	0	6.022297	3.530385	1.722432
72	6	0	-6.129775	-0.223817	-1.778733
73	1	0	-6.765954	0.309253	-2.481735

74	6	0	6.302071	1.239074	-3.026243
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78	1	0	6.704222	0.271750	-2.692353
79	1	0	4.162564	2.780988	-3.987225
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81	1	0	5.139118	3.700679	-2.841911
82	1	0	4.224525	0.798438	-2.672614
83	6	0	6.042720	-1.366019	2.831997
84	1	0	4.550095	-1.773713	1.374417
85	6	0	3.596786	-0.795984	3.022775
86	1	0	6.905500	-1.470257	2.164903
87	1	0	6.306210	-0.630341	3.600871
88	1	0	3.402699	-1.744010	3.543590
89	1	0	2.679976	-0.491690	2.499969
90	1	0	5.885837	-2.324415	3.341217
91	1	0	3.808849	-0.043178	3.793045
92	6	0	-4.451899	0.527389	2.427440
93	6	0	-6.924025	0.147688	2.437327
94	6	0	-3.397721	-2.857318	-1.937655
95	6	0	-2.347235	-2.186556	-2.824747
96	6	0	-4.129485	-3.963927	-2.697232
97	1	0	-2.869753	-3.338697	-1.101334
98	1	0	-5.444464	-1.371268	2.534531
99	1	0	-6.966017	0.204395	3.530119
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101	1	0	-4.462532	0.679662	3.513666
102	1	0	-3.457190	0.157372	2.140696
103	1	0	-4.583945	1.508127	1.949008
104	1	0	-4.658662	-3.564841	-3.570605
105	1	0	-4.868251	-4.471694	-2.066826
106	1	0	-1.560762	-2.905963	-3.088631
107	1	0	-2.792916	-1.826854	-3.760541
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111	6	0	-0.238802	1.754521	1.618486
112	8	0	0.218888	0.576394	1.492809
113	6	0	0.528349	2.699554	2.435558
114	6	0	-0.104385	3.581796	3.324546
115	6	0	1.928844	2.678409	2.355877
116	6	0	0.652597	4.433133	4.119482
117	1	0	-1.187309	3.565946	3.426894

118	6	0	2.675055	3.551083	3.133576
119	1	0	2.419379	2.002355	1.655366
120	6	0	2.041277	4.424963	4.016701
121	1	0	0.160706	5.099747	4.822427
122	1	0	3.758851	3.552305	3.048317
123	1	0	2.633587	5.098784	4.630482
124	6	0	-1.473434	2.093601	0.972418
125	1	0	-2.029208	1.253603	0.552730
126	6	0	-1.889382	3.371200	0.760007
127	1	0	-1.248856	4.180500	1.115055
128	6	0	-3.091593	3.789688	0.080481
129	6	0	-3.359829	5.167197	-0.001531
130	6	0	-4.000293	2.884629	-0.502670
131	6	0	-4.503469	5.633439	-0.634228
132	1	0	-2.655979	5.871318	0.439002
133	6	0	-5.137339	3.354081	-1.136711
134	1	0	-3.807477	1.810883	-0.475873
135	6	0	-5.393710	4.726436	-1.202425
136	1	0	-4.699715	6.700391	-0.688868
137	1	0	-5.828240	2.649462	-1.592786
138	1	0	-6.288158	5.086525	-1.704184
