Theoretical and Experimental Studies on the Structure-property Relationship of Chiral *N,N'*-dioxide-metal Catalysts Probed by Carbonyl-ene Reaction of Isatin

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Supporting Information：

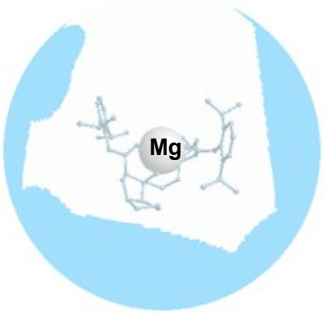
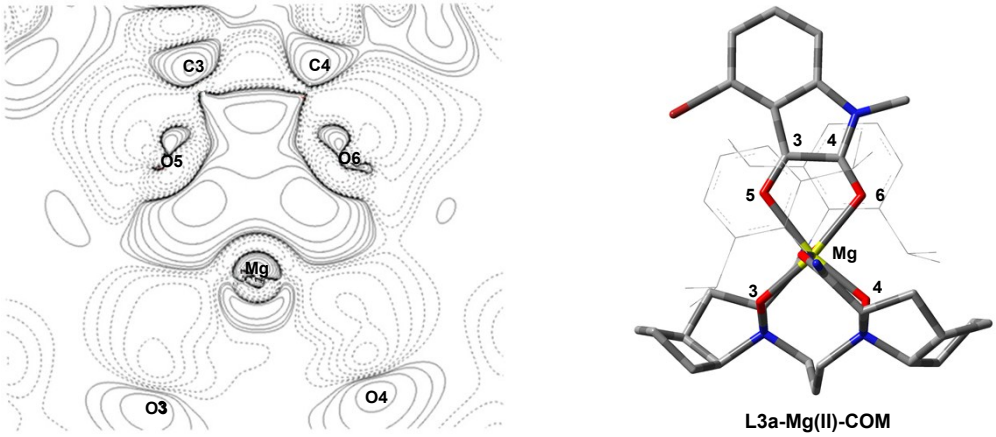


Figure S1. The percent of Mg ion coordination sphere shielded by ligand L3a (blue area) and the corresponding G-parameter G(L3a)=75.72 %.



Scheme S1. Plot of difference map of electron density(DED) for L3a-Mg(II)-COM obtained by Mutilwfn program. The solid and dashed contour lines exhibit where electron density is increased and decreased, respectively.

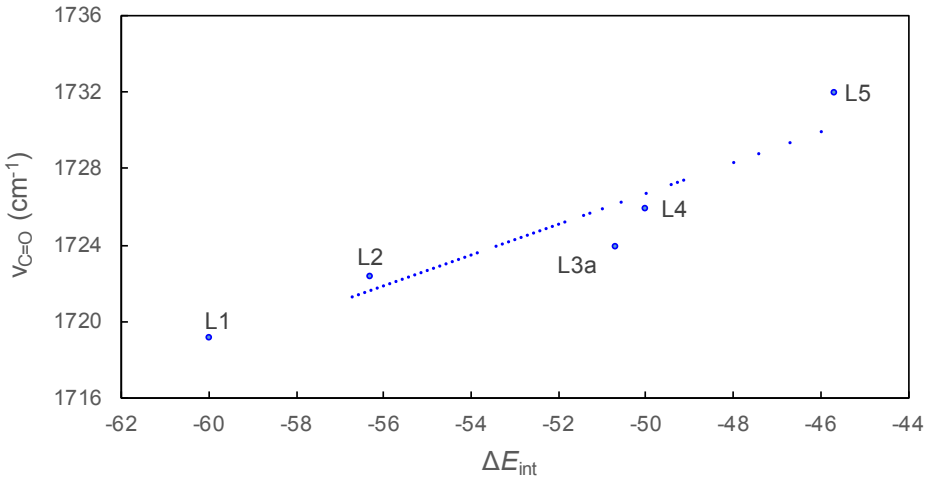
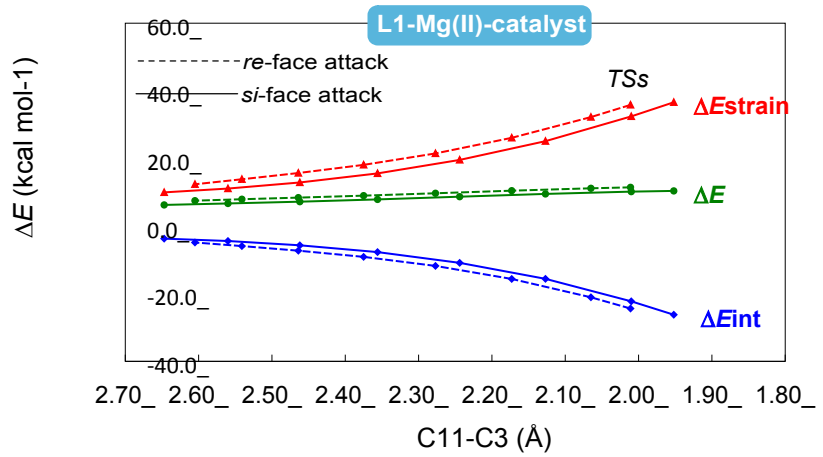


Figure S2. Correlation between interaction energy (ΔE_{int}) of fragments and C=O stretching frequency of R1a ($\nu_{C=O}$, cm^{-1}) in Lm-Mg(II)-COM (m=1~5). The correlation equation is $\nu_{C=O} = 0.80\Delta E_{int} + 1766.80$, R^2=0.90.

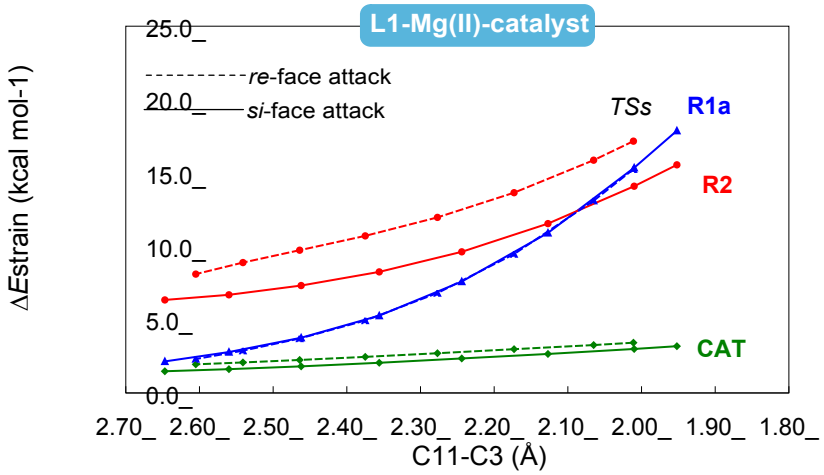
Table S1. Energy Decomposition Analysis (EDA) for two competing TSs in chiral-controlling step (C-C bond formation step) *via* two pathways (*si*-face attack and *re*-face attack) catalyzed by Lm-Mg(II) catalysts(m=1~5). The energies are in kcal mol^{-1}.

Catalyst	Path	$\Delta E^{\neq}_{Pauli}$	$\Delta V^{\neq}_{elstat}$	$\Delta E^{\neq}_{oi}$	$\Delta E^{\neq}_{disp}$	[a]$\Delta\Delta G^{\neq}$
L1-Mg(II)	*si*-face	137.0	-70.2	-86.2	-19.8	-0.7
	re-face	119.5	-63.4	-76.0	-15.7	
L2-Mg(II)	*si*-face	144.3	-73.9	-90.9	-19.7	-0.9
	re-face	128.4	-66.9	-78.9	-20.2	
L3a-Mg(II)	*si*-face	161.6	-81.6	-100.7	-22.3	2.9
	re-face	143.0	-72.9	-86.8	-21.0	
L4-Mg(II)	*si*-face	171.2	-85.6	-106.7	-24.7	5.2
	re-face	162.5	-82.5	-99.3	-20.1	
L5-Mg(II)	*si*-face	159.7	-80.8	-96.2	-26.1	3.2
	re-face	158.2	-80.5	-95.9	-21.1	

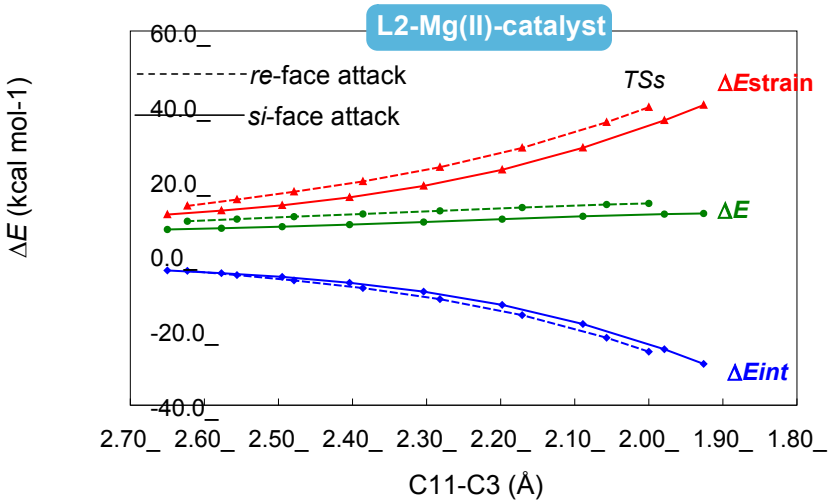
[a] the relative Gibbs energy of transition state for *si*-face attack is set to zero.


L1-Mg(II)-catalyst
60.0
re-face attack
40.0
si-face attack
TSs
ΔEstrain
20.0
ΔE
0.0
-20.0
ΔEint
-40.0
2.70 2.60 2.50 2.40 2.30 2.20 2.10 2.00 1.90 1.80
C11-C3 (Å)
ΔE (kcal mol-1)

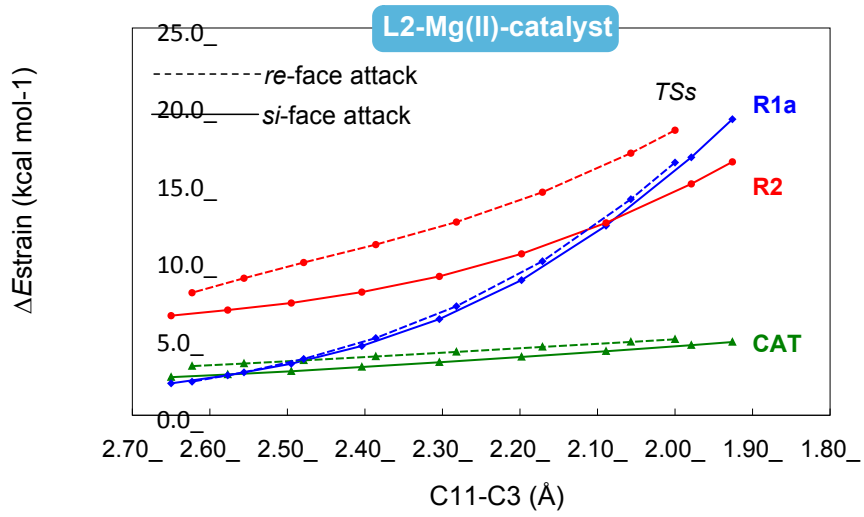
(a)


L1-Mg(II)-catalyst
25.0
re-face attack
20.0
si-face attack
TSs
R1a
15.0
R2
10.0
5.0
CAT
0.0
2.70 2.60 2.50 2.40 2.30 2.20 2.10 2.00 1.90 1.80
C11-C3 (Å)
ΔEstrain (kcal mol-1)

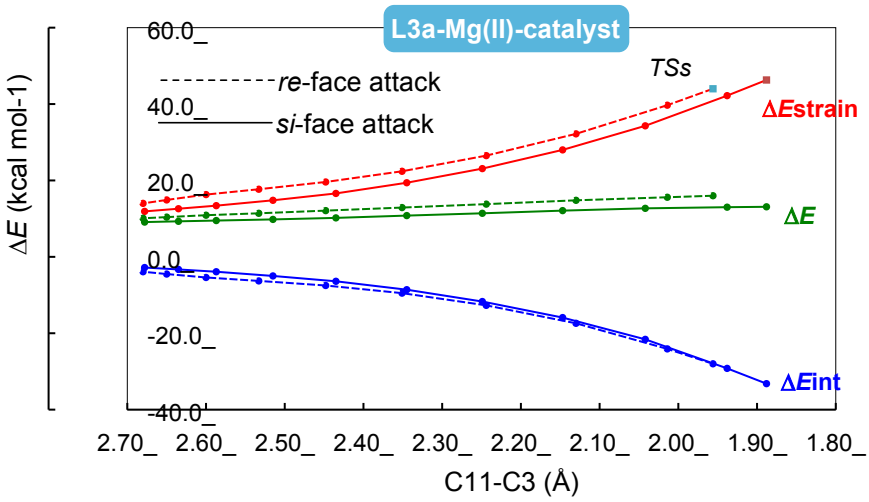
(b)


L2-Mg(II)-catalyst
60.0
re-face attack
40.0
si-face attack
TSs
ΔEstrain
20.0
ΔE
0.0
-20.0
ΔEint
-40.0
2.70 2.60 2.50 2.40 2.30 2.20 2.10 2.00 1.90 1.80
C11-C3 (Å)
ΔE (kcal mol-1)

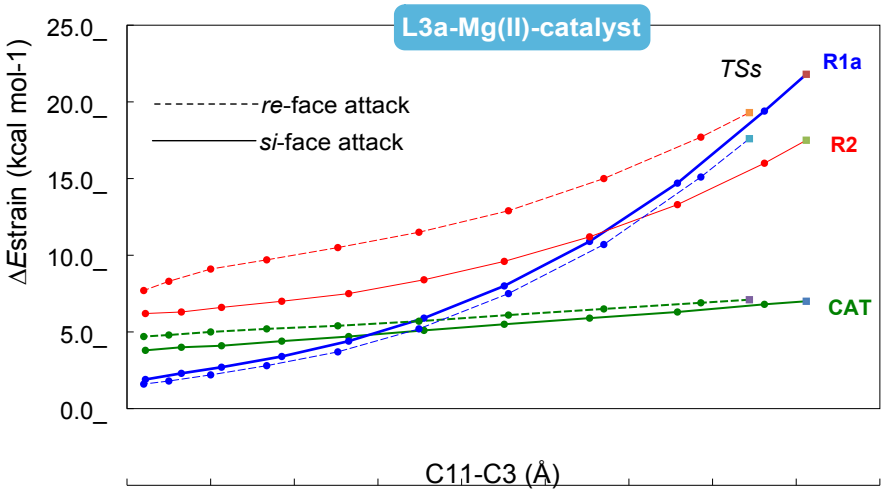
(c)


L2-Mg(II)-catalyst
ΔEstrain (kcal mol-1)
25.0
20.0
15.0
10.0
5.0
0.0
re-face attack
si-face attack
TSs
R1a
R2
CAT
2.70 2.60 2.50 2.40 2.30 2.20 2.10 2.00 1.90 1.80
C11-C3 (Å)

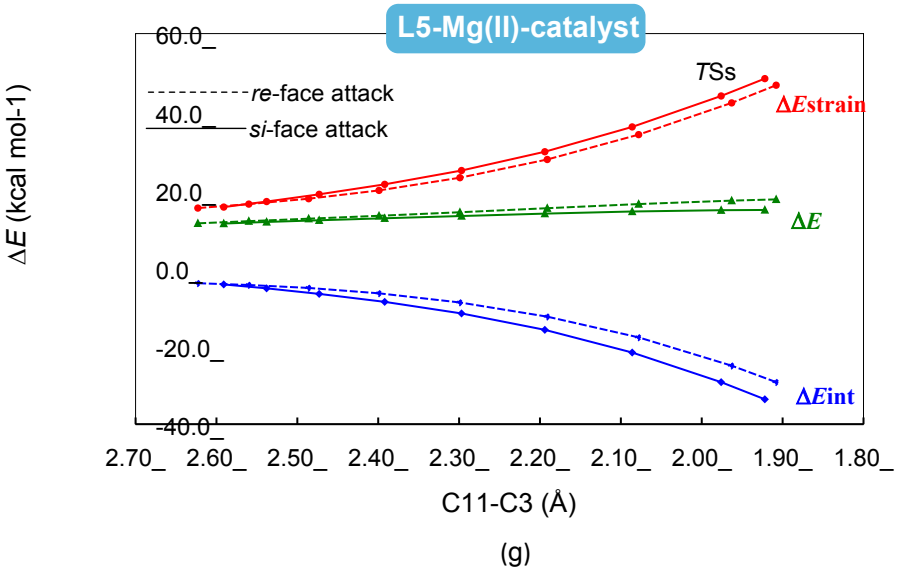
(d)


L3a-Mg(II)-catalyst
ΔE (kcal mol-1)
60.0
40.0
20.0
0.0
-20.0
-40.0
re-face attack
si-face attack
TSs
ΔEstrain
ΔE
ΔEint
2.70 2.60 2.50 2.40 2.30 2.20 2.10 2.00 1.90 1.80
C11-C3 (Å)

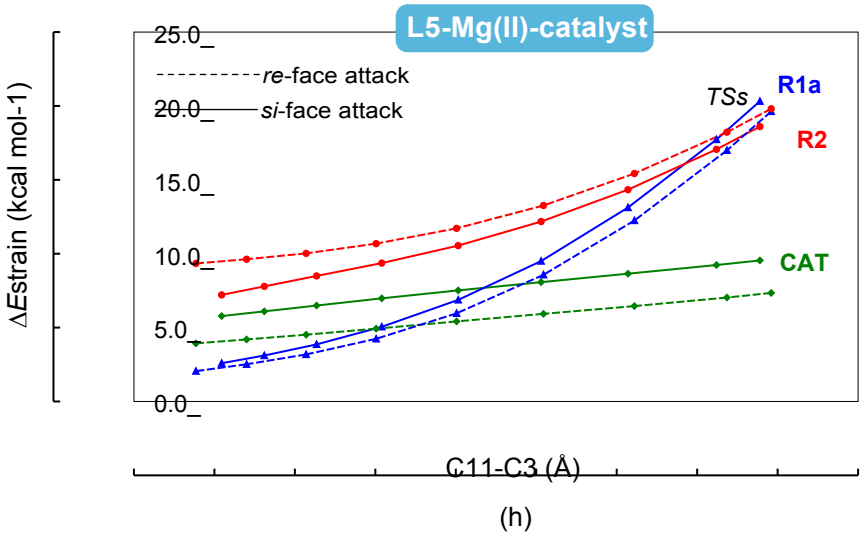
(e)


L3a-Mg(II)-catalyst
ΔEstrain (kcal mol-1)
25.0
20.0
15.0
10.0
5.0
0.0
re-face attack
si-face attack
TSs
R1a
R2
CAT
C11-C3 (Å)

(f)



(g)



(h)

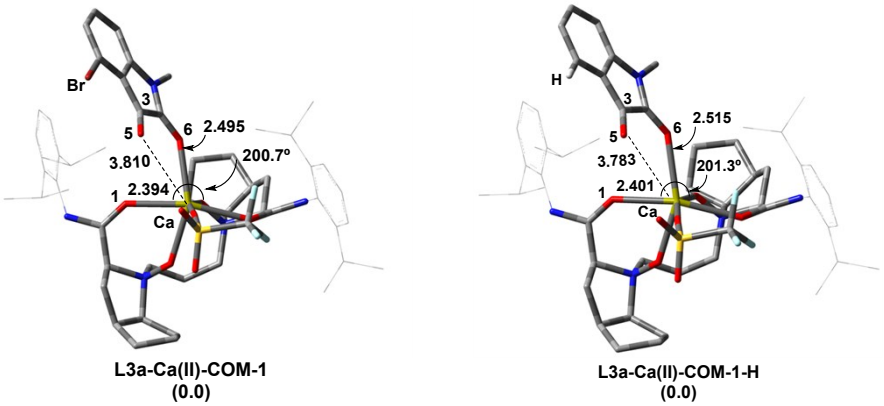
Figure S3. Activation strain analysis of carbonyl-ene reaction between *N*-methyl-protected isatin (R1a) and 2-methoxypropene (R2) catalyzed by L1-Mg(II)~L5-Mg(II) catalyst. i) Evolution of ΔE, ΔE_{int} and ΔE_{strain} along reaction coordinate(a, c, e, g); ii) Evolution of ΔE_{strain} of three energy components along reaction coordinate(b, d, f, h).

Table S2. Results of Energy Decomposition Analysis(EDA) and Activation Strain Model (ASM) as well as the corresponding G-parameter(%) for hexacoordinate complexes(L3a~L3d). The energies are in kcal mol^{-1}.

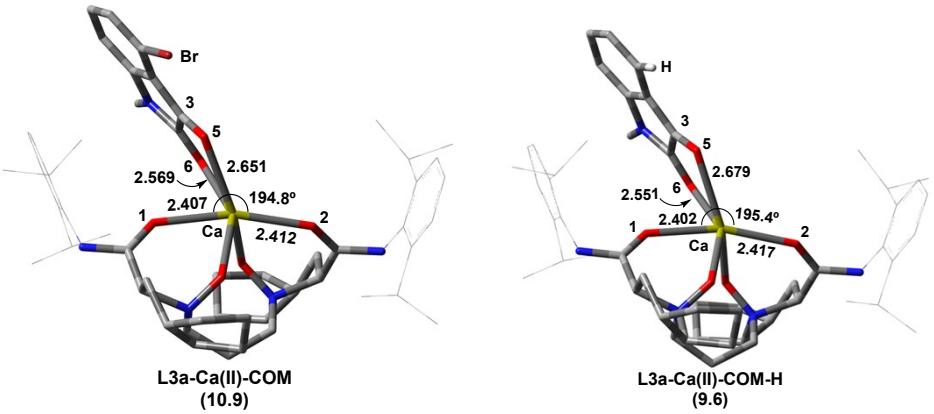
Species	G(L)	ΔE_{int}	ΔE_{strain}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{disp}
L3a-Mg(II)-COM	72.18	-50.7	8.8	41.0	-52.6	-30.1	-17.7
L3b-Mg(II)-COM	72.82	-51.3	7.9	40.8	-53.8	-29.6	-18.3
L3c-Mg(II)-COM	70.34	-54.6	8.2	38.2	-54.0	-30.4	-14.1
L3d-Mg(II)-COM	75.31	-50.2	8.9	43.6	-54.6	-29.9	-20.9

Table S3. Results of Activation Strain Model (ASM) for two competing TSs in chiral-controlling step(C-C bond formation step) *via* two competing pathways(*si*-face attack and *re*-face attack) catalyzed by L3a-Mg(II)~L3d-Mg(II) catalysts. The energies are in kcal mol^{-1}.

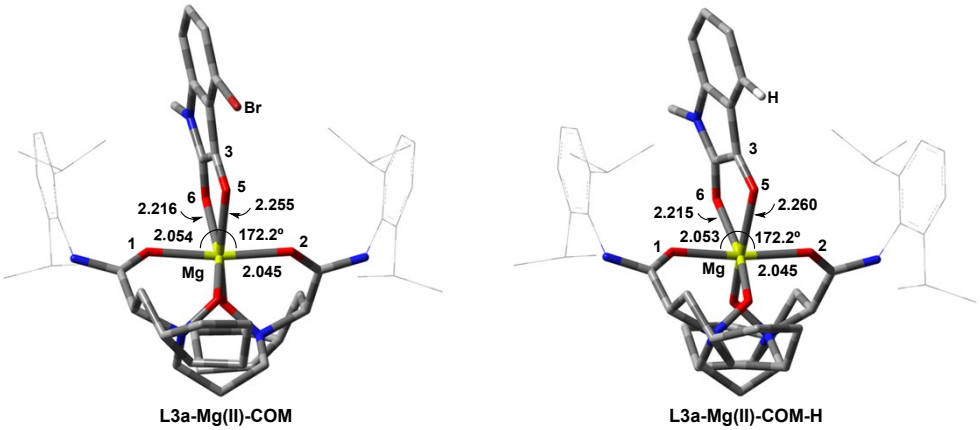
Catalyst	Paths	$\Delta E^{\neq}_{strain}$				$\Delta E^{\neq}_{int}$
		CAT	R1a	R2	Sum	
L3a-Mg(II)	*si*-face	7.0	21.8	17.5	46.3	-33.2
	re-face	7.1	17.6	19.3	44.0	-28.0
L3b-Mg(II)	*si*-face	5.1	18.4	17.7	41.1	-32.8
	re-face	5.7	17.9	18.9	42.5	-29.7
L3c-Mg(II)	*si*-face	5.8	19.6	16.6	41.9	-31.4
	re-face	5.6	17.0	18.3	40.9	-25.5
L3d-Mg(II)	*si*-face	7.9	21.6	17.0	46.6	-33.5
	re-face	7.9	19.0	19.2	46.1	-29.9



L3a-Ca(II) complex (*monodentate model*)
(a)



L3a-Ca(II) complex (*bidentate model*)
(b)



L3a-Mg(II) complex (*bidentate model*)

(c)

Figure S4. Comparison of the optimized geometries of hexacoordinate L3a-Ca(II)(a and b) and L3a-Mg(II) complexes(c) containing 4-bromoisatin or isatin in bidentate model. Their relative Gibbs free energies difference are in kcal mol^{-1}.

Table S4. Selected structural parameter of the monodentate and bidentate complexes formed by 4-bromoisatin(R1a) or isatin (without Br substituent) towards L3a-M(II)(M=Ca and Mg) complexes, and their difference of relative Gibbs free energies ($\Delta\Delta G$, kcal mol^{-1}).

Model	**Substituent**	**Complex**	**Distance(Å)**			**Angle(°)**		**[b]$\Delta\Delta G$**
			$R_{(C)O-M}$	**[a]R_{O-M}**	**$R_{ipr...C3}$**	**$\alpha_{O1-M-O2}$**	**θ_1**	
Mono-dentate	Br	L3a-Ca(II)-COM-1	2.401	2.495	4.429	200.7	37.1	-
	H	L3a-Ca(II)-COM-1-H	2.411	2.515	4.211	201.3	37.3	-
Bidentate	Br	L3a-Ca(II)-COM	2.419	2.610	4.103	194.8	44.5	10.9
	H	L3a-Ca(II)-COM-H	2.410	2.615	4.081	195.4	43.9	9.6
Bidentate	Br	L3a-Mg(II)-COM	2.050	2.221	3.909	172.2	22.4	-
	H	L3a-Mg(II)-COM-H	2.049	2.238	3.939	172.2	20.6	-

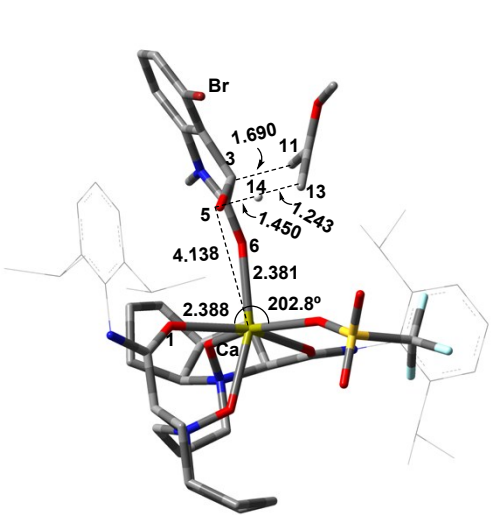
[a] the distance between ligated O atom in carbonyl substrate and metal center in hexacoordinate complexes (O_6-Ca distance for monodentate complex and the average O-metal distance for bidentate complex).

[b] the relative energy of monodentate complexes L3a-Ca(II)-COM-1 or L3a-Ca(II)-COM-1-H are set to zero.

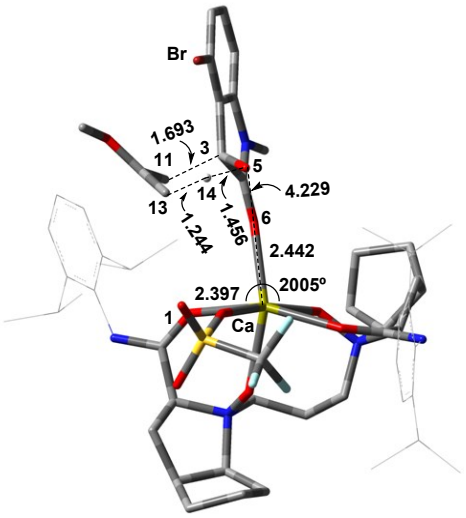
Table S5. Relative Gibbs free energy of transition states (ΔG, kcal mol^{-1}) in asymmetric carbonyl-ene reaction of 2-methoxypropene towards 4-Br-substituted isatin (R1a) or isatin (without Br substituent) catalyzed by L3a-Ca(II) catalyst.

Model	Substituent	Transition state	ΔG	[a]$\Delta\Delta G$	Mechanism
Mono-dentate	Br	L3a-Ca(II)-TS-*si*-1	22.3	1.0	One-step two-stage
		L3a-Ca(II)-TS-*re*-1	23.3		
	H	L3a-Ca(II)-TS-*si*-1-H	23.0	1.4	
		L3a-Ca(II)-TS-*re*-1-H	21.6		
Bidentate	Br	L3a-Ca(II)-TS1-*si*	26.3	2.2	Stepwise
		L3a-Ca(II)-TS1-*re*	28.5		
		L3a-Ca(II)-TS2-*si*	26.5		
		L3a-Ca(II)-TS2-*re*	30.8		
	H	L3a-Ca(II)-TS1-*si*-H	27.7	3.6	
		L3a-Ca(II)-TS1-*re*-H	31.3		
		L3a-Ca(II)-TS2-*si*-H	27.5		
		L3a-Ca(II)-TS2-*re*-H	32.1		

[a] the relative Gibbs free energy difference ($\Delta\Delta G$, kcal mol^{-1}) of two competing transition states in chiral-controlling step (C-C bond formation step).



L3a-Ca(II)-TS-*si*-1 (22.3)



L3a-Ca(II)-TS-*re*-1 (23.3)

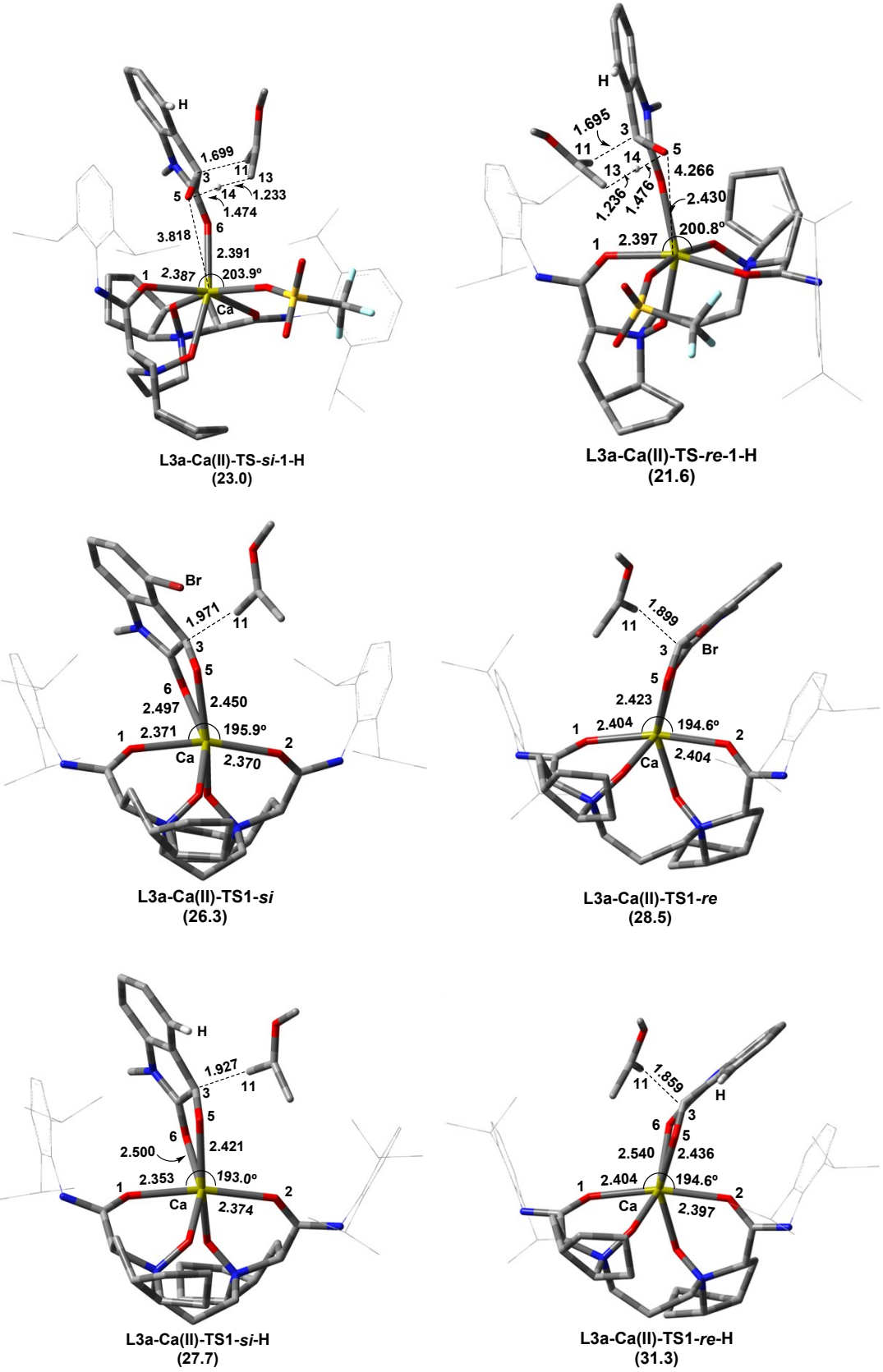


Figure S5. Optimized geometries of competing transition states in the carbonyl-ene reaction between isatin without Br substituent and R2 catalyzed by L3a-Ca(II) complex. Relative energies are in kcal mol^{-1}.

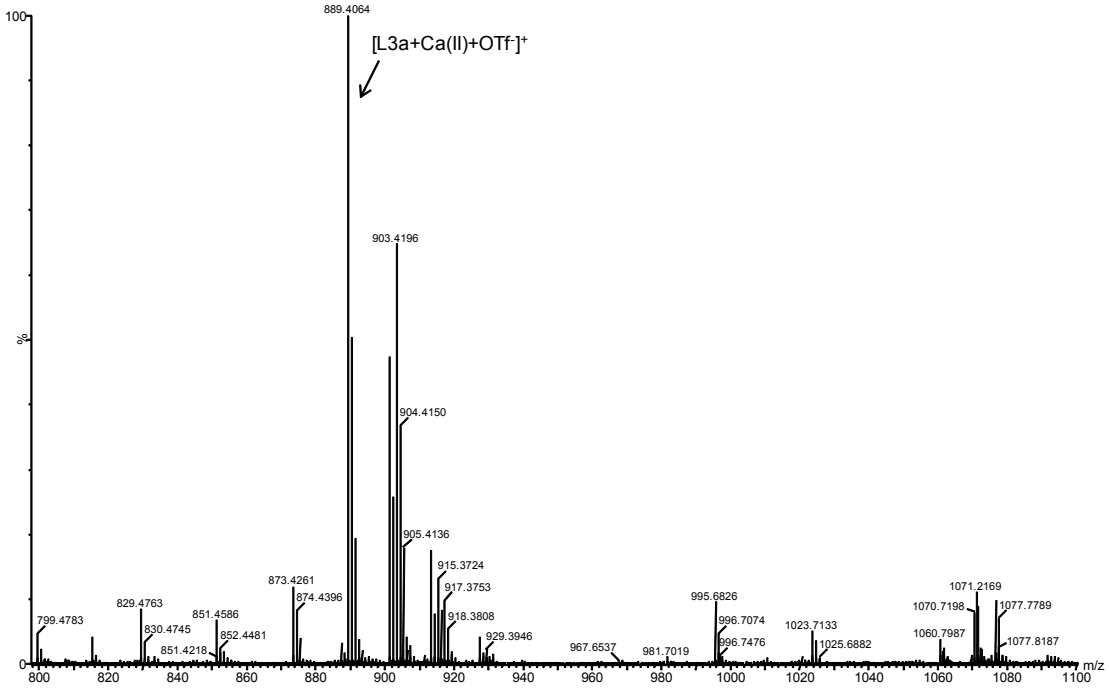


Figure S6. ESI mass spectra in positive-ion mode for the 1:1 L3a:$Ca(OTf)_2$ mixture, HRMS: $[L3a+Ca(II)+OTf]^+$ (m/z=889.4064, calcd:889.4068).

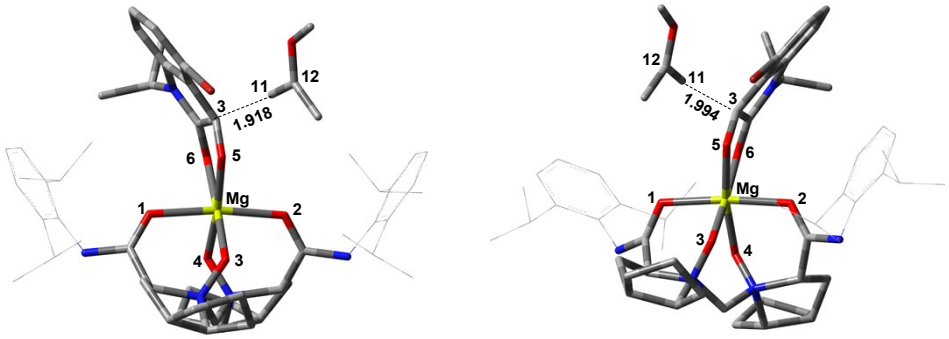


Figure S7. Optimized geometries of two competing transition states in the carbonyl-ene reaction between R1b and R2 catalyzed by L1-Mg(II) complex. Relative energies are in kcal mol^{-1}.

Table S6. Comparison of the results of Activation Strain Model (ASM) and Energy Decomposition Analysis (EDA) for carbonyl-ene reaction of R2 towards R1a or R1b catalyzed by L1-Mg(II). The energies are in kcal mol^{-1}.

Species	Path	$\Delta\Delta G^{\neq}$	$\Delta E^{\neq}$	ASM		EDA			
				$\Delta E^{\neq}_{strain}$	$\Delta E^{\neq}_{int}$	$\Delta E^{\neq}_{Pauli}$	$\Delta V^{\neq}_{elstat}$	$\Delta E^{\neq}_{oi}$	$\Delta E^{\neq}_{disp}$
R1a	*si*-face	0.7	10.4	36.6	-26.2	137.0	-70.2	-86.2	-19.8
	re-face		11.5	35.8	-24.4	119.5	-63.4	-76.0	-15.7
R1b	*si*-face	2.9	10.3	39.6	-29.3	148.4	-75.3	-92.9	-20.4
	re-face		12.9	39.1	-26.2	126.1	-66.4	-79.3	-16.3

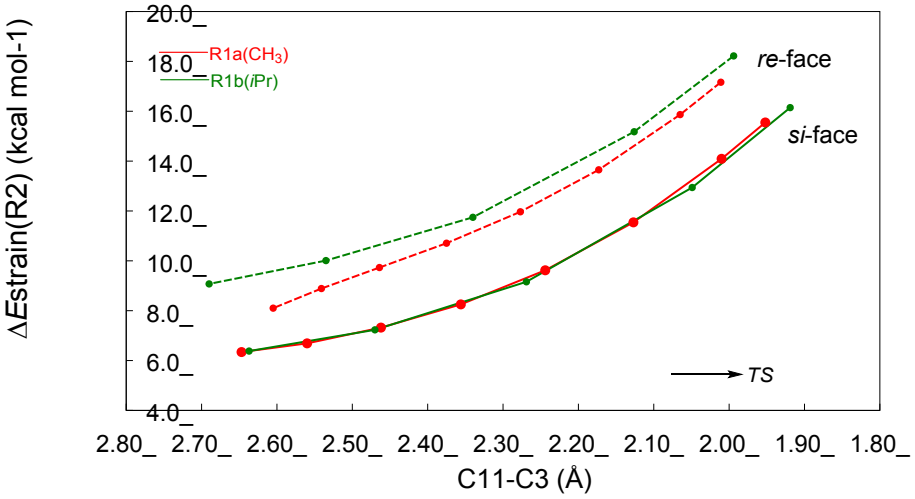


Figure S8. The strain energy($\Delta E_{strain(R2)}$) of R2 along reaction coordinates of two competing pathways (*re*-face attack and *si*-face attack) in the carbonyl-ene reactions of 2-methoxypropene(R2) towards R1a or R1b, respectively.

Cartesian coordinates of all stationary points

R1a

Zero-point correction= 0.13266 a.u.

Thermal correction to Gibbs Free Energy= 0.09442 a.u.

Sum of electronic and zero-point Energies= -3125.98903 a.u.

Sum of electronic and thermal Free Energies= -3126.02726 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.185437	-1.222830	-0.002063
2	6	0	0.628349	-1.339688	-0.002308
3	6	0	0.146046	0.046681	-0.002842
4	6	0	1.286672	0.884533	-0.002641
5	7	0	2.467588	0.124190	-0.002651
6	8	0	0.033245	-2.397430	-0.001448
7	6	0	-1.122773	0.619171	-0.000706
8	6	0	1.173202	2.268016	-0.002034
9	8	0	2.979497	-2.144665	-0.000188
10	6	0	3.811090	0.677536	0.006808
11	1	0	3.973021	1.281457	0.905658
12	1	0	4.511595	-0.158846	0.002451
13	1	0	3.979401	1.296315	-0.880615
14	6	0	-1.264942	2.007733	-0.000533
15	6	0	-0.119497	2.809417	-0.001014
16	35	0	-2.678212	-0.477550	0.001508
17	1	0	-2.250840	2.458605	-0.000203
18	1	0	-0.238121	3.889189	-0.001498
19	1	0	2.045806	2.911531	-0.002924

R1b

Zero-point correction= 0.18854 a.u.

Thermal correction to Gibbs Free Energy= 0.14609 a.u.

Sum of electronic and zero-point Energies= -3204.59664 a.u.

Sum of electronic and thermal Free Energies= -3204.63908 a.u.

The number of imaginary frequencies 0

Standard orientation

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

1	6	0	-1.435591	-1.618773	-0.010835
2	6	0	0.115293	-1.494512	-0.010192
3	6	0	0.374786	-0.052849	-0.005229
4	6	0	-0.881851	0.604795	-0.009181
5	7	0	-1.936865	-0.333663	-0.009790
6	8	0	0.867854	-2.447427	-0.012977
7	6	0	1.551140	0.692684	-0.000869
8	6	0	-0.951962	1.994235	-0.015580
9	8	0	-2.069075	-2.658692	-0.010179
10	6	0	-3.393815	-0.077017	0.007581
11	1	0	-3.816233	-1.085496	0.002899
12	6	0	1.499330	2.085988	-0.003113
13	6	0	0.250735	2.712634	-0.011251
14	35	0	3.247007	-0.173622	0.007496
15	1	0	2.411006	2.672340	0.000612
16	1	0	0.210776	3.798198	-0.015124
17	1	0	-1.895574	2.523468	-0.024292
18	6	0	-3.868371	0.637362	-1.262573
19	1	0	-4.963579	0.667390	-1.269411
20	1	0	-3.506844	1.668270	-1.325900
21	1	0	-3.537714	0.099343	-2.157464
22	6	0	-3.839596	0.611844	1.302392
23	1	0	-4.934210	0.650397	1.330632
24	1	0	-3.496973	0.050924	2.178577
25	1	0	-3.468680	1.638188	1.383993

R2

Zero-point correction= 0.11206 a.u.

Thermal correction to Gibbs Free Energy= 0.08267a.u.

Sum of electronic and zero-point Energies= -232.41202 a.u.

Sum of electronic and thermal Free Energies= -232.44141 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.623987	0.015172	-0.004144
2	6	0	-0.395616	1.461572	-0.000228
3	6	0	-0.474172	0.121744	-0.000676
4	8	0	0.588688	-0.735541	0.000850
5	6	0	1.895702	-0.170658	-0.000279
6	1	0	2.591398	-1.012773	0.000684

7	6	0	-1.760054	-0.654156	-0.000165
8	1	0	2.065436	0.440539	-0.895978
9	1	0	-1.816843	-1.307889	-0.879710
10	1	0	-1.308292	2.047480	0.000085
11	1	0	0.541602	2.006246	0.002556
12	1	0	-1.819564	-1.299835	0.885122
13	1	0	2.065580	0.444371	0.892667

L1-Mg(II)

Zero-point correction= 0.95678 a.u.

Thermal correction to Gibbs Free Energy= 0.87909 a.u.

Sum of electronic and zero-point Energies= -2318.17175 a.u.

Sum of electronic and thermal Free Energies= -2318.24944 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.900115	-0.509639	0.950853
2	12	0	0.022098	-0.019169	0.853086
3	8	0	0.437184	-1.356066	-0.558517
4	8	0	-0.415886	1.380786	-0.492449
5	8	0	1.933373	0.520435	0.952749
6	7	0	-3.826850	-0.623684	-0.241241
7	1	0	-4.266769	-0.792143	-1.140489
8	7	0	-0.364821	-1.209509	-1.668741
9	7	0	3.833210	0.577120	-0.284012
10	1	0	4.261757	0.737472	-1.190249
11	7	0	0.363183	1.277403	-1.623237
12	6	0	-4.651260	-0.164336	0.816461
13	6	0	-5.219311	1.135867	0.750256
14	6	0	-6.040889	1.576705	1.803882
15	1	0	-6.484347	2.563520	1.784735
16	6	0	-6.299957	0.757739	2.896797
17	1	0	-6.930102	1.115734	3.700950
18	6	0	-5.763405	-0.523164	2.955960
19	1	0	-5.999229	-1.139741	3.813264
20	6	0	-4.950394	-1.014477	1.918147
21	6	0	-4.447219	-2.453506	1.988924
22	1	0	-3.860021	-2.708218	1.086191
23	6	0	-3.517197	-2.657385	3.190653
24	1	0	-2.683038	-1.925000	3.160254

25	1	0	-3.078447	-3.677859	3.164575
26	1	0	-4.062434	-2.535837	4.150357
27	6	0	-5.612430	-3.450055	2.023169
28	1	0	-5.225936	-4.490189	1.962331
29	1	0	-6.283749	-3.282682	1.153446
30	1	0	-6.204483	-3.354204	2.957781
31	6	0	-4.949863	2.068270	-0.426817
32	1	0	-4.280502	1.585035	-1.167321
33	6	0	-6.245637	2.405692	-1.173127
34	1	0	-6.757077	1.471892	-1.491161
35	1	0	-6.017496	2.998467	-2.084848
36	1	0	-6.939249	2.995902	-0.537474
37	6	0	-4.234133	3.344022	0.030707
38	1	0	-4.864821	3.939852	0.723194
39	1	0	-3.994860	3.979929	-0.847192
40	1	0	-3.285317	3.083957	0.546218
41	6	0	-2.498421	-0.751796	-0.120843
42	6	0	-1.866389	-1.415448	-1.350480
43	1	0	-2.396837	-1.091860	-2.250313
44	6	0	-1.965303	-2.940112	-1.198869
45	1	0	-3.010201	-3.256755	-1.206922
46	1	0	-1.518923	-3.241076	-0.246248
47	6	0	-1.175114	-3.481680	-2.396312
48	1	0	-1.854068	-3.591564	-3.246162
49	6	0	-0.377409	-4.776509	-2.130278
50	1	0	-0.872893	-5.421017	-1.396608
51	1	0	-0.289815	-5.346689	-3.062399
52	6	0	1.010610	-4.293731	-1.676848
53	1	0	1.781695	-5.058431	-1.810551
54	1	0	0.990440	-4.012355	-0.619045
55	6	0	1.262363	-3.045275	-2.543196
56	1	0	2.007273	-2.361652	-2.132924
57	1	0	1.594694	-3.343319	-3.544811
58	6	0	-0.115757	-2.397037	-2.706107
59	1	0	-0.265588	-1.936363	-3.682679
60	6	0	-0.006593	0.049925	-2.431882
61	1	0	0.848064	-0.182030	-3.063385
62	1	0	-0.873020	0.311510	-3.034141
63	6	0	0.087129	2.498001	-2.606088
64	1	0	0.241204	2.082173	-3.602173
65	6	0	-1.302103	3.111017	-2.408007
66	1	0	-2.035273	2.392950	-2.036162
67	1	0	-1.640934	3.458838	-3.391217
68	6	0	-1.072254	4.310768	-1.469831

69	1	0	-1.045566	3.966076	-0.431443
70	1	0	-1.857759	5.067500	-1.556598
71	6	0	0.306434	4.846344	-1.893327
72	1	0	0.793410	5.446763	-1.117771
73	1	0	0.205760	5.479320	-2.782706
74	6	0	1.127026	3.586939	-2.253350
75	1	0	1.780988	3.763430	-3.111450
76	6	0	1.961319	2.995426	-1.108980
77	1	0	1.547470	3.252618	-0.129398
78	1	0	3.001610	3.324527	-1.144031
79	6	0	1.871229	1.476429	-1.323483
80	1	0	2.388097	1.194227	-2.244233
81	6	0	2.515070	0.759631	-0.129759
82	6	0	4.667721	0.120836	0.767866
83	6	0	5.147263	-1.216148	0.759051
84	6	0	5.961101	-1.656859	1.819094
85	1	0	6.340796	-2.669782	1.842160
86	6	0	6.295056	-0.803939	2.864523
87	1	0	6.917236	-1.162333	3.674728
88	6	0	5.846526	0.511496	2.866418
89	1	0	6.139326	1.152888	3.687233
90	6	0	5.046668	1.002863	1.818631
91	6	0	4.638304	2.472496	1.824631
92	1	0	4.056697	2.718130	0.917086
93	6	0	5.865123	3.392501	1.795977
94	1	0	5.545619	4.451182	1.688253
95	1	0	6.511737	3.140341	0.928233
96	1	0	6.463841	3.304300	2.726836
97	6	0	3.739253	2.794824	3.023891
98	1	0	2.855639	2.121969	3.033954
99	1	0	3.371719	3.841139	2.954680
100	1	0	4.286791	2.678747	3.982986
101	6	0	4.799653	-2.184507	-0.366324
102	1	0	4.148095	-1.695131	-1.118602
103	6	0	6.059069	-2.634979	-1.115546
104	1	0	6.616384	-1.750761	-1.492461
105	1	0	5.779668	-3.261896	-1.989536
106	1	0	6.730629	-3.229483	-0.460754
107	6	0	4.018766	-3.391647	0.165243
108	1	0	4.618611	-3.979661	0.890955
109	1	0	3.745297	-4.064766	-0.673108
110	1	0	3.085643	-3.052193	0.663711

L1-Mg(II)-COM

Zero-point correction= 1.09142 a.u.

Thermal correction to Gibbs Free Energy= 0.99810 a.u.

Sum of electronic and zero-point Energies= -5444.21711 a.u.

Sum of electronic and thermal Free Energies= -5444.31043 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.111709	1.835943	-2.017466
2	6	0	0.630879	2.389171	-0.682051
3	6	0	1.036598	3.744375	-0.950375
4	6	0	0.795351	3.964010	-2.332186
5	7	0	0.247264	2.799834	-2.942576
6	8	0	0.626461	1.664122	0.310923
7	6	0	1.574771	4.768256	-0.166681
8	6	0	1.078330	5.173049	-2.933566
9	8	0	-0.326590	0.683723	-2.111876
10	6	0	-0.093137	2.676945	-4.355368
11	1	0	0.801947	2.823847	-4.966241
12	1	0	-0.487957	1.673970	-4.520179
13	1	0	-0.850872	3.418212	-4.623650
14	6	0	1.869066	5.998302	-0.754174
15	6	0	1.619960	6.182202	-2.117408
16	35	0	1.896439	4.483825	1.675973
17	1	0	2.286944	6.805127	-0.163191
18	1	0	1.853781	7.144399	-2.563044
19	1	0	0.894046	5.348190	-3.987239
20	8	0	1.686471	-0.977034	-0.660141
21	12	0	-0.167736	-0.323923	-0.196514
22	8	0	-0.962743	-2.111883	-0.732955
23	8	0	0.149465	-1.070906	1.667728
24	8	0	-2.043072	0.215750	0.319559
25	7	0	3.340263	-2.494950	-0.362631
26	1	0	3.594762	-3.449940	-0.136283
27	7	0	-0.380022	-3.207054	-0.148770
28	7	0	-4.083870	-0.361247	1.113875
29	1	0	-4.627578	-0.978827	1.707001
30	7	0	-0.788299	-1.973175	2.097581
31	6	0	4.376802	-1.528534	-0.410397
32	6	0	5.068936	-1.178336	0.779800
33	6	0	6.087466	-0.209719	0.717876

34	1	0	6.632970	0.077678	1.607021
35	6	0	6.413959	0.406602	-0.484224
36	1	0	7.195749	1.154945	-0.511259
37	6	0	5.747196	0.060002	-1.653396
38	1	0	6.034046	0.552174	-2.573265
39	6	0	4.733316	-0.915426	-1.645174
40	6	0	4.066011	-1.299826	-2.962639
41	1	0	3.314194	-2.096713	-2.804209
42	6	0	3.322470	-0.105712	-3.575431
43	1	0	2.618018	0.331555	-2.837395
44	1	0	2.733627	-0.434218	-4.458421
45	1	0	4.028152	0.687245	-3.901716
46	6	0	5.084153	-1.877308	-3.953612
47	1	0	4.563317	-2.249171	-4.862130
48	1	0	5.622314	-2.733283	-3.492647
49	1	0	5.827364	-1.114019	-4.266914
50	6	0	4.725834	-1.813601	2.123458
51	1	0	3.889888	-2.534462	2.017573
52	6	0	5.914080	-2.608467	2.677344
53	1	0	6.242020	-3.370273	1.938103
54	1	0	5.618011	-3.139394	3.607484
55	1	0	6.772736	-1.944646	2.912565
56	6	0	4.256366	-0.757399	3.130628
57	1	0	5.065131	-0.037173	3.374473
58	1	0	3.940382	-1.248753	4.074726
59	1	0	3.391095	-0.195677	2.718344
60	6	0	2.042727	-2.151901	-0.468704
61	6	0	1.110980	-3.364529	-0.539377
62	1	0	1.499992	-4.166860	0.093817
63	6	0	1.011942	-3.844680	-1.994864
64	1	0	1.975327	-4.226266	-2.339784
65	1	0	0.722518	-3.005372	-2.633798
66	6	0	-0.075452	-4.928086	-1.953036
67	1	0	0.397395	-5.895430	-1.761573
68	6	0	-1.008823	-4.987223	-3.183871
69	1	0	-0.501740	-4.664933	-4.099601
70	1	0	-1.339921	-6.020801	-3.339442
71	6	0	-2.209792	-4.099613	-2.813092
72	1	0	-3.104203	-4.343645	-3.394820
73	1	0	-1.971721	-3.045059	-2.982073
74	6	0	-2.399638	-4.348839	-1.304644
75	1	0	-2.939070	-3.550450	-0.792326
76	1	0	-2.943910	-5.286727	-1.139965
77	6	0	-0.982674	-4.545588	-0.758575

78	1	0	-0.925647	-5.269448	0.055145
79	6	0	-0.693906	-3.279677	1.334485
80	1	0	-1.654142	-3.780487	1.441090
81	1	0	0.093168	-3.869238	1.800315
82	6	0	-0.520673	-2.383146	3.612387
83	1	0	-0.870316	-3.413710	3.684837
84	6	0	0.946259	-2.207258	4.013757
85	1	0	1.627723	-2.306676	3.167165
86	1	0	1.182082	-2.999010	4.735066
87	6	0	1.004492	-0.829247	4.699224
88	1	0	1.089547	-0.046122	3.939960
89	1	0	1.854650	-0.735039	5.382054
90	6	0	-0.346522	-0.726112	5.427906
91	1	0	-0.636204	0.305362	5.655457
92	1	0	-0.303614	-1.271990	6.377795
93	6	0	-1.357304	-1.417564	4.485319
94	1	0	-2.107936	-1.982164	5.045098
95	6	0	-2.071365	-0.494824	3.488841
96	1	0	-1.479172	0.397831	3.267186
97	1	0	-3.056974	-0.179107	3.837980
98	6	0	-2.198941	-1.347534	2.216836
99	1	0	-2.878504	-2.184830	2.395659
100	6	0	-2.742032	-0.470142	1.084311
101	6	0	-4.789158	0.496770	0.232560
102	6	0	-5.564247	-0.059702	-0.820319
103	6	0	-6.256686	0.803927	-1.688779
104	1	0	-6.856543	0.410612	-2.498868
105	6	0	-6.183859	2.182980	-1.531476
106	1	0	-6.718354	2.832247	-2.213279
107	6	0	-5.436769	2.732075	-0.496189
108	1	0	-5.412812	3.809128	-0.395720
109	6	0	-4.742237	1.909441	0.409332
110	6	0	-3.991502	2.557185	1.570114
111	1	0	-3.526663	1.787312	2.215150
112	6	0	-4.944717	3.342524	2.479424
113	1	0	-4.399378	3.714724	3.373223
114	1	0	-5.767989	2.683632	2.829812
115	1	0	-5.384443	4.215655	1.952640
116	6	0	-2.855231	3.455699	1.064579
117	1	0	-2.193417	2.891478	0.375219
118	1	0	-2.238741	3.809623	1.918571
119	1	0	-3.249502	4.343775	0.526852
120	6	0	-5.657605	-1.567147	-1.037550
121	1	0	-5.032184	-2.112055	-0.301707

122	6	0	-7.094141	-2.062743	-0.836462
123	1	0	-7.460847	-1.771012	0.170893
124	1	0	-7.129043	-3.171110	-0.906852
125	1	0	-7.779939	-1.641510	-1.601853
126	6	0	-5.130501	-1.963412	-2.421603
127	1	0	-5.766592	-1.553415	-3.233727
128	1	0	-5.119311	-3.069501	-2.520287
129	1	0	-4.093954	-1.588033	-2.556908

L2-Mg(II)

Zero-point correction= 0.98510 a.u.

Thermal correction to Gibbs Free Energy= 0.90689 a.u.

Sum of electronic and zero-point Energies= -2357.49701 a.u.

Sum of electronic and thermal Free Energies= -2357.57521a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.987785	0.171903	0.579556
2	12	0	-0.008598	0.022201	0.390290
3	8	0	0.039605	1.613535	-0.775678
4	8	0	-0.026860	-1.556087	-0.780791
5	8	0	-2.011332	-0.139865	0.542392
6	7	0	4.101323	0.632968	-0.088902
7	1	0	4.715071	1.115775	-0.737096
8	7	0	0.921591	1.560258	-1.839064
9	7	0	-4.109337	-0.628942	-0.156037
10	1	0	-4.704570	-1.150984	-0.791317
11	7	0	-0.890408	-1.506687	-1.857655
12	6	0	4.698087	-0.067419	0.985823
13	6	0	5.036595	-1.437228	0.834747
14	6	0	5.601132	-2.123100	1.925787
15	1	0	5.866270	-3.168893	1.844664
16	6	0	5.827987	-1.474318	3.135303
17	1	0	6.259859	-2.018320	3.965672
18	6	0	5.506071	-0.128946	3.281554
19	1	0	5.698072	0.346232	4.234483
20	6	0	4.947851	0.598391	2.214765
21	6	0	4.625127	2.077799	2.401971
22	1	0	4.231700	2.515066	1.461938
23	6	0	3.535254	2.274911	3.461462

24	1	0	2.627380	1.696395	3.186682
25	1	0	3.251156	3.347343	3.522640
26	1	0	3.880204	1.945802	4.464544
27	6	0	5.882985	2.882996	2.749586
28	1	0	5.646903	3.968555	2.771314
29	1	0	6.666897	2.717723	1.979573
30	1	0	6.289534	2.596177	3.742189
31	6	0	4.796627	-2.178739	-0.476736
32	1	0	4.353992	-1.501236	-1.236671
33	6	0	6.113836	-2.689845	-1.071853
34	1	0	6.827707	-1.847534	-1.196804
35	1	0	5.933045	-3.137269	-2.072691
36	1	0	6.579977	-3.462385	-0.424514
37	6	0	3.798383	-3.326195	-0.286539
38	1	0	4.199638	-4.105713	0.394694
39	1	0	3.576107	-3.802658	-1.264809
40	1	0	2.848846	-2.935973	0.137115
41	6	0	2.772469	0.748344	-0.206588
42	6	0	2.358724	1.694030	-1.340432
43	1	0	2.995363	1.493735	-2.208415
44	6	0	2.453344	3.175352	-0.959376
45	1	0	3.494393	3.481806	-0.836647
46	1	0	1.924727	3.348373	-0.017791
47	6	0	1.763827	3.884277	-2.141191
48	1	0	2.519092	4.121111	-2.895424
49	6	0	0.925162	5.128533	-1.770471
50	1	0	1.322867	5.644161	-0.889966
51	1	0	0.944243	5.841887	-2.602801
52	6	0	-0.504726	4.596881	-1.567237
53	1	0	-1.263362	5.378026	-1.680269
54	1	0	-0.611975	4.163295	-0.568184
55	6	0	-0.635503	3.492233	-2.631337
56	1	0	-1.433905	2.776308	-2.428265
57	1	0	-0.834816	3.942367	-3.611439
58	6	0	0.754305	2.849706	-2.718487
59	1	0	1.014286	2.535608	-3.728342
60	6	0	0.737742	0.270388	-2.664283
61	1	0	1.097085	0.475920	-3.671073
62	1	0	1.378585	-0.480734	-2.208408
63	6	0	-0.709541	-0.210004	-2.669190
64	1	0	-1.066480	-0.411154	-3.678338
65	1	0	-1.353658	0.537017	-2.208982
66	6	0	-0.685317	-2.786316	-2.740732
67	1	0	-0.923421	-2.466870	-3.754074

68	6	0	0.711291	-3.411924	-2.625152
69	1	0	1.497048	-2.688694	-2.402437
70	1	0	0.936232	-3.855626	-3.602849
71	6	0	0.572021	-4.523255	-1.569600
72	1	0	0.647208	-4.092492	-0.566483
73	1	0	1.345548	-5.291698	-1.666757
74	6	0	-0.843906	-5.074146	-1.812284
75	1	0	-1.255882	-5.604069	-0.946914
76	1	0	-0.832530	-5.778958	-2.651945
77	6	0	-1.691611	-3.838816	-2.191027
78	1	0	-2.429272	-4.080858	-2.961028
79	6	0	-2.413487	-3.148603	-1.017507
80	1	0	-1.900603	-3.318970	-0.066698
81	1	0	-3.450427	-3.475857	-0.918288
82	6	0	-2.334466	-1.663655	-1.386907
83	1	0	-2.956804	-1.463689	-2.265675
84	6	0	-2.777091	-0.728931	-0.253231
85	6	0	-4.730063	0.033609	0.929000
86	6	0	-5.008413	1.422493	0.843638
87	6	0	-5.591503	2.068992	1.948742
88	1	0	-5.811387	3.127952	1.917343
89	6	0	-5.896973	1.363062	3.107862
90	1	0	-6.342358	1.877129	3.950002
91	6	0	-5.636161	-0.001011	3.188354
92	1	0	-5.885300	-0.520146	4.104351
93	6	0	-5.060486	-0.689561	2.105236
94	6	0	-4.793930	-2.186706	2.222870
95	1	0	-4.389543	-2.587791	1.271694
96	6	0	-6.086495	-2.965730	2.494646
97	1	0	-5.888551	-4.058302	2.453333
98	1	0	-6.847118	-2.726101	1.720884
99	1	0	-6.504794	-2.726935	3.495103
100	6	0	-3.740651	-2.474087	3.297894
101	1	0	-2.806407	-1.915375	3.073740
102	1	0	-3.495871	-3.557756	3.312743
103	1	0	-4.100822	-2.180735	4.306731
104	6	0	-4.693954	2.223250	-0.416108
105	1	0	-4.262916	1.567592	-1.201479
106	6	0	-5.966359	2.831820	-1.018262
107	1	0	-6.722103	2.037301	-1.198100
108	1	0	-5.735028	3.311485	-1.993465
109	1	0	-6.406755	3.600371	-0.348370
110	6	0	-3.648843	3.307548	-0.132144
111	1	0	-4.027358	4.057389	0.594038

112	1	0	-3.388525	3.837305	-1.072548
113	1	0	-2.725139	2.846617	0.278787

L2-Mg(II)-COM

Zero-point correction= 1.11905 a.u.

Thermal correction to Gibbs Free Energy= 1.02563 a.u.

Sum of electronic and zero-point Energies= -5483.54358 a.u.

Sum of electronic and thermal Free Energies= -5483.63700 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.134247	1.261741	-2.028753
2	6	0	0.356749	2.069488	-0.743004
3	6	0	0.642778	3.415566	-1.171265
4	6	0	0.603083	3.396867	-2.590375
5	7	0	0.298702	2.092583	-3.072117
6	8	0	0.271542	1.500901	0.342676
7	6	0	0.927647	4.606741	-0.499921
8	6	0	0.839014	4.532695	-3.337061
9	8	0	-0.128988	0.055381	-1.993200
10	6	0	0.205368	1.722121	-4.479694
11	1	0	1.154751	1.927988	-4.981768
12	1	0	-0.012891	0.655078	-4.533052
13	1	0	-0.597780	2.285216	-4.962735
14	6	0	1.171300	5.766623	-1.234648
15	6	0	1.124642	5.714731	-2.630893
16	35	0	0.977650	4.642535	1.391324
17	1	0	1.395259	6.700115	-0.731480
18	1	0	1.315652	6.624913	-3.191269
19	1	0	0.807683	4.525212	-4.420518
20	8	0	1.876853	-0.982412	0.105830
21	12	0	-0.153420	-0.671604	0.065589
22	8	0	-0.250964	-2.583706	-0.572121
23	8	0	-0.328039	-0.859983	2.068277
24	8	0	-2.188494	-0.420319	0.111267
25	7	0	3.885689	-1.997742	-0.104594
26	1	0	4.401760	-2.845483	-0.312635
27	7	0	0.465038	-3.554215	0.090608
28	7	0	-4.318968	-0.331589	0.859326
29	1	0	-4.968018	-0.439940	1.630983

30	7	0	-1.278860	-1.707532	2.587061
31	6	0	4.588908	-0.770148	-0.131826
32	6	0	4.920336	-0.118932	1.085187
33	6	0	5.563231	1.131448	1.034977
34	1	0	5.822465	1.657190	1.944344
35	6	0	5.876052	1.723448	-0.184222
36	1	0	6.367452	2.687779	-0.204407
37	6	0	5.557967	1.083591	-1.377613
38	1	0	5.809666	1.574649	-2.308351
39	6	0	4.916745	-0.168308	-1.375492
40	6	0	4.562910	-0.832456	-2.702742
41	1	0	4.090496	-1.821303	-2.532629
42	6	0	3.542899	0.005462	-3.481763
43	1	0	2.643540	0.177378	-2.855913
44	1	0	3.223469	-0.533996	-4.399097
45	1	0	3.964856	0.988445	-3.780166
46	6	0	5.815970	-1.098486	-3.544912
47	1	0	5.547732	-1.678248	-4.454054
48	1	0	6.548713	-1.695358	-2.960609
49	1	0	6.299434	-0.152172	-3.866966
50	6	0	4.588539	-0.739597	2.438983
51	1	0	4.107044	-1.731498	2.309538
52	6	0	5.858554	-0.986292	3.261871
53	1	0	6.575186	-1.606059	2.681254
54	1	0	5.608771	-1.535129	4.195118
55	1	0	6.354613	-0.032940	3.541593
56	6	0	3.592056	0.130280	3.214074
57	1	0	4.027108	1.120524	3.465775
58	1	0	3.303607	-0.373021	4.161178
59	1	0	2.673839	0.288205	2.609327
60	6	0	2.541127	-2.021173	-0.053989
61	6	0	1.954290	-3.425958	-0.227968
62	1	0	2.473024	-4.107937	0.454962
63	6	0	2.047368	-3.954706	-1.663087
64	1	0	3.081039	-4.188668	-1.930205
65	1	0	1.670323	-3.198492	-2.357066
66	6	0	1.149380	-5.206986	-1.642010
67	1	0	1.766284	-6.076487	-1.398033
68	6	0	0.316453	-5.449863	-2.922463
69	1	0	0.813558	-5.057946	-3.816418
70	1	0	0.181774	-6.527921	-3.070859
71	6	0	-1.044006	-4.784943	-2.644835
72	1	0	-1.846165	-5.193115	-3.268645
73	1	0	-0.987817	-3.707414	-2.826499

74	6	0	-1.273888	-5.046053	-1.146025
75	1	0	-2.003928	-4.374961	-0.691017
76	1	0	-1.628433	-6.073739	-0.998141
77	6	0	0.116860	-4.963039	-0.503364
78	1	0	0.242544	-5.659623	0.324937
79	6	0	0.222375	-3.496575	1.607728
80	1	0	0.483115	-4.470523	2.019547
81	1	0	0.909181	-2.748125	1.994966
82	6	0	-1.212118	-3.098675	1.935902
83	1	0	-1.688737	-3.801414	2.618595
84	1	0	-1.796140	-3.035428	1.020178
85	6	0	-1.121228	-1.787737	4.144729
86	1	0	-1.464642	-2.786432	4.411694
87	6	0	0.297474	-1.491534	4.649421
88	1	0	1.080105	-1.770427	3.943157
89	1	0	0.439320	-2.091575	5.557192
90	6	0	0.295363	0.004418	5.009078
91	1	0	0.451045	0.599246	4.104076
92	1	0	1.081045	0.264049	5.726237
93	6	0	-1.118675	0.236615	5.570247
94	1	0	-1.430924	1.285924	5.535207
95	1	0	-1.162126	-0.082425	6.618511
96	6	0	-2.038455	-0.668393	4.718620
97	1	0	-2.831168	-1.115174	5.325232
98	6	0	-2.677046	0.010260	3.491933
99	1	0	-2.077266	0.854325	3.140940
100	1	0	-3.691422	0.362330	3.692062
101	6	0	-2.671477	-1.097159	2.433907
102	1	0	-3.384249	-1.882653	2.710574
103	6	0	-3.011410	-0.598293	1.026812
104	6	0	-4.784921	0.303256	-0.315976
105	6	0	-5.135952	-0.476885	-1.448539
106	6	0	-5.533839	0.177142	-2.628710
107	1	0	-5.801964	-0.388672	-3.511108
108	6	0	-5.584407	1.565890	-2.691477
109	1	0	-5.887803	2.052948	-3.609277
110	6	0	-5.242571	2.331882	-1.581796
111	1	0	-5.284069	3.409658	-1.667132
112	6	0	-4.843669	1.720579	-0.379407
113	6	0	-4.457295	2.589692	0.813314
114	1	0	-4.213664	1.960986	1.693376
115	6	0	-5.617757	3.493654	1.245907
116	1	0	-5.356869	4.024139	2.186787
117	1	0	-6.526545	2.883381	1.436975

118	1	0	-5.852386	4.254829	0.472480
119	6	0	-3.201545	3.413689	0.507917
120	1	0	-2.369270	2.740732	0.213067
121	1	0	-2.882682	3.975459	1.411993
122	1	0	-3.382165	4.140251	-0.312495
123	6	0	-5.078734	-2.001191	-1.415927
124	1	0	-4.775567	-2.361204	-0.410578
125	6	0	-6.456763	-2.614926	-1.691509
126	1	0	-7.205309	-2.209226	-0.977587
127	1	0	-6.417415	-3.717193	-1.556471
128	1	0	-6.797493	-2.403830	-2.727101
129	6	0	-4.032452	-2.533695	-2.401903
130	1	0	-4.303916	-2.292750	-3.451419
131	1	0	-3.949843	-3.637304	-2.308502
132	1	0	-3.038862	-2.089301	-2.179485

L3a-Mg(II)

Zero-point correction= 1.01549 a.u.

Thermal correction to Gibbs Free Energy= 0.933070 a.u.

Sum of electronic and zero-point Energies= -2396.81288 a.u.

Sum of electronic and thermal Free Energies= -2396.89530 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.987904	-0.130409	0.393452
2	12	0	-0.015931	0.031528	0.102670
3	8	0	-0.076588	-1.530719	-1.077507
4	8	0	0.080597	1.621797	-1.029215
5	8	0	1.929740	0.233299	0.551038
6	7	0	-4.108229	-0.859162	0.097081
7	1	0	-4.750824	-1.479282	-0.385682
8	7	0	-1.110668	-1.616699	-1.998290
9	7	0	4.079303	0.864066	0.217021
10	1	0	4.743323	1.424299	-0.307256
11	7	0	1.148276	1.746118	-1.902905
12	6	0	-4.620837	-0.070137	1.153423
13	6	0	-4.960874	1.287958	0.920147
14	6	0	-5.415078	2.070234	1.997345
15	1	0	-5.669195	3.112332	1.855318
16	6	0	-5.544150	1.523559	3.270224

17	1	0	-5.894325	2.139796	4.088318
18	6	0	-5.221616	0.189190	3.497537
19	1	0	-5.327197	-0.203101	4.500335
20	6	0	-4.758956	-0.628660	2.450677
21	6	0	-4.390444	-2.081376	2.736632
22	1	0	-4.073500	-2.595313	1.805746
23	6	0	-3.204224	-2.165688	3.703856
24	1	0	-2.340152	-1.596760	3.298513
25	1	0	-2.888707	-3.223391	3.831221
26	1	0	-3.465581	-1.755726	4.702474
27	6	0	-5.593010	-2.868278	3.271380
28	1	0	-5.331804	-3.944123	3.367082
29	1	0	-6.448546	-2.785189	2.567510
30	1	0	-5.911728	-2.498223	4.268672
31	6	0	-4.830965	1.915316	-0.464657
32	1	0	-4.511525	1.157391	-1.209916
33	6	0	-6.176333	2.457548	-0.962240
34	1	0	-6.944267	1.654822	-0.937194
35	1	0	-6.080977	2.808456	-2.012217
36	1	0	-6.527546	3.309721	-0.343017
37	6	0	-3.759312	3.010639	-0.471347
38	1	0	-4.049428	3.865539	0.175591
39	1	0	-3.606931	3.388079	-1.505101
40	1	0	-2.794510	2.598748	-0.106464
41	6	0	-2.804256	-0.873446	-0.199218
42	6	0	-2.438566	-1.880161	-1.289766
43	1	0	-3.203458	-1.824960	-2.071803
44	6	0	-2.296927	-3.331933	-0.826122
45	1	0	-3.259088	-3.747175	-0.518563
46	1	0	-1.606016	-3.387192	0.019867
47	6	0	-1.730207	-4.022283	-2.084843
48	1	0	-2.567697	-4.362724	-2.700289
49	6	0	-0.720372	-5.161204	-1.822063
50	1	0	-0.931719	-5.690908	-0.887106
51	1	0	-0.780337	-5.895253	-2.634307
52	6	0	0.656801	-4.475788	-1.833800
53	1	0	1.476167	-5.175694	-2.027235
54	1	0	0.844553	-3.992565	-0.870161
55	6	0	0.520441	-3.408635	-2.934346
56	1	0	1.247988	-2.599552	-2.857008
57	1	0	0.638599	-3.873131	-3.921053
58	6	0	-0.931906	-2.918320	-2.845219
59	1	0	-1.361964	-2.680382	-3.818244
60	6	0	-1.223091	-0.359167	-2.849705

61	1	0	-2.000857	-0.574525	-3.586956
62	1	0	-1.580674	0.426098	-2.187171
63	6	0	0.041505	0.096961	-3.583880
64	1	0	-0.284684	0.915798	-4.234944
65	1	0	0.384021	-0.696690	-4.257561
66	6	0	1.289024	0.526622	-2.805908
67	1	0	1.639113	-0.287556	-2.173753
68	1	0	2.079310	0.777524	-3.517848
69	6	0	1.000064	3.082989	-2.700347
70	1	0	1.468817	2.882780	-3.663922
71	6	0	-0.447819	3.578407	-2.827864
72	1	0	-1.179795	2.769734	-2.811920
73	1	0	-0.525815	4.082621	-3.798909
74	6	0	-0.629506	4.600532	-1.691600
75	1	0	-0.860274	4.078678	-0.758197
76	1	0	-1.439295	5.309597	-1.891815
77	6	0	0.746340	5.281855	-1.593067
78	1	0	0.918992	5.768790	-0.627329
79	1	0	0.839976	6.050876	-2.369004
80	6	0	1.766341	4.153518	-1.864211
81	1	0	2.626854	4.519670	-2.431133
82	6	0	2.283615	3.411096	-0.614064
83	1	0	1.560356	3.434129	0.205621
84	1	0	3.234173	3.809963	-0.253347
85	6	0	2.445217	1.979079	-1.128976
86	1	0	3.243020	1.952489	-1.877871
87	6	0	2.772211	0.936569	-0.056018
88	6	0	4.590763	-0.017389	1.197286
89	6	0	4.958616	-1.338919	0.833956
90	6	0	5.415944	-2.216685	1.833608
91	1	0	5.687720	-3.235862	1.592530
92	6	0	5.524867	-1.795866	3.155401
93	1	0	5.879638	-2.483791	3.912178
94	6	0	5.178964	-0.495332	3.509505
95	1	0	5.273435	-0.200655	4.546308
96	6	0	4.710250	0.413701	2.543624
97	6	0	4.330582	1.830578	2.963042
98	1	0	4.006226	2.425961	2.084298
99	6	0	5.529998	2.574020	3.562758
100	1	0	5.261855	3.634302	3.759913
101	1	0	6.381820	2.563241	2.849359
102	1	0	5.857694	2.114430	4.519022
103	6	0	3.148197	1.816298	3.938291
104	1	0	2.291023	1.269473	3.489954

105	1	0	2.817260	2.854900	4.153867
106	1	0	3.420337	1.329009	4.898537
107	6	0	4.846835	-1.828875	-0.606735
108	1	0	4.527946	-1.004608	-1.278210
109	6	0	6.200244	-2.311742	-1.141721
110	1	0	6.964763	-1.514208	-1.022789
111	1	0	6.118836	-2.549460	-2.224167
112	1	0	6.547109	-3.223557	-0.611776
113	6	0	3.783458	-2.924634	-0.729337
114	1	0	4.068580	-3.832048	-0.155940
115	1	0	3.650134	-3.209002	-1.794798
116	1	0	2.811423	-2.549885	-0.344612

L3a-Mg(II)-COM

Zero-point correction= 1.15012 a.u.

Thermal correction to Gibbs Free Energy= 1.05414 a.u.

Sum of electronic and zero-point Energies= -5522.85792 a.u.

Sum of electronic and thermal Free Energies= -5522.95390 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.665947	1.065427	-1.868509
2	6	0	-0.586907	1.864244	-0.559525
3	6	0	-1.109024	3.173403	-0.868993
4	6	0	-1.509323	3.129268	-2.230553
5	7	0	-1.229137	1.857245	-2.800154
6	8	0	-0.161569	1.318026	0.454513
7	6	0	-1.302447	4.340655	-0.126521
8	6	0	-2.096584	4.214716	-2.849371
9	8	0	-0.251512	-0.093230	-1.946017
10	6	0	-1.499699	1.482044	-4.182386
11	1	0	-0.915668	2.107487	-4.863614
12	1	0	-1.214672	0.437174	-4.309088
13	1	0	-2.565525	1.598030	-4.397591
14	6	0	-1.892062	5.449750	-0.732074
15	6	0	-2.279002	5.372251	-2.073157
16	35	0	-0.764400	4.416295	1.687176
17	1	0	-2.048726	6.363878	-0.171502
18	1	0	-2.738282	6.242616	-2.531928
19	1	0	-2.404846	4.186134	-3.888165

20	8	0	2.219219	-0.256232	-0.032225
21	12	0	0.268328	-0.861306	0.066405
22	8	0	0.900203	-2.580603	-0.758027
23	8	0	0.239908	-1.341133	2.025537
24	8	0	-1.755347	-1.198726	0.156110
25	7	0	4.389539	-0.182617	-0.663124
26	1	0	5.179713	-0.653802	-1.089968
27	7	0	2.112962	-3.147538	-0.419679
28	7	0	-3.843409	-1.582368	0.929364
29	1	0	-4.433632	-1.833313	1.715452
30	7	0	-0.534164	-2.375913	2.515239
31	6	0	4.507442	1.201268	-0.392990
32	6	0	4.725471	1.646525	0.937858
33	6	0	4.793905	3.028602	1.190379
34	1	0	4.946256	3.400314	2.195066
35	6	0	4.667480	3.949300	0.155170
36	1	0	4.725267	5.009255	0.367016
37	6	0	4.463514	3.514336	-1.150372
38	1	0	4.364740	4.256640	-1.931323
39	6	0	4.374704	2.142260	-1.447491
40	6	0	4.112931	1.700682	-2.884132
41	1	0	4.050792	0.594790	-2.949144
42	6	0	2.769005	2.238172	-3.391858
43	1	0	1.955769	1.951643	-2.693427
44	1	0	2.534290	1.804632	-4.387592
45	1	0	2.781810	3.344514	-3.487084
46	6	0	5.258451	2.124166	-3.810352
47	1	0	5.096569	1.712581	-4.829655
48	1	0	6.223763	1.727152	-3.429467
49	1	0	5.331554	3.229581	-3.887502
50	6	0	4.877671	0.662835	2.094686
51	1	0	4.849556	-0.383771	1.726455
52	6	0	6.232406	0.828319	2.794037
53	1	0	7.057264	0.738693	2.054735
54	1	0	6.367679	0.031636	3.556643
55	1	0	6.311961	1.812000	3.303033
56	6	0	3.722524	0.805537	3.091983
57	1	0	3.741964	1.795257	3.595478
58	1	0	3.790335	0.014669	3.869253
59	1	0	2.750745	0.693620	2.566268
60	6	0	3.222244	-0.827135	-0.499119
61	6	0	3.269468	-2.290166	-0.933598
62	1	0	4.182059	-2.734440	-0.520951
63	6	0	3.225023	-2.526697	-2.444075

64	1	0	4.140777	-2.179106	-2.928034
65	1	0	2.375373	-1.991706	-2.876517
66	6	0	3.047115	-4.055764	-2.537931
67	1	0	4.036363	-4.521378	-2.569143
68	6	0	2.154984	-4.550031	-3.698681
69	1	0	2.208708	-3.886895	-4.568973
70	1	0	2.493001	-5.541586	-4.022570
71	6	0	0.742333	-4.647635	-3.096881
72	1	0	0.089273	-5.321460	-3.661244
73	1	0	0.271527	-3.660101	-3.071081
74	6	0	0.993315	-5.136778	-1.659551
75	1	0	0.165567	-4.931408	-0.979427
76	1	0	1.169616	-6.219765	-1.658579
77	6	0	2.308311	-4.470745	-1.227986
78	1	0	2.917076	-5.107669	-0.585173
79	6	0	2.250248	-3.350121	1.079455
80	1	0	3.213454	-3.845756	1.226787
81	1	0	2.290452	-2.354969	1.516005
82	6	0	1.156523	-4.183704	1.750180
83	1	0	1.504821	-4.355599	2.775197
84	1	0	1.111403	-5.176844	1.288525
85	6	0	-0.287453	-3.677428	1.770042
86	1	0	-0.648433	-3.518471	0.756202
87	1	0	-0.917414	-4.425728	2.259453
88	6	0	-0.301242	-2.514289	4.054086
89	1	0	-0.448175	-3.573622	4.265090
90	6	0	1.060721	-1.992686	4.535182
91	1	0	1.843524	-2.070305	3.779858
92	1	0	1.354378	-2.616837	5.388804
93	6	0	0.800873	-0.551282	5.006699
94	1	0	0.806850	0.122774	4.144994
95	1	0	1.555387	-0.200179	5.718413
96	6	0	-0.607886	-0.620697	5.621622
97	1	0	-1.103511	0.354644	5.677023
98	1	0	-0.551711	-1.017966	6.642164
99	6	0	-1.382457	-1.612757	4.725114
100	1	0	-2.067030	-2.231351	5.312660
101	6	0	-2.171208	-0.977822	3.562879
102	1	0	-1.733239	-0.028505	3.243231
103	1	0	-3.220914	-0.812811	3.815630
104	6	0	-2.022073	-2.019313	2.451138
105	1	0	-2.569028	-2.927216	2.727241
106	6	0	-2.505130	-1.566898	1.077805
107	6	0	-4.447186	-0.955466	-0.188162

108	6	0	-4.464653	-1.613883	-1.447497
109	6	0	-4.954630	-0.923061	-2.570441
110	1	0	-4.973224	-1.393757	-3.544521
111	6	0	-5.421820	0.381870	-2.456349
112	1	0	-5.787626	0.901576	-3.332624
113	6	0	-5.427217	1.020288	-1.220763
114	1	0	-5.797880	2.035317	-1.167888
115	6	0	-4.954356	0.366131	-0.068480
116	6	0	-4.971695	1.100408	1.269427
117	1	0	-4.616331	0.440437	2.085827
118	6	0	-6.393411	1.526004	1.656268
119	1	0	-6.397226	1.953306	2.682005
120	1	0	-7.071138	0.645603	1.650242
121	1	0	-6.793984	2.292901	0.960431
122	6	0	-4.024656	2.303340	1.248861
123	1	0	-2.994030	1.959298	1.026372
124	1	0	-4.011108	2.797568	2.243727
125	1	0	-4.332178	3.051320	0.487897
126	6	0	-3.979793	-3.052346	-1.604442
127	1	0	-3.645686	-3.461339	-0.628144
128	6	0	-5.112924	-3.968304	-2.082285
129	1	0	-5.982601	-3.890655	-1.394864
130	1	0	-4.771943	-5.025918	-2.086602
131	1	0	-5.443412	-3.705200	-3.109463
132	6	0	-2.775514	-3.134624	-2.550414
133	1	0	-3.052374	-2.847694	-3.586699
134	1	0	-2.378790	-4.172073	-2.569540
135	1	0	-1.965168	-2.461990	-2.200365

L3a-TS1-*si*

Zero-point correction= 1.26550 a.u.

Thermal correction to Gibbs Free Energy= 1.16610 a.u.

Sum of electronic and zero-point Energies= -5755.26539 a.u.

Sum of electronic and thermal Free Energies= -5755.36479 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.705600	-0.504800	-1.756800
2	6	0	0.613000	-1.471800	-0.554200
3	6	0	1.700800	-2.473300	-0.889900

4	6	0	2.173300	-2.174500	-2.185400
5	7	0	1.537700	-1.011300	-2.689800
6	8	0	0.447900	-0.872100	0.576400
7	6	0	2.277400	-3.539800	-0.220600
8	6	0	3.166000	-2.913700	-2.811500
9	8	0	0.154800	0.603000	-1.747500
10	6	0	1.908500	-0.334200	-3.925800
11	1	0	1.688100	-0.973300	-4.785800
12	1	0	1.325300	0.584300	-3.995600
13	1	0	2.975300	-0.091100	-3.919200
14	6	0	3.287100	-4.305900	-0.814600
15	6	0	3.715800	-3.990100	-2.102900
16	35	0	1.749800	-3.964500	1.569800
17	1	0	3.736500	-5.129400	-0.271100
18	1	0	4.500300	-4.584800	-2.560800
19	1	0	3.519400	-2.662700	-3.805600
20	6	0	-0.991300	-2.321400	-1.074400
21	6	0	-1.194500	-3.477600	-0.278300
22	8	0	-0.852600	-4.613200	-0.826300
23	6	0	-0.938400	-5.871900	-0.105800
24	1	0	-0.744900	-6.636100	-0.857000
25	6	0	-1.731100	-3.410300	1.107600
26	1	0	-0.165400	-5.892600	0.665100
27	1	0	-1.734800	-2.376500	1.450900
28	1	0	-1.655400	-1.496400	-0.831400
29	1	0	-0.889600	-2.533700	-2.137400
30	1	0	-2.754600	-3.805700	1.123600
31	1	0	-1.933500	-6.001300	0.323900
32	1	0	-1.148900	-4.021000	1.800000
33	8	0	-2.120300	0.882100	0.251700
34	12	0	-0.031500	1.190500	0.364000
35	8	0	-0.523100	3.092500	-0.265700
36	8	0	0.088400	1.619200	2.339600
37	8	0	2.049200	1.537300	0.372500
38	7	0	-4.263000	1.154100	-0.461000
39	1	0	-4.948100	1.782600	-0.866300
40	7	0	-1.656700	3.768400	0.138500
41	7	0	4.170700	1.907100	1.100900
42	1	0	4.755300	2.146900	1.893700
43	7	0	0.946100	2.546500	2.892200
44	6	0	-4.548500	-0.229300	-0.479200
45	6	0	-4.824900	-0.910000	0.735500
46	6	0	-5.062400	-2.295300	0.697400
47	1	0	-5.267000	-2.846200	1.605700

48	6	0	-5.027100	-2.992500	-0.506700
49	1	0	-5.202200	-4.060600	-0.515500
50	6	0	-4.768700	-2.323800	-1.698700
51	1	0	-4.751900	-2.895500	-2.617000
52	6	0	-4.540800	-0.936000	-1.711200
53	6	0	-4.295000	-0.226900	-3.041200
54	1	0	-4.181100	0.865100	-2.890300
55	6	0	-2.995300	-0.703500	-3.698500
56	1	0	-2.133500	-0.475300	-3.038900
57	1	0	-2.831700	-0.167000	-4.657600
58	1	0	-3.018900	-1.793900	-3.906500
59	6	0	-5.486400	-0.402100	-3.990600
60	1	0	-5.344600	0.220300	-4.900100
61	1	0	-6.423600	-0.072400	-3.492700
62	1	0	-5.601400	-1.459700	-4.308700
63	6	0	-4.884200	-0.171400	2.070900
64	1	0	-4.742600	0.919400	1.922800
65	6	0	-6.257000	-0.331700	2.736200
66	1	0	-7.060300	-0.018100	2.035500
67	1	0	-6.320800	0.311300	3.640200
68	1	0	-6.440300	-1.382200	3.045500
69	6	0	-3.763000	-0.633000	3.009300
70	1	0	-3.857200	-1.712200	3.254000
71	1	0	-3.793700	-0.054100	3.957200
72	1	0	-2.774200	-0.454600	2.538600
73	6	0	-3.027100	1.614900	-0.179300
74	6	0	-2.903100	3.113000	-0.440500
75	1	0	-3.756900	3.604800	0.037100
76	6	0	-2.861500	3.520300	-1.913400
77	1	0	-3.816400	3.325500	-2.406900
78	1	0	-2.075500	2.964100	-2.431100
79	6	0	-2.542700	5.024300	-1.825500
80	1	0	-3.482900	5.576400	-1.737600
81	6	0	-1.661700	5.577500	-2.964900
82	1	0	-1.849900	5.066500	-3.915700
83	1	0	-1.879700	6.641800	-3.115800
84	6	0	-0.223700	5.399600	-2.453700
85	1	0	0.496700	6.038600	-2.975200
86	1	0	0.088500	4.358200	-2.578100
87	6	0	-0.329900	5.725300	-0.953500
88	1	0	0.491200	5.318600	-0.363400
89	1	0	-0.347600	6.812600	-0.807600
90	6	0	-1.702700	5.189300	-0.522300
91	1	0	-2.193700	5.826500	0.213600

92	6	0	-1.782600	3.840600	1.651500
93	1	0	-2.706800	4.390100	1.851900
94	1	0	-1.892200	2.813900	1.991600
95	6	0	-0.631400	4.529100	2.382400
96	1	0	-0.942800	4.604700	3.430700
97	1	0	-0.534500	5.563500	2.031700
98	6	0	0.769600	3.929700	2.293000
99	1	0	1.075000	3.841900	1.253300
100	1	0	1.470200	4.581000	2.822300
101	6	0	0.780800	2.526800	4.443400
102	1	0	1.025000	3.538500	4.770000
103	6	0	-0.602000	2.059500	4.921000
104	1	0	-1.402900	2.292100	4.218100
105	1	0	-0.811300	2.592100	5.857500
106	6	0	-0.450400	0.553600	5.199300
107	1	0	-0.549600	-0.002600	4.262500
108	1	0	-1.204400	0.179400	5.900200
109	6	0	0.982200	0.428500	5.748000
110	1	0	1.394600	-0.581600	5.650100
111	1	0	0.998200	0.685700	6.814100
112	6	0	1.806100	1.469200	4.955500
113	1	0	2.549100	1.955700	5.594200
114	6	0	2.517800	0.936600	3.694100
115	1	0	2.010300	0.064200	3.275700
116	1	0	3.560400	0.679400	3.889900
117	6	0	2.405000	2.117800	2.727400
118	1	0	3.005800	2.951500	3.105700
119	6	0	2.831200	1.830100	1.288400
120	6	0	4.787700	1.286200	-0.014100
121	6	0	4.724500	1.895600	-1.297000
122	6	0	5.253000	1.208700	-2.405300
123	1	0	5.219400	1.644600	-3.394800
124	6	0	5.834500	-0.045000	-2.256800
125	1	0	6.224500	-0.564300	-3.122900
126	6	0	5.934700	-0.626000	-0.998500
127	1	0	6.403800	-1.597700	-0.917800
128	6	0	5.439800	0.031700	0.142600
129	6	0	5.601900	-0.629800	1.508500
130	1	0	5.223100	0.025100	2.314700
131	6	0	7.077800	-0.888900	1.836300
132	1	0	7.177600	-1.258300	2.879500
133	1	0	7.659500	0.053800	1.749800
134	1	0	7.520800	-1.647600	1.157300
135	6	0	4.785200	-1.919200	1.591700

136	1	0	3.721100	-1.690700	1.378300
137	1	0	4.846300	-2.348700	2.614500
138	1	0	5.150800	-2.677400	0.868100
139	6	0	4.144800	3.292700	-1.493900
140	1	0	3.764700	3.699800	-0.533900
141	6	0	5.224900	4.270200	-1.972900
142	1	0	6.076800	4.277200	-1.259600
143	1	0	4.813100	5.301100	-2.023500
144	1	0	5.603400	3.995400	-2.980100
145	6	0	2.958900	3.275000	-2.465100
146	1	0	3.268100	2.961800	-3.484200
147	1	0	2.521500	4.292100	-2.537700
148	1	0	2.172500	2.582100	-2.100700

L3a-TS1-*re*

Zero-point correction= 1.26541 a.u.

Thermal correction to Gibbs Free Energy= 1.16689 a.u.

Sum of electronic and zero-point Energies= -5755.26177 a.u.

Sum of electronic and thermal Free Energies= -5755.36029 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.159600	-2.819800	-0.990000
2	6	0	1.226200	-3.734200	0.083900
3	8	0	0.819700	-4.952000	-0.175800
4	6	0	0.751200	-5.979700	0.846300
5	6	0	1.614900	-3.265500	1.436600
6	1	0	1.857300	-1.989800	-0.934700
7	1	0	1.046400	-3.263000	-1.976300
8	1	0	0.468700	-6.884400	0.309400
9	1	0	-0.017200	-5.717700	1.575100
10	1	0	1.725600	-6.109300	1.321600
11	1	0	2.632100	-2.864100	1.413200
12	1	0	1.542700	-4.018200	2.220500
13	1	0	0.952200	-2.410200	1.658200
14	6	0	-0.356800	-0.978900	-1.941800
15	6	0	-0.445900	-1.763900	-0.623500
16	6	0	-1.558500	-2.733500	-0.909200
17	6	0	-1.834400	-2.659700	-2.291600
18	7	0	-1.061500	-1.631900	-2.893800

19	8	0	-0.255300	-1.083600	0.446200
20	8	0	0.221700	0.112800	-2.017500
21	6	0	-1.119000	-1.254300	-4.300200
22	6	0	-2.304200	-3.602300	-0.131400
23	6	0	-2.791900	-3.455800	-2.900500
24	1	0	-0.625500	-2.014600	-4.913900
25	1	0	-0.603300	-0.300300	-4.416400
26	1	0	-2.156100	-1.149600	-4.628700
27	6	0	-3.518100	-4.333800	-2.082300
28	6	0	-3.294300	-4.406800	-0.707800
29	1	0	-2.994100	-3.391500	-3.964100
30	1	0	-4.284000	-4.962300	-2.526600
31	1	0	-3.882100	-5.074700	-0.088100
32	35	0	-2.023800	-3.687400	1.757000
33	8	0	0.250800	2.863600	-0.595800
34	8	0	-1.741700	1.179200	0.223200
35	12	0	0.351700	0.909600	0.058700
36	8	0	0.917600	1.289100	1.976700
37	7	0	-3.833900	2.051400	0.313100
38	1	0	-4.428000	2.856000	0.147600
39	7	0	-0.570500	3.826100	-0.038400
40	7	0	4.695600	0.422000	0.205100
41	1	0	5.421900	0.472900	0.910900
42	7	0	2.066300	1.962000	2.337000
43	6	0	-4.450600	0.785900	0.459400
44	6	0	-4.427300	0.127400	1.716700
45	6	0	-4.939600	-1.179200	1.810700
46	1	0	-4.930000	-1.710800	2.753000
47	6	0	-5.466800	-1.819700	0.693900
48	1	0	-5.846500	-2.829500	0.781400
49	6	0	-5.516400	-1.165000	-0.532400
50	1	0	-5.934200	-1.691500	-1.380200
51	6	0	-5.033400	0.149400	-0.667600
52	6	0	-5.119300	0.846800	-2.021500
53	1	0	-4.782100	1.900100	-1.944300
54	6	0	-4.196900	0.173700	-3.038400
55	1	0	-3.152200	0.203800	-2.664900
56	1	0	-4.229100	0.718300	-4.006200
57	1	0	-4.493400	-0.881600	-3.215900
58	6	0	-6.563000	0.902700	-2.536600
59	1	0	-6.616800	1.529600	-3.452500
60	1	0	-7.225700	1.358600	-1.770000
61	1	0	-6.946700	-0.108200	-2.788400
62	6	0	-3.883200	0.813800	2.965700

63	1	0	-3.537200	1.841700	2.729000
64	6	0	-4.975800	0.967700	4.030400
65	1	0	-5.849500	1.507000	3.605600
66	1	0	-4.591700	1.559500	4.888900
67	1	0	-5.314700	-0.018800	4.411400
68	6	0	-2.672000	0.064700	3.530500
69	1	0	-2.949100	-0.951100	3.882100
70	1	0	-2.251000	0.626500	4.390600
71	1	0	-1.882200	-0.025200	2.755900
72	6	0	-2.503900	2.148500	0.099500
73	6	0	-2.047800	3.538700	-0.315600
74	1	0	-2.607300	4.279200	0.265200
75	6	0	-2.190400	3.865400	-1.800900
76	1	0	-3.240400	3.928800	-2.095800
77	1	0	-1.700000	3.093900	-2.401200
78	6	0	-1.468000	5.223200	-1.899400
79	1	0	-2.191800	6.016700	-1.691300
80	6	0	-0.710900	5.477500	-3.219300
81	1	0	-1.199600	4.995500	-4.073200
82	1	0	-0.681300	6.554600	-3.424700
83	6	0	0.709200	4.951500	-2.956100
84	1	0	1.449700	5.371200	-3.645000
85	1	0	0.730300	3.861600	-3.055200
86	6	0	0.975000	5.339900	-1.490700
87	1	0	1.765600	4.755200	-1.019400
88	1	0	1.255300	6.399100	-1.430300
89	6	0	-0.378600	5.192000	-0.782300
90	1	0	-0.542600	5.953800	-0.019000
91	6	0	-0.369100	3.948500	1.461600
92	1	0	-1.052700	4.733000	1.795800
93	1	0	-0.682800	2.996500	1.883500
94	6	0	1.044600	4.297200	1.921600
95	1	0	0.969400	4.495700	2.997200
96	1	0	1.358900	5.245800	1.471300
97	6	0	2.180200	3.312800	1.651700
98	1	0	2.250700	3.100600	0.587500
99	1	0	3.120100	3.749800	1.999100
100	6	0	2.150200	2.069800	3.897200
101	1	0	2.667600	3.010300	4.089100
102	6	0	0.791200	1.980700	4.608600
103	1	0	-0.039800	2.319700	3.989800
104	1	0	0.845900	2.634100	5.488100
105	6	0	0.661000	0.513200	5.054200
106	1	0	0.299500	-0.092400	4.217500

107	1	0	-0.034300	0.387900	5.890800
108	6	0	2.101200	0.114400	5.413400
109	1	0	2.263600	-0.969100	5.416600
110	1	0	2.355600	0.486200	6.413300
111	6	0	2.974100	0.828000	4.360500
112	1	0	3.930800	1.151100	4.781400
113	6	0	3.252600	0.024100	3.074300
114	1	0	2.442700	-0.673100	2.845000
115	1	0	4.194300	-0.528700	3.121400
116	6	0	3.306700	1.128800	2.020400
117	1	0	4.161600	1.776100	2.240000
118	6	0	3.418600	0.680400	0.562300
119	6	0	5.052400	-0.099700	-1.062400
120	6	0	5.061100	0.745200	-2.205800
121	6	0	5.447000	0.207400	-3.447400
122	1	0	5.454300	0.821100	-4.338400
123	6	0	5.869100	-1.112700	-3.552700
124	1	0	6.185200	-1.502300	-4.512000
125	6	0	5.913700	-1.926300	-2.426600
126	1	0	6.279600	-2.937700	-2.539500
127	6	0	5.492700	-1.446700	-1.172800
128	6	0	5.557900	-2.366100	0.042900
129	1	0	4.998300	-1.920200	0.891200
130	6	0	7.008300	-2.538000	0.503000
131	1	0	7.048500	-3.162400	1.421300
132	1	0	7.452900	-1.547700	0.740600
133	1	0	7.622700	-3.024200	-0.285000
134	6	0	4.909600	-3.732300	-0.227500
135	1	0	3.928800	-3.603100	-0.727000
136	1	0	4.748900	-4.274200	0.729000
137	1	0	5.550500	-4.368900	-0.873200
138	6	0	4.733400	2.232200	-2.110200
139	1	0	4.491700	2.518300	-1.066700
140	6	0	5.939900	3.090600	-2.511100
141	1	0	6.827600	2.809600	-1.904500
142	1	0	5.723900	4.164300	-2.323100
143	1	0	6.187400	2.969600	-3.586900
144	6	0	3.507100	2.586000	-2.956800
145	1	0	3.680900	2.381800	-4.034100
146	1	0	3.275500	3.664900	-2.844100
147	1	0	2.626200	2.000300	-2.619000
148	8	0	2.457300	0.567100	-0.215900

L4-Mg(II)

Zero-point correction= 1.04415 a.u.

Thermal correction to Gibbs Free Energy= 0.96070 a.u.

Sum of electronic and zero-point Energies= -2436.11668 a.u.

Sum of electronic and thermal Free Energies= -2436.20013 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.911886	0.274964	0.531961
2	12	0	-0.026964	0.021182	0.129215
3	8	0	-0.187625	1.901973	-0.389941
4	8	0	0.214806	-1.256198	-1.326565
5	8	0	-1.924707	-0.526431	0.430108
6	7	0	3.944962	1.273063	0.518913
7	1	0	4.514196	2.048235	0.194898
8	7	0	0.822107	2.458547	-1.160630
9	7	0	-3.929218	-1.346317	-0.243414
10	1	0	-4.444397	-1.954525	-0.871884
11	7	0	-0.771173	-1.818426	-2.109626
12	6	0	4.610776	0.144173	1.053433
13	6	0	5.346757	-0.711883	0.192235
14	6	0	5.965850	-1.853197	0.733428
15	1	0	6.523274	-2.532195	0.101803
16	6	0	5.869342	-2.140299	2.090992
17	1	0	6.350598	-3.023827	2.490469
18	6	0	5.160248	-1.295552	2.938740
19	1	0	5.110060	-1.544977	3.990385
20	6	0	4.527358	-0.141466	2.442472
21	6	0	3.783002	0.778295	3.406117
22	1	0	3.367239	1.655782	2.869509
23	6	0	2.594867	0.056364	4.052354
24	1	0	1.922241	-0.353089	3.268718
25	1	0	2.006939	0.767598	4.671352
26	1	0	2.932595	-0.777388	4.703513
27	6	0	4.727139	1.344527	4.473477
28	1	0	4.193023	2.093703	5.096420
29	1	0	5.589197	1.852303	3.989905
30	1	0	5.110847	0.545852	5.142858
31	6	0	5.452565	-0.439111	-1.305532
32	1	0	4.931137	0.503024	-1.572769
33	6	0	6.912416	-0.258850	-1.737882

34	1	0	7.392103	0.542825	-1.136472
35	1	0	6.959318	0.040328	-2.807097
36	1	0	7.493428	-1.196840	-1.613624
37	6	0	4.770659	-1.547974	-2.113625
38	1	0	5.285613	-2.523179	-1.983250
39	1	0	4.770678	-1.291128	-3.194605
40	1	0	3.715845	-1.650533	-1.785791
41	6	0	2.633943	1.257417	0.248251
42	6	0	2.125854	2.559231	-0.366010
43	1	0	2.874441	2.914003	-1.080766
44	6	0	1.826441	3.672188	0.641387
45	1	0	2.741444	4.022316	1.124361
46	1	0	1.142330	3.304683	1.411635
47	6	0	1.169923	4.748478	-0.246160
48	1	0	1.953835	5.404305	-0.635177
49	6	0	0.032491	5.558586	0.416723
50	1	0	0.176842	5.659472	1.497799
51	1	0	0.012914	6.570087	-0.005959
52	6	0	-1.258350	4.808814	0.043418
53	1	0	-2.148681	5.443126	0.104315
54	1	0	-1.408057	3.951330	0.706592
55	6	0	-0.986762	4.315197	-1.387976
56	1	0	-1.621622	3.485988	-1.695147
57	1	0	-1.139224	5.135026	-2.101001
58	6	0	0.506895	3.969399	-1.423694
59	1	0	0.973985	4.183242	-2.385492
60	6	0	1.020968	1.666440	-2.446685
61	1	0	1.822534	2.179457	-2.984371
62	1	0	1.380557	0.680073	-2.147465
63	6	0	-0.211687	1.550482	-3.347937
64	1	0	0.180773	1.242244	-4.325783
65	1	0	-0.635616	2.545873	-3.509705
66	6	0	-1.361581	0.584254	-2.974714
67	1	0	-1.691833	0.750747	-1.948551
68	1	0	-2.211719	0.870573	-3.604114
69	6	0	-0.268852	-3.186891	-2.690692
70	1	0	-0.821340	-3.302614	-3.623802
71	6	0	1.248834	-3.247845	-2.876502
72	1	0	1.689914	-2.275830	-3.106032
73	1	0	1.437220	-3.906559	-3.732872
74	6	0	1.786058	-3.897812	-1.587296
75	1	0	1.887464	-3.139671	-0.805112
76	1	0	2.764652	-4.366549	-1.733365
77	6	0	0.694574	-4.916914	-1.208181

78	1	0	0.702538	-5.179744	-0.144782
79	1	0	0.838175	-5.845357	-1.772791
80	6	0	-0.642151	-4.262917	-1.635954
81	1	0	-1.314168	-4.999164	-2.084833
82	6	0	-1.407900	-3.504889	-0.534095
83	1	0	-0.741680	-3.174958	0.268364
84	1	0	-2.211718	-4.098089	-0.093228
85	6	0	-1.971324	-2.285076	-1.275830
86	1	0	-2.719673	-2.607151	-2.003862
87	6	0	-2.595778	-1.278945	-0.315948
88	6	0	-4.667511	-0.626843	0.726404
89	6	0	-5.243490	0.625160	0.389097
90	6	0	-5.956747	1.334333	1.372677
91	1	0	-6.402364	2.294367	1.148178
92	6	0	-6.098521	0.821864	2.658186
93	1	0	-6.644673	1.383815	3.404941
94	6	0	-5.543427	-0.410412	2.987877
95	1	0	-5.672416	-0.780476	3.996278
96	6	0	-4.835519	-1.160976	2.031526
97	6	0	-4.263697	-2.521551	2.418190
98	1	0	-3.793620	-3.011124	1.541621
99	6	0	-5.363772	-3.478212	2.895795
100	1	0	-4.941323	-4.493038	3.058271
101	1	0	-6.161614	-3.558482	2.126656
102	1	0	-5.817699	-3.136000	3.849544
103	6	0	-3.166127	-2.373767	3.477300
104	1	0	-2.368552	-1.693648	3.108872
105	1	0	-2.702642	-3.361385	3.687837
106	1	0	-3.573136	-1.966842	4.427150
107	6	0	-5.089271	1.223293	-1.005071
108	1	0	-4.497723	0.548082	-1.658017
109	6	0	-6.450468	1.399308	-1.687238
110	1	0	-6.991704	0.429208	-1.714587
111	1	0	-6.310159	1.744061	-2.734210
112	1	0	-7.078603	2.144908	-1.155495
113	6	0	-4.326332	2.551071	-0.950579
114	1	0	-4.915103	3.337943	-0.433592
115	1	0	-4.101061	2.903337	-1.979724
116	1	0	-3.367803	2.412903	-0.407570
117	6	0	-1.109912	-0.903390	-3.280219
118	1	0	-1.981635	-1.357461	-3.755792
119	1	0	-0.261148	-1.010290	-3.958901

L4-Mg(II)-COM

Zero-point correction= 1.17764 a.u.

Thermal correction to Gibbs Free Energy= 1.08520 a.u.

Sum of electronic and zero-point Energies= -5562.15961 a.u.

Sum of electronic and thermal Free Energies= -5562.25205 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.048265	1.328748	-1.990783
2	6	0	0.430637	2.073266	-0.735770
3	6	0	0.671542	3.433118	-1.153902
4	6	0	0.353775	3.483777	-2.536937
5	7	0	-0.070843	2.210794	-3.007569
6	8	0	0.517462	1.462716	0.325573
7	6	0	1.111491	4.586609	-0.500700
8	6	0	0.466213	4.651810	-3.264202
9	8	0	-0.333678	0.129487	-1.960190
10	6	0	-0.477685	1.919050	-4.376856
11	1	0	0.327898	2.179521	-5.068493
12	1	0	-0.688281	0.851391	-4.445127
13	1	0	-1.377897	2.486831	-4.629416
14	6	0	1.234464	5.776795	-1.216396
15	6	0	0.912657	5.793402	-2.577015
16	35	0	1.540042	4.533373	1.344549
17	1	0	1.575353	6.681598	-0.726688
18	1	0	1.012649	6.726483	-3.123230
19	1	0	0.221743	4.697124	-4.319241
20	8	0	1.861634	-1.114134	-0.143632
21	12	0	-0.154356	-0.702784	0.099345
22	8	0	-0.515094	-2.532137	-0.647604
23	8	0	-0.084277	-0.920620	2.099958
24	8	0	-2.128644	-0.120354	0.314211
25	7	0	3.738521	-2.200215	-0.827569
26	1	0	4.149243	-3.067654	-1.153355
27	7	0	0.305762	-3.620805	-0.433441
28	7	0	-4.125709	0.264742	1.327757
29	1	0	-4.642818	0.348575	2.196027
30	7	0	-1.075880	-0.953578	3.050492
31	6	0	4.615480	-1.133120	-0.526285
32	6	0	5.239550	-1.071233	0.746238
33	6	0	6.087152	0.013355	1.036742

34	1	0	6.559773	0.101941	2.006032
35	6	0	6.341737	0.993609	0.082931
36	1	0	7.002867	1.817293	0.320137
37	6	0	5.756539	0.916346	-1.176819
38	1	0	5.983897	1.688688	-1.899706
39	6	0	4.885150	-0.138790	-1.502741
40	6	0	4.257535	-0.192244	-2.891769
41	1	0	3.564377	-1.054710	-2.975012
42	6	0	3.422645	1.062513	-3.170031
43	1	0	2.731984	1.247223	-2.323729
44	1	0	2.818667	0.923800	-4.092137
45	1	0	4.064119	1.959211	-3.302461
46	6	0	5.326496	-0.390349	-3.972020
47	1	0	4.846555	-0.507446	-4.967442
48	1	0	5.913161	-1.310627	-3.763069
49	1	0	6.022105	0.474343	-4.017399
50	6	0	4.996933	-2.142257	1.804896
51	1	0	4.357502	-2.955321	1.401781
52	6	0	6.307352	-2.807780	2.242622
53	1	0	6.850273	-3.201524	1.356561
54	1	0	6.093006	-3.661528	2.920782
55	1	0	6.967510	-2.095346	2.780555
56	6	0	4.247946	-1.557016	3.004012
57	1	0	4.858248	-0.792917	3.530558
58	1	0	3.988126	-2.360902	3.725540
59	1	0	3.306693	-1.086753	2.653240
60	6	0	2.413469	-2.128393	-0.608213
61	6	0	1.686288	-3.396189	-1.046852
62	1	0	2.291169	-4.256990	-0.743232
63	6	0	1.411574	-3.483302	-2.550343
64	1	0	2.340561	-3.576360	-3.117552
65	1	0	0.885116	-2.584746	-2.882975
66	6	0	0.524783	-4.739394	-2.649380
67	1	0	1.170241	-5.611296	-2.790011
68	6	0	-0.592920	-4.689143	-3.715889
69	1	0	-0.314721	-4.065569	-4.572663
70	1	0	-0.779946	-5.700687	-4.095800
71	6	0	-1.833662	-4.171911	-2.966402
72	1	0	-2.771348	-4.440923	-3.464346
73	1	0	-1.798424	-3.082084	-2.875701
74	6	0	-1.705163	-4.808023	-1.571397
75	1	0	-2.270069	-4.288483	-0.800327
76	1	0	-2.050191	-5.849296	-1.599939
77	6	0	-0.201902	-4.839955	-1.274231

78	1	0	0.102623	-5.718519	-0.704095
79	6	0	0.413179	-3.945299	1.048786
80	1	0	1.125955	-4.770849	1.122487
81	1	0	0.841884	-3.058044	1.517553
82	6	0	-0.903437	-4.337501	1.723275
83	1	0	-0.615072	-4.834626	2.659061
84	1	0	-1.406396	-5.107430	1.130837
85	6	0	-1.914200	-3.221178	2.063169
86	1	0	-2.095076	-2.600765	1.185695
87	1	0	-2.865477	-3.711729	2.298193
88	6	0	-0.542446	-0.386446	4.418109
89	1	0	-1.119099	-0.916982	5.176391
90	6	0	0.968904	-0.545153	4.591322
91	1	0	1.357963	-1.431181	4.086457
92	1	0	1.157470	-0.663601	5.665589
93	6	0	1.567755	0.783134	4.095148
94	1	0	1.643385	0.768386	3.004592
95	1	0	2.564826	0.973416	4.506385
96	6	0	0.535242	1.837648	4.535515
97	1	0	0.586332	2.753152	3.935886
98	1	0	0.703676	2.119884	5.581281
99	6	0	-0.839447	1.136686	4.404804
100	1	0	-1.493520	1.389997	5.243557
101	6	0	-1.595332	1.392941	3.087697
102	1	0	-0.915434	1.697807	2.289255
103	1	0	-2.373213	2.153007	3.192204
104	6	0	-2.214274	0.028928	2.755971
105	1	0	-2.994034	-0.208615	3.484556
106	6	0	-2.805792	0.009075	1.351579
107	6	0	-4.829792	0.496714	0.122585
108	6	0	-5.531768	-0.567482	-0.499788
109	6	0	-6.230399	-0.317137	-1.694762
110	1	0	-6.770937	-1.109510	-2.195716
111	6	0	-6.239904	0.952892	-2.261785
112	1	0	-6.779209	1.127187	-3.184095
113	6	0	-5.563040	2.000959	-1.647000
114	1	0	-5.596023	2.978248	-2.110468
115	6	0	-4.859396	1.798396	-0.445869
116	6	0	-4.153975	2.977703	0.216178
117	1	0	-3.657132	2.659254	1.153952
118	6	0	-5.152131	4.071034	0.613508
119	1	0	-4.631729	4.875911	1.175633
120	1	0	-5.940031	3.646427	1.271938
121	1	0	-5.635322	4.524637	-0.277530

122	6	0	-3.053461	3.541365	-0.688672
123	1	0	-2.370829	2.724912	-0.998543
124	1	0	-2.459550	4.303480	-0.140185
125	1	0	-3.476934	4.014780	-1.599456
126	6	0	-5.528783	-1.974467	0.087130
127	1	0	-4.919787	-2.011297	1.014271
128	6	0	-6.943157	-2.414110	0.480667
129	1	0	-7.388136	-1.680474	1.186701
130	1	0	-6.907765	-3.401606	0.988906
131	1	0	-7.603472	-2.501719	-0.407938
132	6	0	-4.894904	-2.971917	-0.888259
133	1	0	-5.530546	-3.123319	-1.786149
134	1	0	-4.754567	-3.955113	-0.390448
135	1	0	-3.903498	-2.597039	-1.218286
136	6	0	-1.533866	-2.384867	3.296904
137	1	0	-2.369916	-2.308796	3.995117
138	1	0	-0.696259	-2.844279	3.826327

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Zero-point correction= 1.29138 a.u.

Thermal correction to Gibbs Free Energy= 1.19163 a.u.

Sum of electronic and zero-point Energies= -5794.57155 a.u.

Sum of electronic and thermal Free Energies= -5794.67129 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542299	0.867775	-2.006540
2	6	0	1.016519	1.671004	-0.776003
3	6	0	0.938792	3.088388	-1.302948
4	6	0	0.727820	3.015266	-2.696279
5	7	0	0.534505	1.667466	-3.096163
6	8	0	0.528768	1.233553	0.338151
7	6	0	1.031815	4.340651	-0.722740
8	6	0	0.650233	4.142573	-3.500026
9	8	0	0.146821	-0.299563	-1.909603
10	6	0	0.102311	1.254766	-4.424796
11	1	0	0.868677	1.505474	-5.163733
12	1	0	-0.048830	0.174955	-4.410142
13	1	0	-0.837186	1.749343	-4.691552
14	6	0	0.946468	5.503719	-1.496912

15	6	0	0.769541	5.391907	-2.875424
16	35	0	1.234216	4.511402	1.174412
17	1	0	1.011390	6.478978	-1.027643
18	1	0	0.706744	6.294899	-3.475145
19	1	0	0.482785	4.068227	-4.568725
20	6	0	2.837059	1.257440	-0.896339
21	6	0	3.582064	2.137646	-0.066100
22	8	0	4.111791	3.167608	-0.665959
23	6	0	4.835169	4.193586	0.066850
24	1	0	5.283738	4.820662	-0.701939
25	6	0	3.722650	1.928087	1.397615
26	1	0	4.128938	4.772943	0.665512
27	1	0	4.727824	1.543177	1.617074
28	1	0	2.781817	0.238717	-0.522484
29	1	0	3.092234	1.347680	-1.949687
30	1	0	3.606917	2.855572	1.961344
31	1	0	5.606989	3.741691	0.692278
32	1	0	2.982502	1.202615	1.733623
33	8	0	1.566064	-1.751289	0.234124
34	12	0	-0.295221	-0.723391	0.249122
35	8	0	-1.068314	-2.533785	-0.319183
36	8	0	-0.497309	-0.839505	2.268853
37	8	0	-2.250497	0.062096	0.181988
38	7	0	3.124547	-3.291690	-0.389484
39	1	0	3.294404	-4.215836	-0.770680
40	7	0	-0.560541	-3.769947	0.020186
41	7	0	-4.240531	0.822842	0.997154
42	1	0	-4.794824	1.020431	1.821762
43	7	0	-1.547968	-0.562212	3.106569
44	6	0	4.204423	-2.378976	-0.374592
45	6	0	4.776320	-1.981432	0.861794
46	6	0	5.785311	-1.002179	0.860562
47	1	0	6.230290	-0.666156	1.787704
48	6	0	6.230078	-0.437710	-0.330472
49	1	0	7.001351	0.321481	-0.311688
50	6	0	5.699210	-0.855237	-1.546148
51	1	0	6.078487	-0.406718	-2.454783
52	6	0	4.693744	-1.837783	-1.594230
53	6	0	4.157459	-2.293973	-2.948557
54	1	0	3.398720	-3.089955	-2.820522
55	6	0	3.456569	-1.150236	-3.688925
56	1	0	2.612044	-0.771785	-3.079685
57	1	0	3.038239	-1.515876	-4.651047
58	1	0	4.154727	-0.314535	-3.905199

59	6	0	5.271868	-2.901828	-3.808907
60	1	0	4.842904	-3.340144	-4.735511
61	1	0	5.784526	-3.715050	-3.251511
62	1	0	6.023061	-2.138059	-4.101189
63	6	0	4.330681	-2.600665	2.183340
64	1	0	3.577043	-3.396760	2.007749
65	6	0	5.500934	-3.279025	2.906449
66	1	0	5.985737	-4.021471	2.236908
67	1	0	5.131701	-3.818411	3.804999
68	1	0	6.262076	-2.540053	3.234182
69	6	0	3.662580	-1.556005	3.081927
70	1	0	4.369484	-0.745656	3.358750
71	1	0	3.291427	-2.033356	4.013703
72	1	0	2.793807	-1.114203	2.554192
73	6	0	1.852667	-2.885621	-0.185429
74	6	0	0.839547	-3.962246	-0.550384
75	1	0	1.200158	-4.917818	-0.155771
76	6	0	0.581208	-4.109552	-2.052830
77	1	0	1.459843	-4.504438	-2.567396
78	1	0	0.322937	-3.138304	-2.481953
79	6	0	-0.604446	-5.092813	-2.087492
80	1	0	-0.209370	-6.111380	-2.143493
81	6	0	-1.657273	-4.841702	-3.191034
82	1	0	-1.218864	-4.367845	-4.076337
83	1	0	-2.084659	-5.799052	-3.512470
84	6	0	-2.742976	-3.981887	-2.519883
85	1	0	-3.711257	-4.057729	-3.026275
86	1	0	-2.446090	-2.929048	-2.509776
87	6	0	-2.790037	-4.512539	-1.075642
88	1	0	-3.207582	-3.801605	-0.365571
89	1	0	-3.388187	-5.431380	-1.029843
90	6	0	-1.346139	-4.892596	-0.732809
91	1	0	-1.276227	-5.767116	-0.084740
92	6	0	-0.565227	-3.979923	1.526963
93	1	0	-0.039044	-4.922819	1.700602
94	1	0	0.016991	-3.155909	1.941203
95	6	0	-1.952674	-4.044765	2.167050
96	1	0	-1.794790	-4.467100	3.168420
97	1	0	-2.568265	-4.778631	1.638063
98	6	0	-2.744193	-2.728955	2.309985
99	1	0	-2.731897	-2.190843	1.362425
100	1	0	-3.787534	-2.998340	2.509414
101	6	0	-1.036597	0.094359	4.441671
102	1	0	-1.740369	-0.241437	5.203148

103	6	0	0.414533	-0.262325	4.772982
104	1	0	0.706720	-1.240501	4.385793
105	1	0	0.501921	-0.291260	5.866188
106	6	0	1.239679	0.904580	4.205417
107	1	0	1.364027	0.761426	3.129137
108	1	0	2.230097	0.989204	4.665891
109	6	0	0.352621	2.136646	4.452935
110	1	0	0.602720	2.975729	3.795259
111	1	0	0.460575	2.483722	5.487554
112	6	0	-1.090202	1.631431	4.219919
113	1	0	-1.789185	2.082530	4.930250
114	6	0	-1.639617	1.816590	2.791403
115	1	0	-0.840626	1.879039	2.047848
116	1	0	-2.273334	2.702843	2.700441
117	6	0	-2.465301	0.543585	2.574876
118	1	0	-3.321873	0.545059	3.255031
119	6	0	-2.963984	0.408088	1.137667
120	6	0	-4.885134	0.934849	-0.257645
121	6	0	-5.830774	-0.047675	-0.651906
122	6	0	-6.532120	0.124124	-1.859208
123	1	0	-7.268571	-0.600847	-2.179695
124	6	0	-6.295598	1.228920	-2.669227
125	1	0	-6.839236	1.342003	-3.598505
126	6	0	-5.373869	2.196015	-2.284113
127	1	0	-5.227582	3.052247	-2.929091
128	6	0	-4.668436	2.078975	-1.072333
129	6	0	-3.722448	3.198221	-0.650909
130	1	0	-3.247608	2.967247	0.323168
131	6	0	-4.478100	4.517359	-0.453594
132	1	0	-3.792619	5.292657	-0.048501
133	1	0	-5.306102	4.377299	0.274141
134	1	0	-4.900866	4.891053	-1.410080
135	6	0	-2.582489	3.365846	-1.659541
136	1	0	-2.053922	2.399049	-1.795139
137	1	0	-1.856045	4.115914	-1.283817
138	1	0	-2.955110	3.710081	-2.647033
139	6	0	-6.107284	-1.277061	0.206340
140	1	0	-5.386312	-1.333437	1.048593
141	6	0	-7.506587	-1.204179	0.824767
142	1	0	-7.605816	-0.280673	1.434578
143	1	0	-7.676247	-2.076603	1.491619
144	1	0	-8.293698	-1.199934	0.040732
145	6	0	-5.932341	-2.571316	-0.598320
146	1	0	-6.774812	-2.730275	-1.304085

147	1	0	-5.886138	-3.444657	0.087112
148	1	0	-4.991664	-2.528764	-1.183696
149	6	0	-2.282158	-1.841882	3.476208
150	1	0	-3.127564	-1.531556	4.095068
151	1	0	-1.577262	-2.379016	4.115105

L4-TS1-*re*

Zero-point correction= 1.29181 a.u.

Thermal correction to Gibbs Free Energy= 1.18811 a.u.

Sum of electronic and zero-point Energies= -5794.55933 a.u.

Sum of electronic and thermal Free Energies= -5794.66302 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.466837	-3.049800	-1.599163
2	6	0	-1.090085	-4.148359	-0.951993
3	8	0	-2.038406	-4.741908	-1.622112
4	6	0	-2.846292	-5.806771	-1.049360
5	6	0	-0.711740	-4.521690	0.433721
6	1	0	0.524369	-2.822734	-1.221471
7	1	0	-0.551904	-3.063311	-2.683874
8	1	0	-3.496145	-6.125658	-1.862606
9	1	0	-3.438204	-5.406386	-0.224183
10	1	0	-2.210060	-6.631277	-0.723732
11	1	0	0.301509	-4.943307	0.419334
12	1	0	-1.384222	-5.233267	0.910032
13	1	0	-0.666511	-3.595208	1.019283
14	6	0	-0.742119	-0.568593	-2.120456
15	6	0	-1.300652	-1.465584	-0.997341
16	6	0	-2.734940	-1.635392	-1.440243
17	6	0	-2.825920	-1.171628	-2.770069
18	7	0	-1.599389	-0.579911	-3.168657
19	8	0	-0.874969	-1.185417	0.187291
20	8	0	0.293644	0.090913	-1.978092
21	6	0	-1.334630	0.018204	-4.470556
22	6	0	-3.871102	-2.151665	-0.843852
23	6	0	-3.999090	-1.249355	-3.505147
24	1	0	-2.194295	0.600872	-4.808944
25	1	0	-1.123820	-0.762534	-5.208807
26	1	0	-0.466345	0.671914	-4.375614

27	6	0	-5.130110	-1.775903	-2.864567
28	6	0	-5.082957	-2.215463	-1.542091
29	1	0	-4.052958	-0.898190	-4.529950
30	1	0	-6.069052	-1.834048	-3.406861
31	1	0	-5.972483	-2.602565	-1.058138
32	35	0	-3.803079	-2.784856	0.959656
33	8	0	1.388888	2.231016	-0.054832
34	8	0	-1.260418	1.577398	0.380309
35	12	0	0.532202	0.398544	0.250346
36	8	0	0.886066	0.162758	2.239976
37	7	0	-2.703508	3.336272	0.522424
38	1	0	-2.809558	4.342340	0.456406
39	7	0	1.015326	3.442227	0.486222
40	7	0	4.507406	-1.317300	0.529296
41	1	0	5.116231	-1.546914	1.306664
42	7	0	1.962214	-0.264592	2.974066
43	6	0	-3.871581	2.542599	0.419844
44	6	0	-4.328748	1.803030	1.540827
45	6	0	-5.407426	0.914432	1.377366
46	1	0	-5.771962	0.327050	2.209637
47	6	0	-6.031038	0.770810	0.142431
48	1	0	-6.851828	0.074175	0.030905
49	6	0	-5.619538	1.535671	-0.943888
50	1	0	-6.136346	1.411609	-1.886272
51	6	0	-4.561265	2.453998	-0.818403
52	6	0	-4.173738	3.320083	-2.012284
53	1	0	-3.404626	4.062007	-1.724033
54	6	0	-3.558964	2.471038	-3.123434
55	1	0	-2.672429	1.935042	-2.726622
56	1	0	-3.222351	3.118420	-3.961358
57	1	0	-4.290080	1.733909	-3.516716
58	6	0	-5.365621	4.133570	-2.533259
59	1	0	-5.024590	4.856060	-3.305646
60	1	0	-5.826257	4.712206	-1.704092
61	1	0	-6.139188	3.480956	-2.989763
62	6	0	-3.704336	1.981585	2.919688
63	1	0	-2.882535	2.727707	2.884112
64	6	0	-4.729932	2.521635	3.923611
65	1	0	-5.179460	3.463149	3.541292
66	1	0	-4.234298	2.748097	4.892113
67	1	0	-5.541767	1.787109	4.110458
68	6	0	-3.087416	0.673865	3.419987
69	1	0	-3.855959	-0.115707	3.553735
70	1	0	-2.589891	0.841198	4.398420

71	1	0	-2.328419	0.319759	2.693033
72	6	0	-1.473169	2.798549	0.351566
73	6	0	-0.399631	3.836738	0.061479
74	1	0	-0.629502	4.758734	0.605715
75	6	0	-0.225296	4.163024	-1.423924
76	1	0	-1.095579	4.688251	-1.822262
77	1	0	-0.077255	3.239915	-1.990002
78	6	0	1.038829	5.044168	-1.418679
79	1	0	0.733589	6.087805	-1.299065
80	6	0	1.985898	4.872048	-2.627717
81	1	0	1.446149	4.581849	-3.536022
82	1	0	2.485526	5.825558	-2.837217
83	6	0	3.020972	3.826125	-2.177487
84	1	0	3.954556	3.887178	-2.747056
85	1	0	2.619242	2.814915	-2.291646
86	6	0	3.222184	4.130258	-0.682391
87	1	0	3.607499	3.282213	-0.118692
88	1	0	3.916945	4.970121	-0.556968
89	6	0	1.852103	4.588548	-0.170335
90	1	0	1.915727	5.364415	0.593588
91	6	0	1.127606	3.437499	2.003599
92	1	0	0.686335	4.379328	2.340196
93	1	0	0.504649	2.606785	2.339591
94	6	0	2.547532	3.316325	2.555958
95	1	0	2.478866	3.605022	3.613045
96	1	0	3.191568	4.070383	2.093336
97	6	0	3.232761	1.940290	2.462438
98	1	0	3.123586	1.557200	1.448008
99	1	0	4.302567	2.097322	2.636719
100	6	0	1.489523	-1.113508	4.215541
101	1	0	2.209727	-0.885885	5.000647
102	6	0	0.047421	-0.816201	4.630256
103	1	0	-0.254034	0.194038	4.351764
104	1	0	-0.004840	-0.899761	5.722683
105	6	0	-0.793387	-1.927854	3.974648
106	1	0	-0.999523	-1.673734	2.930566
107	1	0	-1.751169	-2.085696	4.482089
108	6	0	0.126699	-3.159441	4.045954
109	1	0	-0.149807	-3.949396	3.339028
110	1	0	0.094565	-3.596263	5.051579
111	6	0	1.541557	-2.601913	3.775805
112	1	0	2.302199	-3.138366	4.350417
113	6	0	1.974635	-2.559565	2.299639
114	1	0	1.119265	-2.451759	1.628838

115	1	0	2.555344	-3.435422	1.998785
116	6	0	2.824188	-1.290519	2.230956
117	1	0	3.713658	-1.415218	2.852710
118	6	0	3.233783	-0.953692	0.798208
119	6	0	5.122285	-1.173086	-0.739460
120	6	0	6.099769	-0.158708	-0.929905
121	6	0	6.841537	-0.135819	-2.124636
122	1	0	7.610841	0.607374	-2.286005
123	6	0	6.614522	-1.075712	-3.121650
124	1	0	7.195772	-1.044388	-4.034337
125	6	0	5.662131	-2.071154	-2.941587
126	1	0	5.538455	-2.805670	-3.726007
127	6	0	4.906576	-2.145806	-1.755836
128	6	0	3.941297	-3.312293	-1.567580
129	1	0	3.362891	-3.197543	-0.629276
130	6	0	4.706016	-4.634795	-1.445104
131	1	0	4.000423	-5.466714	-1.233111
132	1	0	5.431818	-4.579373	-0.605634
133	1	0	5.257752	-4.871279	-2.379821
134	6	0	2.914595	-3.382693	-2.706481
135	1	0	2.397157	-2.406521	-2.818747
136	1	0	2.156331	-4.163798	-2.486162
137	1	0	3.391153	-3.643494	-3.674111
138	6	0	6.392096	0.875231	0.151434
139	1	0	5.590828	0.859724	0.917506
140	6	0	7.704797	0.545859	0.868347
141	1	0	7.650307	-0.469465	1.316419
142	1	0	7.887587	1.274516	1.687105
143	1	0	8.563850	0.578431	0.164387
144	6	0	6.421979	2.304188	-0.411000
145	1	0	7.368826	2.509579	-0.953694
146	1	0	6.335483	3.041671	0.415413
147	1	0	5.578727	2.460024	-1.114410
148	8	0	2.439374	-0.525234	-0.053762
149	6	0	2.748248	0.922570	3.506502
150	1	0	3.588365	0.498767	4.062696
151	1	0	2.068722	1.386635	4.225285

L5-Mg(II)

Zero-point correction= 1.07239 a.u.

Thermal correction to Gibbs Free Energy= 0.98827 a.u.

Sum of electronic and zero-point Energies= -2475.42278 a.u.

Sum of electronic and thermal Free Energies= -2475.50691 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.799885	0.406981	0.723451
2	12	0	-0.007247	0.039940	-0.030289
3	8	0	-0.155858	1.857527	-0.721484
4	8	0	0.255953	-1.547173	-1.131368
5	8	0	-1.872953	-0.556018	0.379741
6	7	0	3.818570	1.432305	0.772851
7	1	0	4.374365	2.248861	0.539771
8	7	0	0.902059	2.675322	-1.073134
9	7	0	-3.829232	-1.650741	0.070140
10	1	0	-4.339219	-2.395937	-0.393463
11	7	0	-0.748008	-2.089950	-1.912324
12	6	0	4.505144	0.253993	1.149935
13	6	0	5.094534	-0.565966	0.152651
14	6	0	5.693615	-1.779505	0.536344
15	1	0	6.126118	-2.440943	-0.202500
16	6	0	5.733166	-2.162840	1.873204
17	1	0	6.198027	-3.100252	2.150882
18	6	0	5.174486	-1.349389	2.854195
19	1	0	5.219802	-1.678110	3.884015
20	6	0	4.554539	-0.133117	2.514304
21	6	0	3.942420	0.732416	3.611017
22	1	0	3.531672	1.671424	3.185085
23	6	0	2.772248	0.011167	4.289159
24	1	0	2.016004	-0.285642	3.531068
25	1	0	2.278110	0.687129	5.019602
26	1	0	3.114300	-0.897677	4.828144
27	6	0	4.996882	1.158278	4.639935
28	1	0	4.555491	1.877973	5.362538
29	1	0	5.846805	1.661047	4.130539
30	1	0	5.384673	0.288184	5.210395
31	6	0	5.045425	-0.182440	-1.323448
32	1	0	4.618709	0.834065	-1.451450
33	6	0	6.447115	-0.132801	-1.943906
34	1	0	7.104701	0.537408	-1.349761
35	1	0	6.391035	0.270245	-2.977792
36	1	0	6.910106	-1.140715	-1.991407
37	6	0	4.131573	-1.136045	-2.097086
38	1	0	4.531181	-2.172224	-2.092585

39	1	0	4.028166	-0.800434	-3.151121
40	1	0	3.122415	-1.137237	-1.634487
41	6	0	2.504439	1.425046	0.523951
42	6	0	1.942020	2.763274	0.054794
43	1	0	2.758742	3.359024	-0.359062
44	6	0	1.218161	3.584936	1.119501
45	1	0	1.913220	3.927412	1.889545
46	1	0	0.435399	2.987982	1.596369
47	6	0	0.633252	4.743917	0.285619
48	1	0	1.371520	5.549532	0.245201
49	6	0	-0.746335	5.265430	0.745624
50	1	0	-0.887838	5.152872	1.825865
51	1	0	-0.826488	6.334100	0.514937
52	6	0	-1.767799	4.470970	-0.086665
53	1	0	-2.737032	4.975187	-0.158640
54	1	0	-1.932667	3.483693	0.356238
55	6	0	-1.080344	4.321904	-1.455455
56	1	0	-1.485930	3.517803	-2.069299
57	1	0	-1.181427	5.255150	-2.023448
58	6	0	0.413943	4.159355	-1.145038
59	1	0	1.058733	4.621454	-1.893172
60	6	0	1.554515	2.195444	-2.365366
61	1	0	2.424165	2.841682	-2.513005
62	1	0	1.912296	1.186065	-2.148125
63	6	0	-0.500453	1.238758	-3.715387
64	6	0	-1.248240	-1.084864	-2.957348
65	1	0	-1.926743	-0.425722	-2.411538
66	1	0	-1.846153	-1.653887	-3.671726
67	6	0	-0.250443	-3.432635	-2.525934
68	1	0	-0.850316	-3.561832	-3.426990
69	6	0	1.255608	-3.488971	-2.795707
70	1	0	1.678774	-2.524831	-3.079672
71	1	0	1.392734	-4.168688	-3.645905
72	6	0	1.875863	-4.108599	-1.530325
73	1	0	2.020944	-3.335521	-0.770766
74	1	0	2.846683	-4.574382	-1.729330
75	6	0	0.818528	-5.129744	-1.065429
76	1	0	0.885499	-5.357800	0.003752
77	1	0	0.949013	-6.073910	-1.606571
78	6	0	-0.551318	-4.512247	-1.441987
79	1	0	-1.217377	-5.270022	-1.863295
80	6	0	-1.303359	-3.775041	-0.309284
81	1	0	-0.624910	-3.438579	0.479011
82	1	0	-2.086518	-4.386419	0.143787

83	6	0	-1.904370	-2.570897	-1.038973
84	1	0	-2.671790	-2.913197	-1.740099
85	6	0	-2.519233	-1.494030	-0.145561
86	6	0	-4.565278	-0.734409	0.857406
87	6	0	-5.118709	0.426136	0.256028
88	6	0	-5.772854	1.367933	1.070566
89	1	0	-6.183983	2.274718	0.647054
90	6	0	-5.901059	1.157715	2.440125
91	1	0	-6.409153	1.891847	3.052386
92	6	0	-5.376833	0.010056	3.027111
93	1	0	-5.491288	-0.121516	4.094938
94	6	0	-4.702850	-0.951380	2.252407
95	6	0	-4.120996	-2.190169	2.925631
96	1	0	-3.646842	-2.856819	2.175553
97	6	0	-5.216385	-3.021478	3.603672
98	1	0	-4.788610	-3.969208	3.995330
99	1	0	-6.008213	-3.280730	2.868462
100	1	0	-5.678994	-2.472643	4.450835
101	6	0	-3.021778	-1.808407	3.923285
102	1	0	-2.237763	-1.206910	3.415005
103	1	0	-2.541435	-2.723520	4.331291
104	1	0	-3.430715	-1.219633	4.771545
105	6	0	-4.988949	0.684660	-1.242165
106	1	0	-4.521290	-0.184471	-1.749616
107	6	0	-6.359513	0.873987	-1.904413
108	1	0	-7.018915	0.010133	-1.673637
109	1	0	-6.243652	0.931175	-3.007971
110	1	0	-6.855136	1.805924	-1.560313
111	6	0	-4.077122	1.886304	-1.508364
112	1	0	-4.509853	2.820981	-1.093195
113	1	0	-3.928759	2.021074	-2.601023
114	1	0	-3.084426	1.712039	-1.043505
115	1	0	-1.207265	1.494922	-2.922905
116	1	0	-1.015084	1.425466	-4.665538
117	6	0	0.693334	2.207883	-3.633208
118	1	0	1.402455	1.979332	-4.440592
119	1	0	0.341837	3.227215	-3.828303
120	6	0	-0.129699	-0.259898	-3.609817
121	1	0	0.764860	-0.375731	-2.995125
122	1	0	0.112905	-0.664475	-4.597771

L5-Mg(II)-COM

Zero-point correction= 1.20620 a.u.

Thermal correction to Gibbs Free Energy= 1.10988 a.u.
Sum of electronic and zero-point Energies= -5601.46167 a.u.
Sum of electronic and thermal Free Energies= -5601.55799 a.u.
The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.326518	1.475459	-1.862599
2	6	0	0.102879	2.161875	-0.557829
3	6	0	0.177582	3.572675	-0.862976
4	6	0	-0.164695	3.700142	-2.234107
5	7	0	-0.458783	2.429882	-2.803383
6	8	0	0.304075	1.481833	0.441071
7	6	0	0.495109	4.710090	-0.119157
8	6	0	-0.189618	4.927898	-2.864705
9	8	0	-0.493001	0.255278	-1.929073
10	6	0	-0.872574	2.214436	-4.184192
11	1	0	-1.806152	2.748893	-4.382296
12	1	0	-0.094441	2.565919	-4.867487
13	1	0	-1.028219	1.144631	-4.326931
14	6	0	0.474050	5.961371	-0.734365
15	6	0	0.136008	6.052717	-2.087689
16	35	0	0.946384	4.554561	1.715212
17	1	0	0.716535	6.855888	-0.172462
18	1	0	0.124469	7.032747	-2.554955
19	1	0	-0.449425	5.030178	-3.912169
20	8	0	1.925982	-0.782992	-0.469703
21	12	0	-0.072799	-0.781543	0.029152
22	8	0	-0.181123	-2.611159	-0.821847
23	8	0	0.109105	-0.998602	2.024122
24	8	0	-2.071413	-0.381511	0.399127
25	7	0	3.892564	-1.452095	-1.384146
26	1	0	4.392987	-2.142449	-1.932500
27	7	0	0.817361	-3.449112	-1.271366
28	7	0	-3.981359	0.120009	1.516864
29	1	0	-4.441335	0.265132	2.408429
30	7	0	-0.885054	-1.296951	2.929143
31	6	0	4.656843	-0.491458	-0.682338
32	6	0	5.165596	-0.801092	0.605393
33	6	0	5.833651	0.201242	1.331770
34	1	0	6.205377	0.007283	2.329139
35	6	0	6.030227	1.465486	0.784607

36	1	0	6.550025	2.224314	1.355505
37	6	0	5.567117	1.757146	-0.494943
38	1	0	5.743546	2.747153	-0.894657
39	6	0	4.876323	0.790667	-1.248410
40	6	0	4.378114	1.140417	-2.647227
41	1	0	3.860147	0.272291	-3.105986
42	6	0	3.355764	2.280141	-2.598681
43	1	0	2.551882	2.026182	-1.880757
44	1	0	2.895964	2.426724	-3.599454
45	1	0	3.824250	3.236163	-2.282648
46	6	0	5.543668	1.488101	-3.580044
47	1	0	5.170224	1.648217	-4.614344
48	1	0	6.275448	0.652312	-3.604907
49	1	0	6.066085	2.411313	-3.251708
50	6	0	4.980780	-2.185176	1.220418
51	1	0	4.529093	-2.883195	0.485130
52	6	0	6.321920	-2.810733	1.623070
53	1	0	7.017250	-2.814274	0.756390
54	1	0	6.169127	-3.863500	1.944301
55	1	0	6.795716	-2.259514	2.462302
56	6	0	4.019412	-2.124456	2.409115
57	1	0	4.434131	-1.504510	3.231937
58	1	0	3.823416	-3.146272	2.798724
59	1	0	3.053091	-1.687658	2.081212
60	6	0	2.564916	-1.563447	-1.201458
61	6	0	1.926133	-2.685284	-2.009122
62	1	0	2.692792	-3.432596	-2.228623
63	6	0	1.254856	-2.283467	-3.320013
64	1	0	1.993082	-1.930951	-4.044837
65	1	0	0.523797	-1.491663	-3.146518
66	6	0	0.584087	-3.604138	-3.749760
67	1	0	1.294887	-4.178243	-4.351081
68	6	0	-0.774664	-3.459260	-4.470945
69	1	0	-0.840325	-2.524734	-5.039254
70	1	0	-0.900150	-4.283892	-5.182844
71	6	0	-1.827512	-3.565078	-3.353800
72	1	0	-2.814318	-3.856778	-3.728598
73	1	0	-1.930484	-2.604982	-2.839342
74	6	0	-1.230393	-4.608283	-2.393090
75	1	0	-1.650733	-4.573620	-1.389026
76	1	0	-1.398537	-5.617317	-2.790300
77	6	0	0.283786	-4.367326	-2.421964
78	1	0	0.862658	-5.286854	-2.330811
79	6	0	1.426532	-4.242471	-0.120467

80	1	0	2.292119	-4.764280	-0.538794
81	1	0	1.785864	-3.483790	0.576400
82	6	0	-0.679739	-4.742813	1.374121
83	6	0	-1.424342	-2.709695	2.710965
84	1	0	-2.030381	-2.632600	1.807204
85	1	0	-2.087162	-2.928898	3.551151
86	6	0	-0.373878	-1.044933	4.378909
87	1	0	-0.985149	-1.696448	5.004610
88	6	0	1.127643	-1.265125	4.576957
89	1	0	1.529810	-2.062131	3.951875
90	1	0	1.262715	-1.569433	5.622653
91	6	0	1.776983	0.111314	4.348377
92	1	0	1.911539	0.282259	3.277413
93	1	0	2.755134	0.196620	4.834024
94	6	0	0.746583	1.103520	4.922515
95	1	0	0.832620	2.103579	4.484110
96	1	0	0.890268	1.209923	6.004127
97	6	0	-0.639692	0.468369	4.649022
98	1	0	-1.291949	0.569053	5.521021
99	6	0	-1.396405	0.988980	3.404783
100	1	0	-0.717747	1.425856	2.670135
101	1	0	-2.163650	1.724440	3.658287
102	6	0	-2.027831	-0.289265	2.849932
103	1	0	-2.784683	-0.650415	3.553372
104	6	0	-2.675946	-0.194474	1.472795
105	6	0	-4.761147	0.238592	0.342987
106	6	0	-5.289857	-0.925163	-0.275039
107	6	0	-6.006438	-0.790501	-1.477852
108	1	0	-6.401042	-1.659896	-1.986826
109	6	0	-6.233770	0.464221	-2.034677
110	1	0	-6.795537	0.550929	-2.955940
111	6	0	-5.749544	1.608556	-1.408713
112	1	0	-5.950407	2.569585	-1.863527
113	6	0	-5.004911	1.518470	-0.218576
114	6	0	-4.465973	2.789972	0.429282
115	1	0	-3.872982	2.546463	1.335440
116	6	0	-5.608494	3.701479	0.889801
117	1	0	-5.199901	4.581320	1.431565
118	1	0	-6.279024	3.151539	1.584399
119	1	0	-6.207152	4.068070	0.029183
120	6	0	-3.520207	3.534957	-0.519191
121	1	0	-2.748729	2.837197	-0.900690
122	1	0	-3.008905	4.361382	0.019392
123	1	0	-4.065910	3.965777	-1.384966

124	6	0	-5.101351	-2.309502	0.339120
125	1	0	-4.591679	-2.235474	1.321821
126	6	0	-6.447842	-2.990706	0.614631
127	1	0	-7.091300	-2.329309	1.233894
128	1	0	-6.288690	-3.936594	1.175682
129	1	0	-6.983750	-3.233525	-0.327036
130	6	0	-4.213113	-3.185054	-0.549382
131	1	0	-4.688051	-3.373145	-1.535347
132	1	0	-4.022710	-4.162361	-0.056658
133	1	0	-3.236937	-2.682963	-0.711298
134	1	0	-1.363059	-4.256220	0.674913
135	1	0	-1.213317	-5.608417	1.785780
136	6	0	0.530392	-5.265490	0.583934
137	1	0	1.209706	-5.794459	1.266932
138	1	0	0.192132	-6.017934	-0.138110
139	6	0	-0.323800	-3.753281	2.504933
140	1	0	0.583578	-3.208647	2.240800
141	1	0	-0.119667	-4.289159	3.438072

L3b-Mg(II)

Zero-point correction= 0.88856 a.u.

Thermal correction to Gibbs Free Energy= 0.81418 a.u.

Sum of electronic and zero-point Energies= -2163.37597 a.u.

Sum of electronic and thermal Free Energies= -2163.45035 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.940466	0.227075	0.406001
2	12	0	-0.013367	0.054987	0.005963
3	8	0	0.030360	1.711499	-1.042197
4	8	0	-0.028515	-1.341730	-1.375132
5	8	0	-1.972634	-0.225831	0.305693
6	7	0	4.091400	0.698149	-0.131044
7	1	0	4.741102	1.316160	-0.607130
8	7	0	1.113031	1.923618	-1.889666
9	7	0	-4.110107	-0.705900	-0.265307
10	1	0	-4.746660	-1.238384	-0.850002
11	7	0	-1.088293	-1.361314	-2.276610
12	6	0	4.628648	-0.271571	0.749439
13	6	0	4.633927	-1.643317	0.379306

14	6	0	5.142478	-2.590781	1.286224
15	1	0	5.152837	-3.643846	1.037968
16	6	0	5.647597	-2.195906	2.520759
17	1	0	6.036218	-2.938290	3.206118
18	6	0	5.658436	-0.851481	2.877769
19	1	0	6.058084	-0.578450	3.845401
20	6	0	5.155584	0.130245	2.004815
21	6	0	5.167396	1.594368	2.434198
22	1	0	4.751855	2.241814	1.634992
23	6	0	4.283740	1.814832	3.667472
24	1	0	3.252279	1.452734	3.467912
25	1	0	4.225802	2.898516	3.906555
26	1	0	4.685056	1.281690	4.555120
27	6	0	6.597380	2.086890	2.686635
28	1	0	6.594625	3.179241	2.889406
29	1	0	7.226828	1.906740	1.788797
30	1	0	7.057745	1.572467	3.556482
31	6	0	4.113152	-2.108935	-0.977619
32	1	0	3.773971	-1.245167	-1.585116
33	6	0	5.218179	-2.790967	-1.793400
34	1	0	6.091817	-2.112058	-1.895644
35	1	0	4.847433	-3.028615	-2.813704
36	1	0	5.552830	-3.736162	-1.316328
37	6	0	2.901155	-3.033919	-0.816879
38	1	0	3.185278	-3.993502	-0.335688
39	1	0	2.460567	-3.258515	-1.811700
40	1	0	2.123556	-2.543151	-0.194372
41	6	0	2.776381	0.926825	-0.212395
42	6	0	2.402258	2.116346	-1.092357
43	1	0	3.182352	2.255518	-1.844103
44	6	0	2.156706	3.438452	-0.343475
45	1	0	3.111156	3.929739	-0.144068
46	1	0	1.659957	3.252662	0.610462
47	6	0	1.245943	4.252237	-1.306659
48	1	0	1.746963	5.149972	-1.675622
49	6	0	0.931687	3.310391	-2.477958
50	1	0	1.643551	3.412158	-3.299690
51	6	0	1.269626	0.819359	-2.921353
52	1	0	2.056491	1.158438	-3.600883
53	1	0	1.622363	-0.058064	-2.383066
54	6	0	0.016753	0.472328	-3.731180
55	1	0	0.350761	-0.258026	-4.477073
56	1	0	-0.312292	1.350805	-4.298186
57	6	0	-1.240783	-0.049915	-3.028290

58	1	0	-1.598282	0.681251	-2.307355
59	1	0	-2.022636	-0.224214	-3.772247
60	6	0	-0.867440	-2.565646	-3.174256
61	1	0	-1.568582	-2.483433	-4.008098
62	6	0	-1.175836	-3.762519	-2.264878
63	1	0	-1.639454	-4.562115	-2.846977
64	6	0	-2.132607	-3.220450	-1.165110
65	1	0	-1.669985	-3.270172	-0.177549
66	1	0	-3.081133	-3.759744	-1.126255
67	6	0	-2.386089	-1.755594	-1.573826
68	1	0	-3.157911	-1.713286	-2.346100
69	6	0	-2.788862	-0.823652	-0.433618
70	6	0	-4.660013	0.030535	0.811237
71	6	0	-4.756268	1.445719	0.727936
72	6	0	-5.270109	2.158482	1.826421
73	1	0	-5.349775	3.237107	1.797311
74	6	0	-5.687951	1.494133	2.974815
75	1	0	-6.081839	2.058303	3.810525
76	6	0	-5.602297	0.107943	3.054602
77	1	0	-5.932073	-0.376859	3.964126
78	6	0	-5.088431	-0.645521	1.983502
79	6	0	-4.975963	-2.161216	2.117319
80	1	0	-4.561865	-2.609353	1.190475
81	6	0	-6.351785	-2.804042	2.327758
82	1	0	-6.259559	-3.911334	2.326687
83	1	0	-7.037865	-2.516287	1.502439
84	1	0	-6.802998	-2.494163	3.293839
85	6	0	-4.012245	-2.543953	3.246562
86	1	0	-3.018580	-2.076908	3.074664
87	1	0	-3.872779	-3.645984	3.272766
88	1	0	-4.395562	-2.217124	4.236348
89	6	0	-4.320480	2.205823	-0.521759
90	1	0	-3.974009	1.503103	-1.307065
91	6	0	-5.490329	2.982432	-1.138255
92	1	0	-6.336847	2.294397	-1.349332
93	1	0	-5.176849	3.444407	-2.099021
94	1	0	-5.844718	3.790379	-0.463920
95	6	0	-3.141613	3.138369	-0.216833
96	1	0	-3.442001	3.959153	0.468445
97	1	0	-2.758287	3.589533	-1.156985
98	1	0	-2.313106	2.568673	0.254832
99	1	0	0.156278	-2.513459	-3.539497
100	1	0	-0.262446	-4.154230	-1.814559
101	1	0	-0.087399	3.370958	-2.855511

102	1	0	0.330967	4.557215	-0.796896

L3b-Mg(II)-COM

Zero-point correction= 1.02277 a.u.

Thermal correction to Gibbs Free Energy= 0.93509 a.u.

Sum of electronic and zero-point Energies= -5289.42058 a.u.

Sum of electronic and thermal Free Energies= -5289.50826 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.170404	1.058966	-1.648957
2	6	0	0.459181	1.585394	-0.235301
3	6	0	1.025645	2.900131	-0.416713
4	6	0	1.038497	3.137745	-1.815530
5	7	0	0.505284	2.025677	-2.523568
6	8	0	0.191681	0.884581	0.735041
7	6	0	1.520323	3.870819	0.456165
8	6	0	1.534682	4.309938	-2.348664
9	8	0	-0.274928	-0.076174	-1.840338
10	6	0	0.362253	1.954282	-3.972835
11	1	0	1.330691	2.117105	-4.453547
12	1	0	-0.010800	0.961673	-4.227023
13	1	0	-0.348893	2.711553	-4.315102
14	6	0	2.029190	5.062445	-0.059592
15	6	0	2.029092	5.265007	-1.442830
16	35	0	1.506951	3.564345	2.323370
17	1	0	2.420471	5.825222	0.603666
18	1	0	2.427001	6.197532	-1.831316
19	1	0	1.546208	4.495598	-3.416596
20	8	0	1.632816	-1.419345	0.075340
21	12	0	-0.403332	-1.200049	0.054369
22	8	0	-0.420953	-2.996636	-0.859976
23	8	0	-0.731953	-1.749987	1.964686
24	8	0	-2.397179	-0.729029	0.010858
25	7	0	3.726332	-2.169741	-0.318603
26	1	0	4.318954	-2.899258	-0.701102
27	7	0	0.458751	-3.997865	-0.468492
28	7	0	-4.455194	-0.140600	0.747592
29	1	0	-5.112578	-0.124263	1.520313
30	7	0	-1.909763	-2.396883	2.313008

31	6	0	4.292530	-0.888806	-0.104461
32	6	0	4.397991	-0.370125	1.214744
33	6	0	4.846587	0.950929	1.393429
34	1	0	4.929484	1.377632	2.384255
35	6	0	5.185638	1.742466	0.301651
36	1	0	5.518647	2.760785	0.457089
37	6	0	5.102748	1.230840	-0.988836
38	1	0	5.372489	1.874883	-1.815273
39	6	0	4.668540	-0.088188	-1.215967
40	6	0	4.572371	-0.608612	-2.647337
41	1	0	4.265262	-1.673850	-2.661099
42	6	0	3.505110	0.155706	-3.435798
43	1	0	2.525383	0.055241	-2.926596
44	1	0	3.403294	-0.267780	-4.457838
45	1	0	3.760056	1.232793	-3.524124
46	6	0	5.930300	-0.548334	-3.357511
47	1	0	5.863204	-1.041491	-4.351133
48	1	0	6.698188	-1.084652	-2.759804
49	1	0	6.263388	0.499302	-3.513187
50	6	0	4.041212	-1.211852	2.436688
51	1	0	3.712322	-2.226735	2.130514
52	6	0	5.262252	-1.415219	3.341346
53	1	0	6.098338	-1.859875	2.760083
54	1	0	5.011059	-2.112227	4.169566
55	1	0	5.604781	-0.456273	3.784508
56	6	0	2.877847	-0.591185	3.221091
57	1	0	3.166992	0.379620	3.675870
58	1	0	2.557998	-1.276112	4.035370
59	1	0	2.006598	-0.424536	2.553773
60	6	0	2.388928	-2.323057	-0.322039
61	6	0	1.897644	-3.657692	-0.862046
62	1	0	2.520440	-4.457349	-0.448682
63	6	0	1.875249	-3.740546	-2.402363
64	1	0	2.861917	-4.028575	-2.771207
65	1	0	1.618127	-2.771075	-2.833080
66	6	0	0.782436	-4.796919	-2.718263
67	1	0	1.197500	-5.675674	-3.217542
68	6	0	0.191142	-5.196117	-1.361349
69	1	0	0.706608	-6.053121	-0.920450
70	6	0	0.356241	-4.319738	1.009610
71	1	0	1.024879	-5.168783	1.174486
72	1	0	0.736981	-3.451250	1.541827
73	6	0	-1.046049	-4.684710	1.505258
74	1	0	-0.908342	-5.053219	2.528330

75	1	0	-1.431803	-5.538263	0.935813
76	6	0	-2.162324	-3.636671	1.479507
77	1	0	-2.343645	-3.293663	0.463702
78	1	0	-3.078452	-4.082611	1.875941
79	6	0	-1.838143	-2.680752	3.802508
80	1	0	-2.655214	-3.365876	4.045366
81	6	0	-2.019802	-1.305995	4.454015
82	1	0	-2.552457	-1.407616	5.402452
83	6	0	-2.821082	-0.463105	3.425116
84	1	0	-2.238404	0.394740	3.084585
85	1	0	-3.769195	-0.097505	3.824708
86	6	0	-3.089757	-1.432587	2.252549
87	1	0	-3.982004	-2.033689	2.454906
88	6	0	-3.265000	-0.746962	0.903045
89	6	0	-4.685726	0.738907	-0.337778
90	6	0	-5.024838	0.217348	-1.615043
91	6	0	-5.185702	1.106852	-2.692799
92	1	0	-5.439299	0.740654	-3.678963
93	6	0	-5.021813	2.476795	-2.517114
94	1	0	-5.146394	3.146589	-3.358367
95	6	0	-4.698146	2.990535	-1.265788
96	1	0	-4.573413	4.060553	-1.165108
97	6	0	-4.527580	2.139404	-0.158911
98	6	0	-4.147979	2.736612	1.193323
99	1	0	-4.066405	1.944220	1.964141
100	6	0	-5.221960	3.710011	1.693239
101	1	0	-4.981248	4.045694	2.724808
102	1	0	-6.212269	3.206619	1.718960
103	1	0	-5.292238	4.607307	1.043221
104	6	0	-2.775829	3.417262	1.130559
105	1	0	-2.012014	2.697659	0.769848
106	1	0	-2.471373	3.759539	2.142765
107	1	0	-2.787701	4.296076	0.451708
108	6	0	-5.221114	-1.279042	-1.842261
109	1	0	-5.074372	-1.841851	-0.897310
110	6	0	-6.650896	-1.587232	-2.303197
111	1	0	-7.384006	-1.177874	-1.575494
112	1	0	-6.803247	-2.686383	-2.362788
113	1	0	-6.858748	-1.152435	-3.303750
114	6	0	-4.193652	-1.827545	-2.840019
115	1	0	-4.347046	-1.402693	-3.854620
116	1	0	-4.280402	-2.933275	-2.907905
117	1	0	-3.162893	-1.585978	-2.504446
118	1	0	-0.878229	-3.155757	3.995070

119	1	0	-1.052598	-0.842376	4.653658
120	1	0	-0.883934	-5.362653	-1.364159
121	1	0	0.015481	-4.369286	-3.365756

L3c-Mg(II)

Zero-point correction= 0.94536 a.u.

Thermal correction to Gibbs Free Energy= 0.86128 a.u.

Sum of electronic and zero-point Energies= -2241.99392 a.u.

Sum of electronic and thermal Free Energies= -2242.07800a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.975591	-0.264114	0.524810
2	12	0	0.003882	0.009437	0.289334
3	8	0	0.114445	-1.550108	-0.902499
4	8	0	-0.099186	1.589299	-0.876619
5	8	0	1.975079	0.310964	0.573684
6	7	0	-4.059359	-0.896980	-0.108226
7	1	0	-4.639157	-1.521414	-0.659144
8	7	0	-0.932854	-1.771804	-1.788565
9	7	0	4.062083	0.856597	-0.125175
10	1	0	4.649979	1.438617	-0.712872
11	7	0	0.944255	1.824079	-1.762585
12	6	0	-4.708850	0.051735	0.716564
13	6	0	-4.911533	1.376061	0.246691
14	6	0	-5.518141	2.315705	1.099557
15	1	0	-5.674641	3.336125	0.775348
16	6	0	-5.928954	1.955541	2.379082
17	1	0	-6.393521	2.691493	3.022693
18	6	0	-5.748733	0.653036	2.833772
19	1	0	-6.080552	0.405469	3.833453
20	6	0	-5.145621	-0.319264	2.015096
21	6	0	-4.964350	-1.738753	2.542463
22	1	0	-4.506391	-2.387850	1.768602
23	6	0	-4.015560	-1.761631	3.745800
24	1	0	-3.044339	-1.294764	3.474281
25	1	0	-3.817080	-2.809922	4.056142
26	1	0	-4.445857	-1.215074	4.611366
27	6	0	-6.313225	-2.379076	2.892063
28	1	0	-6.169782	-3.446186	3.166933

29	1	0	-6.993128	-2.339575	2.014162
30	1	0	-6.800329	-1.862845	3.746107
31	6	0	-4.482060	1.800281	-1.154451
32	1	0	-4.046095	0.942596	-1.707531
33	6	0	-5.680572	2.274252	-1.984850
34	1	0	-6.459666	1.482606	-2.016424
35	1	0	-5.362011	2.484893	-3.028398
36	1	0	-6.127839	3.199532	-1.564327
37	6	0	-3.395394	2.879358	-1.091727
38	1	0	-3.795797	3.835157	-0.692313
39	1	0	-2.985397	3.066896	-2.107260
40	1	0	-2.564491	2.543575	-0.436664
41	6	0	-2.727509	-1.005278	-0.150283
42	6	0	-2.216292	-2.149428	-1.032412
43	1	0	-2.955317	-2.350731	-1.812335
44	6	0	-1.993336	-3.409897	-0.177617
45	1	0	-2.936901	-3.633125	0.329975
46	1	0	-1.246341	-3.192101	0.591609
47	6	0	-1.551340	-4.592886	-1.044297
48	1	0	-2.372426	-4.880169	-1.714442
49	6	0	-0.314636	-4.222629	-1.864544
50	1	0	-0.064975	-5.017766	-2.575934
51	6	0	-1.203143	-0.542882	-2.658195
52	1	0	-1.963989	-0.855808	-3.377726
53	1	0	-1.626673	0.218370	-2.007377
54	6	0	-0.005364	0.041691	-3.417278
55	1	0	-0.436746	0.802577	-4.076313
56	1	0	0.418150	-0.709692	-4.091903
57	6	0	1.200686	0.611811	-2.658675
58	1	0	1.624972	-0.161727	-2.023492
59	1	0	1.957077	0.933380	-3.379363
60	6	0	0.343370	4.279573	-1.776982
61	1	0	0.091973	5.093732	-2.466004
62	6	0	1.587634	4.623356	-0.956458
63	1	0	2.404801	4.924212	-1.625647
64	6	0	2.030788	3.418055	-0.122413
65	1	0	1.292260	3.187986	0.651317
66	1	0	2.981714	3.626944	0.377678
67	6	0	2.236329	2.173659	-1.004913
68	1	0	2.974738	2.385061	-1.783548
69	6	0	2.734590	1.013380	-0.134880
70	6	0	4.698740	-0.091091	0.711011
71	6	0	4.899758	-1.418128	0.249871
72	6	0	5.492938	-2.356651	1.113430

73	1	0	5.647536	-3.379615	0.796128
74	6	0	5.891762	-1.992270	2.395528
75	1	0	6.345238	-2.727457	3.047997
76	6	0	5.712990	-0.686867	2.842059
77	1	0	6.037946	-0.435178	3.843056
78	6	0	5.126206	0.284751	2.011236
79	6	0	4.959409	1.711220	2.524216
80	1	0	4.515443	2.357683	1.740975
81	6	0	6.313788	2.338822	2.875165
82	1	0	6.180188	3.409434	3.140984
83	1	0	6.997141	2.285430	2.000385
84	1	0	6.791192	1.824132	3.735542
85	6	0	4.002653	1.759972	3.720390
86	1	0	3.023182	1.314104	3.443364
87	1	0	3.824895	2.813817	4.024086
88	1	0	4.414869	1.208778	4.591957
89	6	0	4.473216	-1.848539	-1.149675
90	1	0	4.042928	-0.991648	-1.707880
91	6	0	5.671975	-2.335386	-1.972123
92	1	0	6.460413	-1.552752	-1.997304
93	1	0	5.358470	-2.541157	-3.017995
94	1	0	6.105091	-3.266288	-1.548916
95	6	0	3.380275	-2.920696	-1.083460
96	1	0	3.773883	-3.875851	-0.675678
97	1	0	2.973029	-3.113897	-2.098884
98	1	0	2.549195	-2.575376	-0.433654
99	1	0	-1.340976	-5.454620	-0.402111
100	1	0	0.551052	-4.087617	-1.209826
101	6	0	-0.543115	-2.953775	-2.673613
102	1	0	0.363002	-2.642758	-3.191231
103	1	0	-1.353207	-3.076482	-3.398961
104	1	0	-0.518677	4.129447	-1.120548
105	1	0	1.386131	5.469978	-0.291834
106	6	0	0.560874	3.029821	-2.618696
107	1	0	1.369514	3.162913	-3.343003
108	1	0	-0.348683	2.737986	-3.141182

L3c-Mg(II)-COM

Zero-point correction= 1.08016 a.u.

Thermal correction to Gibbs Free Energy= 0.98621 a.u.

Sum of electronic and zero-point Energies= -5368.03774 a.u.

Sum of electronic and thermal Free Energies= -5368.13169 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.024636	1.767553	-1.719119
2	6	0	0.513191	2.213976	-0.332805
3	6	0	0.884150	3.600430	-0.476555
4	6	0	0.639532	3.937651	-1.833822
5	7	0	0.129300	2.819424	-2.550584
6	8	0	0.519254	1.404618	0.590574
7	6	0	1.392128	4.564444	0.397100
8	6	0	0.890793	5.203618	-2.322743
9	8	0	-0.367811	0.615300	-1.925132
10	6	0	-0.222326	2.824619	-3.965495
11	1	0	0.651493	3.094627	-4.564927
12	1	0	-0.553461	1.821076	-4.233949
13	1	0	-1.030961	3.538192	-4.147538
14	6	0	1.655025	5.849639	-0.075751
15	6	0	1.403254	6.149466	-1.417707
16	35	0	1.719719	4.126191	2.209265
17	1	0	2.050941	6.609911	0.587503
18	1	0	1.612212	7.153607	-1.774159
19	1	0	0.706546	5.467357	-3.357882
20	8	0	1.745810	-1.040932	-0.536922
21	12	0	-0.214044	-0.606776	-0.095513
22	8	0	-0.735218	-2.307566	-1.040458
23	8	0	-0.078705	-1.337441	1.780359
24	8	0	-2.151417	-0.078183	0.334415
25	7	0	3.567122	-2.281344	-1.066613
26	1	0	3.930506	-3.163777	-1.409557
27	7	0	0.093380	-3.415476	-1.051684
28	7	0	-4.190916	-0.190942	1.315313
29	1	0	-4.748907	-0.520297	2.095447
30	7	0	-1.164500	-1.896231	2.429427
31	6	0	4.459537	-1.415476	-0.391382
32	6	0	4.825629	-1.688548	0.952928
33	6	0	5.675814	-0.790137	1.622639
34	1	0	5.965105	-0.964674	2.650543
35	6	0	6.153843	0.349475	0.983643
36	1	0	6.804138	1.032428	1.515155
37	6	0	5.794238	0.619595	-0.332860
38	1	0	6.176227	1.518788	-0.797789
39	6	0	4.949052	-0.252619	-1.042445

40	6	0	4.564475	0.078614	-2.480933
41	1	0	3.918925	-0.717050	-2.906194
42	6	0	3.754054	1.377853	-2.545443
43	1	0	2.882645	1.310630	-1.862724
44	1	0	3.372571	1.542709	-3.575906
45	1	0	4.367688	2.255733	-2.251937
46	6	0	5.799656	0.154553	-3.385904
47	1	0	5.488605	0.287259	-4.444389
48	1	0	6.382611	-0.788796	-3.315520
49	1	0	6.458048	1.004599	-3.108047
50	6	0	4.286279	-2.908251	1.694554
51	1	0	3.652371	-3.526227	1.025793
52	6	0	5.422656	-3.822534	2.166705
53	1	0	6.067042	-4.105406	1.306812
54	1	0	5.004707	-4.755174	2.602938
55	1	0	6.050276	-3.328499	2.938042
56	6	0	3.393835	-2.486346	2.868253
57	1	0	3.979143	-1.967237	3.656513
58	1	0	2.909682	-3.378546	3.319819
59	1	0	2.594771	-1.803005	2.511581
60	6	0	2.241751	-2.062291	-1.048787
61	6	0	1.411321	-3.115680	-1.785171
62	1	0	1.957674	-4.062245	-1.789937
63	6	0	1.137219	-2.656331	-3.226766
64	1	0	2.106452	-2.463189	-3.698554
65	1	0	0.585730	-1.712510	-3.197372
66	6	0	0.357384	-3.720436	-4.005745
67	1	0	0.990406	-4.607378	-4.144426
68	6	0	-0.920380	-4.107456	-3.257563
69	1	0	-1.415628	-4.955446	-3.744226
70	6	0	0.421047	-3.896219	0.360296
71	1	0	1.013882	-4.806069	0.232202
72	1	0	1.036123	-3.123372	0.813062
73	6	0	-0.768828	-4.195520	1.276744
74	1	0	-0.329474	-4.637991	2.177524
75	1	0	-1.392873	-4.986705	0.847411
76	6	0	-1.744373	-3.074632	1.650708
77	1	0	-2.175597	-2.658415	0.744279
78	1	0	-2.539967	-3.484988	2.278835
79	6	0	-0.158868	-1.204549	4.639806
80	1	0	0.139897	-1.614987	5.611130
81	6	0	-1.206503	-0.102028	4.812418
82	1	0	-2.035868	-0.470024	5.431708
83	6	0	-1.747346	0.343925	3.450360

84	1	0	-0.969507	0.844996	2.867496
85	1	0	-2.576989	1.048168	3.575832
86	6	0	-2.277372	-0.854710	2.646036
87	1	0	-3.053419	-1.373720	3.215998
88	6	0	-2.859610	-0.368317	1.317653
89	6	0	-4.870133	0.233817	0.148877
90	6	0	-5.439191	-0.729255	-0.725101
91	6	0	-6.067715	-0.290477	-1.904458
92	1	0	-6.503938	-1.000021	-2.595171
93	6	0	-6.129911	1.063646	-2.217722
94	1	0	-6.611976	1.383274	-3.132663
95	6	0	-5.570340	2.008626	-1.363644
96	1	0	-5.629982	3.053036	-1.640120
97	6	0	-4.938818	1.616000	-0.169770
98	6	0	-4.337054	2.677402	0.746280
99	1	0	-3.913813	2.210583	1.658863
100	6	0	-5.403008	3.666488	1.232076
101	1	0	-4.964320	4.362738	1.978770
102	1	0	-6.236715	3.118683	1.721642
103	1	0	-5.812625	4.269084	0.394224
104	6	0	-3.182057	3.409586	0.054189
105	1	0	-2.432158	2.675899	-0.307314
106	1	0	-2.676705	4.092726	0.770287
107	1	0	-3.539968	4.007666	-0.810316
108	6	0	-5.348093	-2.224234	-0.433113
109	1	0	-4.836645	-2.406387	0.534339
110	6	0	-6.740763	-2.852639	-0.305062
111	1	0	-7.330355	-2.319303	0.471012
112	1	0	-6.652277	-3.916607	0.003007
113	1	0	-7.295337	-2.813981	-1.266268
114	6	0	-4.515082	-2.942811	-1.501183
115	1	0	-5.019340	-2.923247	-2.490527
116	1	0	-4.353262	-4.002859	-1.210235
117	1	0	-3.521720	-2.456330	-1.598484
118	1	0	0.115261	-3.338529	-5.003433
119	1	0	-1.628234	-3.273512	-3.252671
120	6	0	-0.621363	-4.521000	-1.823130
121	1	0	-1.537776	-4.718653	-1.269197
122	1	0	0.025406	-5.403277	-1.782431
123	1	0	0.740467	-0.805236	4.161972
124	1	0	-0.772642	0.758547	5.332809
125	6	0	-0.695677	-2.360368	3.805693
126	1	0	-1.554123	-2.843558	4.282473
127	1	0	0.077233	-3.103526	3.616328

L3c-TS1-*si*

Zero-point correction= 1.19362 a.u.

Thermal correction to Gibbs Free Energy= 1.08855 a.u.

Sum of electronic and zero-point Energies= -5600.45051 a.u.

Sum of electronic and thermal Free Energies= -5600.55559 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.786347	0.950521	-1.955770
2	6	0	-0.295418	1.833748	-0.793430
3	6	0	-1.180981	3.044374	-0.916485
4	6	0	-1.927344	2.904027	-2.105274
5	7	0	-1.650762	1.653860	-2.718948
6	8	0	-0.035667	1.193931	0.293130
7	6	0	-1.418369	4.147289	-0.115075
8	6	0	-2.841730	3.857595	-2.525727
9	8	0	-0.451925	-0.236665	-2.053939
10	6	0	-2.367481	1.125491	-3.872020
11	1	0	-3.443111	1.105585	-3.670064
12	1	0	-2.174115	1.743888	-4.753163
13	1	0	-2.013676	0.110098	-4.053861
14	6	0	-2.338142	5.128650	-0.502379
15	6	0	-3.026491	4.980701	-1.706491
16	35	0	-0.547974	4.312102	1.581220
17	1	0	-2.519849	5.988535	0.132622
18	1	0	-3.738931	5.743894	-2.004702
19	1	0	-3.410433	3.736044	-3.441035
20	8	0	2.196131	-0.838562	-0.255469
21	12	0	0.076481	-0.873697	0.037862
22	8	0	0.167849	-2.805078	-0.597129
23	8	0	0.225144	-1.280560	2.028162
24	8	0	-2.003244	-1.046916	0.280211
25	7	0	4.310755	-1.676525	-0.440820
26	1	0	4.887851	-2.445311	-0.763363
27	7	0	1.252199	-3.630508	-0.378091
28	7	0	-4.019050	-1.490832	1.225250
29	1	0	-4.546650	-1.642962	2.077283
30	7	0	-0.708459	-2.036582	2.711587
31	6	0	4.964225	-0.467557	-0.102729

32	6	0	5.067064	-0.072604	1.258157
33	6	0	5.713276	1.137552	1.569744
34	1	0	5.795688	1.472730	2.595066
35	6	0	6.267285	1.928046	0.568738
36	1	0	6.762782	2.855147	0.826959
37	6	0	6.191661	1.530716	-0.761690
38	1	0	6.642772	2.164113	-1.513964
39	6	0	5.547369	0.332990	-1.121591
40	6	0	5.500652	-0.078313	-2.589943
41	1	0	4.944266	-1.028538	-2.713439
42	6	0	4.763564	0.963228	-3.439831
43	1	0	3.747736	1.138582	-3.031268
44	1	0	4.652290	0.595775	-4.482465
45	1	0	5.309598	1.929549	-3.467346
46	6	0	6.911445	-0.330127	-3.134858
47	1	0	6.856007	-0.721870	-4.173265
48	1	0	7.432217	-1.086836	-2.509686
49	1	0	7.515209	0.602004	-3.144918
50	6	0	4.511336	-0.934727	2.386607
51	1	0	4.071229	-1.869431	1.985215
52	6	0	5.619728	-1.372578	3.351979
53	1	0	6.431980	-1.885920	2.793974
54	1	0	5.213428	-2.087108	4.099741
55	1	0	6.051059	-0.506946	3.897505
56	6	0	3.389265	-0.206872	3.134156
57	1	0	3.768221	0.697154	3.655946
58	1	0	2.939893	-0.884099	3.890909
59	1	0	2.592959	0.100389	2.424046
60	6	0	2.970783	-1.768846	-0.547036
61	6	0	2.496720	-3.110178	-1.112307
62	1	0	3.269511	-3.864390	-0.937278
63	6	0	2.220201	-2.982259	-2.618373
64	1	0	3.126606	-2.593504	-3.093261
65	1	0	1.422329	-2.249838	-2.767974
66	6	0	0.653776	-4.940297	-2.454185
67	1	0	0.448602	-5.962527	-2.792119
68	6	0	0.921349	-5.003640	-0.955704
69	1	0	1.769429	-5.656622	-0.724017
70	6	0	1.580698	-3.754523	1.107558
71	1	0	2.429694	-4.441077	1.171186
72	1	0	1.883870	-2.763803	1.432302
73	6	0	0.454336	-4.254836	2.015513
74	1	0	0.915800	-4.385686	3.000174
75	1	0	0.138531	-5.259858	1.715770

76	6	0	-0.839140	-3.441629	2.128322
77	1	0	-1.273383	-3.320723	1.139693
78	1	0	-1.543337	-3.970331	2.777034
79	6	0	-0.262035	-2.116040	4.169289
80	1	0	-0.980562	-2.760642	4.685023
81	6	0	-0.177224	-0.737299	4.812183
82	1	0	0.134036	-0.880429	5.853467
83	6	0	-2.016613	0.047769	3.290491
84	1	0	-1.364859	0.661026	2.661364
85	1	0	-3.020683	0.481657	3.252336
86	6	0	-2.095866	-1.368752	2.695265
87	1	0	-2.729499	-2.003077	3.322430
88	6	0	-2.684322	-1.303190	1.285900
89	6	0	-4.737704	-1.211498	0.037808
90	6	0	-4.782894	-2.173836	-1.004911
91	6	0	-5.397315	-1.830991	-2.222863
92	1	0	-5.442186	-2.540335	-3.038594
93	6	0	-5.951076	-0.568914	-2.410760
94	1	0	-6.407896	-0.316557	-3.359231
95	6	0	-5.926063	0.368629	-1.383527
96	1	0	-6.363049	1.341649	-1.564293
97	6	0	-5.343674	0.060416	-0.140621
98	6	0	-5.344937	1.105566	0.969781
99	1	0	-4.962359	0.669547	1.913475
100	6	0	-6.762669	1.600259	1.284445
101	1	0	-6.749281	2.240434	2.192631
102	1	0	-7.433763	0.737434	1.483392
103	1	0	-7.183225	2.198112	0.448716
104	6	0	-4.418839	2.271233	0.616426
105	1	0	-3.392562	1.888057	0.440191
106	1	0	-4.374546	2.997596	1.455875
107	1	0	-4.770082	2.801253	-0.293868
108	6	0	-4.189965	-3.567908	-0.829064
109	1	0	-3.752025	-3.681705	0.184239
110	6	0	-5.270652	-4.648817	-0.949120
111	1	0	-6.082672	-4.459938	-0.214498
112	1	0	-4.836604	-5.648141	-0.730310
113	1	0	-5.709249	-4.675217	-1.968966
114	6	0	-3.053877	-3.815100	-1.827200
115	1	0	-3.432362	-3.864356	-2.869985
116	1	0	-2.546401	-4.775118	-1.592713
117	1	0	-2.304626	-2.998741	-1.760785
118	1	0	0.711550	-2.603114	4.150925
119	1	0	0.601361	-0.155626	4.312134

120	1	0	0.041099	-5.345107	-0.412686
121	1	0	-0.246695	-4.347647	-2.634767
122	6	0	1.835970	-4.338920	-3.216705
123	1	0	2.698938	-5.016994	-3.167599
124	1	0	1.583037	-4.215447	-4.275382
125	6	0	-1.512603	0.004540	4.735808
126	1	0	-1.403735	1.025578	5.117598
127	1	0	-2.257138	-0.499030	5.367669
128	6	0	1.322439	2.345920	-1.682877
129	6	0	1.999997	3.237344	-0.821510
130	8	0	1.874005	4.510586	-1.094273
131	6	0	2.437069	5.536980	-0.236199
132	1	0	2.165619	6.477057	-0.714361
133	6	0	2.723779	2.758731	0.384079
134	1	0	1.993128	5.476107	0.758508
135	1	0	2.906937	1.688727	0.307863
136	1	0	1.761458	1.354474	-1.730524
137	1	0	1.024514	2.767539	-2.640501
138	1	0	3.661732	3.299806	0.539160
139	1	0	3.523504	5.435235	-0.191521
140	1	0	2.087935	2.928454	1.263945

L3c-TS1-*re*

Zero-point correction= 1.19472 a.u.

Thermal correction to Gibbs Free Energy= 1.09896 a.u.

Sum of electronic and zero-point Energies= -5600.44400 a.u.

Sum of electronic and thermal Free Energies= -5600.53975 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.666178	3.025580	-1.104761
2	6	0	-0.453189	4.031623	-0.140610
3	8	0	0.175895	5.102510	-0.559163
4	6	0	0.557137	6.176802	0.338661
5	6	0	-0.831275	3.803768	1.277660
6	1	0	-1.489081	2.347470	-0.899893
7	1	0	-0.566326	3.338802	-2.140999
8	1	0	0.977143	6.943801	-0.310986
9	1	0	1.314481	5.816662	1.036829
10	1	0	-0.317576	6.564343	0.864721

11	1	0	-0.477150	4.567538	1.968773
12	1	0	-0.423289	2.819743	1.556491
13	6	0	0.434110	0.903410	-2.037568
14	6	0	0.745186	1.700124	-0.760633
15	6	0	2.007465	2.420445	-1.135910
16	6	0	2.204616	2.232294	-2.520376
17	7	0	1.218885	1.353488	-3.042785
18	8	0	0.486213	1.108480	0.346190
19	8	0	-0.362495	-0.043973	-2.039027
20	6	0	1.175997	0.871824	-4.417037
21	6	0	2.945881	3.149163	-0.426103
22	6	0	3.277706	2.789404	-3.198638
23	1	0	0.912185	1.689571	-5.094574
24	1	0	0.417357	0.090548	-4.477759
25	1	0	2.146736	0.461969	-4.710188
26	6	0	4.200985	3.532467	-2.448294
27	6	0	4.054979	3.706987	-1.072314
28	1	0	3.419873	2.638638	-4.263340
29	1	0	5.059565	3.971075	-2.947748
30	1	0	4.791747	4.266285	-0.506532
31	35	0	2.759274	3.370544	1.462721
32	8	0	-0.899300	-2.649583	-0.585257
33	8	0	1.543639	-1.447490	0.010710
34	12	0	-0.451144	-0.760773	0.080548
35	8	0	-0.705558	-1.129239	2.065438
36	7	0	3.345214	-2.825626	0.068139
37	1	0	3.732493	-3.733213	-0.164348
38	7	0	-0.179574	-3.777179	-0.230530
39	7	0	-4.648830	-0.000503	0.793003
40	1	0	-5.289249	-0.002749	1.578756
41	7	0	-1.899888	-1.550547	2.618372
42	6	0	4.242938	-1.779123	0.391406
43	6	0	4.307338	-1.285803	1.721237
44	6	0	5.110683	-0.163831	1.993682
45	1	0	5.172629	0.241938	2.994874
46	6	0	5.834596	0.456826	0.980945
47	1	0	6.435355	1.329049	1.204705
48	6	0	5.793894	-0.040974	-0.317197
49	1	0	6.367375	0.466482	-1.081532
50	6	0	5.022232	-1.174786	-0.629953
51	6	0	5.013352	-1.706470	-2.058791
52	1	0	4.441242	-2.653264	-2.118516
53	6	0	4.322705	-0.718459	-3.000526
54	1	0	3.290419	-0.525386	-2.641595

55	1	0	4.257357	-1.145818	-4.023750
56	1	0	4.876848	0.242305	-3.052509
57	6	0	6.428164	-2.040706	-2.548381
58	1	0	6.378202	-2.552335	-3.533723
59	1	0	6.929317	-2.726277	-1.831928
60	1	0	7.047934	-1.126966	-2.665370
61	6	0	3.533242	-1.948964	2.855658
62	1	0	2.958378	-2.821042	2.480045
63	6	0	4.482745	-2.495717	3.928118
64	1	0	5.214212	-3.195635	3.470100
65	1	0	3.907559	-3.055098	4.696802
66	1	0	5.038578	-1.678522	4.434608
67	6	0	2.514030	-0.982902	3.468900
68	1	0	3.015089	-0.145568	3.998809
69	1	0	1.871885	-1.523561	4.196334
70	1	0	1.864234	-0.559381	2.675376
71	6	0	2.045733	-2.566155	-0.180791
72	6	0	1.257480	-3.727839	-0.781152
73	1	0	1.714629	-4.677593	-0.487292
74	6	0	1.243678	-3.598449	-2.314212
75	1	0	2.283072	-3.551301	-2.654834
76	1	0	0.761167	-2.652718	-2.578122
77	6	0	0.517519	-4.781916	-2.959045
78	1	0	1.087194	-5.703666	-2.778096
79	6	0	-0.890417	-4.912868	-2.377636
80	1	0	-1.384247	-5.821358	-2.741133
81	6	0	-0.109928	-3.950565	1.284498
82	1	0	0.452869	-4.871717	1.458511
83	1	0	0.456390	-3.102938	1.661302
84	6	0	-1.452155	-4.035106	2.015306
85	1	0	-1.205839	-4.294043	3.050117
86	1	0	-2.038621	-4.883815	1.647528
87	6	0	-2.404037	-2.837173	1.969638
88	1	0	-2.616351	-2.590969	0.933188
89	1	0	-3.332376	-3.094139	2.486798
90	6	0	-1.238876	-0.504441	4.823322
91	1	0	-1.109417	-0.751568	5.883211
92	6	0	-2.263310	0.616183	4.642436
93	1	0	-3.198107	0.356918	5.158024
94	6	0	-2.545012	0.834920	3.153420
95	1	0	-1.654873	1.210365	2.642546
96	1	0	-3.348625	1.566147	3.015040
97	6	0	-2.985311	-0.472684	2.475010
98	1	0	-3.861872	-0.877162	2.988792

99	6	0	-3.334710	-0.210391	1.005307
100	6	0	-5.166526	0.368215	-0.471997
101	6	0	-5.401334	-0.625352	-1.460369
102	6	0	-5.923586	-0.236799	-2.707320
103	1	0	-6.102078	-0.968255	-3.484482
104	6	0	-6.248008	1.091074	-2.961516
105	1	0	-6.662963	1.370153	-3.921548
106	6	0	-6.061433	2.058725	-1.980544
107	1	0	-6.349229	3.077526	-2.202814
108	6	0	-5.512277	1.721945	-0.729750
109	6	0	-5.325062	2.810338	0.322711
110	1	0	-4.782430	2.410031	1.202883
111	6	0	-6.680738	3.310229	0.831645
112	1	0	-6.534686	4.059720	1.638673
113	1	0	-7.265911	2.463860	1.250997
114	1	0	-7.268329	3.781743	0.015110
115	6	0	-4.480776	3.975982	-0.210160
116	1	0	-3.543069	3.595757	-0.663393
117	1	0	-4.214201	4.664330	0.620211
118	1	0	-5.030338	4.562237	-0.976133
119	6	0	-5.142056	-2.103326	-1.187787
120	1	0	-4.766004	-2.251359	-0.155861
121	6	0	-6.435401	-2.921638	-1.285216
122	1	0	-7.205752	-2.501532	-0.603178
123	1	0	-6.244834	-3.973218	-0.980714
124	1	0	-6.837358	-2.926070	-2.320319
125	6	0	-4.070545	-2.659921	-2.130371
126	1	0	-4.420118	-2.666317	-3.184198
127	1	0	-3.818237	-3.701544	-1.839183
128	1	0	-3.148870	-2.044179	-2.066432
129	8	0	-2.482509	-0.146411	0.101773
130	1	0	-0.265432	-0.189961	4.437408
131	1	0	-1.895669	1.546829	5.088384
132	6	0	-1.671845	-1.778254	4.110554
133	1	0	-2.609857	-2.170780	4.516466
134	1	0	-0.900740	-2.543877	4.176922
135	1	0	0.471049	-4.638362	-4.044049
136	1	0	-1.501443	-4.060518	-2.686170
137	6	0	-0.866460	-4.988000	-0.856828
138	1	0	-0.328453	-5.873775	-0.503524
139	1	0	-1.876574	-4.992421	-0.451206
140	1	0	-1.921260	3.728297	1.358153

L3d-Mg(II)

Zero-point correction= 1.01630 a.u.

Thermal correction to Gibbs Free Energy= 0.93528 a.u.

Sum of electronic and zero-point Energies= -2396.80953 a.u.

Sum of electronic and thermal Free Energies= -2396.89055 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.249661	1.492346	-1.379989
2	8	0	1.982884	-0.001312	0.217146
3	12	0	0.008633	-0.018947	-0.146125
4	8	0	-0.247905	-1.613871	-1.263213
5	7	0	4.182837	0.432704	-0.086241
6	1	0	4.899698	0.963928	-0.570396
7	7	0	1.332784	1.432321	-2.255820
8	7	0	-4.160338	-0.360791	-0.106000
9	1	0	-4.879826	-0.890350	-0.587866
10	7	0	-1.316203	-1.607260	-2.155467
11	6	0	4.591452	-0.435717	0.954350
12	6	0	4.627020	-1.838918	0.734691
13	6	0	4.965015	-2.687039	1.804690
14	1	0	4.984207	-3.761022	1.674109
15	6	0	5.279378	-2.165477	3.055433
16	1	0	5.535924	-2.832928	3.868104
17	6	0	5.266609	-0.790442	3.266389
18	1	0	5.514292	-0.417881	4.251543
19	6	0	4.930174	0.095227	2.226345
20	6	0	4.910569	1.596173	2.494475
21	1	0	4.667989	2.154663	1.568035
22	6	0	3.828566	1.956926	3.518669
23	1	0	2.837086	1.595605	3.170585
24	1	0	3.768956	3.059513	3.641222
25	1	0	4.044339	1.506536	4.510598
26	6	0	6.286571	2.101135	2.945408
27	1	0	6.278787	3.209542	3.024167
28	1	0	7.060342	1.815773	2.200651
29	1	0	6.569891	1.685074	3.935151
30	6	0	4.300512	-2.443422	-0.628056
31	1	0	4.107602	-1.645647	-1.374555
32	6	0	5.478519	-3.257394	-1.177218
33	1	0	6.396328	-2.631399	-1.202668

34	1	0	5.260919	-3.589829	-2.214989
35	1	0	5.676513	-4.158299	-0.559190
36	6	0	3.028388	-3.295159	-0.557072
37	1	0	3.179851	-4.198020	0.071737
38	1	0	2.725186	-3.620822	-1.575242
39	1	0	2.198912	-2.698023	-0.125337
40	6	0	2.891972	0.615199	-0.385903
41	6	0	2.654723	1.621418	-1.510550
42	1	0	3.427898	1.456544	-2.267272
43	6	0	2.675286	3.118357	-1.115151
44	1	0	3.714113	3.453151	-1.164708
45	6	0	1.816344	3.816213	-2.232348
46	1	0	2.454697	4.461051	-2.841703
47	6	0	2.057019	3.553633	0.234908
48	1	0	1.296255	2.841160	0.565438
49	1	0	2.809282	3.637012	1.024722
50	6	0	1.388107	4.899713	-0.092882
51	1	0	2.146834	5.691469	-0.144940
52	1	0	0.651822	5.198375	0.660780
53	6	0	0.766513	4.667566	-1.479568
54	1	0	-0.163665	4.101818	-1.377940
55	1	0	0.539071	5.598441	-2.009108
56	6	0	1.283677	2.683775	-3.120603
57	1	0	1.929958	2.501599	-3.982517
58	6	0	1.338391	0.143378	-3.064056
59	1	0	2.157642	0.244093	-3.779793
60	1	0	1.577520	-0.658669	-2.369155
61	6	0	0.050504	-0.179863	-3.828635
62	1	0	0.288118	-1.068132	-4.425772
63	1	0	-0.156723	0.615116	-4.553642
64	6	0	-1.270049	-0.400070	-3.084147
65	1	0	-1.517125	0.469698	-2.478796
66	1	0	-2.067110	-0.556593	-3.814572
67	6	0	-1.295022	-2.935923	-2.907837
68	1	0	-1.797935	-2.774051	-3.863067
69	6	0	-1.190719	-4.991440	-1.276417
70	1	0	-0.295498	-5.279981	-1.838373
71	1	0	-1.786688	-5.899958	-1.127467
72	6	0	-0.871034	-4.346168	0.081511
73	1	0	-0.013910	-3.678363	-0.018563
74	1	0	-0.637855	-5.089112	0.851420
75	6	0	-2.132321	-3.529331	0.424723
76	1	0	-1.911529	-2.670016	1.065734
77	1	0	-2.846481	-4.154866	0.971368

78	6	0	-2.053636	-3.962459	-2.038742
79	1	0	-2.775434	-4.469587	-2.683243
80	6	0	-2.784769	-3.131211	-0.930373
81	1	0	-3.853359	-3.356458	-0.907046
82	6	0	-2.653108	-1.672747	-1.427348
83	1	0	-3.402023	-1.519557	-2.210794
84	6	0	-2.869312	-0.594858	-0.365970
85	6	0	-4.566373	0.512070	0.930915
86	6	0	-4.593484	1.914560	0.708234
87	6	0	-4.958165	2.764535	1.768006
88	1	0	-4.978436	3.838028	1.633990
89	6	0	-5.305062	2.244777	3.011110
90	1	0	-5.585364	2.913103	3.815133
91	6	0	-5.295525	0.869945	3.225438
92	1	0	-5.569335	0.498613	4.204144
93	6	0	-4.928704	-0.016864	2.197065
94	6	0	-4.904700	-1.517559	2.470586
95	1	0	-4.608716	-2.077184	1.559856
96	6	0	-6.294657	-2.035249	2.858586
97	1	0	-6.278520	-3.143059	2.943862
98	1	0	-7.035654	-1.762528	2.077064
99	1	0	-6.628805	-1.615372	3.830819
100	6	0	-3.868669	-1.864182	3.545983
101	1	0	-2.870553	-1.470697	3.257421
102	1	0	-3.785026	-2.966538	3.656163
103	1	0	-4.148866	-1.435167	4.531270
104	6	0	-4.248317	2.514070	-0.651931
105	1	0	-4.030279	1.713816	-1.389039
106	6	0	-5.428219	3.306800	-1.227271
107	1	0	-6.336885	2.668113	-1.262135
108	1	0	-5.198580	3.633211	-2.264468
109	1	0	-5.647819	4.209892	-0.619746
110	6	0	-2.990096	3.385456	-0.568275
111	1	0	-3.157146	4.279378	0.069176
112	1	0	-2.698880	3.727814	-1.584250
113	1	0	-2.146632	2.799163	-0.145769
114	8	0	-1.953716	0.014095	0.235791
115	1	0	-0.245312	-3.170309	-3.075783
116	1	0	0.251188	2.801013	-3.447053

L3d-Mg(II)-COM

Zero-point correction= 1.14934 a.u.

Thermal correction to Gibbs Free Energy= 1.05687 a.u.

Sum of electronic and zero-point Energies= -5522.85777 a.u.

Sum of electronic and thermal Free Energies= -5522.95023 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.398858	-0.731892	-1.941601
2	6	0	-0.802587	-1.602342	-0.743049
3	6	0	-1.576412	-2.689813	-1.291109
4	6	0	-1.601897	-2.489580	-2.695947
5	7	0	-0.878783	-1.317904	-3.054299
6	8	0	-0.442391	-1.279586	0.383627
7	8	0	0.245992	0.310954	-1.796977
8	6	0	-0.703613	-0.832205	-4.418211
9	6	0	-2.248195	-3.778211	-0.731519
10	6	0	-2.277224	-3.349507	-3.538340
11	1	0	-0.115523	-1.549321	-4.997868
12	1	0	-0.175892	0.120858	-4.371328
13	1	0	-1.678482	-0.688185	-4.891959
14	6	0	-2.942874	-4.435608	-2.943694
15	6	0	-2.938150	-4.659338	-1.563709
16	1	0	-2.302647	-3.200597	-4.611777
17	1	0	-3.484275	-5.128447	-3.580518
18	1	0	-3.466706	-5.509155	-1.147756
19	35	0	-2.229348	-4.046159	1.143022
20	8	0	0.760550	2.781671	0.127620
21	8	0	-1.516936	1.281961	0.368718
22	12	0	0.479751	0.789941	0.357763
23	8	0	0.857475	0.598583	2.330060
24	7	0	-3.481028	2.394301	0.336179
25	1	0	-3.975512	3.276905	0.262719
26	7	0	-0.015320	3.692572	0.836239
27	7	0	4.481988	-0.641340	0.491748
28	1	0	5.196313	-0.907594	1.160698
29	7	0	2.085071	0.957379	2.867245
30	6	0	-4.231191	1.193193	0.279155
31	6	0	-4.366424	0.384433	1.440794
32	6	0	-4.994788	-0.868993	1.329154
33	1	0	-5.097859	-1.514471	2.191296
34	6	0	-5.489366	-1.312175	0.107414
35	1	0	-5.961666	-2.283637	0.037894
36	6	0	-5.383852	-0.511154	-1.024407

37	1	0	-5.780272	-0.886228	-1.958727
38	6	0	-4.768175	0.752297	-0.959503
39	6	0	-4.663931	1.599666	-2.222750
40	1	0	-4.204812	2.582495	-1.995410
41	6	0	-3.764198	0.923930	-3.262907
42	1	0	-2.759066	0.748206	-2.828769
43	1	0	-3.644769	1.578297	-4.152630
44	1	0	-4.188338	-0.046628	-3.596030
45	6	0	-6.048004	1.905405	-2.808152
46	1	0	-5.954189	2.620105	-3.653947
47	1	0	-6.695503	2.372517	-2.035349
48	1	0	-6.544502	0.986145	-3.184094
49	6	0	-3.846700	0.842490	2.800845
50	1	0	-3.410202	1.860155	2.729819
51	6	0	-4.982790	0.942266	3.825458
52	1	0	-5.786005	1.607073	3.441352
53	1	0	-4.602164	1.376707	4.774650
54	1	0	-5.418734	-0.054214	4.049611
55	6	0	-2.733051	-0.082391	3.306408
56	1	0	-3.120733	-1.097218	3.537103
57	1	0	-2.273350	0.336699	4.227178
58	1	0	-1.938261	-0.174392	2.538936
59	6	0	-2.136359	2.360813	0.339621
60	6	0	-1.458214	3.725360	0.322952
61	1	0	-1.995725	4.370872	1.024095
62	6	0	-1.379259	4.450068	-1.043701
63	1	0	-2.288706	5.046879	-1.150029
64	6	0	-0.120028	5.382397	-0.909608
65	1	0	-0.428358	6.430821	-0.940848
66	6	0	-1.153297	3.611577	-2.324163
67	1	0	-0.668273	2.662000	-2.087209
68	1	0	-2.091715	3.397714	-2.843889
69	6	0	-0.200832	4.477795	-3.166782
70	1	0	-0.760725	5.286620	-3.655018
71	1	0	0.303010	3.905520	-3.953294
72	6	0	0.773866	5.057513	-2.130041
73	1	0	1.514427	4.301213	-1.854690
74	1	0	1.309891	5.941667	-2.491454
75	6	0	0.468531	5.088572	0.474500
76	1	0	0.079751	5.771466	1.234119
77	6	0	0.020174	3.435231	2.333697
78	1	0	-0.578526	4.228124	2.789474
79	1	0	-0.468956	2.478075	2.496495
80	6	0	1.415060	3.441940	2.963895

81	1	0	1.250342	3.381898	4.046166
82	1	0	1.892087	4.413913	2.793464
83	6	0	2.447208	2.395617	2.537042
84	1	0	2.604163	2.433894	1.461751
85	1	0	3.392556	2.597983	3.047449
86	6	0	2.033835	0.699609	4.370553
87	1	0	2.766349	1.361423	4.837822
88	6	0	1.227809	-1.737091	4.922821
89	1	0	0.453425	-1.249429	5.525898
90	1	0	1.619438	-2.574003	5.514347
91	6	0	0.710675	-2.245360	3.568252
92	1	0	0.028301	-1.518093	3.128947
93	1	0	0.182902	-3.201501	3.651571
94	6	0	1.972243	-2.351087	2.690215
95	1	0	1.740184	-2.221089	1.629948
96	1	0	2.430151	-3.340837	2.800774
97	6	0	2.396985	-0.783834	4.592632
98	1	0	3.156621	-0.823984	5.377188
99	6	0	2.975857	-1.291816	3.228148
100	1	0	3.959901	-1.746465	3.363697
101	6	0	3.192173	0.007779	2.419412
102	1	0	4.121603	0.468205	2.769500
103	6	0	3.303736	-0.147143	0.905995
104	6	0	4.725056	-0.887768	-0.880364
105	6	0	5.135078	0.175372	-1.727850
106	6	0	5.293436	-0.073203	-3.103271
107	1	0	5.591003	0.718669	-3.777706
108	6	0	5.060932	-1.339871	-3.629618
109	1	0	5.182749	-1.512574	-4.691232
110	6	0	4.662087	-2.382994	-2.800012
111	1	0	4.473308	-3.351445	-3.243927
112	6	0	4.489919	-2.179515	-1.418948
113	6	0	4.005345	-3.330893	-0.543930
114	1	0	3.968194	-3.022295	0.520771
115	6	0	4.962914	-4.527047	-0.604837
116	1	0	4.647692	-5.302853	0.125593
117	1	0	5.993324	-4.206177	-0.340622
118	1	0	4.978461	-4.987339	-1.615114
119	6	0	2.581241	-3.746311	-0.930471
120	1	0	1.906215	-2.865287	-0.900233
121	1	0	2.194409	-4.502756	-0.214656
122	1	0	2.550397	-4.181106	-1.952025
123	6	0	5.380269	1.580279	-1.184345
124	1	0	5.264541	1.598745	-0.080729

125	6	0	6.813361	2.048336	-1.466266
126	1	0	7.542257	1.310216	-1.067901
127	1	0	7.001870	3.021491	-0.964180
128	1	0	6.993752	2.179961	-2.553782
129	6	0	4.356094	2.572513	-1.748808
130	1	0	4.477245	2.698876	-2.845572
131	1	0	4.477715	3.565031	-1.264205
132	1	0	3.324570	2.215077	-1.544599
133	8	0	2.404021	0.152685	0.099175
134	1	0	1.030169	0.974301	4.690623
135	1	0	1.556462	5.067725	0.515327

L3a-Ca(II)

Zero-point correction= 1.01274 a.u.

Thermal correction to Gibbs Free Energy= 0.92994 a.u.

Sum of electronic and zero-point Energies= -2874.36708 a.u.

Sum of electronic and thermal Free Energies= -2874.44988 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.357775	0.408479	0.875875
2	8	0	0.319114	1.676329	-0.614872
3	8	0	-0.253917	-1.485451	-0.667138
4	8	0	-2.413185	-0.110065	0.559456
5	7	0	4.457784	0.775309	0.082140
6	1	0	5.028885	1.183935	-0.648402
7	7	0	1.304137	1.767562	-1.563564
8	7	0	-4.465733	-0.745080	-0.180066
9	1	0	-5.004443	-1.376648	-0.762446
10	7	0	-1.157009	-1.524456	-1.702912
11	6	0	5.063174	-0.183907	0.926386
12	6	0	5.344551	-1.484275	0.430347
13	6	0	5.932494	-2.428361	1.291743
14	1	0	6.154393	-3.429457	0.946207
15	6	0	6.237157	-2.099310	2.608634
16	1	0	6.686138	-2.839502	3.258511
17	6	0	5.971265	-0.822696	3.092976
18	1	0	6.226155	-0.597876	4.120148
19	6	0	5.391302	0.155991	2.265241
20	6	0	5.145487	1.557111	2.816897

21	1	0	4.713436	2.216415	2.035833
22	6	0	4.135464	1.527213	3.969802
23	1	0	3.190409	1.046933	3.637765
24	1	0	3.897122	2.562263	4.295857
25	1	0	4.533076	0.968216	4.843177
26	6	0	6.458231	2.218951	3.253556
27	1	0	6.274014	3.273641	3.550551
28	1	0	7.182786	2.221304	2.411071
29	1	0	6.914265	1.689516	4.116655
30	6	0	5.008956	-1.883708	-1.003825
31	1	0	4.550586	-1.035362	-1.552913
32	6	0	6.272692	-2.267545	-1.782398
33	1	0	7.010668	-1.437758	-1.744664
34	1	0	6.021727	-2.454745	-2.848662
35	1	0	6.742746	-3.184586	-1.368354
36	6	0	3.980311	-3.019600	-1.033229
37	1	0	4.392925	-3.954049	-0.598065
38	1	0	3.676497	-3.229958	-2.080668
39	1	0	3.076730	-2.727327	-0.457471
40	6	0	3.124182	0.981139	0.086263
41	6	0	2.677123	2.029582	-0.929688
42	1	0	3.384738	2.034888	-1.764329
43	6	0	2.529732	3.456654	-0.409565
44	1	0	3.494476	3.876296	-0.114912
45	1	0	1.859639	3.468477	0.453993
46	6	0	1.915765	4.173247	-1.631895
47	1	0	2.732587	4.542973	-2.258717
48	6	0	0.898131	5.292634	-1.319817
49	1	0	1.108207	5.785314	-0.364035
50	1	0	0.950928	6.061238	-2.100052
51	6	0	-0.476358	4.602410	-1.357083
52	1	0	-1.296648	5.305638	-1.536102
53	1	0	-0.669007	4.088366	-0.410570
54	6	0	-0.332523	3.562898	-2.483236
55	1	0	-1.061814	2.754479	-2.423453
56	1	0	-0.452673	4.051403	-3.458618
57	6	0	1.119432	3.072402	-2.403186
58	1	0	1.549822	2.847645	-3.380503
59	6	0	1.376651	0.503333	-2.401583
60	1	0	2.216019	0.636160	-3.090308
61	1	0	1.608259	-0.296066	-1.699643
62	6	0	0.130815	0.147126	-3.212963
63	1	0	0.433044	-0.670734	-3.876770
64	1	0	-0.126731	0.979338	-3.878096

65	6	0	-1.165513	-0.226285	-2.493827
66	1	0	-1.439805	0.547862	-1.780437
67	1	0	-1.958913	-0.329364	-3.239419
68	6	0	-0.902192	-2.788076	-2.586458
69	1	0	-1.253875	-2.517055	-3.583352
70	6	0	0.551661	-3.276680	-2.574208
71	1	0	1.270059	-2.471031	-2.424045
72	1	0	0.748866	-3.723896	-3.556669
73	6	0	0.609294	-4.362268	-1.484800
74	1	0	0.719124	-3.886542	-0.505941
75	1	0	1.445475	-5.055469	-1.624817
76	6	0	-0.760596	-5.054989	-1.588865
77	1	0	-1.044903	-5.588104	-0.674915
78	1	0	-0.746425	-5.789363	-2.403001
79	6	0	-1.754389	-3.923947	-1.935049
80	1	0	-2.512659	-4.267222	-2.644771
81	6	0	-2.473413	-3.264306	-0.738996
82	1	0	-1.883456	-3.323446	0.179417
83	1	0	-3.460286	-3.694845	-0.553742
84	6	0	-2.574969	-1.811617	-1.199594
85	1	0	-3.215600	-1.771476	-2.085878
86	6	0	-3.117329	-0.807305	-0.186102
87	6	0	-5.160674	0.011183	0.791861
88	6	0	-5.343591	1.406762	0.604841
89	6	0	-5.989511	2.148983	1.610278
90	1	0	-6.135186	3.215660	1.502968
91	6	0	-6.459940	1.528410	2.763155
92	1	0	-6.957382	2.114344	3.525424
93	6	0	-6.296840	0.158134	2.939606
94	1	0	-6.673992	-0.293064	3.847957
95	6	0	-5.648550	-0.621935	1.964874
96	6	0	-5.467975	-2.118878	2.198308
97	1	0	-4.955537	-2.592495	1.336043
98	6	0	-6.821149	-2.826938	2.333326
99	1	0	-6.671997	-3.926585	2.390664
100	1	0	-7.454416	-2.613394	1.445603
101	1	0	-7.362450	-2.500807	3.246465
102	6	0	-4.583912	-2.384320	3.422107
103	1	0	-3.606042	-1.869946	3.304842
104	1	0	-4.387474	-3.473368	3.521878
105	1	0	-5.066158	-2.028213	4.356883
106	6	0	-4.868868	2.111662	-0.662855
107	1	0	-4.428037	1.383906	-1.375372
108	6	0	-6.038390	2.772464	-1.403156

109	1	0	-6.833843	2.023745	-1.606893
110	1	0	-5.691909	3.178177	-2.377923
111	1	0	-6.474024	3.607635	-0.815282
112	6	0	-3.770742	3.133726	-0.348689
113	1	0	-4.150411	3.950936	0.300222
114	1	0	-3.391259	3.583076	-1.290801
115	1	0	-2.921092	2.635728	0.164670
116	20	0	-0.037829	0.095809	1.064883

L3a-Ca(II)-COM

Zero-point correction= 1.14739 a.u.

Thermal correction to Gibbs Free Energy= 1.05059 a.u.

Sum of electronic and zero-point Energies= -6000.39210 a.u.

Sum of electronic and thermal Free Energies= -6000.48890 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.855315	1.211585	-1.893857
2	6	0	-2.025725	2.048628	-0.603925
3	6	0	-3.286362	2.743605	-0.758868
4	6	0	-3.840100	2.305840	-1.988439
5	7	0	-2.966732	1.398173	-2.640711
6	8	0	-1.190619	2.013508	0.290861
7	6	0	-3.986194	3.659971	0.028712
8	6	0	-5.076884	2.742062	-2.423539
9	8	0	-0.861080	0.528626	-2.135867
10	6	0	-3.195253	0.826921	-3.962219
11	1	0	-3.195845	1.617271	-4.718923
12	1	0	-2.386704	0.125986	-4.169936
13	1	0	-4.152878	0.301327	-3.984758
14	6	0	-5.237439	4.112027	-0.389175
15	6	0	-5.764363	3.646503	-1.597547
16	35	0	-3.232755	4.308722	1.643966
17	1	0	-5.796315	4.819852	0.211911
18	1	0	-6.740533	4.004084	-1.910831
19	1	0	-5.507307	2.406405	-3.359837
20	8	0	2.901045	0.619343	-0.378109
21	8	0	1.495986	-1.643724	-1.365189
22	8	0	0.956307	-1.314738	1.802590
23	8	0	-1.508614	-1.035988	0.427888

24	7	0	5.118686	0.620570	-0.864779
25	1	0	5.908360	0.132023	-1.269972
26	7	0	2.748493	-2.200661	-1.318762
27	7	0	-3.166876	-2.387996	1.191065
28	1	0	-3.473433	-3.051932	1.893332
29	7	0	0.444729	-2.559747	2.072511
30	6	0	5.374924	1.817270	-0.157598
31	6	0	5.778137	1.761090	1.201953
32	6	0	5.994683	2.964695	1.897159
33	1	0	6.294580	2.956495	2.936754
34	6	0	5.820361	4.192940	1.266986
35	1	0	5.987911	5.109471	1.818062
36	6	0	5.429053	4.248648	-0.067196
37	1	0	5.299462	5.219719	-0.526398
38	6	0	5.204681	3.070178	-0.801682
39	6	0	4.780406	3.163038	-2.264303
40	1	0	4.679924	2.151007	-2.708534
41	6	0	3.408642	3.833782	-2.396854
42	1	0	2.656880	3.288668	-1.786645
43	1	0	3.072234	3.810504	-3.455633
44	1	0	3.441302	4.892274	-2.062379
45	6	0	5.834541	3.893773	-3.104832
46	1	0	5.560119	3.852483	-4.180772
47	1	0	6.824775	3.404198	-2.984262
48	1	0	5.923818	4.960447	-2.809444
49	6	0	5.958184	0.430228	1.926574
50	1	0	5.773001	-0.421343	1.238926
51	6	0	7.394420	0.263608	2.437029
52	1	0	8.113902	0.383873	1.598984
53	1	0	7.532385	-0.753175	2.863547
54	1	0	7.635247	1.007265	3.225750
55	6	0	4.948227	0.287965	3.070949
56	1	0	5.120932	1.047968	3.861989
57	1	0	5.034246	-0.719380	3.531170
58	1	0	3.914624	0.406703	2.681745
59	6	0	3.881242	0.087441	-0.921211
60	6	0	3.823628	-1.195122	-1.748366
61	1	0	4.777001	-1.720432	-1.634166
62	6	0	3.536254	-1.028510	-3.238541
63	1	0	4.348106	-0.502240	-3.746092
64	1	0	2.608416	-0.467061	-3.375053
65	6	0	3.400853	-2.497094	-3.695753
66	1	0	4.393369	-2.861129	-3.977469
67	6	0	2.367364	-2.767287	-4.810764

68	1	0	2.248222	-1.906994	-5.478662
69	1	0	2.705284	-3.611085	-5.424402
70	6	0	1.072182	-3.142803	-4.070311
71	1	0	0.383790	-3.721755	-4.695281
72	1	0	0.552266	-2.241547	-3.732804
73	6	0	1.566104	-3.935479	-2.846338
74	1	0	0.840465	-3.969441	-2.033159
75	1	0	1.795076	-4.968650	-3.137101
76	6	0	2.892359	-3.277261	-2.441518
77	1	0	3.626164	-3.991263	-2.064012
78	6	0	3.079036	-2.720747	0.069409
79	1	0	4.104012	-3.099809	0.020719
80	1	0	3.047154	-1.850179	0.721697
81	6	0	2.177101	-3.826595	0.619626
82	1	0	2.677545	-4.196000	1.521873
83	1	0	2.168781	-4.674907	-0.074175
84	6	0	0.710187	-3.529636	0.933140
85	1	0	0.216297	-3.101237	0.062790
86	1	0	0.214781	-4.465677	1.206030
87	6	0	0.972924	-3.061917	3.455089
88	1	0	0.978287	-4.150984	3.383912
89	6	0	2.335738	-2.477912	3.851798
90	1	0	2.969943	-2.248956	2.995408
91	1	0	2.847280	-3.238941	4.454750
92	6	0	2.016686	-1.249885	4.722505
93	1	0	1.793113	-0.396273	4.076179
94	1	0	2.847298	-0.972945	5.380608
95	6	0	0.758354	-1.673223	5.500043
96	1	0	0.179773	-0.823658	5.879201
97	1	0	1.041852	-2.286071	6.364205
98	6	0	-0.054612	-2.531606	4.505368
99	1	0	-0.533664	-3.375681	5.010095
100	6	0	-1.127216	-1.780507	3.688303
101	1	0	-0.877176	-0.724888	3.553912
102	1	0	-2.121704	-1.853321	4.134768
103	6	0	-1.064101	-2.502325	2.344002
104	1	0	-1.377094	-3.541446	2.485277
105	6	0	-1.908022	-1.899055	1.223925
106	6	0	-4.144431	-1.825837	0.337491
107	6	0	-4.213186	-2.230118	-1.021435
108	6	0	-5.131635	-1.592993	-1.874990
109	1	0	-5.204741	-1.874511	-2.917085
110	6	0	-5.971971	-0.592181	-1.397967
111	1	0	-6.670882	-0.110311	-2.069454

112	6	0	-5.925943	-0.215747	-0.059406
113	1	0	-6.596845	0.562021	0.280622
114	6	0	-5.026273	-0.829671	0.831057
115	6	0	-5.013251	-0.408136	2.297212
116	1	0	-4.279293	-1.008294	2.872842
117	6	0	-6.375399	-0.650742	2.958413
118	1	0	-6.312249	-0.445505	4.048576
119	1	0	-6.681194	-1.710743	2.826230
120	1	0	-7.160623	0.005163	2.526556
121	6	0	-4.584798	1.053718	2.445290
122	1	0	-3.587828	1.201933	1.980128
123	1	0	-4.502493	1.322950	3.519989
124	1	0	-5.317149	1.737806	1.967470
125	6	0	-3.337112	-3.355394	-1.563642
126	1	0	-2.693848	-3.773431	-0.761293
127	6	0	-4.190828	-4.522373	-2.074553
128	1	0	-4.877476	-4.871965	-1.273729
129	1	0	-3.538872	-5.374943	-2.362348
130	1	0	-4.792247	-4.229559	-2.961017
131	6	0	-2.392926	-2.847705	-2.657939
132	1	0	-2.955449	-2.474286	-3.539285
133	1	0	-1.727022	-3.670551	-2.993113
134	1	0	-1.756986	-2.030326	-2.260217
135	20	0	0.575620	0.066757	-0.056242

L3a- Ca(II) -IM1-*si*

Zero-point correction= 1.26049 a.u.

Thermal correction to Gibbs Free Energy= 1.15521 a.u.

Sum of electronic and zero-point Energies= -6232.80768 a.u.

Sum of electronic and thermal Free Energies= -6232.91296 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.650590	0.839993	-2.070397
2	6	0	-1.729163	1.754369	-0.825032
3	6	0	-2.811981	2.674912	-1.092002
4	6	0	-3.359136	2.305735	-2.346439
5	7	0	-2.654258	1.204607	-2.898106
6	8	0	-0.976378	1.601348	0.129478
7	6	0	-3.361290	3.743900	-0.382624

8	6	0	-4.442361	2.971738	-2.887451
9	8	0	-0.799326	-0.036696	-2.219148
10	6	0	-2.908942	0.619279	-4.209239
11	1	0	-2.598325	1.309496	-4.999703
12	1	0	-2.334515	-0.304420	-4.282991
13	1	0	-3.972780	0.398028	-4.317478
14	6	0	-4.452506	4.433046	-0.909238
15	6	0	-4.976724	4.037099	-2.143820
16	35	0	-2.625996	4.260624	1.288440
17	1	0	-4.891366	5.264743	-0.370197
18	1	0	-5.828874	4.577940	-2.543922
19	1	0	-4.869388	2.691972	-3.843669
20	6	0	2.137686	3.349061	-1.043440
21	6	0	1.744198	4.349368	-0.239776
22	8	0	1.387759	5.535445	-0.826561
23	6	0	0.569654	6.454528	-0.101280
24	1	0	0.430047	7.311262	-0.764609
25	6	0	1.736080	4.257980	1.261220
26	1	0	-0.411332	6.022752	0.134038
27	1	0	2.105016	3.279043	1.576800
28	1	0	2.505749	2.417920	-0.628482
29	1	0	2.138544	3.474391	-2.122404
30	1	0	2.374091	5.028032	1.712373
31	1	0	1.048160	6.797598	0.822809
32	1	0	0.727611	4.386004	1.671882
33	8	0	2.813903	-0.208941	-0.207117
34	8	0	1.380290	-2.537208	-0.847404
35	8	0	0.387278	-1.486469	2.086307
36	8	0	-1.780521	-1.348280	0.313834
37	7	0	5.068848	-0.381473	-0.385943
38	1	0	5.861911	-0.941884	-0.678786
39	7	0	2.557203	-3.140203	-0.477302
40	7	0	-3.673259	-2.383466	1.015513
41	1	0	-4.151759	-2.870920	1.765046
42	7	0	-0.258010	-2.621234	2.511375
43	6	0	5.276894	1.000682	-0.164968
44	6	0	5.192711	1.527068	1.151360
45	6	0	5.296693	2.917640	1.336319
46	1	0	5.221689	3.351306	2.324859
47	6	0	5.496978	3.767485	0.253345
48	1	0	5.569124	4.835688	0.413089
49	6	0	5.605791	3.250936	-1.033972
50	1	0	5.757770	3.940069	-1.854021
51	6	0	5.504255	1.866962	-1.266785

52	6	0	5.609974	1.335074	-2.693273
53	1	0	5.559014	0.227634	-2.705378
54	6	0	4.441743	1.827340	-3.554015
55	1	0	3.478124	1.505195	-3.105225
56	1	0	4.504726	1.386158	-4.571906
57	1	0	4.446726	2.933657	-3.650152
58	6	0	6.956518	1.704735	-3.327397
59	1	0	7.061768	1.209569	-4.316418
60	1	0	7.790748	1.358320	-2.680299
61	1	0	7.049348	2.800944	-3.477736
62	6	0	5.007484	0.618725	2.363723
63	1	0	4.986946	-0.447316	2.054887
64	6	0	6.181473	0.752875	3.341607
65	1	0	7.141410	0.564526	2.814606
66	1	0	6.085859	0.004664	4.157656
67	1	0	6.216276	1.763860	3.799588
68	6	0	3.674604	0.895668	3.068402
69	1	0	3.641424	1.924357	3.484943
70	1	0	3.533716	0.177302	3.903210
71	1	0	2.831128	0.767729	2.358163
72	6	0	3.819510	-0.884414	-0.474407
73	6	0	3.776216	-2.333744	-0.949242
74	1	0	4.651601	-2.855714	-0.549768
75	6	0	3.732629	-2.532506	-2.463743
76	1	0	4.659701	-2.204157	-2.938883
77	1	0	2.898199	-1.966035	-2.885842
78	6	0	3.518295	-4.056250	-2.577758
79	1	0	4.499254	-4.540299	-2.594406
80	6	0	2.639600	-4.526930	-3.757159
81	1	0	2.711782	-3.853401	-4.618206
82	1	0	2.974079	-5.516942	-4.089465
83	6	0	1.217252	-4.620049	-3.178830
84	1	0	0.570121	-5.287472	-3.757938
85	1	0	0.751806	-3.630110	-3.153644
86	6	0	1.439910	-5.117203	-1.739074
87	1	0	0.601266	-4.905602	-1.075469
88	1	0	1.603377	-6.202396	-1.739869
89	6	0	2.752362	-4.465895	-1.280844
90	1	0	3.344083	-5.110754	-0.629533
91	6	0	2.634596	-3.333005	1.027932
92	1	0	3.620698	-3.759268	1.232917
93	1	0	2.580352	-2.333627	1.455900
94	6	0	1.575221	-4.240558	1.656075
95	1	0	1.905214	-4.410661	2.687099

96	1	0	1.605258	-5.226317	1.178116
97	6	0	0.104496	-3.820385	1.652530
98	1	0	-0.216707	-3.566989	0.643532
99	1	0	-0.496396	-4.655865	2.022205
100	6	0	0.012667	-2.845351	4.034910
101	1	0	-0.036272	-3.925721	4.180783
102	6	0	1.330174	-2.230508	4.529007
103	1	0	2.097550	-2.183944	3.755655
104	1	0	1.702153	-2.873825	5.336428
105	6	0	0.950820	-0.849768	5.093295
106	1	0	0.883989	-0.128560	4.272878
107	1	0	1.682052	-0.476207	5.817870
108	6	0	-0.436324	-1.079228	5.717392
109	1	0	-1.015518	-0.156466	5.833933
110	1	0	-0.328551	-1.524396	6.713731
111	6	0	-1.133080	-2.086450	4.775968
112	1	0	-1.744513	-2.798342	5.338081
113	6	0	-2.003453	-1.467989	3.662663
114	1	0	-1.658364	-0.470515	3.377074
115	1	0	-3.058312	-1.409333	3.940280
116	6	0	-1.782476	-2.440520	2.505413
117	1	0	-2.200166	-3.415879	2.775112
118	6	0	-2.384476	-2.006898	1.172642
119	6	0	-4.451869	-1.850603	-0.039563
120	6	0	-4.344509	-2.398310	-1.345219
121	6	0	-5.021619	-1.768612	-2.405329
122	1	0	-4.950185	-2.153814	-3.413793
123	6	0	-5.798735	-0.636324	-2.181804
124	1	0	-6.308377	-0.160305	-3.009568
125	6	0	-5.932282	-0.118736	-0.897934
126	1	0	-6.547328	0.760605	-0.758908
127	6	0	-5.276960	-0.718749	0.192808
128	6	0	-5.453615	-0.131715	1.589970
129	1	0	-4.922510	-0.745450	2.345088
130	6	0	-6.928679	-0.125898	2.010082
131	1	0	-7.021520	0.187931	3.071941
132	1	0	-7.356943	-1.146913	1.916284
133	1	0	-7.527034	0.573062	1.388369
134	6	0	-4.851675	1.273174	1.676025
135	1	0	-3.773202	1.234653	1.415712
136	1	0	-4.937600	1.664970	2.712083
137	1	0	-5.369678	1.976772	0.991116
138	6	0	-3.532891	-3.662310	-1.615606
139	1	0	-3.093645	-4.054468	-0.674416

140	6	0	-4.422477	-4.782954	-2.167601
141	1	0	-5.274202	-4.969546	-1.479110
142	1	0	-3.840517	-5.725572	-2.254008
143	1	0	-4.821988	-4.527901	-3.171747
144	6	0	-2.360992	-3.380951	-2.561627
145	1	0	-2.714466	-3.047100	-3.559744
146	1	0	-1.755441	-4.301735	-2.696813
147	1	0	-1.703577	-2.597606	-2.131628
148	20	0	0.443899	-0.542341	-0.053203

L3a-Ca(II)-TS1-*si*

Zero-point correction= 1.26080 a.u.

Thermal correction to Gibbs Free Energy= 1.15595 a.u.

Sum of electronic and zero-point Energies= -6232.80092 a.u.

Sum of electronic and thermal Free Energies= -6232.90578 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888586	1.229499	-1.832219
2	6	0	-1.072042	2.047323	-0.531317
3	6	0	-2.365128	2.772300	-0.783874
4	6	0	-2.772912	2.474805	-2.099513
5	7	0	-1.861235	1.576183	-2.705659
6	8	0	-0.738958	1.476054	0.565062
7	6	0	-3.182919	3.572539	-0.004555
8	6	0	-3.943387	2.976813	-2.648199
9	8	0	-0.012953	0.368076	-1.981222
10	6	0	-2.012342	1.013742	-4.039967
11	1	0	-1.904120	1.797798	-4.795674
12	1	0	-1.233066	0.264180	-4.179625
13	1	0	-2.994889	0.546119	-4.145500
14	6	0	-4.375259	4.093055	-0.520062
15	6	0	-4.738020	3.795770	-1.833942
16	35	0	-2.715469	3.946980	1.811604
17	1	0	-5.013634	4.713213	0.099179
18	1	0	-5.664688	4.199590	-2.230330
19	1	0	-4.246157	2.736255	-3.661569
20	6	0	0.323212	3.342050	-1.044604
21	6	0	0.331942	4.325416	-0.036293
22	8	0	-0.250902	5.462784	-0.328302

23	6	0	-0.357742	6.543438	0.632702
24	1	0	-0.735509	7.388609	0.058383
25	6	0	0.893915	4.003322	1.300352
26	1	0	-1.072823	6.268584	1.410587
27	1	0	0.472746	3.024410	1.585235
28	1	0	1.135593	2.625242	-0.976777
29	1	0	0.088374	3.686401	-2.049163
30	1	0	1.978455	3.866286	1.219574
31	1	0	0.620677	6.779283	1.055343
32	1	0	0.685940	4.742921	2.072091
33	8	0	2.875958	-0.177827	0.357240
34	8	0	1.648184	-2.352057	-0.885193
35	8	0	0.327271	-1.926491	2.161567
36	8	0	-1.586003	-1.621132	0.112714
37	7	0	5.016091	0.120547	-0.322795
38	1	0	5.805624	-0.255711	-0.836622
39	7	0	2.822626	-2.955737	-0.503125
40	7	0	-3.544839	-2.703278	0.475143
41	1	0	-4.096670	-3.273003	1.107162
42	7	0	-0.280800	-3.151515	2.268928
43	6	0	4.983629	1.517353	-0.091671
44	6	0	5.044341	2.020289	1.236174
45	6	0	4.944931	3.408024	1.444016
46	1	0	4.981779	3.821806	2.443027
47	6	0	4.786638	4.280274	0.372541
48	1	0	4.702430	5.344451	0.552107
49	6	0	4.727190	3.791159	-0.927687
50	1	0	4.592307	4.496825	-1.736774
51	6	0	4.833319	2.412248	-1.185621
52	6	0	4.753755	1.913332	-2.626327
53	1	0	4.910762	0.818092	-2.673795
54	6	0	3.366690	2.171942	-3.224357
55	1	0	2.594865	1.642453	-2.627487
56	1	0	3.317021	1.779648	-4.262679
57	1	0	3.127988	3.256414	-3.246276
58	6	0	5.853419	2.535700	-3.495332
59	1	0	5.856885	2.063811	-4.501413
60	1	0	6.849229	2.363739	-3.033459
61	1	0	5.701038	3.627626	-3.626280
62	6	0	5.213584	1.094342	2.437391
63	1	0	5.294398	0.037166	2.109832
64	6	0	6.509190	1.404058	3.197123
65	1	0	7.378149	1.351120	2.506679
66	1	0	6.666704	0.657017	4.004379

67	1	0	6.479450	2.413517	3.659188
68	6	0	3.998553	1.172524	3.371124
69	1	0	3.914880	2.173910	3.843865
70	1	0	4.085415	0.411777	4.176409
71	1	0	3.063516	0.967813	2.807759
72	6	0	3.894576	-0.622423	-0.190861
73	6	0	4.022991	-2.034186	-0.761775
74	1	0	4.890170	-2.512403	-0.292281
75	6	0	4.171288	-2.094270	-2.283790
76	1	0	5.130592	-1.687067	-2.611965
77	1	0	3.366441	-1.520656	-2.752297
78	6	0	4.049025	-3.599617	-2.577792
79	1	0	5.045027	-4.048530	-2.521607
80	6	0	3.340566	-3.956175	-3.902669
81	1	0	3.514763	-3.202087	-4.678139
82	1	0	3.727550	-4.909972	-4.281337
83	6	0	1.858557	-4.105107	-3.520396
84	1	0	1.290526	-4.695729	-4.247111
85	1	0	1.386501	-3.120819	-3.437416
86	6	0	1.908326	-4.764637	-2.131450
87	1	0	0.990923	-4.626540	-1.560128
88	1	0	2.086331	-5.842448	-2.235632
89	6	0	3.145090	-4.167223	-1.443565
90	1	0	3.670450	-4.886369	-0.814280
91	6	0	2.791612	-3.368968	0.959784
92	1	0	3.788657	-3.756409	1.186351
93	1	0	2.627073	-2.455301	1.526819
94	6	0	1.762280	-4.439115	1.335671
95	1	0	2.017339	-4.752875	2.353744
96	1	0	1.919315	-5.328881	0.715257
97	6	0	0.265281	-4.131865	1.247377
98	1	0	0.020888	-3.708351	0.274890
99	1	0	-0.293185	-5.061467	1.387708
100	6	0	-0.169907	-3.664156	3.740080
101	1	0	-0.175488	-4.752758	3.669104
102	6	0	1.049328	-3.115742	4.495806
103	1	0	1.895178	-2.897725	3.842659
104	1	0	1.361364	-3.891214	5.206916
105	6	0	0.537800	-1.880086	5.257420
106	1	0	0.531704	-1.017065	4.584777
107	1	0	1.160915	-1.633617	6.124081
108	6	0	-0.899719	-2.262980	5.652205
109	1	0	-1.535510	-1.394932	5.858643
110	1	0	-0.886019	-2.879396	6.559070

111	6	0	-1.430842	-3.102264	4.467799
112	1	0	-2.054629	-3.930204	4.817338
113	6	0	-2.214646	-2.321482	3.392219
114	1	0	-1.910399	-1.272421	3.344497
115	1	0	-3.294600	-2.368190	3.549083
116	6	0	-1.802119	-3.036823	2.105587
117	1	0	-2.183753	-4.063729	2.129572
118	6	0	-2.274065	-2.380747	0.806993
119	6	0	-4.224733	-1.999215	-0.547855
120	6	0	-3.990469	-2.324925	-1.910899
121	6	0	-4.638815	-1.577474	-2.910687
122	1	0	-4.479449	-1.798650	-3.957636
123	6	0	-5.496476	-0.534200	-2.578185
124	1	0	-5.980785	0.035321	-3.360960
125	6	0	-5.733138	-0.218393	-1.244837
126	1	0	-6.401380	0.602718	-1.021505
127	6	0	-5.111769	-0.942263	-0.210854
128	6	0	-5.384780	-0.557836	1.240030
129	1	0	-4.846758	-1.232729	1.934695
130	6	0	-6.873579	-0.692763	1.580992
131	1	0	-7.033680	-0.519152	2.666801
132	1	0	-7.228383	-1.718463	1.342178
133	1	0	-7.488951	0.039927	1.017483
134	6	0	-4.876296	0.855568	1.538709
135	1	0	-3.792851	0.921539	1.304612
136	1	0	-5.008107	1.090979	2.616311
137	1	0	-5.424599	1.616239	0.944581
138	6	0	-3.066006	-3.470315	-2.313937
139	1	0	-2.652630	-3.976659	-1.417109
140	6	0	-3.827224	-4.548061	-3.095088
141	1	0	-4.698590	-4.904014	-2.504587
142	1	0	-3.165004	-5.419436	-3.287513
143	1	0	-4.189017	-4.164068	-4.072055
144	6	0	-1.865968	-2.956008	-3.118249
145	1	0	-2.184144	-2.518203	-4.087709
146	1	0	-1.165297	-3.791724	-3.327393
147	1	0	-1.317336	-2.183881	-2.539273
148	20	0	0.543554	-0.588415	0.257644

L3a-Ca(II)-IM2-*si*

Zero-point correction= 1.26257 a.u.

Thermal correction to Gibbs Free Energy= 1.15789 a.u.

Sum of electronic and zero-point Energies= -6232.80267 a.u.

Sum of electronic and thermal Free Energies= -6232.90736 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.655990	1.308567	-1.931916
2	6	0	-0.686507	2.204139	-0.653430
3	6	0	-1.951791	3.022068	-0.919924
4	6	0	-2.416209	2.720015	-2.213406
5	7	0	-1.604778	1.718855	-2.802771
6	8	0	-0.567729	1.496655	0.461077
7	6	0	-2.689383	3.909560	-0.158231
8	6	0	-3.550305	3.302735	-2.761273
9	8	0	0.101052	0.337045	-2.058233
10	6	0	-1.872230	1.089855	-4.088500
11	1	0	-1.774392	1.822955	-4.894577
12	1	0	-1.143700	0.291349	-4.231294
13	1	0	-2.881699	0.669073	-4.104479
14	6	0	-3.841357	4.519978	-0.669569
15	6	0	-4.254283	4.216989	-1.966314
16	35	0	-2.184821	4.285299	1.653161
17	1	0	-4.410827	5.211000	-0.058180
18	1	0	-5.149030	4.688505	-2.361215
19	1	0	-3.893478	3.053033	-3.759305
20	6	0	0.659963	3.176797	-0.944082
21	6	0	0.900459	4.089330	0.159528
22	8	0	0.657258	5.335680	-0.077727
23	6	0	0.807971	6.370676	0.939208
24	1	0	0.660839	7.304784	0.399973
25	6	0	1.321256	3.539416	1.457170
26	1	0	0.033032	6.238699	1.695028
27	1	0	0.615795	2.700405	1.635783
28	1	0	1.463634	2.438798	-0.992127
29	1	0	0.544701	3.702796	-1.892895
30	1	0	2.302430	3.065463	1.344763
31	1	0	1.808508	6.327187	1.372042
32	1	0	1.342658	4.248602	2.282965
33	8	0	2.746174	-0.371862	0.323511
34	8	0	1.376421	-2.562151	-0.800738
35	8	0	0.058282	-1.869495	2.204540
36	8	0	-1.768963	-1.615579	0.069168
37	7	0	4.913598	-0.294944	-0.339999

38	1	0	5.674159	-0.766468	-0.817658
39	7	0	2.507607	-3.210162	-0.367338
40	7	0	-3.850662	-2.387910	0.517738
41	1	0	-4.467011	-2.825513	1.193761
42	7	0	-0.632704	-3.044803	2.363852
43	6	0	5.004238	1.109271	-0.184217
44	6	0	5.113627	1.674233	1.115089
45	6	0	5.144792	3.074420	1.248235
46	1	0	5.220834	3.535741	2.223854
47	6	0	5.061625	3.898980	0.131443
48	1	0	5.074864	4.974400	0.253906
49	6	0	4.957538	3.348663	-1.141307
50	1	0	4.888921	4.019445	-1.987544
51	6	0	4.937489	1.954008	-1.325142
52	6	0	4.822037	1.387785	-2.738227
53	1	0	4.873153	0.281727	-2.724554
54	6	0	3.472136	1.744406	-3.370022
55	1	0	2.646870	1.323819	-2.758737
56	1	0	3.395714	1.302969	-4.386697
57	1	0	3.338226	2.843731	-3.452886
58	6	0	5.984548	1.854070	-3.623119
59	1	0	5.951227	1.331509	-4.603331
60	1	0	6.954845	1.611674	-3.138988
61	1	0	5.940162	2.947252	-3.812044
62	6	0	5.195728	0.801435	2.364267
63	1	0	5.183143	-0.274511	2.092903
64	6	0	6.511559	1.033846	3.116535
65	1	0	7.374186	0.871540	2.435104
66	1	0	6.601151	0.316485	3.960232
67	1	0	6.568819	2.063287	3.528907
68	6	0	3.989544	1.035028	3.283249
69	1	0	3.985424	2.067404	3.692168
70	1	0	4.014885	0.321517	4.134885
71	1	0	3.042279	0.868073	2.727976
72	6	0	3.731029	-0.931432	-0.180933
73	6	0	3.760647	-2.380050	-0.671357
74	1	0	4.597142	-2.886142	-0.176071
75	6	0	3.901766	-2.533882	-2.188107
76	1	0	4.884546	-2.207333	-2.536331
77	1	0	3.134456	-1.936565	-2.688900
78	6	0	3.684138	-4.042761	-2.399274
79	1	0	4.651532	-4.548469	-2.326607
80	6	0	2.941427	-4.428066	-3.697716
81	1	0	3.142119	-3.722021	-4.511108

82	1	0	3.277408	-5.416688	-4.033132
83	6	0	1.457808	-4.486699	-3.295636
84	1	0	0.856797	-5.091093	-3.983531
85	1	0	1.030504	-3.479492	-3.263793
86	6	0	1.492775	-5.070384	-1.872921
87	1	0	0.586776	-4.863759	-1.304075
88	1	0	1.623419	-6.159019	-1.919092
89	6	0	2.761618	-4.493095	-1.227856
90	1	0	3.254074	-5.195918	-0.555044
91	6	0	2.437922	-3.527233	1.117650
92	1	0	3.408120	-3.956812	1.381712
93	1	0	2.322654	-2.571241	1.624173
94	6	0	1.340786	-4.507149	1.544908
95	1	0	1.563634	-4.768771	2.584976
96	1	0	1.450655	-5.443084	0.985304
97	6	0	-0.133411	-4.115847	1.411443
98	1	0	-0.338219	-3.737917	0.411835
99	1	0	-0.750292	-4.999553	1.597693
100	6	0	-0.582846	-3.484938	3.861512
101	1	0	-0.654552	-4.573425	3.846044
102	6	0	0.653031	-2.974219	4.616487
103	1	0	1.524249	-2.844052	3.973306
104	1	0	0.900470	-3.729212	5.373747
105	6	0	0.204459	-1.671140	5.301543
106	1	0	0.265228	-0.846427	4.585064
107	1	0	0.824508	-1.417643	6.168294
108	6	0	-1.261675	-1.943734	5.682545
109	1	0	-1.846114	-1.028479	5.827203
110	1	0	-1.305013	-2.508827	6.621409
111	6	0	-1.820167	-2.812858	4.532388
112	1	0	-2.497066	-3.583757	4.912238
113	6	0	-2.538878	-2.046458	3.402918
114	1	0	-2.180716	-1.017210	3.312906
115	1	0	-3.622701	-2.031812	3.538469
116	6	0	-2.141112	-2.842493	2.159291
117	1	0	-2.588422	-3.840973	2.215530
118	6	0	-2.543329	-2.218900	0.822518
119	6	0	-4.439757	-1.644501	-0.534493
120	6	0	-4.264733	-2.058896	-1.882757
121	6	0	-4.800652	-1.266198	-2.913804
122	1	0	-4.680583	-1.551927	-3.950331
123	6	0	-5.492080	-0.094273	-2.626900
124	1	0	-5.890221	0.507834	-3.433480
125	6	0	-5.669526	0.310827	-1.308682

126	1	0	-6.205018	1.232157	-1.121316
127	6	0	-5.155257	-0.451548	-0.244247
128	6	0	-5.346320	0.040495	1.187198
129	1	0	-4.904932	-0.672061	1.911049
130	6	0	-6.833173	0.150846	1.545607
131	1	0	-6.948394	0.402947	2.621671
132	1	0	-7.342802	-0.819903	1.364621
133	1	0	-7.339356	0.938211	0.948153
134	6	0	-4.626446	1.373863	1.410466
135	1	0	-3.552096	1.270706	1.149078
136	1	0	-4.690795	1.669962	2.479274
137	1	0	-5.075052	2.181898	0.795897
138	6	0	-3.516255	-3.340943	-2.236745
139	1	0	-3.171742	-3.860538	-1.318644
140	6	0	-4.430301	-4.331776	-2.967929
141	1	0	-5.340339	-4.531191	-2.362189
142	1	0	-3.901783	-5.297175	-3.120615
143	1	0	-4.739843	-3.943837	-3.961269
144	6	0	-2.261019	-3.038989	-3.065848
145	1	0	-2.522097	-2.612120	-4.057139
146	1	0	-1.681082	-3.971894	-3.230106
147	1	0	-1.609068	-2.318178	-2.529214
148	20	0	0.387776	-0.669699	0.213847

L3a-Ca(II)-TS2-*si*

Zero-point correction= 1.25926 a.u.

Thermal correction to Gibbs Free Energy= 1.15635 a.u.

Sum of electronic and zero-point Energies= -6232.80262 a.u.

Sum of electronic and thermal Free Energies= -6232.90553 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022913	1.330989	-2.053056
2	6	0	-0.675265	2.327771	-0.920381
3	6	0	-1.890396	3.247265	-0.960528
4	6	0	-2.643722	2.925141	-2.103968
5	7	0	-2.078238	1.799108	-2.754364
6	8	0	-0.406002	1.662822	0.246285
7	6	0	-2.368268	4.240614	-0.124328
8	6	0	-3.804954	3.597882	-2.456059

9	8	0	-0.411212	0.270572	-2.238941
10	6	0	-2.644954	1.152212	-3.929480
11	1	0	-2.528320	1.796411	-4.806388
12	1	0	-2.113182	0.214454	-4.092263
13	1	0	-3.706972	0.947716	-3.773780
14	6	0	-3.540136	4.940407	-0.438979
15	6	0	-4.236949	4.622755	-1.603953
16	35	0	-1.489522	4.636925	1.529746
17	1	0	-3.906046	5.714123	0.226525
18	1	0	-5.143712	5.169698	-1.844058
19	1	0	-4.368823	3.335623	-3.344559
20	6	0	0.653535	3.081326	-1.503001
21	6	0	1.346583	3.763696	-0.393124
22	8	0	1.252274	5.070732	-0.392667
23	6	0	1.880547	5.840805	0.661877
24	1	0	1.813149	6.877266	0.333876
25	6	0	1.811473	2.953322	0.661566
26	1	0	1.333951	5.705631	1.596923
27	1	0	0.662377	2.329344	0.761427
28	1	0	1.287680	2.276197	-1.882807
29	1	0	0.382429	3.761344	-2.311042
30	1	0	2.357845	2.063729	0.342581
31	1	0	2.925056	5.540229	0.774300
32	1	0	2.197835	3.419281	1.563775
33	8	0	2.573176	-0.328388	-0.276715
34	8	0	1.095822	-2.570348	-1.132553
35	8	0	0.148385	-1.940228	1.965015
36	8	0	-1.935216	-1.594951	0.066547
37	7	0	4.822362	-0.614039	-0.326049
38	1	0	5.607679	-1.183801	-0.620758
39	7	0	2.257267	-3.248962	-0.870600
40	7	0	-3.976222	-2.119882	0.900455
41	1	0	-4.503032	-2.487066	1.685596
42	7	0	-0.559012	-3.100795	2.173175
43	6	0	5.086106	0.709926	0.097463
44	6	0	4.969272	1.050017	1.470936
45	6	0	5.156023	2.389164	1.858875
46	1	0	5.062496	2.682948	2.896020
47	6	0	5.456278	3.368466	0.917518
48	1	0	5.591549	4.395025	1.232706
49	6	0	5.584139	3.034474	-0.426701
50	1	0	5.816010	3.820560	-1.133033
51	6	0	5.411288	1.707069	-0.859331
52	6	0	5.553049	1.375489	-2.341731

53	1	0	5.418221	0.288582	-2.515638
54	6	0	4.473913	2.080677	-3.169763
55	1	0	3.467290	1.793363	-2.801284
56	1	0	4.546701	1.773749	-4.235152
57	1	0	4.575167	3.185153	-3.114362
58	6	0	6.955778	1.719663	-2.857297
59	1	0	7.074492	1.367083	-3.904381
60	1	0	7.725471	1.213278	-2.236160
61	1	0	7.140415	2.814500	-2.836541
62	6	0	4.644284	-0.000736	2.528283
63	1	0	4.573170	-1.009339	2.070555
64	6	0	5.754775	-0.091752	3.582023
65	1	0	6.734676	-0.272815	3.090601
66	1	0	5.556632	-0.939711	4.272527
67	1	0	5.821603	0.838174	4.185103
68	6	0	3.287358	0.278206	3.184245
69	1	0	3.286303	1.251534	3.718717
70	1	0	3.052388	-0.521693	3.917135
71	1	0	2.484316	0.289493	2.417076
72	6	0	3.560274	-1.029194	-0.556361
73	6	0	3.488428	-2.401292	-1.223269
74	1	0	4.357138	-2.985079	-0.903954
75	6	0	3.437038	-2.371891	-2.749881
76	1	0	4.371053	-1.997741	-3.175661
77	1	0	2.615459	-1.728484	-3.075715
78	6	0	3.179603	-3.853627	-3.096663
79	1	0	4.144583	-4.357452	-3.204337
80	6	0	2.273389	-4.104070	-4.323194
81	1	0	2.360170	-3.305419	-5.068154
82	1	0	2.570918	-5.039491	-4.812264
83	6	0	0.854496	-4.243779	-3.744924
84	1	0	0.177389	-4.786907	-4.413171
85	1	0	0.422905	-3.257703	-3.548707
86	6	0	1.077932	-4.975373	-2.410253
87	1	0	0.250236	-4.854797	-1.711588
88	1	0	1.213262	-6.049556	-2.590438
89	6	0	2.412634	-4.440679	-1.870234
90	1	0	2.990115	-5.195023	-1.334140
91	6	0	2.329775	-3.674399	0.585644
92	1	0	3.296912	-4.169835	0.714341
93	1	0	2.319639	-2.751533	1.164415
94	6	0	1.227332	-4.621923	1.064968
95	1	0	1.544913	-4.971692	2.053772
96	1	0	1.220355	-5.516543	0.432018

97	6	0	-0.229008	-4.150480	1.125776
98	1	0	-0.532511	-3.721609	0.173702
99	1	0	-0.862175	-5.013135	1.352769
100	6	0	-0.326965	-3.615807	3.632572
101	1	0	-0.407526	-4.701880	3.570816
102	6	0	0.997807	-3.144566	4.248798
103	1	0	1.770677	-2.962588	3.501734
104	1	0	1.348660	-3.943654	4.913948
105	6	0	0.640812	-1.894915	5.073531
106	1	0	0.596525	-1.023152	4.412813
107	1	0	1.371579	-1.687900	5.862642
108	6	0	-0.758151	-2.212589	5.627677
109	1	0	-1.316836	-1.319891	5.930036
110	1	0	-0.673714	-2.858291	6.510140
111	6	0	-1.464627	-2.982853	4.490573
112	1	0	-2.113701	-3.770357	4.884887
113	6	0	-2.282237	-2.118769	3.511130
114	1	0	-1.893987	-1.098430	3.441455
115	1	0	-3.340137	-2.073394	3.781082
116	6	0	-2.071126	-2.840993	2.180049
117	1	0	-2.546428	-3.826920	2.229113
118	6	0	-2.626404	-2.119542	0.951411
119	6	0	-4.663435	-1.320244	-0.044675
120	6	0	-4.817374	-1.775433	-1.382074
121	6	0	-5.465960	-0.944470	-2.313411
122	1	0	-5.594279	-1.259530	-3.340392
123	6	0	-5.951189	0.304197	-1.938766
124	1	0	-6.441684	0.933376	-2.670392
125	6	0	-5.799236	0.752912	-0.631583
126	1	0	-6.177212	1.734398	-0.377371
127	6	0	-5.160131	-0.044608	0.334971
128	6	0	-4.985361	0.494352	1.751701
129	1	0	-4.485889	-0.253222	2.399511
130	6	0	-6.339717	0.791895	2.405668
131	1	0	-6.195045	1.073469	3.470861
132	1	0	-6.985928	-0.111598	2.374704
133	1	0	-6.864346	1.626455	1.894483
134	6	0	-4.087152	1.735867	1.759905
135	1	0	-3.107577	1.497423	1.294437
136	1	0	-3.898137	2.065428	2.803793
137	1	0	-4.556956	2.576349	1.207797
138	6	0	-4.298811	-3.139571	-1.829111
139	1	0	-3.836857	-3.681785	-0.978560
140	6	0	-5.441379	-4.031562	-2.329123

141	1	0	-6.226045	-4.121467	-1.547432
142	1	0	-5.059680	-5.051434	-2.550443
143	1	0	-5.901567	-3.624400	-3.254054
144	6	0	-3.208054	-2.993851	-2.898472
145	1	0	-3.614792	-2.558484	-3.835607
146	1	0	-2.770172	-3.987233	-3.135313
147	1	0	-2.390343	-2.340403	-2.527971
148	20	0	0.237913	-0.696329	-0.029449

L3a-Ca(II)-IM3-*si*

Zero-point correction= 1.26501 a.u.

Thermal correction to Gibbs Free Energy= 1.16719 a.u.

Sum of electronic and zero-point Energies= -6232.82385 a.u.

Sum of electronic and thermal Free Energies= -6232.92167 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.286796	1.185182	-1.941674
2	6	0	-1.258757	2.275918	-0.849061
3	6	0	-2.654839	2.855647	-0.972637
4	6	0	-3.230811	2.342063	-2.148199
5	7	0	-2.368468	1.374421	-2.723145
6	8	0	-0.964004	1.629676	0.387966
7	6	0	-3.417843	3.701648	-0.185544
8	6	0	-4.494594	2.703161	-2.588795
9	8	0	-0.418090	0.311685	-2.066331
10	6	0	-2.673916	0.596293	-3.915602
11	1	0	-2.686901	1.248555	-4.793852
12	1	0	-1.900533	-0.162523	-4.034656
13	1	0	-3.649421	0.115766	-3.809957
14	6	0	-4.702533	4.084581	-0.590688
15	6	0	-5.218995	3.598377	-1.791124
16	35	0	-2.784773	4.285697	1.521966
17	1	0	-5.295084	4.744194	0.033423
18	1	0	-6.214338	3.902376	-2.100426
19	1	0	-4.916904	2.296949	-3.501108
20	6	0	-0.088845	3.235540	-1.260220
21	6	0	0.328607	4.215256	-0.194452
22	8	0	-0.322358	5.394689	-0.326620
23	6	0	-0.021999	6.426916	0.614089

24	1	0	-0.627787	7.285363	0.320372
25	6	0	1.230558	3.901824	0.756247
26	1	0	-0.287640	6.121044	1.631799
27	1	0	-0.608585	2.313723	0.994575
28	1	0	0.764349	2.592517	-1.492760
29	1	0	-0.371808	3.770382	-2.171184
30	1	0	1.731196	2.940384	0.715987
31	1	0	1.041396	6.691172	0.575704
32	1	0	1.534475	4.587292	1.538450
33	8	0	2.793886	0.038571	-0.240311
34	8	0	1.578299	-2.327703	-1.110374
35	8	0	0.643998	-1.811779	2.005114
36	8	0	-1.557533	-1.667962	0.233443
37	7	0	5.041925	0.128990	-0.477502
38	1	0	5.886144	-0.290689	-0.851119
39	7	0	2.824256	-2.851184	-0.871178
40	7	0	-3.417225	-2.736501	0.963290
41	1	0	-3.861433	-3.264608	1.706486
42	7	0	0.099123	-3.048657	2.250123
43	6	0	5.096574	1.476913	-0.049071
44	6	0	5.061851	1.778800	1.338021
45	6	0	4.993234	3.124939	1.740137
46	1	0	4.952489	3.387415	2.789047
47	6	0	4.965340	4.149106	0.798852
48	1	0	4.903721	5.179325	1.125307
49	6	0	5.011252	3.855201	-0.560143
50	1	0	4.977450	4.674615	-1.265757
51	6	0	5.084627	2.523537	-1.007650
52	6	0	5.105900	2.232780	-2.505037
53	1	0	5.227600	1.145980	-2.690961
54	6	0	3.781620	2.639119	-3.160402
55	1	0	2.939591	2.097914	-2.679031
56	1	0	3.788662	2.368316	-4.238101
57	1	0	3.603479	3.731890	-3.072578
58	6	0	6.294566	2.916166	-3.192207
59	1	0	6.361590	2.588816	-4.251864
60	1	0	7.242817	2.633530	-2.686648
61	1	0	6.195107	4.021946	-3.177195
62	6	0	5.085820	0.677628	2.394387
63	1	0	5.182322	-0.319805	1.916980
64	6	0	6.298102	0.823055	3.322336
65	1	0	7.234660	0.854966	2.725122
66	1	0	6.359238	-0.048034	4.009555
67	1	0	6.232507	1.745522	3.937052

68	6	0	3.780108	0.652235	3.197421
69	1	0	3.644762	1.586600	3.782145
70	1	0	3.786246	-0.205192	3.903632
71	1	0	2.913087	0.530618	2.514548
72	6	0	3.852025	-0.492852	-0.609519
73	6	0	3.934322	-1.864833	-1.268855
74	1	0	4.876017	-2.337866	-0.974107
75	6	0	3.835009	-1.860357	-2.793794
76	1	0	4.703246	-1.379006	-3.250232
77	1	0	2.931679	-1.326897	-3.101564
78	6	0	3.757421	-3.367525	-3.115551
79	1	0	4.776617	-3.744660	-3.241514
80	6	0	2.863261	-3.756572	-4.313636
81	1	0	2.822272	-2.965527	-5.070447
82	1	0	3.273263	-4.650390	-4.799221
83	6	0	1.490307	-4.078076	-3.697882
84	1	0	0.881789	-4.724079	-4.339594
85	1	0	0.929925	-3.156796	-3.511570
86	6	0	1.839752	-4.743108	-2.354264
87	1	0	1.020573	-4.713702	-1.636026
88	1	0	2.108777	-5.794780	-2.515964
89	6	0	3.105296	-4.027758	-1.860843
90	1	0	3.791073	-4.691243	-1.331972
91	6	0	2.989202	-3.244453	0.587438
92	1	0	4.016709	-3.603590	0.695590
93	1	0	2.869251	-2.325714	1.158909
94	6	0	2.041508	-4.329157	1.106992
95	1	0	2.430969	-4.616707	2.090024
96	1	0	2.142482	-5.225604	0.484928
97	6	0	0.536852	-4.061370	1.206396
98	1	0	0.152380	-3.691783	0.257797
99	1	0	0.032551	-4.998144	1.459503
100	6	0	0.434255	-3.495494	3.711744
101	1	0	0.477602	-4.584834	3.677711
102	6	0	1.714425	-2.858178	4.269819
103	1	0	2.442408	-2.620817	3.493788
104	1	0	2.169322	-3.588660	4.950595
105	6	0	1.244876	-1.624933	5.061892
106	1	0	1.088946	-0.788821	4.372860
107	1	0	1.969483	-1.310875	5.820734
108	6	0	-0.094984	-2.073369	5.670908
109	1	0	-0.742532	-1.236658	5.955426
110	1	0	0.086530	-2.666798	6.575078
111	6	0	-0.742203	-2.967062	4.589753

112	1	0	-1.278665	-3.809115	5.036830
113	6	0	-1.692057	-2.246668	3.611525
114	1	0	-1.435086	-1.190059	3.494970
115	1	0	-2.739067	-2.322161	3.914388
116	6	0	-1.433460	-2.987935	2.300520
117	1	0	-1.769676	-4.024528	2.404739
118	6	0	-2.115764	-2.394294	1.068361
119	6	0	-4.247849	-2.142336	-0.017332
120	6	0	-4.217038	-2.616974	-1.356546
121	6	0	-5.020641	-1.983720	-2.321755
122	1	0	-5.015530	-2.316936	-3.351222
123	6	0	-5.833539	-0.908342	-1.978949
124	1	0	-6.438926	-0.427380	-2.736525
125	6	0	-5.865679	-0.442451	-0.669108
126	1	0	-6.501269	0.402282	-0.439060
127	6	0	-5.082039	-1.047030	0.330712
128	6	0	-5.117498	-0.487895	1.749622
129	1	0	-4.459971	-1.075851	2.421183
130	6	0	-6.526943	-0.573045	2.347007
131	1	0	-6.509290	-0.255945	3.411776
132	1	0	-6.895455	-1.620415	2.307214
133	1	0	-7.240621	0.079798	1.801653
134	6	0	-4.590852	0.950529	1.785718
135	1	0	-3.570000	0.989364	1.350478
136	1	0	-4.529521	1.309194	2.835335
137	1	0	-5.253693	1.638128	1.219645
138	6	0	-3.334396	-3.791001	-1.770952
139	1	0	-2.793495	-4.204525	-0.894745
140	6	0	-4.171234	-4.945743	-2.334699
141	1	0	-4.951083	-5.245612	-1.602352
142	1	0	-3.523932	-5.828713	-2.525014
143	1	0	-4.663885	-4.664512	-3.289147
144	6	0	-2.264922	-3.347944	-2.776968
145	1	0	-2.721154	-3.006325	-3.730092
146	1	0	-1.580737	-4.193825	-3.000432
147	1	0	-1.659886	-2.519034	-2.353370
148	20	0	0.511975	-0.570708	0.016829

L3a-Ca(11)-IM1-*re*

Zero-point correction= 1.25973 a.u.

Thermal correction to Gibbs Free Energy= 1.15652 a.u.

Sum of electronic and zero-point Energies= -6232.81267 a.u.

Sum of electronic and thermal Free Energies= -6232.91588 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.369937	-3.957875	-2.136836
2	6	0	-0.745975	-4.652391	-1.044936
3	8	0	-1.749153	-5.564331	-1.197631
4	6	0	-2.287822	-6.238443	-0.057343
5	6	0	-0.117838	-4.479872	0.309387
6	1	0	0.454616	-3.257977	-2.091921
7	1	0	-0.840004	-4.135980	-3.099303
8	1	0	-3.033722	-6.930866	-0.453390
9	1	0	-2.781042	-5.540789	0.629318
10	1	0	-1.524410	-6.808917	0.482832
11	1	0	0.325937	-5.416726	0.666600
12	1	0	-0.853019	-4.157882	1.055211
13	1	0	0.666747	-3.722031	0.263576
14	6	0	-1.520343	-0.959540	-2.256307
15	6	0	-1.898661	-1.443452	-0.838865
16	6	0	-3.226993	-2.014147	-0.971068
17	6	0	-3.599538	-1.865251	-2.329682
18	7	0	-2.558352	-1.255714	-3.072738
19	8	0	-1.163465	-1.245079	0.121422
20	8	0	-0.466993	-0.376630	-2.520271
21	6	0	-2.574172	-1.054490	-4.516439
22	6	0	-4.118857	-2.598413	-0.073684
23	6	0	-4.839710	-2.267506	-2.790798
24	1	0	-2.503701	-2.018156	-5.030713
25	1	0	-1.716713	-0.435245	-4.781945
26	1	0	-3.495555	-0.550890	-4.816886
27	6	0	-5.721329	-2.832555	-1.855569
28	6	0	-5.378181	-3.006562	-0.511513
29	1	0	-5.128589	-2.153045	-3.829100
30	1	0	-6.704621	-3.151783	-2.187645
31	1	0	-6.081667	-3.455358	0.180087
32	35	0	-3.611771	-2.870159	1.734591
33	8	0	1.357218	2.730751	-0.284376
34	8	0	-1.296223	1.766149	-0.226857
35	8	0	1.199755	0.364981	1.922014
36	7	0	-2.860776	3.356538	0.193244
37	1	0	-3.075650	4.338949	0.319676
38	7	0	0.817852	3.763611	0.437283

39	7	0	4.979198	-1.146773	0.555697
40	1	0	5.562438	-1.415763	1.340085
41	7	0	2.382758	0.606410	2.575527
42	6	0	-3.939319	2.445897	0.121172
43	6	0	-4.311293	1.700554	1.269228
44	6	0	-5.333344	0.740773	1.155575
45	1	0	-5.634007	0.149065	2.009987
46	6	0	-5.983050	0.532819	-0.057415
47	1	0	-6.766424	-0.210665	-0.128341
48	6	0	-5.636897	1.282698	-1.177292
49	1	0	-6.165678	1.100326	-2.103348
50	6	0	-4.623485	2.255904	-1.106885
51	6	0	-4.284374	3.083546	-2.342633
52	1	0	-3.494649	3.828099	-2.112386
53	6	0	-3.730791	2.199323	-3.463313
54	1	0	-2.836253	1.650383	-3.101269
55	1	0	-3.419889	2.824882	-4.327251
56	1	0	-4.491697	1.470726	-3.812849
57	6	0	-5.499335	3.885935	-2.823367
58	1	0	-5.205857	4.563071	-3.654002
59	1	0	-5.894605	4.511779	-1.994552
60	1	0	-6.309619	3.219701	-3.187645
61	6	0	-3.640347	1.933403	2.619557
62	1	0	-2.879498	2.738333	2.546036
63	6	0	-4.656053	2.401724	3.668954
64	1	0	-5.192033	3.304908	3.305981
65	1	0	-4.134097	2.668770	4.612910
66	1	0	-5.401241	1.610206	3.895787
67	6	0	-2.900823	0.680027	3.095785
68	1	0	-3.606567	-0.151479	3.300747
69	1	0	-2.347367	0.902676	4.032047
70	1	0	-2.169240	0.354085	2.326926
71	6	0	-1.592180	2.954656	-0.030933
72	6	0	-0.594827	4.111923	-0.050008
73	1	0	-0.955965	4.888641	0.631253
74	6	0	-0.326251	4.736724	-1.416868
75	1	0	-1.212741	5.243927	-1.804943
76	1	0	-0.024286	3.960701	-2.125365
77	6	0	0.826399	5.713998	-1.100935
78	1	0	0.393635	6.676422	-0.812849
79	6	0	1.885677	5.884539	-2.212351
80	1	0	1.459950	5.742173	-3.211816
81	1	0	2.294532	6.901458	-2.174978
82	6	0	2.986126	4.864596	-1.871881

83	1	0	3.950852	5.119007	-2.323668
84	1	0	2.700728	3.866351	-2.217831
85	6	0	3.031879	4.878617	-0.333538
86	1	0	3.485649	3.984159	0.094134
87	1	0	3.605274	5.747329	0.014359
88	6	0	1.579355	5.089519	0.116718
89	1	0	1.495654	5.695824	1.019726
90	6	0	0.767008	3.439660	1.920771
91	1	0	0.279239	4.291730	2.402512
92	1	0	0.129377	2.561183	2.005743
93	6	0	2.107482	3.188724	2.613565
94	1	0	1.887210	3.163002	3.686953
95	1	0	2.762396	4.056767	2.476072
96	6	0	2.950570	1.972338	2.227061
97	1	0	3.110841	1.953867	1.151185
98	1	0	3.916556	2.042031	2.735545
99	6	0	2.197343	0.380019	4.110396
100	1	0	2.927114	1.033892	4.590096
101	6	0	0.764210	0.613054	4.607091
102	1	0	0.221444	1.350075	4.014567
103	1	0	0.838489	0.993530	5.633870
104	6	0	0.100238	-0.775834	4.609001
105	1	0	-0.256458	-1.008430	3.601654
106	1	0	-0.751768	-0.833124	5.295038
107	6	0	1.242632	-1.726813	5.006501
108	1	0	1.066231	-2.763932	4.700288
109	1	0	1.367775	-1.726145	6.096029
110	6	0	2.505767	-1.133431	4.344032
111	1	0	3.379282	-1.235451	4.994320
112	6	0	2.866481	-1.698802	2.953850
113	1	0	1.984631	-2.060770	2.419179
114	1	0	3.604276	-2.502861	3.006057
115	6	0	3.427950	-0.464963	2.250251
116	1	0	4.340334	-0.151014	2.767423
117	6	0	3.756433	-0.618562	0.766288
118	6	0	5.450873	-1.432440	-0.746146
119	6	0	6.039041	-0.402829	-1.527304
120	6	0	6.468134	-0.700879	-2.833428
121	1	0	6.910251	0.063747	-3.458362
122	6	0	6.336246	-1.985528	-3.351072
123	1	0	6.671942	-2.197795	-4.358109
124	6	0	5.774338	-2.998701	-2.580899
125	1	0	5.684017	-3.985937	-3.014714
126	6	0	5.326810	-2.745011	-1.271556

127	6	0	4.694808	-3.872846	-0.461822
128	1	0	4.408606	-3.518279	0.550008
129	6	0	5.681055	-5.027303	-0.249852
130	1	0	5.237522	-5.788759	0.427077
131	1	0	6.613708	-4.650087	0.221942
132	1	0	5.939627	-5.523480	-1.209150
133	6	0	3.405336	-4.365662	-1.126579
134	1	0	2.713921	-3.511099	-1.278182
135	1	0	2.900572	-5.112876	-0.477760
136	1	0	3.609609	-4.838600	-2.110276
137	6	0	6.215579	1.011658	-0.981953
138	1	0	5.868279	1.073452	0.070355
139	6	0	7.693038	1.421821	-0.964536
140	1	0	8.289551	0.676326	-0.396240
141	1	0	7.809242	2.406988	-0.463955
142	1	0	8.105598	1.503503	-1.992175
143	6	0	5.375994	2.017654	-1.777563
144	1	0	5.715293	2.084579	-2.832779
145	1	0	5.459133	3.026070	-1.319973
146	1	0	4.306901	1.716762	-1.764928
147	8	0	2.995621	-0.301332	-0.160340
148	20	0	0.723818	0.472085	-0.370507

L3a-Ca(II)-TS1-*re*

Zero-point correction= 1.26050 a.u.

Thermal correction to Gibbs Free Energy= 1.15561 a.u.

Sum of electronic and zero-point Energies= -6232.79729 a.u.

Sum of electronic and thermal Free Energies= -6232.90219 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.586749	-3.513763	-1.376662
2	6	0	-0.898144	-4.348852	-0.275268
3	8	0	-1.816840	-5.254788	-0.484423
4	6	0	-2.295321	-6.136414	0.565409
5	6	0	-0.275508	-4.081049	1.041875
6	1	0	0.427045	-3.122906	-1.363280
7	1	0	-0.911616	-3.890354	-2.344343
8	1	0	-2.937994	-6.851106	0.052937
9	1	0	-2.874314	-5.558955	1.288152

10	1	0	-1.460192	-6.652356	1.042707
11	1	0	0.804475	-4.259527	0.977881
12	1	0	-0.688259	-4.655332	1.869923
13	1	0	-0.407945	-2.996857	1.213931
14	6	0	-1.008658	-1.251785	-2.418795
15	6	0	-1.476885	-1.863825	-1.073840
16	6	0	-2.925046	-2.174334	-1.359989
17	6	0	-3.152255	-1.950051	-2.731661
18	7	0	-1.982092	-1.433513	-3.343326
19	8	0	-1.041703	-1.303912	-0.000960
20	8	0	0.071204	-0.664038	-2.562551
21	6	0	-1.878237	-1.052111	-4.745158
22	6	0	-3.984223	-2.587042	-0.572298
23	6	0	-4.386756	-2.166637	-3.325729
24	1	0	-1.930416	-1.940438	-5.382524
25	1	0	-0.917860	-0.556141	-4.889544
26	1	0	-2.685892	-0.367593	-5.018226
27	6	0	-5.431886	-2.605488	-2.500157
28	6	0	-5.247685	-2.808694	-1.132496
29	1	0	-4.549929	-1.989665	-4.383196
30	1	0	-6.413265	-2.778168	-2.931395
31	1	0	-6.074815	-3.125973	-0.507203
32	35	0	-3.745350	-2.825912	1.311260
33	8	0	1.248829	2.716463	-0.300531
34	8	0	-1.386492	1.749362	-0.449677
35	8	0	1.152571	0.418201	1.978070
36	7	0	-2.954575	3.233519	0.256412
37	1	0	-3.161989	4.162870	0.602608
38	7	0	0.692487	3.763641	0.385155
39	7	0	4.940134	-1.030517	0.553469
40	1	0	5.555259	-1.229253	1.334292
41	7	0	2.347176	0.702242	2.588484
42	6	0	-3.998086	2.278931	0.254931
43	6	0	-4.343956	1.608129	1.456360
44	6	0	-5.353470	0.629066	1.422526
45	1	0	-5.636954	0.095511	2.320048
46	6	0	-6.006400	0.319569	0.233741
47	1	0	-6.777461	-0.439970	0.224811
48	6	0	-5.674794	0.983049	-0.942981
49	1	0	-6.201356	0.717778	-1.850154
50	6	0	-4.682217	1.979802	-0.952132
51	6	0	-4.367022	2.716581	-2.250128
52	1	0	-3.611894	3.511102	-2.076902
53	6	0	-3.768088	1.763506	-3.288256

54	1	0	-2.855084	1.283629	-2.876991
55	1	0	-3.476153	2.325631	-4.200976
56	1	0	-4.494588	0.975469	-3.578154
57	6	0	-5.607614	3.426639	-2.805798
58	1	0	-5.329232	4.050555	-3.682056
59	1	0	-6.042717	4.096455	-2.033454
60	1	0	-6.382972	2.700841	-3.129814
61	6	0	-3.642751	1.920541	2.774553
62	1	0	-2.885673	2.720663	2.637444
63	6	0	-4.636040	2.443392	3.819442
64	1	0	-5.187721	3.320171	3.417535
65	1	0	-4.093077	2.768654	4.732790
66	1	0	-5.369161	1.661776	4.110850
67	6	0	-2.885928	0.697362	3.302366
68	1	0	-3.578627	-0.133111	3.552590
69	1	0	-2.325829	0.969119	4.221573
70	1	0	-2.158452	0.342300	2.542326
71	6	0	-1.696089	2.896310	-0.099300
72	6	0	-0.729553	4.077776	-0.111241
73	1	0	-1.105413	4.857199	0.558076
74	6	0	-0.469204	4.682931	-1.486613
75	1	0	-1.366493	5.159086	-1.889707
76	1	0	-0.144654	3.898931	-2.176263
77	6	0	0.657432	5.692842	-1.186030
78	1	0	0.201441	6.646449	-0.904259
79	6	0	1.705019	5.877473	-2.305246
80	1	0	1.273714	5.728346	-3.301339
81	1	0	2.101508	6.899550	-2.271419
82	6	0	2.819082	4.871451	-1.969990
83	1	0	3.776019	5.130868	-2.435231
84	1	0	2.538577	3.867808	-2.304504
85	6	0	2.882050	4.898910	-0.432477
86	1	0	3.350397	4.012719	-0.003632
87	1	0	3.449370	5.777047	-0.098585
88	6	0	1.431955	5.096401	0.031558
89	1	0	1.351396	5.716276	0.925676
90	6	0	0.651893	3.481424	1.876787
91	1	0	0.152538	4.337523	2.339633
92	1	0	0.029079	2.595076	1.992037
93	6	0	2.003693	3.274213	2.563198
94	1	0	1.794962	3.266380	3.639169
95	1	0	2.635287	4.155235	2.400743
96	6	0	2.873437	2.071090	2.191861
97	1	0	3.011746	2.028757	1.113524

98	1	0	3.846541	2.180727	2.679729
99	6	0	2.213363	0.516585	4.135088
100	1	0	2.938163	1.204009	4.573424
101	6	0	0.788110	0.727345	4.663113
102	1	0	0.210782	1.426443	4.057220
103	1	0	0.876827	1.146768	5.673255
104	6	0	0.164537	-0.678577	4.730551
105	1	0	-0.212974	-0.954029	3.741708
106	1	0	-0.666128	-0.736806	5.442063
107	6	0	1.344409	-1.583602	5.125501
108	1	0	1.188148	-2.635886	4.862428
109	1	0	1.502156	-1.539980	6.209949
110	6	0	2.568994	-0.980001	4.403326
111	1	0	3.466346	-1.040470	5.025851
112	6	0	2.896708	-1.578245	3.019118
113	1	0	2.006871	-1.976009	2.524476
114	1	0	3.655368	-2.362884	3.070189
115	6	0	3.404673	-0.354111	2.259536
116	1	0	4.323794	-0.003206	2.738276
117	6	0	3.695308	-0.557189	0.771180
118	6	0	5.389925	-1.371843	-0.742308
119	6	0	5.923544	-0.368081	-1.592171
120	6	0	6.341212	-0.724945	-2.887214
121	1	0	6.740158	0.018789	-3.564221
122	6	0	6.257706	-2.043091	-3.324724
123	1	0	6.587873	-2.301324	-4.322819
124	6	0	5.755763	-3.031692	-2.484195
125	1	0	5.709813	-4.047848	-2.853337
126	6	0	5.315002	-2.717907	-1.185644
127	6	0	4.764684	-3.823689	-0.290082
128	1	0	4.441938	-3.413021	0.688946
129	6	0	5.840587	-4.871770	0.014610
130	1	0	5.451146	-5.619315	0.738764
131	1	0	6.730261	-4.384208	0.467936
132	1	0	6.156251	-5.408621	-0.904926
133	6	0	3.524253	-4.475492	-0.911364
134	1	0	2.766386	-3.699852	-1.146611
135	1	0	3.072460	-5.196103	-0.196441
136	1	0	3.776103	-5.022796	-1.843995
137	6	0	6.057460	1.080260	-1.130063
138	1	0	5.731224	1.188277	-0.074532
139	6	0	7.517978	1.546508	-1.171184
140	1	0	8.156134	0.857906	-0.576894
141	1	0	7.606405	2.562009	-0.729058

142	1	0	7.904199	1.586196	-2.211412
143	6	0	5.162244	2.007234	-1.958796
144	1	0	5.466240	2.017462	-3.026776
145	1	0	5.228018	3.044544	-1.568206
146	1	0	4.104517	1.675443	-1.890548
147	8	0	2.892450	-0.334566	-0.148016
148	20	0	0.619530	0.432851	-0.305658

L3a-Ca(II)-IM2-*re*

Zero-point correction= 1.26152 a.u.

Thermal correction to Gibbs Free Energy= 1.15541 a.u.

Sum of electronic and zero-point Energies= -6232.79668 a.u.

Sum of electronic and thermal Free Energies= -6232.90278 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.484296	-3.402440	-1.337789
2	6	0	-0.691218	-4.265219	-0.200918
3	8	0	-1.472552	-5.281064	-0.394408
4	6	0	-1.819708	-6.209691	0.673542
5	6	0	-0.106992	-3.886641	1.096885
6	1	0	0.538042	-3.024117	-1.365949
7	1	0	-0.774129	-3.869966	-2.278553
8	1	0	-2.341178	-7.022914	0.171432
9	1	0	-2.485026	-5.706568	1.376809
10	1	0	-0.915056	-6.574339	1.161963
11	1	0	0.986976	-3.935738	1.031780
12	1	0	-0.451777	-4.468084	1.950424
13	1	0	-0.358633	-2.810435	1.201905
14	6	0	-0.943637	-1.233021	-2.453456
15	6	0	-1.373175	-1.930659	-1.127538
16	6	0	-2.831195	-2.253323	-1.438150
17	6	0	-3.065427	-1.979725	-2.798540
18	7	0	-1.909749	-1.406434	-3.386338
19	8	0	-1.018426	-1.286590	-0.040638
20	8	0	0.112180	-0.599225	-2.576437
21	6	0	-1.827919	-0.940225	-4.763640
22	6	0	-3.884376	-2.720422	-0.675294
23	6	0	-4.292873	-2.201159	-3.406653
24	1	0	-1.835011	-1.791716	-5.451420

25	1	0	-0.895017	-0.387230	-4.878400
26	1	0	-2.671136	-0.284805	-4.997914
27	6	0	-5.330330	-2.695950	-2.603988
28	6	0	-5.142842	-2.948411	-1.245464
29	1	0	-4.455458	-1.986843	-4.457495
30	1	0	-6.306627	-2.873871	-3.044730
31	1	0	-5.962233	-3.308802	-0.633603
32	35	0	-3.652154	-3.031651	1.201146
33	8	0	1.155373	2.781602	-0.268601
34	8	0	-1.447902	1.763782	-0.466165
35	8	0	1.151907	0.449013	1.995623
36	7	0	-3.047653	3.159348	0.341510
37	1	0	-3.276565	4.061357	0.742343
38	7	0	0.578978	3.806140	0.434246
39	7	0	4.952014	-0.892591	0.502707
40	1	0	5.580359	-1.096194	1.271931
41	7	0	2.346686	0.766012	2.590186
42	6	0	-4.052745	2.164030	0.326997
43	6	0	-4.355713	1.447919	1.513904
44	6	0	-5.319539	0.424397	1.464010
45	1	0	-5.569746	-0.143709	2.350118
46	6	0	-5.968217	0.113899	0.273187
47	1	0	-6.702656	-0.680879	0.251393
48	6	0	-5.679897	0.821799	-0.888846
49	1	0	-6.203022	0.555439	-1.797656
50	6	0	-4.735375	1.864149	-0.881138
51	6	0	-4.471448	2.649780	-2.161675
52	1	0	-3.750654	3.472727	-1.975508
53	6	0	-3.845498	1.754142	-3.234716
54	1	0	-2.910419	1.297605	-2.847247
55	1	0	-3.585248	2.356172	-4.131449
56	1	0	-4.543021	0.947195	-3.543157
57	6	0	-5.750667	3.318300	-2.680230
58	1	0	-5.513689	3.978941	-3.541610
59	1	0	-6.204282	3.945211	-1.882860
60	1	0	-6.497300	2.567433	-3.014616
61	6	0	-3.656233	1.758436	2.833521
62	1	0	-2.934015	2.592059	2.709749
63	6	0	-4.661627	2.215059	3.897809
64	1	0	-5.250995	3.078644	3.521646
65	1	0	-4.125284	2.539277	4.815398
66	1	0	-5.360677	1.397656	4.174222
67	6	0	-2.845119	0.555910	3.327318
68	1	0	-3.500518	-0.308271	3.563555

69	1	0	-2.289601	0.830127	4.248458
70	1	0	-2.110066	0.248159	2.553937
71	6	0	-1.786324	2.881935	-0.056431
72	6	0	-0.856726	4.091817	-0.044913
73	1	0	-1.248638	4.845566	0.643982
74	6	0	-0.624395	4.730033	-1.409910
75	1	0	-1.537466	5.189147	-1.796905
76	1	0	-0.285279	3.967296	-2.116335
77	6	0	0.477662	5.763483	-1.100908
78	1	0	-0.000005	6.698572	-0.793936
79	6	0	1.506025	5.998247	-2.228335
80	1	0	1.065482	5.861824	-3.222258
81	1	0	1.879311	7.028325	-2.175751
82	6	0	2.647019	5.011310	-1.929665
83	1	0	3.591173	5.303020	-2.401736
84	1	0	2.385277	4.008537	-2.282486
85	6	0	2.730383	5.007054	-0.392992
86	1	0	3.223414	4.121857	0.009275
87	1	0	3.282994	5.889951	-0.047487
88	6	0	1.282454	5.162424	0.094313
89	1	0	1.200833	5.764153	1.000557
90	6	0	0.561143	3.502434	1.921639
91	1	0	0.042506	4.336764	2.402550
92	1	0	-0.034908	2.596806	2.030163
93	6	0	1.927249	3.325485	2.588183
94	1	0	1.734312	3.300423	3.666828
95	1	0	2.530970	4.226017	2.426960
96	6	0	2.824838	2.151259	2.190690
97	1	0	2.941205	2.119007	1.109437
98	1	0	3.804689	2.286806	2.657889
99	6	0	2.242682	0.575265	4.139115
100	1	0	2.949966	1.287347	4.566241
101	6	0	0.819127	0.736709	4.688611
102	1	0	0.207948	1.410865	4.087767
103	1	0	0.907372	1.164446	5.695223
104	6	0	0.248292	-0.690559	4.771725
105	1	0	-0.134978	-0.983458	3.789938
106	1	0	-0.568413	-0.776039	5.496582
107	6	0	1.466393	-1.550530	5.150129
108	1	0	1.343306	-2.609520	4.896349
109	1	0	1.642015	-1.494206	6.231200
110	6	0	2.654562	-0.907347	4.402423
111	1	0	3.566253	-0.936107	5.006148
112	6	0	2.974436	-1.496493	3.012881

113	1	0	2.088149	-1.921152	2.534227
114	1	0	3.756992	-2.258031	3.052065
115	6	0	3.431526	-0.257849	2.243772
116	1	0	4.348234	0.121095	2.705731
117	6	0	3.698157	-0.455874	0.751269
118	6	0	5.355190	-1.275316	-0.797738
119	6	0	5.783260	-0.288853	-1.724792
120	6	0	6.143336	-0.687533	-3.024817
121	1	0	6.464570	0.041076	-3.757356
122	6	0	6.102936	-2.027614	-3.396135
123	1	0	6.387873	-2.317306	-4.399523
124	6	0	5.702861	-2.997537	-2.482631
125	1	0	5.685341	-4.031070	-2.802453
126	6	0	5.321452	-2.643309	-1.175746
127	6	0	4.870249	-3.729627	-0.204304
128	1	0	4.589384	-3.289322	0.773970
129	6	0	6.002888	-4.722761	0.078898
130	1	0	5.687306	-5.448660	0.858821
131	1	0	6.898284	-4.183187	0.455166
132	1	0	6.283614	-5.290345	-0.833492
133	6	0	3.622037	-4.453681	-0.722049
134	1	0	2.821707	-3.718211	-0.944334
135	1	0	3.241535	-5.157251	0.049094
136	1	0	3.840424	-5.032067	-1.644509
137	6	0	5.877040	1.184141	-1.336891
138	1	0	5.604935	1.328193	-0.270694
139	6	0	7.311553	1.707381	-1.481571
140	1	0	8.011456	1.071498	-0.898083
141	1	0	7.380843	2.743683	-1.086506
142	1	0	7.636739	1.718614	-2.543311
143	6	0	4.898587	2.034232	-2.154361
144	1	0	5.143338	2.006588	-3.237067
145	1	0	4.942451	3.090247	-1.814637
146	1	0	3.860403	1.665423	-2.012730
147	8	0	2.869493	-0.257880	-0.149321
148	20	0	0.580733	0.479353	-0.290387

L3a-Ca(II)-TS2-*re*

Zero-point correction= 1.25802 a.u.

Thermal correction to Gibbs Free Energy= 1.15590 a.u.

Sum of electronic and zero-point Energies= -6232.79671 a.u.

Sum of electronic and thermal Free Energies= -6232.89883 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.799178	-3.490653	-1.502607
2	6	0	-0.849300	-4.235253	-0.234926
3	8	0	-1.770646	-5.165427	-0.174000
4	6	0	-1.962536	-5.926935	1.043369
5	6	0	-0.120332	-3.695652	0.846286
6	1	0	0.238104	-3.287969	-1.775963
7	1	0	-1.311991	-4.004644	-2.315250
8	1	0	-2.648963	-6.727538	0.770313
9	1	0	-2.411706	-5.291022	1.807760
10	1	0	-1.009923	-6.337541	1.385240
11	1	0	0.904208	-3.410843	0.603410
12	1	0	-0.232923	-4.132325	1.835278
13	1	0	-0.634526	-2.507440	0.671199
14	6	0	-1.004931	-1.238254	-2.498553
15	6	0	-1.480573	-2.009619	-1.245346
16	6	0	-2.976764	-2.105270	-1.516192
17	6	0	-3.194007	-1.742160	-2.857851
18	7	0	-1.985069	-1.268769	-3.430783
19	8	0	-1.039247	-1.442249	-0.090337
20	8	0	0.103815	-0.693878	-2.591312
21	6	0	-1.853167	-0.762910	-4.790378
22	6	0	-4.069672	-2.467646	-0.751172
23	6	0	-4.443695	-1.794571	-3.457888
24	1	0	-1.992023	-1.579227	-5.506036
25	1	0	-0.851462	-0.347362	-4.901983
26	1	0	-2.595167	0.015179	-4.988128
27	6	0	-5.521679	-2.205522	-2.662003
28	6	0	-5.349933	-2.528489	-1.316768
29	1	0	-4.590844	-1.512989	-4.494832
30	1	0	-6.516072	-2.254897	-3.095247
31	1	0	-6.199979	-2.814204	-0.707339
32	35	0	-3.878214	-2.830493	1.118894
33	8	0	1.278429	2.606212	-0.220908
34	8	0	-1.384400	1.680927	-0.369442
35	8	0	1.135913	0.240464	1.971647
36	7	0	-2.910276	3.188811	0.386349
37	1	0	-3.096355	4.127798	0.718029
38	7	0	0.736782	3.640745	0.496361
39	7	0	4.953580	-1.111592	0.534752

40	1	0	5.624785	-1.155964	1.292813
41	7	0	2.325388	0.487693	2.608910
42	6	0	-3.991944	2.279716	0.340078
43	6	0	-4.352742	1.551196	1.502385
44	6	0	-5.410232	0.626922	1.425022
45	1	0	-5.707817	0.052888	2.292411
46	6	0	-6.094401	0.425502	0.230559
47	1	0	-6.903030	-0.292515	0.187590
48	6	0	-5.745185	1.143720	-0.908529
49	1	0	-6.295090	0.960766	-1.822112
50	6	0	-4.707272	2.092193	-0.870883
51	6	0	-4.374970	2.896400	-2.123356
52	1	0	-3.589609	3.650441	-1.908975
53	6	0	-3.818560	1.987709	-3.221941
54	1	0	-2.926038	1.445588	-2.844312
55	1	0	-3.505261	2.594468	-4.098276
56	1	0	-4.578117	1.250703	-3.557517
57	6	0	-5.591445	3.685204	-2.623198
58	1	0	-5.294782	4.352676	-3.460568
59	1	0	-5.996678	4.320151	-1.806355
60	1	0	-6.395080	3.010705	-2.986532
61	6	0	-3.620547	1.748374	2.825692
62	1	0	-2.827921	2.519184	2.725851
63	6	0	-4.573465	2.250924	3.916997
64	1	0	-5.088000	3.176038	3.579441
65	1	0	-4.002882	2.492864	4.839424
66	1	0	-5.338894	1.487632	4.172028
67	6	0	-2.916789	0.460277	3.264521
68	1	0	-3.644826	-0.353046	3.466245
69	1	0	-2.341310	0.645957	4.195215
70	1	0	-2.209854	0.124531	2.476543
71	6	0	-1.666811	2.828466	0.003140
72	6	0	-0.676696	3.990769	0.005278
73	1	0	-1.036561	4.764941	0.688930
74	6	0	-0.403061	4.617985	-1.357586
75	1	0	-1.289729	5.121600	-1.750262
76	1	0	-0.095185	3.842247	-2.063635
77	6	0	0.745218	5.597993	-1.036174
78	1	0	0.309889	6.559298	-0.747808
79	6	0	1.808066	5.771582	-2.144115
80	1	0	1.385421	5.630326	-3.144964
81	1	0	2.216456	6.788624	-2.103861
82	6	0	2.907161	4.751301	-1.801254
83	1	0	3.873389	5.002611	-2.251715

84	1	0	2.619642	3.753183	-2.145221
85	6	0	2.949404	4.768054	-0.262999
86	1	0	3.406490	3.877352	0.168457
87	1	0	3.517203	5.640310	0.084886
88	6	0	1.495075	4.971772	0.182479
89	1	0	1.405284	5.574021	1.087773
90	6	0	0.682921	3.313926	1.978307
91	1	0	0.192171	4.162777	2.462626
92	1	0	0.046751	2.433769	2.061739
93	6	0	2.024085	3.064154	2.669580
94	1	0	1.804054	3.020726	3.742451
95	1	0	2.671690	3.939632	2.545070
96	6	0	2.875432	1.860291	2.263122
97	1	0	3.019338	1.852869	1.184446
98	1	0	3.847641	1.935282	2.758588
99	6	0	2.169967	0.252685	4.147319
100	1	0	2.893034	0.921392	4.616214
101	6	0	0.739566	0.454832	4.664196
102	1	0	0.172667	1.173464	4.071379
103	1	0	0.817718	0.845477	5.686722
104	6	0	0.110322	-0.950158	4.685203
105	1	0	-0.256703	-1.196890	3.684417
106	1	0	-0.728642	-1.025678	5.385218
107	6	0	1.282099	-1.870098	5.068143
108	1	0	1.123892	-2.915064	4.778314
109	1	0	1.430235	-1.853493	6.154688
110	6	0	2.514873	-1.253970	4.372146
111	1	0	3.408572	-1.339764	4.996845
112	6	0	2.845410	-1.811054	2.971654
113	1	0	1.952558	-2.175283	2.456789
114	1	0	3.591199	-2.609099	2.999923
115	6	0	3.379662	-0.569509	2.261818
116	1	0	4.293220	-0.243064	2.768505
117	6	0	3.683766	-0.720414	0.771748
118	6	0	5.434948	-1.309211	-0.779841
119	6	0	6.083365	-0.246782	-1.462113
120	6	0	6.533193	-0.457477	-2.778291
121	1	0	7.025267	0.333942	-3.328061
122	6	0	6.351575	-1.686036	-3.405357
123	1	0	6.701258	-1.830161	-4.419619
124	6	0	5.720872	-2.729704	-2.735607
125	1	0	5.592117	-3.671144	-3.253104
126	6	0	5.256098	-2.563994	-1.418275
127	6	0	4.559878	-3.725198	-0.715362

128	1	0	4.274645	-3.444536	0.319796
129	6	0	5.487816	-4.939126	-0.587692
130	1	0	4.995578	-5.733815	0.013027
131	1	0	6.426298	-4.649335	-0.068441
132	1	0	5.743997	-5.362908	-1.581533
133	6	0	3.261165	-4.098267	-1.437717
134	1	0	2.624661	-3.196479	-1.553077
135	1	0	2.696943	-4.852746	-0.848706
136	1	0	3.464330	-4.520178	-2.444781
137	6	0	6.287997	1.115445	-0.806087
138	1	0	5.894041	1.115720	0.231663
139	6	0	7.777625	1.462549	-0.698767
140	1	0	8.320012	0.655054	-0.161885
141	1	0	7.909316	2.404556	-0.124222
142	1	0	8.237535	1.598541	-1.700306
143	6	0	5.521743	2.209411	-1.557843
144	1	0	5.913714	2.346465	-2.587560
145	1	0	5.614177	3.176188	-1.018726
146	1	0	4.444675	1.944852	-1.618131
147	8	0	2.854271	-0.552935	-0.134955
148	20	0	0.622644	0.341898	-0.323617

L3a-Ca(II)-IM3-*re*

Zero-point correction= 1.26328 a.u.

Thermal correction to Gibbs Free Energy= 1.16221 a.u.

Sum of electronic and zero-point Energies= -6232.82367 a.u.

Sum of electronic and thermal Free Energies= -6232.924747 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.587306	-3.262214	-1.488408
2	6	0	-0.553387	-4.243089	-0.347118
3	8	0	-1.530669	-5.172415	-0.467012
4	6	0	-1.621525	-6.173121	0.548487
5	6	0	0.341685	-4.150594	0.654701
6	1	0	0.422970	-2.883272	-1.662883
7	1	0	-0.926203	-3.761562	-2.400337
8	1	0	-2.454030	-6.816869	0.260993
9	1	0	-1.825621	-5.722559	1.525615
10	1	0	-0.697563	-6.761169	0.597784

11	1	0	1.117746	-3.395324	0.603656
12	1	0	0.372369	-4.839173	1.490913
13	1	0	-0.936906	-2.040552	0.649394
14	6	0	-1.201606	-1.064356	-2.411213
15	6	0	-1.491163	-2.005647	-1.226438
16	6	0	-2.973033	-2.266843	-1.413456
17	6	0	-3.314498	-1.844729	-2.710743
18	7	0	-2.212936	-1.171289	-3.299608
19	8	0	-1.089921	-1.350482	-0.029979
20	8	0	-0.179227	-0.373387	-2.515834
21	6	0	-2.206266	-0.598875	-4.639372
22	6	0	-3.964541	-2.807369	-0.614187
23	6	0	-4.581126	-2.017386	-3.247259
24	1	0	-2.097831	-1.394379	-5.383382
25	1	0	-1.364998	0.090591	-4.715638
26	1	0	-3.138842	-0.062414	-4.826152
27	6	0	-5.550245	-2.605574	-2.423561
28	6	0	-5.261092	-2.983228	-1.112674
29	1	0	-4.823984	-1.693905	-4.253335
30	1	0	-6.556422	-2.750952	-2.804883
31	1	0	-6.035442	-3.400153	-0.478684
32	35	0	-3.611129	-3.251099	1.210826
33	8	0	1.208638	2.796580	-0.132888
34	8	0	-1.398342	1.722446	-0.100261
35	8	0	1.169034	0.277074	1.935093
36	7	0	-3.022579	3.206254	0.458858
37	1	0	-3.278814	4.172236	0.628948
38	7	0	0.638410	3.760452	0.658230
39	7	0	4.962289	-1.027309	0.417463
40	1	0	5.570927	-1.311803	1.176759
41	7	0	2.356838	0.535516	2.576760
42	6	0	-4.063649	2.259706	0.318389
43	6	0	-4.379213	1.391825	1.395391
44	6	0	-5.365659	0.406512	1.208778
45	1	0	-5.623691	-0.276387	2.007329
46	6	0	-6.034060	0.288963	-0.005787
47	1	0	-6.790542	-0.474581	-0.132475
48	6	0	-5.739155	1.152354	-1.056071
49	1	0	-6.277086	1.033611	-1.987289
50	6	0	-4.762347	2.154329	-0.911836
51	6	0	-4.468599	3.093954	-2.076644
52	1	0	-3.706516	3.848055	-1.791530
53	6	0	-3.890699	2.324865	-3.267317
54	1	0	-2.979187	1.774135	-2.951890

55	1	0	-3.601989	3.029715	-4.076257
56	1	0	-4.629706	1.604022	-3.675624
57	6	0	-5.718069	3.884312	-2.483634
58	1	0	-5.457841	4.638428	-3.257214
59	1	0	-6.130882	4.423673	-1.604251
60	1	0	-6.504577	3.218971	-2.898194
61	6	0	-3.682066	1.514358	2.746496
62	1	0	-2.958251	2.356097	2.740158
63	6	0	-4.686925	1.826109	3.861955
64	1	0	-5.271695	2.735448	3.605640
65	1	0	-4.150599	2.020537	4.815598
66	1	0	-5.389757	0.981920	4.024488
67	6	0	-2.878015	0.251555	3.070265
68	1	0	-3.539698	-0.631929	3.187208
69	1	0	-2.320734	0.393935	4.019437
70	1	0	-2.144062	0.049752	2.261855
71	6	0	-1.743132	2.880248	0.178084
72	6	0	-0.796207	4.078806	0.214110
73	1	0	-1.176387	4.796882	0.947410
74	6	0	-0.576311	4.796157	-1.115270
75	1	0	-1.489091	5.289158	-1.458416
76	1	0	-0.255139	4.078222	-1.874773
77	6	0	0.540659	5.799609	-0.756240
78	1	0	0.073472	6.722813	-0.401157
79	6	0	1.571753	6.084314	-1.870587
80	1	0	1.134062	5.988388	-2.870395
81	1	0	1.939898	7.112838	-1.774051
82	6	0	2.718357	5.091092	-1.613425
83	1	0	3.663654	5.413178	-2.063061
84	1	0	2.466947	4.105823	-2.018064
85	6	0	2.791960	5.009423	-0.078285
86	1	0	3.288237	4.108089	0.282473
87	1	0	3.337478	5.876486	0.315456
88	6	0	1.340670	5.132963	0.407909
89	1	0	1.249760	5.679174	1.347740
90	6	0	0.626404	3.344593	2.119169
91	1	0	0.119370	4.147643	2.661485
92	1	0	0.019950	2.441085	2.161445
93	6	0	1.989083	3.099733	2.768582
94	1	0	1.794691	3.001381	3.842741
95	1	0	2.610298	3.997424	2.670735
96	6	0	2.863690	1.939776	2.289888
97	1	0	2.995497	1.988391	1.211112
98	1	0	3.840142	2.016293	2.776505

99	6	0	2.220221	0.231262	4.104512
100	1	0	2.924651	0.903453	4.596224
101	6	0	0.789244	0.365021	4.642210
102	1	0	0.192228	1.089805	4.087690
103	1	0	0.866820	0.714016	5.679569
104	6	0	0.205791	-1.059231	4.611499
105	1	0	-0.165697	-1.277954	3.605912
106	1	0	-0.622507	-1.190024	5.315935
107	6	0	1.410508	-1.956538	4.943214
108	1	0	1.282748	-2.991825	4.607695
109	1	0	1.568224	-1.983587	6.027999
110	6	0	2.616620	-1.270452	4.265232
111	1	0	3.517206	-1.351251	4.880806
112	6	0	2.955128	-1.758799	2.841651
113	1	0	2.071876	-2.137680	2.321737
114	1	0	3.728488	-2.530462	2.834360
115	6	0	3.435526	-0.471820	2.174285
116	1	0	4.348549	-0.138656	2.677715
117	6	0	3.728665	-0.550128	0.675850
118	6	0	5.412214	-1.243823	-0.904850
119	6	0	5.946494	-0.163791	-1.655657
120	6	0	6.366325	-0.397222	-2.977755
121	1	0	6.766229	0.406980	-3.581050
122	6	0	6.284058	-1.668576	-3.537485
123	1	0	6.616740	-1.831922	-4.554571
124	6	0	5.776573	-2.731244	-2.796182
125	1	0	5.727717	-3.707223	-3.260881
126	6	0	5.329990	-2.540351	-1.475976
127	6	0	4.755338	-3.720540	-0.698056
128	1	0	4.418293	-3.400899	0.309994
129	6	0	5.816601	-4.803601	-0.477008
130	1	0	5.407867	-5.613813	0.164494
131	1	0	6.701266	-4.371179	0.037589
132	1	0	6.145639	-5.251348	-1.438547
133	6	0	3.520350	-4.298009	-1.399596
134	1	0	2.785279	-3.490644	-1.599229
135	1	0	3.032851	-5.058833	-0.752853
136	1	0	3.788365	-4.780462	-2.363106
137	6	0	6.077416	1.235779	-1.059758
138	1	0	5.752547	1.243151	0.001544
139	6	0	7.536705	1.707213	-1.057337
140	1	0	8.176684	0.966149	-0.532086
141	1	0	7.623248	2.676103	-0.520097
142	1	0	7.921776	1.847082	-2.089260

143	6	0	5.178778	2.235301	-1.796747
144	1	0	5.487370	2.352685	-2.856992
145	1	0	5.234056	3.229526	-1.304878
146	1	0	4.122657	1.892682	-1.767649
147	8	0	2.937208	-0.221835	-0.221913
148	20	0	0.657778	0.528504	-0.339391

L3a-Ca(II)-COM-1

Zero-point correction= 1.17582 a.u.

Thermal correction to Gibbs Free Energy= 1.06975 a.u.

Sum of electronic and zero-point Energies= -6962.19294 a.u.

Sum of electronic and thermal Free Energies= -6962.29900 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.895454	-1.332716	1.663511
2	6	0	-2.688942	-1.950301	0.473001
3	6	0	-3.912280	-2.483462	1.079670
4	6	0	-3.850313	-2.195647	2.460493
5	7	0	-2.646326	-1.519931	2.776533
6	8	0	-2.290126	-1.939762	-0.671288
7	8	0	-0.794473	-0.789678	1.597856
8	6	0	-2.250998	-1.139502	4.124563
9	6	0	-5.024948	-3.144239	0.566614
10	6	0	-4.869386	-2.543448	3.328947
11	6	0	-5.980272	-3.203434	2.780299
12	6	0	-6.069831	-3.507562	1.420335
13	1	0	-2.064160	-2.032285	4.730032
14	1	0	-1.337824	-0.547580	4.055571
15	1	0	-3.038360	-0.543633	4.593672
16	1	0	-4.821087	-2.319866	4.388647
17	1	0	-6.798396	-3.489963	3.434248
18	1	0	-6.941457	-4.021166	1.031100
19	8	0	1.163366	1.622439	1.929623
20	8	0	2.976198	0.001232	0.490735
21	8	0	1.186346	2.309650	-1.298219
22	7	0	4.473432	-0.892538	1.946685
23	1	0	5.012200	-0.782340	2.797793
24	7	0	2.361095	2.215576	2.253208

25	7	0	-3.057704	2.936676	-1.104877
26	1	0	-3.326135	3.712721	-1.699838
27	7	0	0.621003	3.555830	-1.248023
28	6	0	4.765952	-2.002101	1.120617
29	6	0	5.882790	-1.956857	0.246742
30	6	0	6.141626	-3.061788	-0.584588
31	1	0	6.977359	-3.053031	-1.271715
32	6	0	5.322394	-4.185769	-0.551869
33	1	0	5.533030	-5.024741	-1.202543
34	6	0	4.228452	-4.232471	0.306688
35	1	0	3.606951	-5.118000	0.301038
36	6	0	3.931171	-3.150255	1.154977
37	6	0	2.721942	-3.231869	2.082685
38	1	0	2.655888	-2.327534	2.721756
39	6	0	1.416620	-3.296033	1.280966
40	1	0	1.327921	-2.405367	0.622380
41	1	0	0.546181	-3.302665	1.971099
42	1	0	1.370624	-4.212372	0.655456
43	6	0	2.834533	-4.420996	3.044469
44	1	0	2.007780	-4.390546	3.786470
45	1	0	3.795569	-4.373714	3.600076
46	1	0	2.779420	-5.389194	2.503762
47	6	0	6.783634	-0.728381	0.167863
48	1	0	6.469814	0.037533	0.907424
49	6	0	8.237285	-1.079857	0.507047
50	1	0	8.288179	-1.582567	1.496574
51	1	0	8.850732	-0.154774	0.560138
52	1	0	8.684609	-1.748707	-0.258096
53	6	0	6.685069	-0.065014	-1.210645
54	1	0	7.053642	-0.739115	-2.012563
55	1	0	7.289885	0.866898	-1.230672
56	1	0	5.630145	0.207953	-1.428336
57	6	0	3.576438	0.045388	1.573532
58	6	0	3.399076	1.150079	2.617954
59	1	0	4.359304	1.669460	2.717909
60	6	0	2.927858	0.683026	3.995577
61	1	0	3.687708	0.090614	4.510375
62	1	0	2.025599	0.075221	3.883939
63	6	0	2.637120	2.008843	4.720703
64	1	0	3.555046	2.348464	5.209945
65	6	0	1.450101	1.978757	5.707804
66	1	0	1.332146	0.997541	6.181325
67	1	0	1.620251	2.708646	6.508684
68	6	0	0.233981	2.400216	4.866303

69	1	0	-0.593443	2.776358	5.477331
70	1	0	-0.134685	1.554851	4.276270
71	6	0	0.802752	3.469067	3.917041
72	1	0	0.191730	3.617817	3.027256
73	1	0	0.881382	4.430230	4.441020
74	6	0	2.233116	3.009234	3.596735
75	1	0	2.935139	3.839157	3.509042
76	6	0	2.889297	3.091127	1.126960
77	1	0	3.876410	3.436085	1.449594
78	1	0	2.998277	2.434148	0.267976
79	6	0	2.039125	4.313225	0.771283
80	1	0	2.655564	4.921806	0.100245
81	1	0	1.890062	4.932238	1.663097
82	6	0	0.650735	4.117879	0.159328
83	1	0	0.066427	3.424719	0.761420
84	1	0	0.141139	5.085084	0.118089
85	6	0	1.295240	4.490884	-2.301746
86	1	0	1.200880	5.499623	-1.895313
87	6	0	2.744627	4.108654	-2.635417
88	1	0	3.257637	3.613977	-1.810295
89	1	0	3.280379	5.040782	-2.857243
90	6	0	2.658790	3.234290	-3.898952
91	1	0	2.433304	2.202302	-3.617862
92	1	0	3.593210	3.234585	-4.471194
93	6	0	1.485066	3.840761	-4.688100
94	1	0	1.040688	3.137301	-5.400742
95	1	0	1.825175	4.713529	-5.259431
96	6	0	0.471715	4.293709	-3.613442
97	1	0	-0.006883	5.237677	-3.892174
98	6	0	-0.631975	3.275374	-3.254687
99	1	0	-0.306244	2.244326	-3.413147
100	1	0	-1.555733	3.444788	-3.813204
101	6	0	-0.822931	3.533227	-1.760161
102	1	0	-1.205235	4.549994	-1.620958
103	6	0	-1.755950	2.575197	-1.023336
104	6	0	-4.075358	2.065109	-0.650670
105	6	0	-4.416739	2.036437	0.727390
106	6	0	-5.371481	1.104740	1.173024
107	1	0	-5.644374	1.048433	2.218602
108	6	0	-5.987236	0.234020	0.280115
109	1	0	-6.719970	-0.476655	0.639973
110	6	0	-5.663612	0.269691	-1.072443
111	1	0	-6.154991	-0.427394	-1.737945
112	6	0	-4.712094	1.182585	-1.562548

113	6	0	-4.361953	1.178290	-3.047872
114	1	0	-3.647769	1.992325	-3.285867
115	6	0	-5.600200	1.432921	-3.916483
116	1	0	-5.301278	1.551939	-4.980079
117	1	0	-6.106659	2.368561	-3.595948
118	1	0	-6.323746	0.593167	-3.853147
119	6	0	-3.670302	-0.130375	-3.444164
120	1	0	-2.751531	-0.273132	-2.836975
121	1	0	-3.368001	-0.095487	-4.512785
122	1	0	-4.340726	-1.003017	-3.297245
123	6	0	-3.784045	3.001901	1.725971
124	1	0	-3.089773	3.699313	1.212041
125	6	0	-4.846886	3.880603	2.396661
126	1	0	-5.454148	4.401574	1.625486
127	1	0	-4.359012	4.653148	3.029020
128	1	0	-5.523974	3.281303	3.041353
129	6	0	-2.954140	2.251901	2.773515
130	1	0	-3.591923	1.582264	3.386780
131	1	0	-2.455572	2.976216	3.451786
132	1	0	-2.166803	1.648041	2.276413
133	8	0	-1.388353	1.569661	-0.401864
134	20	0	0.662855	0.386168	-0.051289
135	8	0	0.949626	-0.889941	-2.006807
136	16	0	1.339865	-1.422514	-3.351700
137	8	0	0.343679	-2.332615	-3.940675
138	8	0	1.926853	-0.411472	-4.250375
139	6	0	2.765787	-2.524124	-2.901920
140	9	0	2.366405	-3.488683	-2.057991
141	9	0	3.279482	-3.108381	-3.995510
142	9	0	3.740792	-1.818511	-2.307216
143	35	0	-5.134507	-3.560054	-1.281887

L3a-Ca(II)-IM1-*si*-1

Zero-point correction= 1.28765 a.u.

Thermal correction to Gibbs Free Energy= 1.17095 a.u.

Sum of electronic and zero-point Energies= -7194.60971a.u.

Sum of electronic and thermal Free Energies= -7194.72642 a.u.

The number of imaginary frequencies 0

Standard orientation

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

1	6	0	1.916751	0.780998	1.484799
2	6	0	3.081253	0.994688	0.467020
3	6	0	4.240055	1.333447	1.304062
4	6	0	3.816977	1.279663	2.648268
5	7	0	2.441267	0.953380	2.722822
6	8	0	2.971467	0.853832	-0.730092
7	8	0	0.750123	0.502276	1.218321
8	6	0	1.687182	0.851792	3.963028
9	6	0	5.564509	1.645856	1.017818
10	6	0	4.684121	1.515105	3.700890
11	6	0	6.016709	1.816080	3.378634
12	6	0	6.465221	1.886889	2.057921
13	1	0	1.661889	1.821052	4.470733
14	1	0	0.671705	0.545052	3.712870
15	1	0	2.142634	0.107105	4.622103
16	1	0	4.356426	1.471146	4.733409
17	1	0	6.723136	2.004418	4.181526
18	1	0	7.499445	2.129436	1.841584
19	6	0	1.637296	4.471988	-0.110788
20	6	0	2.790762	4.711244	-0.755048
21	8	0	3.702509	5.530369	-0.135000
22	6	0	5.042018	5.593655	-0.621453
23	6	0	3.109319	4.161856	-2.117728
24	1	0	0.854945	3.890853	-0.584244
25	1	0	1.452077	4.897573	0.871612
26	1	0	5.554968	6.312303	0.022769
27	1	0	5.550304	4.625187	-0.545447
28	1	0	5.094674	5.949858	-1.656735
29	1	0	3.336665	4.964139	-2.830993
30	1	0	3.974983	3.489591	-2.089088
31	1	0	2.257257	3.594227	-2.499171
32	8	0	-1.812625	-1.643890	1.931388
33	8	0	-3.241999	0.269123	0.414664
34	8	0	-1.919766	-2.350856	-1.280321
35	7	0	-4.703261	1.391528	1.742812
36	1	0	-5.215272	1.429239	2.616493
37	7	0	-3.111209	-1.986616	2.231644
38	7	0	2.102284	-3.848562	-0.986773
39	1	0	2.207322	-4.671166	-1.570254
40	7	0	-1.617010	-3.685255	-1.222679
41	6	0	-4.719221	2.540609	0.920411
42	6	0	-5.646047	2.630264	-0.149664
43	6	0	-5.612381	3.761673	-0.985241
44	1	0	-6.297021	3.855106	-1.817789

45	6	0	-4.691728	4.782014	-0.766274
46	1	0	-4.675513	5.642950	-1.422100
47	6	0	-3.787498	4.697988	0.288091
48	1	0	-3.079686	5.504696	0.425897
49	6	0	-3.786189	3.585220	1.148711
50	6	0	-2.771473	3.512642	2.286343
51	1	0	-2.931789	2.602087	2.898984
52	6	0	-1.342585	3.421716	1.739965
53	1	0	-1.249682	2.546031	1.063029
54	1	0	-0.619488	3.289025	2.573426
55	1	0	-1.072042	4.341682	1.181336
56	6	0	-2.920309	4.699883	3.245310
57	1	0	-2.256768	4.563432	4.126199
58	1	0	-3.967265	4.766163	3.611332
59	1	0	-2.650231	5.657780	2.753073
60	6	0	-6.658733	1.521588	-0.420608
61	1	0	-6.584706	0.726015	0.350276
62	6	0	-8.096446	2.050460	-0.350423
63	1	0	-8.270829	2.555775	0.623902
64	1	0	-8.816794	1.208614	-0.433692
65	1	0	-8.306611	2.769463	-1.169966
66	6	0	-6.385584	0.845264	-1.768996
67	1	0	-6.495121	1.560476	-2.611480
68	1	0	-7.096348	0.006189	-1.927465
69	1	0	-5.357054	0.425580	-1.783206
70	6	0	-3.902762	0.341781	1.460466
71	6	0	-3.937876	-0.737938	2.543289
72	1	0	-4.977654	-1.071076	2.638761
73	6	0	-3.416360	-0.325102	3.919772
74	1	0	-4.061362	0.417310	4.396024
75	1	0	-2.412027	0.095799	3.819965
76	6	0	-3.404728	-1.662453	4.683463
77	1	0	-4.383994	-1.804833	5.150187
78	6	0	-2.262538	-1.836552	5.707033
79	1	0	-1.969609	-0.884993	6.164593
80	1	0	-2.593631	-2.498727	6.516212
81	6	0	-1.128102	-2.505997	4.913825
82	1	0	-0.406018	-3.018528	5.558528
83	1	0	-0.587092	-1.760794	4.322276
84	6	0	-1.864660	-3.469157	3.966089
85	1	0	-1.271058	-3.751338	3.096560
86	1	0	-2.138729	-4.385425	4.504128
87	6	0	-3.171595	-2.753252	3.594404
88	1	0	-4.017377	-3.435940	3.503597

89	6	0	-3.777430	-2.766564	1.108268
90	1	0	-4.817609	-2.906493	1.417244
91	1	0	-3.741850	-2.117345	0.237297
92	6	0	-3.178832	-4.137106	0.785723
93	1	0	-3.897761	-4.626966	0.119466
94	1	0	-3.157846	-4.755306	1.690421
95	6	0	-1.775698	-4.224673	0.185836
96	1	0	-1.071427	-3.658810	0.792799
97	1	0	-1.467295	-5.273485	0.153561
98	6	0	-2.450985	-4.460255	-2.290614
99	1	0	-2.574290	-5.468006	-1.889472
100	6	0	-3.784391	-3.785611	-2.644786
101	1	0	-4.206221	-3.209562	-1.820679
102	1	0	-4.491960	-4.586836	-2.894963
103	6	0	-3.493957	-2.932215	-3.892143
104	1	0	-3.057178	-1.976533	-3.589082
105	1	0	-4.397052	-2.725207	-4.476851
106	6	0	-2.463500	-3.766975	-4.672357
107	1	0	-1.871228	-3.170113	-5.374293
108	1	0	-2.973667	-4.545082	-5.253662
109	6	0	-1.583642	-4.429819	-3.588899
110	1	0	-1.309364	-5.450739	-3.871324
111	6	0	-0.295994	-3.667305	-3.206621
112	1	0	-0.390937	-2.590478	-3.367425
113	1	0	0.580103	-4.029927	-3.749285
114	6	0	-0.189748	-3.959764	-1.710598
115	1	0	-0.030241	-5.034254	-1.568605
116	6	0	0.906217	-3.214050	-0.951853
117	6	0	3.278466	-3.200470	-0.539724
118	6	0	3.576240	-3.148183	0.849277
119	6	0	4.731227	-2.465905	1.272700
120	1	0	4.983020	-2.401137	2.323049
121	6	0	5.581161	-1.864295	0.351641
122	1	0	6.468916	-1.349375	0.695130
123	6	0	5.294514	-1.918430	-1.008266
124	1	0	5.975147	-1.436342	-1.697139
125	6	0	4.144466	-2.578308	-1.477777
126	6	0	3.848733	-2.593366	-2.975054
127	1	0	2.918670	-3.157168	-3.189233
128	6	0	4.965754	-3.298389	-3.753232
129	1	0	4.681434	-3.397859	-4.822739
130	1	0	5.129179	-4.319091	-3.345896
131	1	0	5.919747	-2.732876	-3.698136
132	6	0	3.615810	-1.175236	-3.508678

133	1	0	2.771024	-0.699891	-2.966504
134	1	0	3.348668	-1.211063	-4.586631
135	1	0	4.520911	-0.542414	-3.394395
136	6	0	2.687877	-3.829670	1.886517
137	1	0	1.841714	-4.353601	1.395715
138	6	0	3.460897	-4.905739	2.658670
139	1	0	3.911888	-5.634404	1.951280
140	1	0	2.771946	-5.462615	3.329699
141	1	0	4.267229	-4.461579	3.279575
142	6	0	2.070988	-2.805954	2.846707
143	1	0	2.852054	-2.265709	3.421532
144	1	0	1.402287	-3.320553	3.567841
145	1	0	1.464673	-2.068635	2.281562
146	8	0	0.742004	-2.145653	-0.350743
147	20	0	-1.026797	-0.571817	-0.042196
148	8	0	-0.599812	0.647328	-1.998687
149	16	0	-0.856585	1.432348	-3.249542
150	8	0	0.291185	2.248119	-3.681887
151	8	0	-1.562480	0.671329	-4.295359
152	6	0	-2.103526	2.671557	-2.649329
153	9	0	-1.609639	3.374358	-1.614558
154	9	0	-2.433763	3.531963	-3.622356
155	9	0	-3.218469	2.049070	-2.236820
156	35	0	6.161669	1.766483	-0.782150

L3a-Ca(II)-TS-*si*-1

Zero-point correction= 1.28694 a.u.

Thermal correction to Gibbs Free Energy= 1.17025 a.u.

Sum of electronic and zero-point Energies= -7194.58814 a.u.

Sum of electronic and thermal Free Energies= -7194.70483a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.689490	-1.049431	1.442790
2	6	0	-2.802911	-1.515168	0.453230
3	6	0	-3.976719	-1.717069	1.421426
4	6	0	-3.523720	-1.497680	2.731906
5	7	0	-2.158098	-1.133865	2.712604
6	8	0	-2.997000	-0.717247	-0.581978
7	8	0	-0.546430	-0.690186	1.138276

8	6	0	-1.380440	-0.817435	3.899413
9	6	0	-5.326686	-1.957076	1.239166
10	6	0	-4.348882	-1.576923	3.845839
11	6	0	-5.701456	-1.864577	3.623100
12	6	0	-6.198802	-2.041878	2.332814
13	1	0	-1.247439	-1.711971	4.517257
14	1	0	-0.407788	-0.449313	3.573875
15	1	0	-1.883899	-0.046251	4.490104
16	1	0	-3.970233	-1.408414	4.848306
17	1	0	-6.380545	-1.933344	4.468014
18	1	0	-7.253847	-2.234472	2.172233
19	6	0	-2.157055	-3.025789	0.011345
20	6	0	-2.897404	-3.510505	-1.141533
21	8	0	-3.714978	-4.518846	-0.915216
22	6	0	-4.514046	-5.059997	-1.990775
23	6	0	-2.871223	-2.691017	-2.305009
24	1	0	-1.138114	-2.765481	-0.279823
25	1	0	-2.171396	-3.709319	0.861250
26	1	0	-4.942115	-5.979444	-1.591378
27	1	0	-5.310977	-4.363082	-2.255567
28	1	0	-3.885843	-5.278265	-2.857900
29	1	0	-1.868782	-2.437188	-2.659345
30	1	0	-3.550959	-2.935927	-3.118789
31	1	0	-3.120640	-1.633326	-1.709407
32	8	0	1.768840	1.551732	1.964749
33	8	0	3.127355	-0.383291	0.434358
34	8	0	1.900152	2.456424	-1.231495
35	7	0	4.586333	-1.551621	1.721773
36	1	0	5.116464	-1.609433	2.583486
37	7	0	3.069054	1.851590	2.296052
38	7	0	-2.152935	3.818677	-0.909956
39	1	0	-2.292917	4.629712	-1.502291
40	7	0	1.600722	3.783499	-1.065761
41	6	0	4.601649	-2.673444	0.861378
42	6	0	5.528939	-2.728782	-0.210915
43	6	0	5.507556	-3.840861	-1.072668
44	1	0	6.193554	-3.907859	-1.906598
45	6	0	4.593741	-4.872862	-0.881769
46	1	0	4.585720	-5.717653	-1.558382
47	6	0	3.679999	-4.816727	0.166096
48	1	0	2.971788	-5.627210	0.276934
49	6	0	3.668674	-3.725726	1.054116
50	6	0	2.632971	-3.677280	2.172752
51	1	0	2.779324	-2.777098	2.804365

52	6	0	1.215895	-3.577103	1.597538
53	1	0	1.157815	-2.721025	0.893139
54	1	0	0.483050	-3.405091	2.414968
55	1	0	0.931109	-4.504858	1.057472
56	6	0	2.764388	-4.881504	3.112192
57	1	0	2.077743	-4.765678	3.978189
58	1	0	3.802197	-4.948516	3.503390
59	1	0	2.513253	-5.831698	2.595507
60	6	0	6.516958	-1.595567	-0.467458
61	1	0	6.436130	-0.818555	0.321164
62	6	0	7.965947	-2.095634	-0.425861
63	1	0	8.162217	-2.618332	0.534941
64	1	0	8.667450	-1.236969	-0.498646
65	1	0	8.181350	-2.791849	-1.263520
66	6	0	6.211354	-0.897001	-1.797365
67	1	0	6.348825	-1.585896	-2.657745
68	1	0	6.885409	-0.024664	-1.935069
69	1	0	5.164194	-0.523982	-1.800569
70	6	0	3.800181	-0.483145	1.469274
71	6	0	3.859194	0.570589	2.577030
72	1	0	4.906947	0.870440	2.693881
73	6	0	3.309284	0.129371	3.934063
74	1	0	3.928274	-0.646479	4.391668
75	1	0	2.295805	-0.260965	3.807881
76	6	0	3.321346	1.440470	4.741299
77	1	0	4.297565	1.543161	5.224595
78	6	0	2.169588	1.608697	5.755437
79	1	0	1.847403	0.649433	6.176119
80	1	0	2.505663	2.234477	6.591177
81	6	0	1.062269	2.331926	4.970868
82	1	0	0.345525	2.842112	5.623469
83	1	0	0.509962	1.620362	4.349622
84	6	0	1.834796	3.306093	4.064374
85	1	0	1.258071	3.630395	3.198571
86	1	0	2.124001	4.197660	4.634978
87	6	0	3.129015	2.570743	3.685680
88	1	0	3.991691	3.235766	3.629239
89	6	0	3.761836	2.660264	1.209889
90	1	0	4.803941	2.763479	1.526800
91	1	0	3.717331	2.049916	0.311102
92	6	0	3.196033	4.058942	0.946451
93	1	0	3.919558	4.553575	0.288583
94	1	0	3.208919	4.640782	1.875098
95	6	0	1.785274	4.216129	0.375375

96	1	0	1.076310	3.624499	0.950588
97	1	0	1.500740	5.271592	0.418526
98	6	0	2.426546	4.640106	-2.076534
99	1	0	2.566526	5.608042	-1.591911
100	6	0	3.748690	3.986740	-2.505713
101	1	0	4.166381	3.328773	-1.743071
102	1	0	4.465532	4.798454	-2.685445
103	6	0	3.435801	3.257321	-3.824272
104	1	0	2.994787	2.280813	-3.604962
105	1	0	4.330106	3.097767	-4.436790
106	6	0	2.404349	4.169876	-4.510635
107	1	0	1.800132	3.647524	-5.260552
108	1	0	2.915307	4.996345	-5.020181
109	6	0	1.541630	4.731812	-3.359308
110	1	0	1.265857	5.774876	-3.542701
111	6	0	0.258291	3.938974	-3.031374
112	1	0	0.350006	2.880486	-3.288423
113	1	0	-0.623071	4.348426	-3.530828
114	6	0	0.166491	4.094745	-1.513806
115	1	0	-0.000553	5.150367	-1.272815
116	6	0	-0.916798	3.275900	-0.813953
117	6	0	-3.294042	3.076815	-0.518612
118	6	0	-3.645244	2.987157	0.856188
119	6	0	-4.757226	2.209174	1.226024
120	1	0	-5.047106	2.114819	2.264427
121	6	0	-5.512352	1.544631	0.266699
122	1	0	-6.367409	0.954695	0.569550
123	6	0	-5.170189	1.629059	-1.078785
124	1	0	-5.770016	1.085949	-1.796842
125	6	0	-4.063054	2.390285	-1.496373
126	6	0	-3.695227	2.425370	-2.977444
127	1	0	-2.832475	3.098204	-3.153953
128	6	0	-4.847642	2.977900	-3.825557
129	1	0	-4.515573	3.114743	-4.877040
130	1	0	-5.169142	3.967634	-3.435969
131	1	0	-5.720289	2.291405	-3.825000
132	6	0	-3.263306	1.039568	-3.471634
133	1	0	-2.388795	0.682680	-2.886982
134	1	0	-2.955983	1.092551	-4.538037
135	1	0	-4.087670	0.300937	-3.381408
136	6	0	-2.856866	3.724462	1.935556
137	1	0	-2.033101	4.316651	1.485759
138	6	0	-3.743749	4.730497	2.678841
139	1	0	-4.221592	5.425350	1.955225

140	1	0	-3.129408	5.334433	3.380586
141	1	0	-4.537896	4.219830	3.263451
142	6	0	-2.205274	2.740930	2.915811
143	1	0	-2.969500	2.162351	3.475764
144	1	0	-1.579935	3.293805	3.648470
145	1	0	-1.548860	2.032190	2.369224
146	8	0	-0.705404	2.227813	-0.193803
147	20	0	1.009031	0.605623	-0.093975
148	8	0	0.553036	-0.462293	-2.160569
149	16	0	0.983549	-1.201377	-3.391653
150	8	0	-0.145329	-1.736300	-4.175338
151	8	0	2.064840	-0.545345	-4.146964
152	6	0	1.786144	-2.704494	-2.650308
153	9	0	0.904701	-3.400448	-1.907099
154	9	0	2.263377	-3.517057	-3.602396
155	9	0	2.802196	-2.335708	-1.856098
156	35	0	-6.070923	-2.126179	-0.519762

L3a-Ca(II)-IM2-*si*-1

Zero-point correction= 1.29294 a.u.

Thermal correction to Gibbs Free Energy= 1.17737 a.u.

Sum of electronic and zero-point Energies= -7194.62430 a.u.

Sum of electronic and thermal Free Energies= -7194.73987 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.731036	-0.986723	1.453462
2	6	0	-2.774008	-1.545632	0.452025
3	6	0	-4.002766	-1.666348	1.346053
4	6	0	-3.606245	-1.440969	2.673929
5	7	0	-2.239777	-1.080204	2.706309
6	8	0	-2.918300	-0.661177	-0.628654
7	8	0	-0.591527	-0.602905	1.175731
8	6	0	-1.495655	-0.780016	3.918852
9	6	0	-5.348679	-1.877363	1.097627
10	6	0	-4.481265	-1.502362	3.749133
11	6	0	-5.826494	-1.768269	3.463880
12	6	0	-6.268713	-1.936611	2.152486
13	1	0	-1.385478	-1.684158	4.526544
14	1	0	-0.512250	-0.412609	3.627073

15	1	0	-2.013226	-0.015575	4.505179
16	1	0	-4.145806	-1.333892	4.766635
17	1	0	-6.545255	-1.822486	4.276175
18	1	0	-7.319921	-2.103639	1.945337
19	6	0	-2.158942	-2.915595	-0.002303
20	6	0	-2.951781	-3.649868	-1.049288
21	8	0	-3.866329	-4.477816	-0.473545
22	6	0	-4.678789	-5.268456	-1.338066
23	6	0	-2.759912	-3.475928	-2.368540
24	1	0	-1.171815	-2.678655	-0.406784
25	1	0	-2.031570	-3.557865	0.875370
26	1	0	-5.320003	-5.864995	-0.686168
27	1	0	-5.300732	-4.639289	-1.983680
28	1	0	-4.062021	-5.931486	-1.957074
29	1	0	-1.961946	-2.833053	-2.724263
30	1	0	-3.348546	-3.990283	-3.119748
31	1	0	-3.217328	-1.187869	-1.394943
32	8	0	1.826561	1.521851	1.983990
33	8	0	3.142438	-0.408845	0.406805
34	8	0	1.948194	2.463274	-1.202324
35	7	0	4.565152	-1.639358	1.677077
36	1	0	5.091408	-1.726457	2.538580
37	7	0	3.135985	1.794724	2.304252
38	7	0	-2.077344	3.893968	-0.854261
39	1	0	-2.201391	4.724400	-1.422900
40	7	0	1.675474	3.793901	-1.018999
41	6	0	4.528114	-2.758754	0.813825
42	6	0	5.443268	-2.848524	-0.266393
43	6	0	5.370181	-3.956927	-1.130182
44	1	0	6.046657	-4.049937	-1.969398
45	6	0	4.416139	-4.950922	-0.934991
46	1	0	4.368031	-5.792393	-1.614169
47	6	0	3.514755	-4.861181	0.121019
48	1	0	2.774948	-5.642533	0.235138
49	6	0	3.556431	-3.774250	1.013172
50	6	0	2.536004	-3.690190	2.143951
51	1	0	2.730936	-2.804522	2.782709
52	6	0	1.119100	-3.520088	1.585370
53	1	0	1.090935	-2.652917	0.892831
54	1	0	0.402589	-3.327652	2.412663
55	1	0	0.789631	-4.427380	1.036051
56	6	0	2.621202	-4.908556	3.070859
57	1	0	1.953144	-4.766931	3.947455
58	1	0	3.659570	-5.031211	3.446572

59	1	0	2.315898	-5.839912	2.549369
60	6	0	6.475175	-1.756266	-0.528419
61	1	0	6.426882	-0.973880	0.257621
62	6	0	7.902660	-2.314764	-0.487755
63	1	0	8.080577	-2.838610	0.475980
64	1	0	8.638423	-1.485978	-0.568770
65	1	0	8.086577	-3.024936	-1.321174
66	6	0	6.195913	-1.050588	-1.860551
67	1	0	6.304677	-1.746875	-2.718892
68	1	0	6.904102	-0.206367	-2.002303
69	1	0	5.164697	-0.635774	-1.863793
70	6	0	3.813071	-0.543333	1.439658
71	6	0	3.905911	0.495543	2.559664
72	1	0	4.960732	0.773833	2.666051
73	6	0	3.363328	0.047256	3.917878
74	1	0	3.975683	-0.740714	4.362906
75	1	0	2.343314	-0.327422	3.797281
76	6	0	3.402472	1.347539	4.740976
77	1	0	4.383062	1.427819	5.219554
78	6	0	2.260069	1.522642	5.765018
79	1	0	1.922608	0.564176	6.175259
80	1	0	2.613164	2.130654	6.606695
81	6	0	1.161883	2.278652	4.998263
82	1	0	0.458791	2.792454	5.662689
83	1	0	0.592365	1.588058	4.368779
84	6	0	1.948707	3.251290	4.102715
85	1	0	1.372910	3.603684	3.247398
86	1	0	2.261644	4.126596	4.686017
87	6	0	3.223796	2.494465	3.701791
88	1	0	4.099412	3.141823	3.644378
89	6	0	3.830628	2.606675	1.221209
90	1	0	4.878483	2.685252	1.526284
91	1	0	3.762873	2.012388	0.313324
92	6	0	3.287538	4.019075	0.985094
93	1	0	4.013440	4.511887	0.328118
94	1	0	3.318428	4.587005	1.921926
95	6	0	1.875004	4.206168	0.426944
96	1	0	1.160003	3.618277	0.998711
97	1	0	1.606669	5.265278	0.484727
98	6	0	2.514666	4.646894	-2.022303
99	1	0	2.674024	5.605942	-1.526221
100	6	0	3.822268	3.973515	-2.464336
101	1	0	4.232703	3.300113	-1.711413
102	1	0	4.552834	4.773964	-2.639173

103	6	0	3.490321	3.264193	-3.789218
104	1	0	3.032039	2.293707	-3.579182
105	1	0	4.379112	3.094785	-4.407053
106	6	0	2.473526	4.203017	-4.461785
107	1	0	1.854183	3.698321	-5.211516
108	1	0	2.997173	5.022864	-4.968995
109	6	0	1.628284	4.772960	-3.300894
110	1	0	1.375564	5.823747	-3.472309
111	6	0	0.329486	4.004792	-2.977293
112	1	0	0.397309	2.948670	-3.251222
113	1	0	-0.544511	4.440959	-3.466829
114	6	0	0.245923	4.137838	-1.456619
115	1	0	0.096942	5.191461	-1.196060
116	6	0	-0.852027	3.324054	-0.773577
117	6	0	-3.232484	3.160244	-0.489641
118	6	0	-3.592204	3.037715	0.880286
119	6	0	-4.711358	2.257920	1.223685
120	1	0	-5.006838	2.138038	2.257624
121	6	0	-5.466023	1.624195	0.243202
122	1	0	-6.326977	1.032839	0.525986
123	6	0	-5.117159	1.743125	-1.097918
124	1	0	-5.717970	1.224870	-1.833315
125	6	0	-4.003070	2.507797	-1.489309
126	6	0	-3.629951	2.583035	-2.967544
127	1	0	-2.760574	3.252482	-3.121425
128	6	0	-4.773308	3.172125	-3.802841
129	1	0	-4.436496	3.333176	-4.849379
130	1	0	-5.083149	4.155036	-3.387228
131	1	0	-5.654350	2.496832	-3.822762
132	6	0	-3.210077	1.208116	-3.500395
133	1	0	-2.349078	0.819806	-2.915660
134	1	0	-2.887979	1.290788	-4.560546
135	1	0	-4.045229	0.478296	-3.443951
136	6	0	-2.801841	3.737650	1.982483
137	1	0	-1.971783	4.335294	1.551718
138	6	0	-3.682855	4.728968	2.752416
139	1	0	-4.154232	5.448041	2.048663
140	1	0	-3.065418	5.308175	3.472228
141	1	0	-4.481794	4.208010	3.321332
142	6	0	-2.161930	2.720844	2.935556
143	1	0	-2.934058	2.141071	3.482873
144	1	0	-1.526281	3.245366	3.680235
145	1	0	-1.517191	2.017026	2.369403
146	8	0	-0.664380	2.254674	-0.182569

147	20	0	1.034328	0.614164	-0.078057
148	8	0	0.506776	-0.448069	-2.126604
149	16	0	0.913899	-1.156906	-3.384406
150	8	0	-0.229521	-1.648967	-4.173475
151	8	0	1.998166	-0.492499	-4.128504
152	6	0	1.705688	-2.689505	-2.693413
153	9	0	0.831533	-3.389874	-1.947440
154	9	0	2.152019	-3.485803	-3.673604
155	9	0	2.743134	-2.351948	-1.911930
156	35	0	-6.013822	-2.013670	-0.690618

L3a-Ca(II)-IM1-*re*-1

Zero-point correction= 1.28751 a.u.

Thermal correction to Gibbs Free Energy= 1.17295 a.u.

Sum of electronic and zero-point Energies= -7194.61521 a.u.

Sum of electronic and thermal Free Energies= -7194.72978 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.588330	-0.075213	-0.313972
2	6	0	4.623956	0.507188	-0.941640
3	8	0	5.803546	0.617233	-0.251016
4	6	0	7.016256	0.798896	-0.980773
5	6	0	4.532143	1.102771	-2.318545
6	1	0	2.625204	-0.155499	-0.800856
7	1	0	3.707937	-0.495290	0.679857
8	1	0	7.810786	0.832991	-0.231509
9	1	0	7.022958	1.736957	-1.547388
10	1	0	7.208852	-0.037909	-1.663703
11	1	0	5.261158	0.660898	-3.008173
12	1	0	4.720146	2.184208	-2.292892
13	1	0	3.532571	0.945036	-2.729899
14	6	0	1.795286	1.619198	1.579443
15	6	0	1.993000	2.631723	0.415412
16	6	0	3.144706	3.445461	0.826342
17	6	0	3.537761	2.993430	2.104076
18	7	0	2.716108	1.921354	2.528421
19	8	0	1.260274	2.692790	-0.548113
20	8	0	0.938237	0.737026	1.633670
21	6	0	2.893420	1.198357	3.779212

22	6	0	3.842414	4.487411	0.224919
23	6	0	4.595552	3.566238	2.789772
24	1	0	3.834962	0.639743	3.766267
25	1	0	2.058274	0.506940	3.892981
26	1	0	2.898737	1.900401	4.617702
27	6	0	5.272210	4.622631	2.160632
28	6	0	4.913257	5.086244	0.893106
29	1	0	4.899379	3.217296	3.769942
30	1	0	6.106870	5.092321	2.672591
31	1	0	5.462544	5.897943	0.429982
32	8	0	-1.581434	-0.926166	2.405756
33	8	0	-2.530292	1.045916	0.633001
34	8	0	-1.992946	-2.312759	-0.467976
35	7	0	-4.471432	2.037637	1.262993
36	1	0	-5.249580	2.048408	1.912021
37	7	0	-2.877806	-0.918126	2.843070
38	7	0	1.782244	-4.328545	-0.183200
39	1	0	1.688552	-5.213762	-0.668643
40	7	0	-1.908261	-3.626290	-0.083873
41	6	0	-4.629151	2.705508	0.025655
42	6	0	-5.480574	2.156267	-0.969002
43	6	0	-5.559665	2.790137	-2.222341
44	1	0	-6.186889	2.387973	-3.006955
45	6	0	-4.822265	3.939353	-2.487875
46	1	0	-4.890368	4.410156	-3.460153
47	6	0	-3.995298	4.484397	-1.511000
48	1	0	-3.432544	5.376627	-1.751663
49	6	0	-3.888196	3.886917	-0.242150
50	6	0	-2.974070	4.511118	0.808043
51	1	0	-3.039428	3.953465	1.765394
52	6	0	-1.508528	4.448176	0.364077
53	1	0	-1.228361	3.397234	0.144419
54	1	0	-0.845176	4.818030	1.175062
55	1	0	-1.332005	5.062996	-0.543825
56	6	0	-3.390827	5.951660	1.128662
57	1	0	-2.783897	6.344901	1.972406
58	1	0	-4.459317	5.981459	1.431986
59	1	0	-3.246197	6.622412	0.255880
60	6	0	-6.272589	0.874966	-0.724334
61	1	0	-6.129841	0.515940	0.315623
62	6	0	-7.778992	1.108127	-0.893011
63	1	0	-8.112591	1.942539	-0.239784
64	1	0	-8.341179	0.196422	-0.597347
65	1	0	-8.039125	1.350177	-1.944974

66	6	0	-5.784732	-0.253693	-1.639395
67	1	0	-5.958737	-0.014085	-2.709563
68	1	0	-6.320272	-1.197226	-1.400274
69	1	0	-4.698947	-0.422895	-1.482429
70	6	0	-3.435835	1.191160	1.463304
71	6	0	-3.470921	0.500039	2.824035
72	1	0	-4.515550	0.386501	3.130272
73	6	0	-2.696025	1.188685	3.943518
74	1	0	-3.145903	2.148674	4.208502
75	1	0	-1.663912	1.354867	3.624922
76	6	0	-2.790339	0.150023	5.082220
77	1	0	-3.693457	0.356611	5.664066
78	6	0	-1.549309	0.037653	5.995952
79	1	0	-1.007310	0.987017	6.071892
80	1	0	-1.864996	-0.238346	7.009500
81	6	0	-0.705875	-1.094205	5.383181
82	1	0	-0.015403	-1.544470	6.104818
83	1	0	-0.122915	-0.720467	4.536290
84	6	0	-1.755556	-2.093475	4.867395
85	1	0	-1.364598	-2.768351	4.106006
86	1	0	-2.132466	-2.702930	5.698934
87	6	0	-2.927307	-1.234268	4.371434
88	1	0	-3.899961	-1.700219	4.539759
89	6	0	-3.750032	-1.836625	2.008063
90	1	0	-4.771318	-1.723183	2.384196
91	1	0	-3.689828	-1.448393	0.992734
92	6	0	-3.380260	-3.321420	2.025707
93	1	0	-4.212075	-3.841785	1.537575
94	1	0	-3.379758	-3.687819	3.058881
95	6	0	-2.052669	-3.782267	1.419669
96	1	0	-1.225034	-3.222885	1.849697
97	1	0	-1.924101	-4.847942	1.631549
98	6	0	-2.939055	-4.483101	-0.885283
99	1	0	-3.189260	-5.320845	-0.232177
100	6	0	-4.170939	-3.695407	-1.350228
101	1	0	-4.429548	-2.876527	-0.679539
102	1	0	-5.015102	-4.397376	-1.365804
103	6	0	-3.844461	-3.233078	-2.781462
104	1	0	-3.234282	-2.326842	-2.743246
105	1	0	-4.744654	-3.015148	-3.367047
106	6	0	-3.029081	-4.401771	-3.362604
107	1	0	-2.400586	-4.104864	-4.208813
108	1	0	-3.704162	-5.190834	-3.716776
109	6	0	-2.191136	-4.934131	-2.177326

110	1	0	-2.123912	-6.026050	-2.199866
111	6	0	-0.765933	-4.355713	-2.051533
112	1	0	-0.681744	-3.366245	-2.507686
113	1	0	-0.015448	-5.012798	-2.498142
114	6	0	-0.586967	-4.254809	-0.535626
115	1	0	-0.577788	-5.263927	-0.109375
116	6	0	0.682974	-3.545337	-0.059506
117	6	0	3.088969	-3.802507	-0.032114
118	6	0	3.621301	-3.577151	1.267424
119	6	0	4.933122	-3.082903	1.389913
120	1	0	5.362393	-2.889116	2.363836
121	6	0	5.712255	-2.838956	0.264155
122	1	0	6.720241	-2.460289	0.377430
123	6	0	5.198033	-3.066921	-1.007199
124	1	0	5.828595	-2.859200	-1.861418
125	6	0	3.882859	-3.535524	-1.181047
126	6	0	3.339021	-3.720793	-2.594884
127	1	0	2.279561	-4.042708	-2.570282
128	6	0	4.110317	-4.814442	-3.341332
129	1	0	3.645314	-5.000459	-4.333271
130	1	0	4.079797	-5.763378	-2.764031
131	1	0	5.170837	-4.525774	-3.499999
132	6	0	3.356823	-2.402276	-3.378261
133	1	0	2.807938	-1.620277	-2.815159
134	1	0	2.852311	-2.533763	-4.359350
135	1	0	4.393485	-2.051516	-3.565060
136	6	0	2.814004	-3.867820	2.530280
137	1	0	1.821267	-4.290892	2.274554
138	6	0	3.506148	-4.920222	3.405123
139	1	0	3.701222	-5.840737	2.814116
140	1	0	2.851576	-5.195169	4.259858
141	1	0	4.468425	-4.544580	3.812471
142	6	0	2.552353	-2.581821	3.324371
143	1	0	3.495902	-2.153980	3.723786
144	1	0	1.874145	-2.792336	4.178677
145	1	0	2.063427	-1.824593	2.676820
146	8	0	0.722616	-2.405454	0.416755
147	20	0	-0.687894	-0.480917	0.248061
148	8	0	0.394399	-0.327989	-1.899172
149	16	0	0.108032	-0.098368	-3.354411
150	8	0	1.126735	0.712677	-4.042533
151	8	0	-0.362358	-1.302513	-4.066041
152	6	0	-1.393802	1.000243	-3.276523
153	9	0	-1.128346	2.133489	-2.611771

154	9	0	-1.825142	1.316464	-4.504420
155	9	0	-2.395087	0.366703	-2.629108
156	35	0	3.367945	5.084051	-1.516070

L3a-Ca(II)-TS-*re*-1

Zero-point correction= 1.28559 a.u.

Thermal correction to Gibbs Free Energy= 1.17449 a.u.

Sum of electronic and zero-point Energies= -7194.59210 a.u.

Sum of electronic and thermal Free Energies= -7194.70320 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.608770	-0.347138	-0.565505
2	6	0	-3.996808	-0.808363	-1.889909
3	8	0	-5.286124	-0.755784	-2.154831
4	6	0	-5.780142	-1.212772	-3.433887
5	6	0	-3.011838	-1.505792	-2.639266
6	1	0	-2.690219	0.240650	-0.616259
7	1	0	-4.398191	0.194644	-0.044493
8	1	0	-6.817652	-0.880858	-3.472202
9	1	0	-5.735901	-2.302084	-3.485507
10	1	0	-5.205500	-0.762246	-4.246744
11	1	0	-2.058896	-0.985205	-2.749291
12	1	0	-3.321312	-2.004038	-3.555520
13	1	0	-2.667198	-2.258632	-1.710756
14	6	0	-2.466990	-0.965015	1.543177
15	6	0	-3.143428	-1.697869	0.344617
16	6	0	-4.382471	-2.288986	1.028831
17	6	0	-4.422981	-1.829214	2.354741
18	7	0	-3.287998	-1.031721	2.623519
19	8	0	-2.344360	-2.524789	-0.315913
20	8	0	-1.375249	-0.388706	1.514061
21	6	0	-2.988104	-0.480302	3.934437
22	6	0	-5.357743	-3.184303	0.627407
23	6	0	-5.427481	-2.176040	3.248951
24	1	0	-3.800117	0.175058	4.262654
25	1	0	-2.062981	0.089129	3.861366
26	1	0	-2.860054	-1.285406	4.665825
27	6	0	-6.423987	-3.046752	2.789498
28	6	0	-6.390198	-3.564369	1.495269

29	1	0	-5.438084	-1.802084	4.267084
30	1	0	-7.227268	-3.342104	3.458246
31	1	0	-7.150318	-4.262781	1.162689
32	8	0	1.489204	0.519031	2.648895
33	8	0	2.575131	-1.132862	0.615381
34	8	0	2.203832	2.077601	-0.138541
35	7	0	4.220114	-2.526370	1.324401
36	1	0	4.900185	-2.738593	2.045316
37	7	0	2.776741	0.428010	3.112033
38	7	0	-1.407099	4.315593	-0.410478
39	1	0	-1.201709	5.194942	-0.871677
40	7	0	2.171474	3.378563	0.296132
41	6	0	4.434458	-3.067197	0.035126
42	6	0	5.483217	-2.560606	-0.777385
43	6	0	5.633350	-3.060750	-2.083676
44	1	0	6.410028	-2.682283	-2.734938
45	6	0	4.781256	-4.045862	-2.572164
46	1	0	4.909513	-4.417196	-3.580818
47	6	0	3.760995	-4.551712	-1.772904
48	1	0	3.111566	-5.311930	-2.186111
49	6	0	3.567547	-4.074964	-0.463680
50	6	0	2.430688	-4.640977	0.382456
51	1	0	2.440712	-4.196472	1.399344
52	6	0	1.066430	-4.300754	-0.229698
53	1	0	0.966028	-3.201727	-0.355137
54	1	0	0.250723	-4.643163	0.442565
55	1	0	0.932852	-4.788424	-1.218501
56	6	0	2.582066	-6.154174	0.580309
57	1	0	1.814859	-6.523616	1.294302
58	1	0	3.583150	-6.386330	1.002729
59	1	0	2.459783	-6.704691	-0.376276
60	6	0	6.421581	-1.464206	-0.279835
61	1	0	6.205997	-1.211639	0.778654
62	6	0	7.885410	-1.919682	-0.319875
63	1	0	8.004564	-2.872165	0.239962
64	1	0	8.534607	-1.156431	0.160401
65	1	0	8.238226	-2.069162	-1.361954
66	6	0	6.225447	-0.169979	-1.076815
67	1	0	6.478728	-0.308842	-2.149147
68	1	0	6.870076	0.635404	-0.664380
69	1	0	5.169990	0.162553	-0.996167
70	6	0	3.325903	-1.530090	1.515591
71	6	0	3.331448	-0.992079	2.946836
72	1	0	4.373500	-0.940147	3.279381

73	6	0	2.523068	-1.780521	3.974573
74	1	0	2.946341	-2.774067	4.140044
75	1	0	1.492392	-1.888775	3.626286
76	6	0	2.622221	-0.874339	5.221163
77	1	0	3.512584	-1.163225	5.787417
78	6	0	1.372386	-0.831654	6.128519
79	1	0	0.809875	-1.771599	6.098819
80	1	0	1.680909	-0.669344	7.168522
81	6	0	0.560670	0.375309	5.626376
82	1	0	-0.134656	0.761522	6.379780
83	1	0	-0.013026	0.099245	4.737992
84	6	0	1.633317	1.402278	5.227328
85	1	0	1.266295	2.150300	4.523654
86	1	0	2.005284	1.925092	6.117658
87	6	0	2.797721	0.574466	4.666596
88	1	0	3.774118	0.998039	4.905912
89	6	0	3.698805	1.407116	2.410017
90	1	0	4.696566	1.239658	2.827091
91	1	0	3.685389	1.117047	1.362024
92	6	0	3.347091	2.891018	2.545952
93	1	0	4.242918	3.437387	2.229738
94	1	0	3.211857	3.149721	3.601799
95	6	0	2.125380	3.452850	1.813374
96	1	0	1.221939	2.921017	2.104782
97	1	0	2.022351	4.511574	2.072203
98	6	0	3.368839	4.187284	-0.307030
99	1	0	3.586724	4.965638	0.426176
100	6	0	4.595133	3.331628	-0.653393
101	1	0	4.707183	2.457361	-0.013301
102	1	0	5.478575	3.967498	-0.508123
103	6	0	4.443199	2.980574	-2.143495
104	1	0	3.770325	2.126339	-2.253942
105	1	0	5.400284	2.724210	-2.611720
106	6	0	3.807083	4.244130	-2.748402
107	1	0	3.288201	4.051400	-3.693499
108	1	0	4.580953	4.996180	-2.946730
109	6	0	2.845828	4.767561	-1.656662
110	1	0	2.851406	5.860889	-1.613764
111	6	0	1.386091	4.285734	-1.769356
112	1	0	1.311610	3.322848	-2.281512
113	1	0	0.749934	5.010319	-2.283839
114	6	0	0.979187	4.127785	-0.303421
115	1	0	0.965428	5.112438	0.175214
116	6	0	-0.389426	3.487601	-0.076880

117	6	0	-2.748087	3.863050	-0.416996
118	6	0	-3.473956	3.780504	0.801453
119	6	0	-4.789737	3.283717	0.777945
120	1	0	-5.364265	3.196070	1.690588
121	6	0	-5.384701	2.897345	-0.418301
122	1	0	-6.398215	2.517155	-0.417710
123	6	0	-4.680136	2.987777	-1.614037
124	1	0	-5.169493	2.668983	-2.524926
125	6	0	-3.358110	3.468368	-1.637589
126	6	0	-2.605086	3.520838	-2.963414
127	1	0	-1.582359	3.923480	-2.819915
128	6	0	-3.299304	4.454688	-3.961357
129	1	0	-2.681646	4.558375	-4.879290
130	1	0	-3.423523	5.464746	-3.515382
131	1	0	-4.297534	4.067009	-4.255205
132	6	0	-2.431286	2.117094	-3.551767
133	1	0	-1.922055	1.465962	-2.812418
134	1	0	-1.802026	2.160141	-4.466205
135	1	0	-3.408430	1.663734	-3.820933
136	6	0	-2.863285	4.224047	2.127900
137	1	0	-1.842442	4.631361	1.974535
138	6	0	-3.677612	5.355865	2.766260
139	1	0	-3.785462	6.199133	2.050807
140	1	0	-3.156254	5.737458	3.670304
141	1	0	-4.688607	5.010457	3.068748
142	6	0	-2.721861	3.039762	3.089980
143	1	0	-3.714603	2.637768	3.382587
144	1	0	-2.184513	3.354346	4.010194
145	1	0	-2.132703	2.231064	2.610117
146	8	0	-0.577720	2.353767	0.382055
147	20	0	0.693080	0.322349	0.428645
148	8	0	0.373863	-0.015031	-1.905961
149	16	0	0.767499	-0.000636	-3.352721
150	8	0	-0.190332	-0.702870	-4.225780
151	8	0	1.255674	1.305209	-3.833939
152	6	0	2.269383	-1.093639	-3.348846
153	9	0	1.947494	-2.321680	-2.917515
154	9	0	2.785291	-1.199614	-4.581707
155	9	0	3.214810	-0.593400	-2.536459
156	35	0	-5.298321	-3.992784	-1.110142

L3a-Ca(II)-IM2-*re*-1

Zero-point correction= 1.29130 a.u.

Thermal correction to Gibbs Free Energy= 1.17629 a.u.
Sum of electronic and zero-point Energies= -7194.62803 a.u.
Sum of electronic and thermal Free Energies= -7194.74304 a.u.
The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.366500	-0.376470	-0.419068
2	6	0	-4.309809	-0.352435	-1.590448
3	8	0	-5.600906	-0.263189	-1.167231
4	6	0	-6.617111	-0.167213	-2.160680
5	6	0	-3.895789	-0.422716	-2.866915
6	1	0	-2.421963	0.089004	-0.711308
7	1	0	-3.799094	0.198991	0.405117
8	1	0	-7.555281	-0.029676	-1.619182
9	1	0	-6.671242	-1.084129	-2.757621
10	1	0	-6.443500	0.690944	-2.821345
11	1	0	-2.835377	-0.442490	-3.094572
12	1	0	-4.580453	-0.433479	-3.707427
13	1	0	-2.761595	-2.386690	-1.719878
14	6	0	-2.019707	-1.517152	1.285486
15	6	0	-2.992443	-1.801220	0.111981
16	6	0	-4.123421	-2.525663	0.835128
17	6	0	-3.885794	-2.448496	2.216516
18	7	0	-2.641173	-1.820567	2.450705
19	8	0	-2.332584	-2.572367	-0.862432
20	8	0	-0.891971	-1.024043	1.186104
21	6	0	-2.053931	-1.639661	3.767853
22	6	0	-5.232084	-3.238088	0.408094
23	6	0	-4.749709	-2.973818	3.167439
24	1	0	-2.717884	-1.041355	4.398675
25	1	0	-1.103549	-1.123164	3.642681
26	1	0	-1.882930	-2.611133	4.243496
27	6	0	-5.891928	-3.634629	2.698697
28	6	0	-6.128941	-3.787633	1.333275
29	1	0	-4.545864	-2.891979	4.229425
30	1	0	-6.594531	-4.059347	3.409575
31	1	0	-6.995860	-4.337937	0.984705
32	8	0	1.714011	0.523868	2.497223
33	8	0	2.658358	-1.194559	0.478186
34	8	0	2.259918	2.150344	-0.249330
35	7	0	4.354957	-2.560952	1.089030

36	1	0	5.088862	-2.760804	1.759508
37	7	0	3.014493	0.408877	2.919874
38	7	0	-1.425594	4.302979	0.207903
39	1	0	-1.295464	5.258637	-0.104870
40	7	0	2.227273	3.427263	0.246948
41	6	0	4.477038	-3.095794	-0.215273
42	6	0	5.429963	-2.548649	-1.114454
43	6	0	5.467880	-3.024601	-2.437671
44	1	0	6.166670	-2.612937	-3.153788
45	6	0	4.595865	-4.022006	-2.861886
46	1	0	4.635906	-4.372831	-3.885029
47	6	0	3.662169	-4.559637	-1.981722
48	1	0	2.988288	-5.322476	-2.348488
49	6	0	3.582329	-4.108570	-0.651706
50	6	0	2.522383	-4.693108	0.277964
51	1	0	2.617914	-4.265791	1.297874
52	6	0	1.109652	-4.347293	-0.211330
53	1	0	0.999438	-3.247701	-0.321603
54	1	0	0.354202	-4.693551	0.526311
55	1	0	0.891046	-4.827658	-1.188483
56	6	0	2.692907	-6.208908	0.436183
57	1	0	1.987868	-6.593637	1.203937
58	1	0	3.725903	-6.445000	0.770482
59	1	0	2.493341	-6.743532	-0.516326
60	6	0	6.364586	-1.416696	-0.695393
61	1	0	6.259884	-1.200222	0.387722
62	6	0	7.836270	-1.790766	-0.913084
63	1	0	8.066974	-2.751174	-0.404479
64	1	0	8.495466	-1.007616	-0.480910
65	1	0	8.078166	-1.888597	-1.992206
66	6	0	6.011212	-0.118199	-1.429340
67	1	0	6.138415	-0.224612	-2.527503
68	1	0	6.662516	0.710512	-1.078129
69	1	0	4.958339	0.159932	-1.214613
70	6	0	3.464238	-1.576496	1.336394
71	6	0	3.528771	-1.029064	2.759714
72	1	0	4.578905	-1.007888	3.067768
73	6	0	2.721965	-1.781387	3.816376
74	1	0	3.124944	-2.782795	3.986496
75	1	0	1.682039	-1.868127	3.492391
76	6	0	2.873046	-0.860145	5.047234
77	1	0	3.762770	-1.171630	5.602143
78	6	0	1.645133	-0.757360	5.980696
79	1	0	1.033811	-1.666598	5.958491

80	1	0	1.984257	-0.620582	7.014645
81	6	0	0.882943	0.494507	5.510050
82	1	0	0.245161	0.918877	6.293125
83	1	0	0.253712	0.257008	4.648818
84	6	0	1.991921	1.461526	5.063098
85	1	0	1.634592	2.224293	4.370487
86	1	0	2.422406	1.970446	5.934856
87	6	0	3.093858	0.573589	4.468949
88	1	0	4.097664	0.953282	4.667046
89	6	0	3.933824	1.361964	2.176401
90	1	0	4.945599	1.164787	2.544809
91	1	0	3.863758	1.077613	1.128778
92	6	0	3.634557	2.853952	2.340632
93	1	0	4.498894	3.380571	1.920851
94	1	0	3.629796	3.114582	3.405056
95	6	0	2.343833	3.437912	1.760899
96	1	0	1.480085	2.884690	2.124350
97	1	0	2.263779	4.484659	2.069096
98	6	0	3.318315	4.294148	-0.456732
99	1	0	3.586448	5.066227	0.266587
100	6	0	4.526903	3.488571	-0.953506
101	1	0	4.740484	2.611993	-0.342070
102	1	0	5.398542	4.154348	-0.899901
103	6	0	4.216691	3.146440	-2.421255
104	1	0	3.570000	2.266120	-2.463246
105	1	0	5.122075	2.933906	-3.000863
106	6	0	3.465906	4.389318	-2.932006
107	1	0	2.842770	4.181879	-3.808329
108	1	0	4.182605	5.169399	-3.217464
109	6	0	2.627082	4.876831	-1.727353
110	1	0	2.617047	5.969550	-1.670422
111	6	0	1.170607	4.368588	-1.676488
112	1	0	1.046761	3.422101	-2.209214
113	1	0	0.466596	5.097465	-2.084147
114	6	0	0.946996	4.157593	-0.177271
115	1	0	0.971499	5.126961	0.331591
116	6	0	-0.363568	3.462911	0.195486
117	6	0	-2.748724	3.796983	0.243336
118	6	0	-3.311938	3.359727	1.473657
119	6	0	-4.618977	2.839075	1.477810
120	1	0	-5.074502	2.494775	2.396763
121	6	0	-5.355684	2.750355	0.301782
122	1	0	-6.358213	2.342640	0.323278
123	6	0	-4.805350	3.170074	-0.903981

124	1	0	-5.400150	3.071173	-1.802245
125	6	0	-3.502708	3.698630	-0.958004
126	6	0	-2.919757	4.106845	-2.307741
127	1	0	-1.900665	4.522026	-2.188040
128	6	0	-3.756009	5.209114	-2.968815
129	1	0	-3.248198	5.573090	-3.887767
130	1	0	-3.868830	6.070443	-2.276008
131	1	0	-4.764881	4.841788	-3.251619
132	6	0	-2.775836	2.893986	-3.233093
133	1	0	-2.165614	2.110183	-2.735984
134	1	0	-2.256506	3.187215	-4.170410
135	1	0	-3.766528	2.469786	-3.500398
136	6	0	-2.537972	3.442983	2.786714
137	1	0	-1.537193	3.893438	2.625839
138	6	0	-3.252384	4.350150	3.795567
139	1	0	-3.429022	5.352372	3.349355
140	1	0	-2.621643	4.484407	4.700562
141	1	0	-4.226680	3.921233	4.111473
142	6	0	-2.300526	2.046742	3.377431
143	1	0	-3.256508	1.561569	3.666346
144	1	0	-1.657864	2.119022	4.280561
145	1	0	-1.783175	1.399697	2.638674
146	8	0	-0.474241	2.261015	0.467163
147	20	0	0.867651	0.326226	0.270765
148	8	0	-0.029050	0.041078	-1.938354
149	16	0	0.312040	0.046974	-3.400245
150	8	0	-0.629642	-0.728516	-4.226626
151	8	0	0.712502	1.368502	-3.918700
152	6	0	1.876041	-0.961607	-3.423924
153	9	0	1.642953	-2.203977	-2.976359
154	9	0	2.378417	-1.041917	-4.662708
155	9	0	2.806024	-0.399760	-2.626678
156	35	0	-5.534805	-3.576690	-1.449799

L1-Mg(II)-TS1-*si*-1

Zero-point correction= 1.26094 a.u.

Thermal correction to Gibbs Free Energy= 1.15804 a.u.

Sum of electronic and zero-point Energies= -5755.24322 a.u.

Sum of electronic and thermal Free Energies= -5755.34612 a.u.

The number of imaginary frequencies 1

Standard orientation

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.733187	1.338027	-1.832094
2	6	0	-0.091299	2.137180	-0.687005
3	6	0	-0.943229	3.374407	-0.660223
4	6	0	-1.815512	3.326369	-1.771071
5	7	0	-1.629474	2.105332	-2.489026
6	8	0	0.253688	1.433874	0.335664
7	6	0	-1.050559	4.426275	0.233021
8	6	0	-2.739595	4.335590	-2.009476
9	8	0	-0.475586	0.136997	-2.004477
10	6	0	-2.426372	1.568620	-3.622289
11	1	0	-1.937734	0.613980	-3.832811
12	6	0	-1.975352	5.453440	0.023709
13	6	0	-2.798276	5.400499	-1.099880
14	35	0	0.023568	4.457524	1.815684
15	1	0	-2.056875	6.271529	0.730533
16	1	0	-3.518740	6.195754	-1.265476
17	1	0	-3.419217	4.304949	-2.851215
18	8	0	2.114121	-0.842876	-0.563173
19	12	0	0.140410	-0.598604	-0.038130
20	8	0	-0.168763	-2.564992	-0.572970
21	8	0	0.664643	-1.291255	1.817841
22	8	0	-1.845153	-0.652366	0.513922
23	7	0	4.092540	-1.919561	-0.307843
24	1	0	4.582709	-2.789816	-0.135899
25	7	0	0.651749	-3.493591	0.005751
26	7	0	-3.640415	-1.716871	1.403307
27	1	0	-3.984990	-2.433279	2.031948
28	7	0	-0.002991	-2.398509	2.267542
29	6	0	4.869494	-0.752537	-0.512192
30	6	0	5.378448	-0.039377	0.604297
31	6	0	6.109193	1.142500	0.383405
32	1	0	6.503543	1.712975	1.213748
33	6	0	6.328573	1.615636	-0.905556
34	1	0	6.882111	2.533618	-1.055652
35	6	0	5.841579	0.913751	-2.002015
36	1	0	6.034888	1.306819	-2.991241
37	6	0	5.128415	-0.286428	-1.831235
38	6	0	4.673189	-1.063049	-3.062307
39	1	0	4.208918	-2.020250	-2.763135
40	6	0	3.612341	-0.286232	-3.849438
41	1	0	2.728453	-0.092535	-3.208011
42	1	0	3.269952	-0.882291	-4.722401

43	1	0	4.009466	0.683011	-4.218284
44	6	0	5.859151	-1.437795	-3.960985
45	1	0	5.522572	-2.117209	-4.773328
46	1	0	6.633973	-1.971466	-3.370054
47	1	0	6.317221	-0.540890	-4.428223
48	6	0	5.138195	-0.513879	2.033160
49	1	0	4.571424	-1.467656	2.039080
50	6	0	6.461800	-0.798791	2.753694
51	1	0	7.070099	-1.519591	2.166509
52	1	0	6.264208	-1.250219	3.749670
53	1	0	7.051904	0.129772	2.904189
54	6	0	4.296318	0.501751	2.814532
55	1	0	4.800454	1.488962	2.876083
56	1	0	4.127212	0.139002	3.849394
57	1	0	3.308080	0.633722	2.325689
58	6	0	2.745504	-1.895354	-0.379269
59	6	0	2.134967	-3.300979	-0.395264
60	1	0	2.709180	-3.959189	0.262299
61	6	0	2.156761	-3.840191	-1.833859
62	1	0	3.180472	-4.023734	-2.163196
63	1	0	1.700483	-3.103956	-2.502248
64	6	0	1.337330	-5.135501	-1.771620
65	1	0	2.012019	-5.970689	-1.565279
66	6	0	0.446930	-5.418346	-3.003205
67	1	0	0.874647	-5.005576	-3.923225
68	1	0	0.353708	-6.501759	-3.143457
69	6	0	-0.922385	-4.813547	-2.646671
70	1	0	-1.736810	-5.259822	-3.225859
71	1	0	-0.923672	-3.735078	-2.831150
72	6	0	-1.057183	-5.076985	-1.135058
73	1	0	-1.764802	-4.412226	-0.637521
74	1	0	-1.377768	-6.110633	-0.957819
75	6	0	0.365932	-4.943006	-0.586316
76	1	0	0.582502	-5.626038	0.235713
77	6	0	0.383113	-3.641883	1.491574
78	1	0	1.291113	-4.036415	1.942715
79	1	0	-0.432125	-4.352858	1.602166
80	6	0	0.405191	-2.729171	3.768537
81	1	0	0.320546	-3.813854	3.847206
82	6	0	1.796434	-2.198758	4.126404
83	1	0	2.454027	-2.123531	3.258821
84	1	0	2.243395	-2.909385	4.832078
85	6	0	1.537080	-0.849133	4.822402
86	1	0	1.406373	-0.068135	4.067179

87	1	0	2.358676	-0.552915	5.482159
88	6	0	0.223412	-1.077246	5.589496
89	1	0	-0.302184	-0.146848	5.829955
90	1	0	0.426346	-1.593218	6.535382
91	6	0	-0.614420	-1.996859	4.673350
92	1	0	-1.185158	-2.728006	5.252996
93	6	0	-1.566681	-1.282684	3.705356
94	1	0	-1.221446	-0.272902	3.464562
95	1	0	-2.584862	-1.220379	4.094961
96	6	0	-1.523959	-2.149433	2.438998
97	1	0	-1.959698	-3.130757	2.647197
98	6	0	-2.315695	-1.466618	1.318989
99	6	0	-4.587938	-1.043845	0.591840
100	6	0	-5.186707	-1.721635	-0.502975
101	6	0	-6.123123	-1.038002	-1.300734
102	1	0	-6.594283	-1.526173	-2.143323
103	6	0	-6.456010	0.285259	-1.034742
104	1	0	-7.168494	0.799678	-1.666803
105	6	0	-5.874821	0.951796	0.037726
106	1	0	-6.157858	1.980562	0.217258
107	6	0	-4.955758	0.300229	0.880629
108	6	0	-4.401752	1.046155	2.090020
109	1	0	-3.753493	0.382637	2.692848
110	6	0	-5.524613	1.501132	3.030948
111	1	0	-5.092326	1.926362	3.962211
112	1	0	-6.161900	0.635570	3.313085
113	1	0	-6.162845	2.278241	2.560172
114	6	0	-3.535713	2.233002	1.656025
115	1	0	-2.713201	1.878398	1.002328
116	1	0	-3.081438	2.720473	2.544845
117	1	0	-4.132050	2.990496	1.105075
118	6	0	-4.826545	-3.163061	-0.845208
119	1	0	-4.071938	-3.558987	-0.135284
120	6	0	-6.048847	-4.081356	-0.730822
121	1	0	-6.493287	-3.999592	0.284264
122	1	0	-5.747450	-5.139046	-0.889014
123	1	0	-6.823615	-3.823208	-1.483387
124	6	0	-4.199081	-3.256416	-2.240718
125	1	0	-4.914280	-2.946622	-3.031348
126	1	0	-3.891461	-4.302402	-2.448641
127	1	0	-3.299847	-2.606317	-2.298267
128	6	0	-2.308522	2.442395	-4.873253
129	1	0	-2.750276	1.906041	-5.720017
130	1	0	-2.832485	3.397908	-4.777881

131	1	0	-1.258511	2.644459	-5.110841
132	6	0	-3.865437	1.269764	-3.193609
133	1	0	-4.388043	0.754014	-4.006346
134	1	0	-3.862207	0.612832	-2.318349
135	1	0	-4.427747	2.176283	-2.951014
136	6	0	1.448816	2.645163	-1.711973
137	6	0	2.212742	3.526702	-0.915125
138	8	0	2.055848	4.802994	-1.152537
139	6	0	2.698062	5.819953	-0.339894
140	1	0	2.514831	6.754659	-0.867925
141	6	0	3.102484	3.037860	0.171293
142	1	0	2.225836	5.843474	0.644552
143	1	0	3.078280	1.949976	0.208501
144	1	0	1.880163	1.653712	-1.810522
145	1	0	1.061116	3.076614	-2.632313
146	1	0	4.129788	3.380132	-0.003530
147	1	0	3.770390	5.631339	-0.260869
148	1	0	2.786701	3.438643	1.140173

L1-Mg(II)-TS1-*re*-1

Zero-point correction= 1.26146 a.u.

Thermal correction to Gibbs Free Energy= 1.15750 a.u.

Sum of electronic and zero-point Energies= -5755.23756 a.u.

Sum of electronic and thermal Free Energies= -5755.34151 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.018515	3.534710	-0.100290
2	6	0	0.424580	4.094958	1.126017
3	8	0	1.277981	5.088304	1.049462
4	6	0	1.841140	5.714384	2.229899
5	6	0	-0.023297	3.492476	2.406802
6	1	0	-0.936279	3.016379	-0.079217
7	1	0	0.205035	4.140576	-0.982910
8	1	0	2.413042	6.559061	1.847617
9	1	0	2.503789	5.011504	2.738412
10	1	0	1.047708	6.065139	2.892891
11	1	0	0.152295	2.407643	2.319021
12	1	0	-1.106310	3.628210	2.513049
13	1	0	0.476601	3.884594	3.291644

14	6	0	0.614329	1.597850	-1.678508
15	6	0	1.153310	1.904665	-0.278472
16	6	0	2.503198	2.469347	-0.581180
17	6	0	2.576912	2.680466	-1.977976
18	7	0	1.387338	2.203739	-2.609019
19	8	0	0.833370	1.083189	0.651037
20	8	0	-0.350348	0.838112	-1.847225
21	6	0	0.966150	2.345242	-4.028390
22	6	0	3.602902	2.759676	0.207623
23	6	0	3.718603	3.207397	-2.567036
24	1	0	-0.057175	1.960299	-4.023959
25	6	0	4.809750	3.500798	-1.735886
26	6	0	4.772089	3.273839	-0.361030
27	1	0	3.790619	3.368295	-3.635302
28	1	0	5.715895	3.902177	-2.179785
29	1	0	5.636583	3.485059	0.258405
30	35	0	3.545887	2.419116	2.086475
31	8	0	-1.520082	-1.980339	-0.885491
32	8	0	1.234508	-1.390129	-0.568508
33	12	0	-0.481250	-0.375617	-0.048651
34	8	0	-0.599464	-1.419186	1.706765
35	7	0	2.549475	-3.138474	0.025525
36	1	0	2.619654	-4.125249	0.246203
37	7	0	-1.200365	-3.230785	-0.418243
38	7	0	-4.510212	-0.236758	0.268815
39	1	0	-5.200623	-0.873267	0.652288
40	7	0	-1.719576	-2.190148	1.876767
41	6	0	3.718516	-2.343100	0.148316
42	6	0	4.210236	-1.997475	1.435047
43	6	0	5.339554	-1.163030	1.534378
44	1	0	5.736159	-0.879481	2.500238
45	6	0	5.966755	-0.672323	0.395537
46	1	0	6.824491	-0.018832	0.491224
47	6	0	5.506771	-1.029897	-0.865668
48	1	0	6.029111	-0.644397	-1.731285
49	6	0	4.401572	-1.887928	-1.013881
50	6	0	3.985847	-2.325917	-2.413011
51	1	0	3.148788	-3.048451	-2.361438
52	6	0	3.494788	-1.134089	-3.238884
53	1	0	2.661070	-0.624872	-2.712206
54	1	0	3.120769	-1.486639	-4.223571
55	1	0	4.307963	-0.398384	-3.413992
56	6	0	5.125761	-3.058258	-3.132441
57	1	0	4.764183	-3.469794	-4.099217

58	1	0	5.485919	-3.907519	-2.513104
59	1	0	5.979371	-2.380014	-3.342393
60	6	0	3.543167	-2.501195	2.708596
61	1	0	2.661077	-3.127897	2.466372
62	6	0	4.496889	-3.391083	3.514035
63	1	0	4.864629	-4.227421	2.881756
64	1	0	3.965818	-3.829031	4.386281
65	1	0	5.369203	-2.815551	3.889616
66	6	0	3.031136	-1.335766	3.562414
67	1	0	3.860225	-0.679944	3.900139
68	1	0	2.521986	-1.726017	4.466957
69	1	0	2.305221	-0.727951	2.981638
70	6	0	1.368958	-2.601577	-0.344517
71	6	0	0.281835	-3.623280	-0.667650
72	1	0	0.439139	-4.547463	-0.105485
73	6	0	0.289033	-3.919323	-2.172595
74	1	0	1.205053	-4.439681	-2.459710
75	1	0	0.231831	-2.978657	-2.727794
76	6	0	-0.962686	-4.783230	-2.381480
77	1	0	-0.688982	-5.834648	-2.256768
78	6	0	-1.727096	-4.552591	-3.704288
79	1	0	-1.063108	-4.228974	-4.513048
80	1	0	-2.195585	-5.491576	-4.021670
81	6	0	-2.809367	-3.513840	-3.360627
82	1	0	-3.651934	-3.546704	-4.058152
83	1	0	-2.385617	-2.505808	-3.379351
84	6	0	-3.223692	-3.871709	-1.921492
85	1	0	-3.698948	-3.050311	-1.383313
86	1	0	-3.922352	-4.717260	-1.931239
87	6	0	-1.935678	-4.361768	-1.254711
88	1	0	-2.100947	-5.165638	-0.536454
89	6	0	-1.679084	-3.419432	1.006545
90	1	0	-2.690771	-3.818089	0.965486
91	1	0	-1.009572	-4.128077	1.489893
92	6	0	-1.793499	-2.770575	3.357073
93	1	0	-2.286186	-3.737523	3.248523
94	6	0	-0.421501	-2.861290	4.029986
95	1	0	0.390654	-2.983308	3.312905
96	1	0	-0.439106	-3.745178	4.679146
97	6	0	-0.313501	-1.580983	4.879429
98	1	0	0.018840	-0.751227	4.248142
99	1	0	0.393198	-1.684644	5.708738
100	6	0	-1.752855	-1.340788	5.363570
101	1	0	-1.940195	-0.304434	5.665285

102	1	0	-1.969849	-1.978368	6.228697
103	6	0	-2.640870	-1.768346	4.174808
104	1	0	-3.564012	-2.247345	4.512907
105	6	0	-2.995339	-0.652357	3.185317
106	1	0	-2.225499	0.123655	3.154699
107	1	0	-3.947899	-0.185030	3.430982
108	6	0	-3.037168	-1.365312	1.825969
109	1	0	-3.838836	-2.107647	1.811917
110	6	0	-3.235369	-0.331185	0.711299
111	6	0	-5.004219	0.941358	-0.352719
112	6	0	-4.862331	1.128435	-1.755237
113	6	0	-5.397635	2.287297	-2.348619
114	1	0	-5.329076	2.445440	-3.416545
115	6	0	-6.023540	3.259860	-1.579634
116	1	0	-6.412749	4.152842	-2.051878
117	6	0	-6.165667	3.083363	-0.209561
118	1	0	-6.664615	3.857459	0.358251
119	6	0	-5.693108	1.918203	0.421095
120	6	0	-5.930643	1.741087	1.916195
121	1	0	-5.591472	0.743402	2.243947
122	6	0	-7.423749	1.802719	2.263861
123	1	0	-7.576550	1.538173	3.332239
124	1	0	-7.991079	1.073610	1.646465
125	1	0	-7.842286	2.817278	2.096978
126	6	0	-5.133084	2.770022	2.724840
127	1	0	-4.053136	2.700045	2.473825
128	1	0	-5.246229	2.573244	3.812664
129	1	0	-5.481437	3.803882	2.516577
130	6	0	-4.193393	0.086912	-2.642290
131	1	0	-3.668071	-0.665028	-2.021493
132	6	0	-5.244511	-0.662902	-3.467046
133	1	0	-5.934519	-1.213947	-2.792557
134	1	0	-4.757106	-1.396931	-4.141048
135	1	0	-5.839508	0.037200	-4.091562
136	6	0	-3.130916	0.716806	-3.556687
137	1	0	-3.593811	1.242097	-4.418788
138	1	0	-2.456266	-0.068408	-3.958277
139	1	0	-2.521282	1.451501	-2.992278
140	8	0	-2.340344	0.456107	0.359836
141	6	0	1.785779	1.477687	-4.986519
142	1	0	1.640183	0.416899	-4.765881
143	1	0	1.437509	1.653502	-6.010138
144	1	0	2.855284	1.705480	-4.951786
145	6	0	0.916013	3.822063	-4.434719

146	1	0	1.911224	4.271017	-4.501245
147	1	0	0.446799	3.901905	-5.420947
148	1	0	0.317677	4.405501	-3.726586

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Zero-point correction= 1.17582 a.u.

Thermal correction to Gibbs Free Energy= 1.06975 a.u.

Sum of electronic and zero-point Energies= -6962.19294 a.u.

Sum of electronic and thermal Free Energies= -6962.29900 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.895454	-1.332716	1.663511
2	6	0	-2.688942	-1.950301	0.473001
3	6	0	-3.912280	-2.483462	1.079670
4	6	0	-3.850313	-2.195647	2.460493
5	7	0	-2.646326	-1.519931	2.776533
6	8	0	-2.290126	-1.939762	-0.671288
7	8	0	-0.794473	-0.789678	1.597856
8	6	0	-2.250998	-1.139502	4.124563
9	6	0	-5.024948	-3.144239	0.566614
10	6	0	-4.869386	-2.543448	3.328947
11	6	0	-5.980272	-3.203434	2.780299
12	6	0	-6.069831	-3.507562	1.420335
13	1	0	-2.064160	-2.032285	4.730032
14	1	0	-1.337824	-0.547580	4.055571
15	1	0	-3.038360	-0.543633	4.593672
16	1	0	-4.821087	-2.319866	4.388647
17	1	0	-6.798396	-3.489963	3.434248
18	1	0	-6.941457	-4.021166	1.031100
19	8	0	1.163366	1.622439	1.929623
20	8	0	2.976198	0.001232	0.490735
21	8	0	1.186346	2.309650	-1.298219
22	7	0	4.473432	-0.892538	1.946685
23	1	0	5.012200	-0.782340	2.797793
24	7	0	2.361095	2.215576	2.253208
25	7	0	-3.057704	2.936676	-1.104877
26	1	0	-3.326135	3.712721	-1.699838
27	7	0	0.621003	3.555830	-1.248023
28	6	0	4.765952	-2.002101	1.120617

29	6	0	5.882790	-1.956857	0.246742
30	6	0	6.141626	-3.061788	-0.584588
31	1	0	6.977359	-3.053031	-1.271715
32	6	0	5.322394	-4.185769	-0.551869
33	1	0	5.533030	-5.024741	-1.202543
34	6	0	4.228452	-4.232471	0.306688
35	1	0	3.606951	-5.118000	0.301038
36	6	0	3.931171	-3.150255	1.154977
37	6	0	2.721942	-3.231869	2.082685
38	1	0	2.655888	-2.327534	2.721756
39	6	0	1.416620	-3.296033	1.280966
40	1	0	1.327921	-2.405367	0.622380
41	1	0	0.546181	-3.302665	1.971099
42	1	0	1.370624	-4.212372	0.655456
43	6	0	2.834533	-4.420996	3.044469
44	1	0	2.007780	-4.390546	3.786470
45	1	0	3.795569	-4.373714	3.600076
46	1	0	2.779420	-5.389194	2.503762
47	6	0	6.783634	-0.728381	0.167863
48	1	0	6.469814	0.037533	0.907424
49	6	0	8.237285	-1.079857	0.507047
50	1	0	8.288179	-1.582567	1.496574
51	1	0	8.850732	-0.154774	0.560138
52	1	0	8.684609	-1.748707	-0.258096
53	6	0	6.685069	-0.065014	-1.210645
54	1	0	7.053642	-0.739115	-2.012563
55	1	0	7.289885	0.866898	-1.230672
56	1	0	5.630145	0.207953	-1.428336
57	6	0	3.576438	0.045388	1.573532
58	6	0	3.399076	1.150079	2.617954
59	1	0	4.359304	1.669460	2.717909
60	6	0	2.927858	0.683026	3.995577
61	1	0	3.687708	0.090614	4.510375
62	1	0	2.025599	0.075221	3.883939
63	6	0	2.637120	2.008843	4.720703
64	1	0	3.555046	2.348464	5.209945
65	6	0	1.450101	1.978757	5.707804
66	1	0	1.332146	0.997541	6.181325
67	1	0	1.620251	2.708646	6.508684
68	6	0	0.233981	2.400216	4.866303
69	1	0	-0.593443	2.776358	5.477331
70	1	0	-0.134685	1.554851	4.276270
71	6	0	0.802752	3.469067	3.917041
72	1	0	0.191730	3.617817	3.027256

73	1	0	0.881382	4.430230	4.441020
74	6	0	2.233116	3.009234	3.596735
75	1	0	2.935139	3.839157	3.509042
76	6	0	2.889297	3.091127	1.126960
77	1	0	3.876410	3.436085	1.449594
78	1	0	2.998277	2.434148	0.267976
79	6	0	2.039125	4.313225	0.771283
80	1	0	2.655564	4.921806	0.100245
81	1	0	1.890062	4.932238	1.663097
82	6	0	0.650735	4.117879	0.159328
83	1	0	0.066427	3.424719	0.761420
84	1	0	0.141139	5.085084	0.118089
85	6	0	1.295240	4.490884	-2.301746
86	1	0	1.200880	5.499623	-1.895313
87	6	0	2.744627	4.108654	-2.635417
88	1	0	3.257637	3.613977	-1.810295
89	1	0	3.280379	5.040782	-2.857243
90	6	0	2.658790	3.234290	-3.898952
91	1	0	2.433304	2.202302	-3.617862
92	1	0	3.593210	3.234585	-4.471194
93	6	0	1.485066	3.840761	-4.688100
94	1	0	1.040688	3.137301	-5.400742
95	1	0	1.825175	4.713529	-5.259431
96	6	0	0.471715	4.293709	-3.613442
97	1	0	-0.006883	5.237677	-3.892174
98	6	0	-0.631975	3.275374	-3.254687
99	1	0	-0.306244	2.244326	-3.413147
100	1	0	-1.555733	3.444788	-3.813204
101	6	0	-0.822931	3.533227	-1.760161
102	1	0	-1.205235	4.549994	-1.620958
103	6	0	-1.755950	2.575197	-1.023336
104	6	0	-4.075358	2.065109	-0.650670
105	6	0	-4.416739	2.036437	0.727390
106	6	0	-5.371481	1.104740	1.173024
107	1	0	-5.644374	1.048433	2.218602
108	6	0	-5.987236	0.234020	0.280115
109	1	0	-6.719970	-0.476655	0.639973
110	6	0	-5.663612	0.269691	-1.072443
111	1	0	-6.154991	-0.427394	-1.737945
112	6	0	-4.712094	1.182585	-1.562548
113	6	0	-4.361953	1.178290	-3.047872
114	1	0	-3.647769	1.992325	-3.285867
115	6	0	-5.600200	1.432921	-3.916483
116	1	0	-5.301278	1.551939	-4.980079

117	1	0	-6.106659	2.368561	-3.595948
118	1	0	-6.323746	0.593167	-3.853147
119	6	0	-3.670302	-0.130375	-3.444164
120	1	0	-2.751531	-0.273132	-2.836975
121	1	0	-3.368001	-0.095487	-4.512785
122	1	0	-4.340726	-1.003017	-3.297245
123	6	0	-3.784045	3.001901	1.725971
124	1	0	-3.089773	3.699313	1.212041
125	6	0	-4.846886	3.880603	2.396661
126	1	0	-5.454148	4.401574	1.625486
127	1	0	-4.359012	4.653148	3.029020
128	1	0	-5.523974	3.281303	3.041353
129	6	0	-2.954140	2.251901	2.773515
130	1	0	-3.591923	1.582264	3.386780
131	1	0	-2.455572	2.976216	3.451786
132	1	0	-2.166803	1.648041	2.276413
133	8	0	-1.388353	1.569661	-0.401864
134	20	0	0.662855	0.386168	-0.051289
135	8	0	0.949626	-0.889941	-2.006807
136	16	0	1.339865	-1.422514	-3.351700
137	8	0	0.343679	-2.332615	-3.940675
138	8	0	1.926853	-0.411472	-4.250375
139	6	0	2.765787	-2.524124	-2.901920
140	9	0	2.366405	-3.488683	-2.057991
141	9	0	3.279482	-3.108381	-3.995510
142	9	0	3.740792	-1.818511	-2.307216
143	35	0	-5.134507	-3.560054	-1.281887

L3a-Ca(II)-COM-H

Zero-point correction= 1.18559 a.u.

Thermal correction to Gibbs Free Energy= 1.08114 a.u.

Sum of electronic and zero-point Energies= -4388.63667 a.u.

Sum of electronic and thermal Free Energies= -4388.74111 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.019242	-2.364729	-0.451202
2	6	0	-2.552737	-1.958069	-1.860706
3	6	0	-3.729473	-2.799251	-2.073081
4	6	0	-3.873751	-3.608075	-0.929766

5	7	0	-2.846428	-3.333762	0.012725
6	8	0	-2.026214	-1.119096	-2.561557
7	8	0	-1.031475	-1.898805	0.116872
8	6	0	-2.675598	-4.047100	1.268631
9	6	0	-4.634771	-2.878689	-3.127948
10	6	0	-4.915532	-4.512728	-0.813275
11	6	0	-5.822933	-4.586541	-1.884171
12	6	0	-5.692729	-3.786948	-3.025096
13	1	0	-2.385809	-5.085956	1.078741
14	1	0	-1.891143	-3.549591	1.839387
15	1	0	-3.609147	-4.034096	1.837568
16	1	0	-5.036069	-5.142009	0.061808
17	1	0	-6.650044	-5.287604	-1.817720
18	1	0	-6.416218	-3.872177	-3.829587
19	8	0	0.496343	-0.321667	2.410123
20	8	0	2.652448	-0.217928	0.575157
21	8	0	0.540083	2.491695	0.681353
22	7	0	4.203371	-1.758068	1.198910
23	1	0	4.662721	-2.254024	1.953754
24	7	0	1.549079	-0.036602	3.248484
25	7	0	-3.752550	2.384101	0.558167
26	1	0	-4.133589	3.319087	0.652014
27	7	0	-0.246696	3.252365	1.504086
28	6	0	4.735330	-1.902801	-0.102848
29	6	0	5.877035	-1.153072	-0.486296
30	6	0	6.376007	-1.293946	-1.794117
31	1	0	7.236360	-0.725876	-2.121928
32	6	0	5.767131	-2.156717	-2.700069
33	1	0	6.160514	-2.248182	-3.704310
34	6	0	4.649638	-2.895538	-2.323797
35	1	0	4.195192	-3.550520	-3.055284
36	6	0	4.116742	-2.786301	-1.026500
37	6	0	2.889412	-3.609547	-0.645123
38	1	0	2.632170	-3.458240	0.423251
39	6	0	1.662534	-3.175040	-1.455212
40	1	0	1.459557	-2.094838	-1.291136
41	1	0	0.768336	-3.747367	-1.128404
42	1	0	1.811304	-3.353229	-2.541045
43	6	0	3.150578	-5.112137	-0.806888
44	1	0	2.290810	-5.693094	-0.409156
45	1	0	4.056802	-5.406284	-0.235017
46	1	0	3.292468	-5.389061	-1.872635
47	6	0	6.550490	-0.179036	0.475413
48	1	0	6.064830	-0.212536	1.473061

49	6	0	8.021534	-0.547398	0.703803
50	1	0	8.103842	-1.603722	1.038235
51	1	0	8.457696	0.098398	1.495938
52	1	0	8.623260	-0.416227	-0.220254
53	6	0	6.415383	1.264099	-0.023320
54	1	0	6.937503	1.408904	-0.992844
55	1	0	6.851607	1.967310	0.718053
56	1	0	5.342786	1.524874	-0.150681
57	6	0	3.174184	-0.920623	1.451789
58	6	0	2.746137	-0.933623	2.920960
59	1	0	3.588676	-0.560060	3.514747
60	6	0	2.303308	-2.292329	3.465517
61	1	0	3.133135	-2.999846	3.528340
62	1	0	1.533178	-2.712209	2.812360
63	6	0	1.742451	-1.933436	4.852682
64	1	0	2.559340	-1.969047	5.579900
65	6	0	0.535337	-2.775291	5.319963
66	1	0	0.573333	-3.800436	4.934650
67	1	0	0.533986	-2.838389	6.414889
68	6	0	-0.696011	-1.989061	4.840163
69	1	0	-1.605033	-2.247897	5.393564
70	1	0	-0.878700	-2.175961	3.777244
71	6	0	-0.284474	-0.518919	5.030482
72	1	0	-0.869418	0.171047	4.423244
73	1	0	-0.403441	-0.231001	6.082873
74	6	0	1.217832	-0.473121	4.715139
75	1	0	1.762902	0.224367	5.352196
76	6	0	1.959364	1.426483	3.175478
77	1	0	2.852479	1.521109	3.800617
78	1	0	2.223213	1.608643	2.136974
79	6	0	0.918914	2.440642	3.657657
80	1	0	1.444392	3.399817	3.723849
81	1	0	0.621770	2.205769	4.685814
82	6	0	-0.382912	2.619373	2.874329
83	1	0	-0.855866	1.654531	2.702549
84	1	0	-1.058528	3.260832	3.447960
85	6	0	0.290376	4.718503	1.549898
86	1	0	-0.007868	5.105600	2.526206
87	6	0	1.799273	4.835991	1.290094
88	1	0	2.355797	3.948501	1.592574
89	1	0	2.163789	5.683489	1.885107
90	6	0	1.935814	5.145600	-0.211127
91	1	0	1.895105	4.215697	-0.784001
92	1	0	2.878859	5.650024	-0.449300

93	6	0	0.706859	6.018497	-0.521361
94	1	0	0.434327	6.010690	-1.582366
95	1	0	0.904749	7.061119	-0.242596
96	6	0	-0.421253	5.454151	0.370723
97	1	0	-1.053226	6.255661	0.765574
98	6	0	-1.332760	4.392956	-0.282887
99	1	0	-0.814237	3.831421	-1.063910
100	1	0	-2.245241	4.823350	-0.702464
101	6	0	-1.636909	3.471849	0.898157
102	1	0	-2.204931	4.031803	1.648908
103	6	0	-2.412695	2.196354	0.578780
104	6	0	-4.619959	1.350165	0.134515
105	6	0	-5.001140	0.330888	1.046815
106	6	0	-5.792195	-0.736077	0.584301
107	1	0	-6.088252	-1.535600	1.250809
108	6	0	-6.213749	-0.787359	-0.739969
109	1	0	-6.822382	-1.615419	-1.079053
110	6	0	-5.853495	0.217901	-1.631768
111	1	0	-6.189573	0.140638	-2.657224
112	6	0	-5.061664	1.303185	-1.213716
113	6	0	-4.672211	2.381854	-2.220264
114	1	0	-4.108985	3.198011	-1.723386
115	6	0	-5.909947	3.038805	-2.844604
116	1	0	-5.606182	3.904406	-3.471628
117	1	0	-6.587388	3.414031	-2.047801
118	1	0	-6.470211	2.326868	-3.486574
119	6	0	-3.745533	1.815175	-3.300611
120	1	0	-2.818415	1.422131	-2.833398
121	1	0	-3.450713	2.615998	-4.012205
122	1	0	-4.238276	1.000472	-3.872649
123	6	0	-4.587239	0.379215	2.514865
124	1	0	-4.005006	1.299720	2.729052
125	6	0	-5.813321	0.430462	3.434331
126	1	0	-6.469034	1.281182	3.149265
127	1	0	-5.493774	0.581382	4.487787
128	1	0	-6.402242	-0.509449	3.381210
129	6	0	-3.682519	-0.803957	2.874839
130	1	0	-4.221462	-1.768111	2.770750
131	1	0	-3.338125	-0.710184	3.926225
132	1	0	-2.788149	-0.816229	2.217238
133	8	0	-1.897419	1.090964	0.365642
134	20	0	0.321943	0.220284	0.085045
135	8	0	1.018829	0.946514	-2.053411
136	16	0	1.583960	1.511469	-3.319549

137	8	0	0.779041	1.217638	-4.517574
138	8	0	2.089571	2.889973	-3.185336
139	6	0	3.111946	0.478167	-3.529474
140	9	0	2.788351	-0.820777	-3.637775
141	9	0	3.782417	0.836453	-4.635525
142	9	0	3.931972	0.623791	-2.477128
143	1	0	-4.515236	-2.244481	-4.001506

L3a-Ca(II)-COM

Zero-point correction= 1.14739 a.u.

Thermal correction to Gibbs Free Energy= 1.05059 a.u.

Sum of electronic and zero-point Energies= -6000.39210 a.u.

Sum of electronic and thermal Free Energies= -6000.48890 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.855315	1.211585	-1.893857
2	6	0	-2.025725	2.048628	-0.603925
3	6	0	-3.286362	2.743605	-0.758868
4	6	0	-3.840100	2.305840	-1.988439
5	7	0	-2.966732	1.398173	-2.640711
6	8	0	-1.190619	2.013508	0.290861
7	6	0	-3.986194	3.659971	0.028712
8	6	0	-5.076884	2.742062	-2.423539
9	8	0	-0.861080	0.528626	-2.135867
10	6	0	-3.195253	0.826921	-3.962219
11	1	0	-3.195845	1.617271	-4.718923
12	1	0	-2.386704	0.125986	-4.169936
13	1	0	-4.152878	0.301327	-3.984758
14	6	0	-5.237439	4.112027	-0.389175
15	6	0	-5.764363	3.646503	-1.597547
16	35	0	-3.232755	4.308722	1.643966
17	1	0	-5.796315	4.819852	0.211911
18	1	0	-6.740533	4.004084	-1.910831
19	1	0	-5.507307	2.406405	-3.359837
20	8	0	2.901045	0.619343	-0.378109
21	8	0	1.495986	-1.643724	-1.365189
22	8	0	0.956307	-1.314738	1.802590
23	8	0	-1.508614	-1.035988	0.427888
24	7	0	5.118686	0.620570	-0.864779

25	1	0	5.908360	0.132023	-1.269972
26	7	0	2.748493	-2.200661	-1.318762
27	7	0	-3.166876	-2.387996	1.191065
28	1	0	-3.473433	-3.051932	1.893332
29	7	0	0.444729	-2.559747	2.072511
30	6	0	5.374924	1.817270	-0.157598
31	6	0	5.778137	1.761090	1.201953
32	6	0	5.994683	2.964695	1.897159
33	1	0	6.294580	2.956495	2.936754
34	6	0	5.820361	4.192940	1.266986
35	1	0	5.987911	5.109471	1.818062
36	6	0	5.429053	4.248648	-0.067196
37	1	0	5.299462	5.219719	-0.526398
38	6	0	5.204681	3.070178	-0.801682
39	6	0	4.780406	3.163038	-2.264303
40	1	0	4.679924	2.151007	-2.708534
41	6	0	3.408642	3.833782	-2.396854
42	1	0	2.656880	3.288668	-1.786645
43	1	0	3.072234	3.810504	-3.455633
44	1	0	3.441302	4.892274	-2.062379
45	6	0	5.834541	3.893773	-3.104832
46	1	0	5.560119	3.852483	-4.180772
47	1	0	6.824775	3.404198	-2.984262
48	1	0	5.923818	4.960447	-2.809444
49	6	0	5.958184	0.430228	1.926574
50	1	0	5.773001	-0.421343	1.238926
51	6	0	7.394420	0.263608	2.437029
52	1	0	8.113902	0.383873	1.598984
53	1	0	7.532385	-0.753175	2.863547
54	1	0	7.635247	1.007265	3.225750
55	6	0	4.948227	0.287965	3.070949
56	1	0	5.120932	1.047968	3.861989
57	1	0	5.034246	-0.719380	3.531170
58	1	0	3.914624	0.406703	2.681745
59	6	0	3.881242	0.087441	-0.921211
60	6	0	3.823628	-1.195122	-1.748366
61	1	0	4.777001	-1.720432	-1.634166
62	6	0	3.536254	-1.028510	-3.238541
63	1	0	4.348106	-0.502240	-3.746092
64	1	0	2.608416	-0.467061	-3.375053
65	6	0	3.400853	-2.497094	-3.695753
66	1	0	4.393369	-2.861129	-3.977469
67	6	0	2.367364	-2.767287	-4.810764
68	1	0	2.248222	-1.906994	-5.478662

69	1	0	2.705284	-3.611085	-5.424402
70	6	0	1.072182	-3.142803	-4.070311
71	1	0	0.383790	-3.721755	-4.695281
72	1	0	0.552266	-2.241547	-3.732804
73	6	0	1.566104	-3.935479	-2.846338
74	1	0	0.840465	-3.969441	-2.033159
75	1	0	1.795076	-4.968650	-3.137101
76	6	0	2.892359	-3.277261	-2.441518
77	1	0	3.626164	-3.991263	-2.064012
78	6	0	3.079036	-2.720747	0.069409
79	1	0	4.104012	-3.099809	0.020719
80	1	0	3.047154	-1.850179	0.721697
81	6	0	2.177101	-3.826595	0.619626
82	1	0	2.677545	-4.196000	1.521873
83	1	0	2.168781	-4.674907	-0.074175
84	6	0	0.710187	-3.529636	0.933140
85	1	0	0.216297	-3.101237	0.062790
86	1	0	0.214781	-4.465677	1.206030
87	6	0	0.972924	-3.061917	3.455089
88	1	0	0.978287	-4.150984	3.383912
89	6	0	2.335738	-2.477912	3.851798
90	1	0	2.969943	-2.248956	2.995408
91	1	0	2.847280	-3.238941	4.454750
92	6	0	2.016686	-1.249885	4.722505
93	1	0	1.793113	-0.396273	4.076179
94	1	0	2.847298	-0.972945	5.380608
95	6	0	0.758354	-1.673223	5.500043
96	1	0	0.179773	-0.823658	5.879201
97	1	0	1.041852	-2.286071	6.364205
98	6	0	-0.054612	-2.531606	4.505368
99	1	0	-0.533664	-3.375681	5.010095
100	6	0	-1.127216	-1.780507	3.688303
101	1	0	-0.877176	-0.724888	3.553912
102	1	0	-2.121704	-1.853321	4.134768
103	6	0	-1.064101	-2.502325	2.344002
104	1	0	-1.377094	-3.541446	2.485277
105	6	0	-1.908022	-1.899055	1.223925
106	6	0	-4.144431	-1.825837	0.337491
107	6	0	-4.213186	-2.230118	-1.021435
108	6	0	-5.131635	-1.592993	-1.874990
109	1	0	-5.204741	-1.874511	-2.917085
110	6	0	-5.971971	-0.592181	-1.397967
111	1	0	-6.670882	-0.110311	-2.069454
112	6	0	-5.925943	-0.215747	-0.059406

113	1	0	-6.596845	0.562021	0.280622
114	6	0	-5.026273	-0.829671	0.831057
115	6	0	-5.013251	-0.408136	2.297212
116	1	0	-4.279293	-1.008294	2.872842
117	6	0	-6.375399	-0.650742	2.958413
118	1	0	-6.312249	-0.445505	4.048576
119	1	0	-6.681194	-1.710743	2.826230
120	1	0	-7.160623	0.005163	2.526556
121	6	0	-4.584798	1.053718	2.445290
122	1	0	-3.587828	1.201933	1.980128
123	1	0	-4.502493	1.322950	3.519989
124	1	0	-5.317149	1.737806	1.967470
125	6	0	-3.337112	-3.355394	-1.563642
126	1	0	-2.693848	-3.773431	-0.761293
127	6	0	-4.190828	-4.522373	-2.074553
128	1	0	-4.877476	-4.871965	-1.273729
129	1	0	-3.538872	-5.374943	-2.362348
130	1	0	-4.792247	-4.229559	-2.961017
131	6	0	-2.392926	-2.847705	-2.657939
132	1	0	-2.955449	-2.474286	-3.539285
133	1	0	-1.727022	-3.670551	-2.993113
134	1	0	-1.756986	-2.030326	-2.260217
135	20	0	0.575620	0.066757	-0.056242

L3a-Ca(II)-COM-H

Zero-point correction= 1.14739 a.u.

Thermal correction to Gibbs Free Energy= 1.05059 a.u.

Sum of electronic and zero-point Energies= -6000.39210 a.u.

Sum of electronic and thermal Free Energies= -6000.48890 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.965125	-2.438559	-0.068837
2	6	0	-2.041778	-2.065488	-1.571766
3	6	0	-3.247408	-2.697835	-2.065247
4	6	0	-3.847176	-3.341958	-0.958245
5	7	0	-3.063932	-3.170590	0.216570
6	8	0	-1.188583	-1.357583	-2.095686
7	6	0	-3.845032	-2.732880	-3.326701
8	6	0	-5.047701	-4.016742	-1.084353

9	8	0	-1.042561	-2.100293	0.673749
10	6	0	-3.370444	-3.753952	1.515813
11	1	0	-3.329358	-4.846023	1.457987
12	1	0	-2.626107	-3.400170	2.229591
13	1	0	-4.367540	-3.445891	1.840738
14	6	0	-5.055408	-3.413463	-3.466097
15	6	0	-5.640819	-4.039000	-2.358543
16	1	0	-5.547086	-3.457425	-4.432149
17	1	0	-6.585252	-4.560922	-2.481737
18	1	0	-5.521879	-4.508905	-0.242555
19	8	0	2.750061	-0.696478	-0.207464
20	8	0	1.067834	0.055243	1.961468
21	8	0	0.694276	2.117839	-0.498446
22	8	0	-1.773649	0.821693	-0.012349
23	7	0	4.932981	-0.954131	0.362142
24	1	0	5.647174	-0.878241	1.076532
25	7	0	2.254130	0.522949	2.465311
26	7	0	-3.544718	2.223401	0.218122
27	1	0	-3.895657	3.173385	0.167743
28	7	0	0.065332	3.142241	0.165424
29	6	0	5.349603	-1.228788	-0.960409
30	6	0	5.805252	-0.171958	-1.790797
31	6	0	6.184803	-0.462155	-3.113865
32	1	0	6.528749	0.322173	-3.775273
33	6	0	6.119483	-1.762442	-3.605066
34	1	0	6.412281	-1.967388	-4.626940
35	6	0	5.677469	-2.799862	-2.789981
36	1	0	5.636315	-3.798844	-3.203557
37	6	0	5.291072	-2.555870	-1.459579
38	6	0	4.816250	-3.714873	-0.588393
39	1	0	4.583053	-3.363983	0.438481
40	6	0	3.524247	-4.325609	-1.142685
41	1	0	2.743498	-3.541265	-1.242385
42	1	0	3.140800	-5.104261	-0.448748
43	1	0	3.690726	-4.792770	-2.136318
44	6	0	5.908187	-4.780665	-0.436033
45	1	0	5.583695	-5.558635	0.287932
46	1	0	6.840929	-4.318182	-0.047618
47	1	0	6.130682	-5.277619	-1.403838
48	6	0	5.870083	1.267264	-1.287677
49	1	0	5.559342	1.327473	-0.223683
50	6	0	7.301494	1.813895	-1.347090
51	1	0	7.989559	1.144048	-0.788236
52	1	0	7.345601	2.819782	-0.876800

53	1	0	7.660194	1.903255	-2.394139
54	6	0	4.905806	2.165978	-2.070149
55	1	0	5.199469	2.244133	-3.138257
56	1	0	4.900382	3.187943	-1.634909
57	1	0	3.874703	1.756706	-2.012801
58	6	0	3.642878	-0.689515	0.653615
59	6	0	3.412081	-0.428683	2.141126
60	1	0	4.307320	0.051904	2.548057
61	6	0	3.081372	-1.646557	3.000724
62	1	0	3.923099	-2.341218	3.050579
63	1	0	2.214612	-2.167056	2.585335
64	6	0	2.768192	-0.990871	4.363337
65	1	0	3.702055	-0.910682	4.927665
66	6	0	1.662422	-1.667098	5.203144
67	1	0	1.604633	-2.745023	5.015751
68	1	0	1.881928	-1.533847	6.269470
69	6	0	0.369046	-0.918596	4.836521
70	1	0	-0.402780	-1.011035	5.608244
71	1	0	-0.038854	-1.301753	3.896747
72	6	0	0.831534	0.536129	4.636593
73	1	0	0.142721	1.128458	4.033568
74	1	0	0.938831	1.031731	5.609981
75	6	0	2.235836	0.438255	4.024645
76	1	0	2.906496	1.229211	4.364595
77	6	0	2.581834	1.906455	1.932055
78	1	0	3.556415	2.175369	2.349994
79	1	0	2.671506	1.788691	0.853922
80	6	0	1.586948	3.020431	2.260619
81	1	0	2.080399	3.954391	1.968435
82	1	0	1.456589	3.089886	3.346490
83	6	0	0.175648	2.981570	1.672790
84	1	0	-0.304431	2.032100	1.902386
85	1	0	-0.407173	3.796813	2.110826
86	6	0	0.596672	4.517751	-0.352778
87	1	0	0.482549	5.205815	0.486675
88	6	0	2.030008	4.467679	-0.899120
89	1	0	2.646963	3.710558	-0.415358
90	1	0	2.483094	5.447337	-0.700760
91	6	0	1.882196	4.258569	-2.416437
92	1	0	1.722470	3.196028	-2.621108
93	1	0	2.765646	4.586097	-2.974916
94	6	0	0.621306	5.065097	-2.772674
95	1	0	0.153815	4.743092	-3.709749
96	1	0	0.875428	6.126110	-2.883077

97	6	0	-0.321445	4.885479	-1.561794
98	1	0	-0.865838	5.808695	-1.343087
99	6	0	-1.341495	3.732379	-1.668415
100	1	0	-0.985422	2.927430	-2.316741
101	1	0	-2.317779	4.067830	-2.026032
102	6	0	-1.414685	3.239257	-0.224733
103	1	0	-1.833840	4.034514	0.399668
104	6	0	-2.234650	1.972523	0.005316
105	6	0	-4.486091	1.169574	0.273217
106	6	0	-4.668995	0.447802	1.481947
107	6	0	-5.545806	-0.651750	1.491388
108	1	0	-5.701197	-1.227294	2.394230
109	6	0	-6.240806	-1.018700	0.343352
110	1	0	-6.911523	-1.867823	0.368151
111	6	0	-6.083521	-0.294823	-0.834444
112	1	0	-6.642543	-0.603329	-1.707865
113	6	0	-5.214481	0.809974	-0.890529
114	6	0	-5.069384	1.587662	-2.195637
115	1	0	-4.367407	2.437282	-2.071356
116	6	0	-6.407451	2.198402	-2.629091
117	1	0	-6.260271	2.848287	-3.518234
118	1	0	-6.824136	2.825143	-1.811819
119	1	0	-7.147533	1.412972	-2.890884
120	6	0	-4.485142	0.706856	-3.304221
121	1	0	-3.513058	0.281319	-2.977892
122	1	0	-4.301086	1.312825	-4.217149
123	1	0	-5.177067	-0.120044	-3.568464
124	6	0	-3.959579	0.855950	2.770011
125	1	0	-3.336011	1.759288	2.605144
126	6	0	-4.969083	1.231075	3.861659
127	1	0	-5.656565	2.021400	3.490507
128	1	0	-4.437780	1.630730	4.751995
129	1	0	-5.569771	0.353032	4.180412
130	6	0	-3.011228	-0.244716	3.256314
131	1	0	-3.563930	-1.171543	3.517044
132	1	0	-2.463255	0.100055	4.158548
133	1	0	-2.264701	-0.476705	2.469183
134	20	0	0.384515	-0.203168	-0.259355
135	1	0	-3.374690	-2.238089	-4.171035

L3a-Mg(II)-COM-H

Zero-point correction= 1.15935 a.u.

Thermal correction to Gibbs Free Energy=1.06820 a.u.

Sum of electronic and zero-point Energies=-2949.30264 a.u.

Sum of electronic and thermal Free Energies= -2949.39379 a.u.

The number of imaginary frequencies 0

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.900462	1.902663	1.080609
2	6	0	0.773826	2.136984	-0.434177
3	6	0	1.409406	3.406966	-0.689461
4	6	0	1.909737	3.854741	0.558314
5	7	0	1.590913	2.934521	1.598771
6	8	0	0.227597	1.284247	-1.131818
7	6	0	1.617030	4.148655	-1.854860
8	6	0	2.617992	5.035713	0.665337
9	8	0	0.408480	0.911592	1.626611
10	6	0	1.945943	3.099829	3.001853
11	1	0	1.439033	3.974901	3.419241
12	1	0	1.630525	2.203995	3.537701
13	1	0	3.027986	3.223108	3.100750
14	6	0	2.330545	5.343585	-1.757278
15	6	0	2.818991	5.771378	-0.516514
16	1	0	2.509610	5.943815	-2.643095
17	1	0	3.373255	6.703498	-0.458502
18	1	0	3.005669	5.389283	1.614212
19	8	0	-2.191159	0.091909	0.016396
20	12	0	-0.250868	-0.549931	0.098097
21	8	0	-0.846921	-1.757756	1.586987
22	8	0	-0.339911	-1.807583	-1.485810
23	8	0	1.759270	-0.961655	0.035848
24	7	0	-4.337613	0.451055	0.631666
25	1	0	-5.123975	0.193955	1.217857
26	7	0	-2.079382	-2.378445	1.579818
27	7	0	3.801309	-1.654326	-0.632886
28	1	0	4.346387	-2.225257	-1.270243
29	7	0	0.397677	-2.976158	-1.535282
30	6	0	-4.483642	1.566158	-0.226024
31	6	0	-4.826649	1.368599	-1.589234
32	6	0	-4.910086	2.486725	-2.438673
33	1	0	-5.155949	2.368757	-3.485717
34	6	0	-4.671908	3.769016	-1.954149
35	1	0	-4.739772	4.618447	-2.621736
36	6	0	-4.339073	3.964098	-0.617450

37	1	0	-4.149737	4.972741	-0.274933
38	6	0	-4.236466	2.874137	0.265816
39	6	0	-3.830660	3.117292	1.716087
40	1	0	-3.807066	2.162579	2.281230
41	6	0	-2.416931	3.704791	1.797472
42	1	0	-1.704506	3.052195	1.251546
43	1	0	-2.085597	3.764727	2.856358
44	1	0	-2.374140	4.723798	1.357990
45	6	0	-4.842612	4.016606	2.435417
46	1	0	-4.582586	4.096300	3.512864
47	1	0	-5.861871	3.580872	2.360281
48	1	0	-4.856945	5.039819	2.004141
49	6	0	-5.081480	-0.026100	-2.153355
50	1	0	-5.030194	-0.789886	-1.349622
51	6	0	-6.487479	-0.138778	-2.755220
52	1	0	-7.249927	0.154328	-2.001879
53	1	0	-6.689932	-1.188645	-3.057484
54	1	0	-6.601554	0.506880	-3.651405
55	6	0	-4.009622	-0.403781	-3.181853
56	1	0	-4.060747	0.249784	-4.078441
57	1	0	-4.147236	-1.457355	-3.506333
58	1	0	-2.999927	-0.308306	-2.729432
59	6	0	-3.174891	-0.216259	0.715010
60	6	0	-3.199580	-1.350872	1.736691
61	1	0	-4.136119	-1.903680	1.604057
62	6	0	-3.064432	-0.920576	3.198087
63	1	0	-3.947588	-0.371900	3.533853
64	1	0	-2.187309	-0.278351	3.313397
65	6	0	-2.887974	-2.268322	3.927499
66	1	0	-3.875598	-2.644644	4.209415
67	6	0	-1.926922	-2.248642	5.137509
68	1	0	-1.918737	-1.274943	5.639464
69	1	0	-2.252370	-2.992703	5.874403
70	6	0	-0.556399	-2.645339	4.561245
71	1	0	0.123794	-3.038001	5.324478
72	1	0	-0.077228	-1.781569	4.090520
73	6	0	-0.903151	-3.691340	3.487238
74	1	0	-0.117920	-3.826459	2.742252
75	1	0	-1.090287	-4.664125	3.959260
76	6	0	-2.236214	-3.226385	2.882472
77	1	0	-2.889914	-4.054186	2.604968
78	6	0	-2.301747	-3.190280	0.316071
79	1	0	-3.272710	-3.677247	0.439358
80	1	0	-2.364031	-2.470158	-0.496486

81	6	0	-1.247691	-4.254526	0.004975
82	1	0	-1.652100	-4.833227	-0.833627
83	1	0	-1.177257	-4.962036	0.839054
84	6	0	0.192721	-3.836380	-0.298805
85	1	0	0.609334	-3.274219	0.533773
86	1	0	0.794111	-4.735857	-0.458598
87	6	0	0.067969	-3.744530	-2.855216
88	1	0	0.194669	-4.797815	-2.604407
89	6	0	-1.318086	-3.433299	-3.438896
90	1	0	-2.054312	-3.160733	-2.682211
91	1	0	-1.666331	-4.350326	-3.931006
92	6	0	-1.079714	-2.335477	-4.490118
93	1	0	-1.028230	-1.360148	-3.996807
94	1	0	-1.875009	-2.294603	-5.241843
95	6	0	0.287579	-2.703321	-5.092550
96	1	0	0.785179	-1.859161	-5.582229
97	1	0	0.165105	-3.492214	-5.844309
98	6	0	1.110302	-3.248408	-3.903338
99	1	0	1.751826	-4.079892	-4.209254
100	6	0	1.975323	-2.207880	-3.165741
101	1	0	1.565091	-1.198608	-3.257774
102	1	0	3.007895	-2.201279	-3.521363
103	6	0	1.889783	-2.672956	-1.709716
104	1	0	2.414790	-3.628169	-1.601509
105	6	0	2.455496	-1.692400	-0.689974
106	6	0	4.451241	-0.590913	0.041189
107	6	0	4.531782	-0.594173	1.460523
108	6	0	5.040440	0.541268	2.116464
109	1	0	5.103235	0.574745	3.196073
110	6	0	5.473792	1.647480	1.393740
111	1	0	5.856308	2.515496	1.915306
112	6	0	5.427696	1.640166	0.003837
113	1	0	5.776354	2.516286	-0.526520
114	6	0	4.928420	0.526486	-0.696019
115	6	0	4.890544	0.557925	-2.221877
116	1	0	4.512129	-0.400969	-2.627498
117	6	0	6.294658	0.742917	-2.810245
118	1	0	6.259713	0.650941	-3.917046
119	1	0	6.978052	-0.042926	-2.422673
120	1	0	6.714538	1.739698	-2.558809
121	6	0	3.936069	1.642186	-2.729439
122	1	0	2.915518	1.453480	-2.337944
123	1	0	3.881911	1.617642	-3.838921
124	1	0	4.267843	2.654398	-2.416324

125	6	0	4.100148	-1.805192	2.283298
126	1	0	3.739419	-2.619020	1.620250
127	6	0	5.282906	-2.388127	3.065873
128	1	0	6.118067	-2.628160	2.373204
129	1	0	4.978145	-3.327766	3.574655
130	1	0	5.649989	-1.678138	3.837009
131	6	0	2.941143	-1.458506	3.226422
132	1	0	3.251482	-0.724728	3.999778
133	1	0	2.581841	-2.376209	3.739204
134	1	0	2.092826	-1.031670	2.653754
135	1	0	1.233118	3.793819	-2.806361

L3a-Ca(II)-TS-*si*-1

Zero-point correction= 1.28694 a.u.

Thermal correction to Gibbs Free Energy= 1.17025 a.u.

Sum of electronic and zero-point Energies= -7194.58814 a.u.

Sum of electronic and thermal Free Energies= -7194.70483a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.689490	-1.049431	1.442790
2	6	0	-2.802911	-1.515168	0.453230
3	6	0	-3.976719	-1.717069	1.421426
4	6	0	-3.523720	-1.497680	2.731906
5	7	0	-2.158098	-1.133865	2.712604
6	8	0	-2.997000	-0.717247	-0.581978
7	8	0	-0.546430	-0.690186	1.138276
8	6	0	-1.380440	-0.817435	3.899413
9	6	0	-5.326686	-1.957076	1.239166
10	6	0	-4.348882	-1.576923	3.845839
11	6	0	-5.701456	-1.864577	3.623100
12	6	0	-6.198802	-2.041878	2.332814
13	1	0	-1.247439	-1.711971	4.517257
14	1	0	-0.407788	-0.449313	3.573875
15	1	0	-1.883899	-0.046251	4.490104
16	1	0	-3.970233	-1.408414	4.848306
17	1	0	-6.380545	-1.933344	4.468014
18	1	0	-7.253847	-2.234472	2.172233
19	6	0	-2.157055	-3.025789	0.011345
20	6	0	-2.897404	-3.510505	-1.141533

21	8	0	-3.714978	-4.518846	-0.915216
22	6	0	-4.514046	-5.059997	-1.990775
23	6	0	-2.871223	-2.691017	-2.305009
24	1	0	-1.138114	-2.765481	-0.279823
25	1	0	-2.171396	-3.709319	0.861250
26	1	0	-4.942115	-5.979444	-1.591378
27	1	0	-5.310977	-4.363082	-2.255567
28	1	0	-3.885843	-5.278265	-2.857900
29	1	0	-1.868782	-2.437188	-2.659345
30	1	0	-3.550959	-2.935927	-3.118789
31	1	0	-3.120640	-1.633326	-1.709407
32	8	0	1.768840	1.551732	1.964749
33	8	0	3.127355	-0.383291	0.434358
34	8	0	1.900152	2.456424	-1.231495
35	7	0	4.586333	-1.551621	1.721773
36	1	0	5.116464	-1.609433	2.583486
37	7	0	3.069054	1.851590	2.296052
38	7	0	-2.152935	3.818677	-0.909956
39	1	0	-2.292917	4.629712	-1.502291
40	7	0	1.600722	3.783499	-1.065761
41	6	0	4.601649	-2.673444	0.861378
42	6	0	5.528939	-2.728782	-0.210915
43	6	0	5.507556	-3.840861	-1.072668
44	1	0	6.193554	-3.907859	-1.906598
45	6	0	4.593741	-4.872862	-0.881769
46	1	0	4.585720	-5.717653	-1.558382
47	6	0	3.679999	-4.816727	0.166096
48	1	0	2.971788	-5.627210	0.276934
49	6	0	3.668674	-3.725726	1.054116
50	6	0	2.632971	-3.677280	2.172752
51	1	0	2.779324	-2.777098	2.804365
52	6	0	1.215895	-3.577103	1.597538
53	1	0	1.157815	-2.721025	0.893139
54	1	0	0.483050	-3.405091	2.414968
55	1	0	0.931109	-4.504858	1.057472
56	6	0	2.764388	-4.881504	3.112192
57	1	0	2.077743	-4.765678	3.978189
58	1	0	3.802197	-4.948516	3.503390
59	1	0	2.513253	-5.831698	2.595507
60	6	0	6.516958	-1.595567	-0.467458
61	1	0	6.436130	-0.818555	0.321164
62	6	0	7.965947	-2.095634	-0.425861
63	1	0	8.162217	-2.618332	0.534941
64	1	0	8.667450	-1.236969	-0.498646

65	1	0	8.181350	-2.791849	-1.263520
66	6	0	6.211354	-0.897001	-1.797365
67	1	0	6.348825	-1.585896	-2.657745
68	1	0	6.885409	-0.024664	-1.935069
69	1	0	5.164194	-0.523982	-1.800569
70	6	0	3.800181	-0.483145	1.469274
71	6	0	3.859194	0.570589	2.577030
72	1	0	4.906947	0.870440	2.693881
73	6	0	3.309284	0.129371	3.934063
74	1	0	3.928274	-0.646479	4.391668
75	1	0	2.295805	-0.260965	3.807881
76	6	0	3.321346	1.440470	4.741299
77	1	0	4.297565	1.543161	5.224595
78	6	0	2.169588	1.608697	5.755437
79	1	0	1.847403	0.649433	6.176119
80	1	0	2.505663	2.234477	6.591177
81	6	0	1.062269	2.331926	4.970868
82	1	0	0.345525	2.842112	5.623469
83	1	0	0.509962	1.620362	4.349622
84	6	0	1.834796	3.306093	4.064374
85	1	0	1.258071	3.630395	3.198571
86	1	0	2.124001	4.197660	4.634978
87	6	0	3.129015	2.570743	3.685680
88	1	0	3.991691	3.235766	3.629239
89	6	0	3.761836	2.660264	1.209889
90	1	0	4.803941	2.763479	1.526800
91	1	0	3.717331	2.049916	0.311102
92	6	0	3.196033	4.058942	0.946451
93	1	0	3.919558	4.553575	0.288583
94	1	0	3.208919	4.640782	1.875098
95	6	0	1.785274	4.216129	0.375375
96	1	0	1.076310	3.624499	0.950588
97	1	0	1.500740	5.271592	0.418526
98	6	0	2.426546	4.640106	-2.076534
99	1	0	2.566526	5.608042	-1.591911
100	6	0	3.748690	3.986740	-2.505713
101	1	0	4.166381	3.328773	-1.743071
102	1	0	4.465532	4.798454	-2.685445
103	6	0	3.435801	3.257321	-3.824272
104	1	0	2.994787	2.280813	-3.604962
105	1	0	4.330106	3.097767	-4.436790
106	6	0	2.404349	4.169876	-4.510635
107	1	0	1.800132	3.647524	-5.260552
108	1	0	2.915307	4.996345	-5.020181

109	6	0	1.541630	4.731812	-3.359308
110	1	0	1.265857	5.774876	-3.542701
111	6	0	0.258291	3.938974	-3.031374
112	1	0	0.350006	2.880486	-3.288423
113	1	0	-0.623071	4.348426	-3.530828
114	6	0	0.166491	4.094745	-1.513806
115	1	0	-0.000553	5.150367	-1.272815
116	6	0	-0.916798	3.275900	-0.813953
117	6	0	-3.294042	3.076815	-0.518612
118	6	0	-3.645244	2.987157	0.856188
119	6	0	-4.757226	2.209174	1.226024
120	1	0	-5.047106	2.114819	2.264427
121	6	0	-5.512352	1.544631	0.266699
122	1	0	-6.367409	0.954695	0.569550
123	6	0	-5.170189	1.629059	-1.078785
124	1	0	-5.770016	1.085949	-1.796842
125	6	0	-4.063054	2.390285	-1.496373
126	6	0	-3.695227	2.425370	-2.977444
127	1	0	-2.832475	3.098204	-3.153953
128	6	0	-4.847642	2.977900	-3.825557
129	1	0	-4.515573	3.114743	-4.877040
130	1	0	-5.169142	3.967634	-3.435969
131	1	0	-5.720289	2.291405	-3.825000
132	6	0	-3.263306	1.039568	-3.471634
133	1	0	-2.388795	0.682680	-2.886982
134	1	0	-2.955983	1.092551	-4.538037
135	1	0	-4.087670	0.300937	-3.381408
136	6	0	-2.856866	3.724462	1.935556
137	1	0	-2.033101	4.316651	1.485759
138	6	0	-3.743749	4.730497	2.678841
139	1	0	-4.221592	5.425350	1.955225
140	1	0	-3.129408	5.334433	3.380586
141	1	0	-4.537896	4.219830	3.263451
142	6	0	-2.205274	2.740930	2.915811
143	1	0	-2.969500	2.162351	3.475764
144	1	0	-1.579935	3.293805	3.648470
145	1	0	-1.548860	2.032190	2.369224
146	8	0	-0.705404	2.227813	-0.193803
147	20	0	1.009031	0.605623	-0.093975
148	8	0	0.553036	-0.462293	-2.160569
149	16	0	0.983549	-1.201377	-3.391653
150	8	0	-0.145329	-1.736300	-4.175338
151	8	0	2.064840	-0.545345	-4.146964
152	6	0	1.786144	-2.704494	-2.650308

153	9	0	0.904701	-3.400448	-1.907099
154	9	0	2.263377	-3.517057	-3.602396
155	9	0	2.802196	-2.335708	-1.856098
156	35	0	-6.070923	-2.126179	-0.519762

L3a-Ca(II)-TS-*re*-1

Zero-point correction= 1.28559 a.u.

Thermal correction to Gibbs Free Energy= 1.17449 a.u.

Sum of electronic and zero-point Energies= -7194.59210 a.u.

Sum of electronic and thermal Free Energies= -7194.70320 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.608770	-0.347138	-0.565505
2	6	0	-3.996808	-0.808363	-1.889909
3	8	0	-5.286124	-0.755784	-2.154831
4	6	0	-5.780142	-1.212772	-3.433887
5	6	0	-3.011838	-1.505792	-2.639266
6	1	0	-2.690219	0.240650	-0.616259
7	1	0	-4.398191	0.194644	-0.044493
8	1	0	-6.817652	-0.880858	-3.472202
9	1	0	-5.735901	-2.302084	-3.485507
10	1	0	-5.205500	-0.762246	-4.246744
11	1	0	-2.058896	-0.985205	-2.749291
12	1	0	-3.321312	-2.004038	-3.555520
13	1	0	-2.667198	-2.258632	-1.710756
14	6	0	-2.466990	-0.965015	1.543177
15	6	0	-3.143428	-1.697869	0.344617
16	6	0	-4.382471	-2.288986	1.028831
17	6	0	-4.422981	-1.829214	2.354741
18	7	0	-3.287998	-1.031721	2.623519
19	8	0	-2.344360	-2.524789	-0.315913
20	8	0	-1.375249	-0.388706	1.514061
21	6	0	-2.988104	-0.480302	3.934437
22	6	0	-5.357743	-3.184303	0.627407
23	6	0	-5.427481	-2.176040	3.248951
24	1	0	-3.800117	0.175058	4.262654
25	1	0	-2.062981	0.089129	3.861366
26	1	0	-2.860054	-1.285406	4.665825
27	6	0	-6.423987	-3.046752	2.789498

28	6	0	-6.390198	-3.564369	1.495269
29	1	0	-5.438084	-1.802084	4.267084
30	1	0	-7.227268	-3.342104	3.458246
31	1	0	-7.150318	-4.262781	1.162689
32	8	0	1.489204	0.519031	2.648895
33	8	0	2.575131	-1.132862	0.615381
34	8	0	2.203832	2.077601	-0.138541
35	7	0	4.220114	-2.526370	1.324401
36	1	0	4.900185	-2.738593	2.045316
37	7	0	2.776741	0.428010	3.112033
38	7	0	-1.407099	4.315593	-0.410478
39	1	0	-1.201709	5.194942	-0.871677
40	7	0	2.171474	3.378563	0.296132
41	6	0	4.434458	-3.067197	0.035126
42	6	0	5.483217	-2.560606	-0.777385
43	6	0	5.633350	-3.060750	-2.083676
44	1	0	6.410028	-2.682283	-2.734938
45	6	0	4.781256	-4.045862	-2.572164
46	1	0	4.909513	-4.417196	-3.580818
47	6	0	3.760995	-4.551712	-1.772904
48	1	0	3.111566	-5.311930	-2.186111
49	6	0	3.567547	-4.074964	-0.463680
50	6	0	2.430688	-4.640977	0.382456
51	1	0	2.440712	-4.196472	1.399344
52	6	0	1.066430	-4.300754	-0.229698
53	1	0	0.966028	-3.201727	-0.355137
54	1	0	0.250723	-4.643163	0.442565
55	1	0	0.932852	-4.788424	-1.218501
56	6	0	2.582066	-6.154174	0.580309
57	1	0	1.814859	-6.523616	1.294302
58	1	0	3.583150	-6.386330	1.002729
59	1	0	2.459783	-6.704691	-0.376276
60	6	0	6.421581	-1.464206	-0.279835
61	1	0	6.205997	-1.211639	0.778654
62	6	0	7.885410	-1.919682	-0.319875
63	1	0	8.004564	-2.872165	0.239962
64	1	0	8.534607	-1.156431	0.160401
65	1	0	8.238226	-2.069162	-1.361954
66	6	0	6.225447	-0.169979	-1.076815
67	1	0	6.478728	-0.308842	-2.149147
68	1	0	6.870076	0.635404	-0.664380
69	1	0	5.169990	0.162553	-0.996167
70	6	0	3.325903	-1.530090	1.515591
71	6	0	3.331448	-0.992079	2.946836

72	1	0	4.373500	-0.940147	3.279381
73	6	0	2.523068	-1.780521	3.974573
74	1	0	2.946341	-2.774067	4.140044
75	1	0	1.492392	-1.888775	3.626286
76	6	0	2.622221	-0.874339	5.221163
77	1	0	3.512584	-1.163225	5.787417
78	6	0	1.372386	-0.831654	6.128519
79	1	0	0.809875	-1.771599	6.098819
80	1	0	1.680909	-0.669344	7.168522
81	6	0	0.560670	0.375309	5.626376
82	1	0	-0.134656	0.761522	6.379780
83	1	0	-0.013026	0.099245	4.737992
84	6	0	1.633317	1.402278	5.227328
85	1	0	1.266295	2.150300	4.523654
86	1	0	2.005284	1.925092	6.117658
87	6	0	2.797721	0.574466	4.666596
88	1	0	3.774118	0.998039	4.905912
89	6	0	3.698805	1.407116	2.410017
90	1	0	4.696566	1.239658	2.827091
91	1	0	3.685389	1.117047	1.362024
92	6	0	3.347091	2.891018	2.545952
93	1	0	4.242918	3.437387	2.229738
94	1	0	3.211857	3.149721	3.601799
95	6	0	2.125380	3.452850	1.813374
96	1	0	1.221939	2.921017	2.104782
97	1	0	2.022351	4.511574	2.072203
98	6	0	3.368839	4.187284	-0.307030
99	1	0	3.586724	4.965638	0.426176
100	6	0	4.595133	3.331628	-0.653393
101	1	0	4.707183	2.457361	-0.013301
102	1	0	5.478575	3.967498	-0.508123
103	6	0	4.443199	2.980574	-2.143495
104	1	0	3.770325	2.126339	-2.253942
105	1	0	5.400284	2.724210	-2.611720
106	6	0	3.807083	4.244130	-2.748402
107	1	0	3.288201	4.051400	-3.693499
108	1	0	4.580953	4.996180	-2.946730
109	6	0	2.845828	4.767561	-1.656662
110	1	0	2.851406	5.860889	-1.613764
111	6	0	1.386091	4.285734	-1.769356
112	1	0	1.311610	3.322848	-2.281512
113	1	0	0.749934	5.010319	-2.283839
114	6	0	0.979187	4.127785	-0.303421
115	1	0	0.965428	5.112438	0.175214

116	6	0	-0.389426	3.487601	-0.076880
117	6	0	-2.748087	3.863050	-0.416996
118	6	0	-3.473956	3.780504	0.801453
119	6	0	-4.789737	3.283717	0.777945
120	1	0	-5.364265	3.196070	1.690588
121	6	0	-5.384701	2.897345	-0.418301
122	1	0	-6.398215	2.517155	-0.417710
123	6	0	-4.680136	2.987777	-1.614037
124	1	0	-5.169493	2.668983	-2.524926
125	6	0	-3.358110	3.468368	-1.637589
126	6	0	-2.605086	3.520838	-2.963414
127	1	0	-1.582359	3.923480	-2.819915
128	6	0	-3.299304	4.454688	-3.961357
129	1	0	-2.681646	4.558375	-4.879290
130	1	0	-3.423523	5.464746	-3.515382
131	1	0	-4.297534	4.067009	-4.255205
132	6	0	-2.431286	2.117094	-3.551767
133	1	0	-1.922055	1.465962	-2.812418
134	1	0	-1.802026	2.160141	-4.466205
135	1	0	-3.408430	1.663734	-3.820933
136	6	0	-2.863285	4.224047	2.127900
137	1	0	-1.842442	4.631361	1.974535
138	6	0	-3.677612	5.355865	2.766260
139	1	0	-3.785462	6.199133	2.050807
140	1	0	-3.156254	5.737458	3.670304
141	1	0	-4.688607	5.010457	3.068748
142	6	0	-2.721861	3.039762	3.089980
143	1	0	-3.714603	2.637768	3.382587
144	1	0	-2.184513	3.354346	4.010194
145	1	0	-2.132703	2.231064	2.610117
146	8	0	-0.577720	2.353767	0.382055
147	20	0	0.693080	0.322349	0.428645
148	8	0	0.373863	-0.015031	-1.905961
149	16	0	0.767499	-0.000636	-3.352721
150	8	0	-0.190332	-0.702870	-4.225780
151	8	0	1.255674	1.305209	-3.833939
152	6	0	2.269383	-1.093639	-3.348846
153	9	0	1.947494	-2.321680	-2.917515
154	9	0	2.785291	-1.199614	-4.581707
155	9	0	3.214810	-0.593400	-2.536459
156	35	0	-5.298321	-3.992784	-1.110142

L3a-Ca(II)-TS-*si*-1-H

Zero-point correction= 1.29660 a.u.
Thermal correction to Gibbs Free Energy= 1.17990 a.u.
Sum of electronic and zero-point Energies= -4621.02918 a.u.
Sum of electronic and thermal Free Energies= -4621.14587 a.u.
The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.760566	1.725774	1.455226
2	6	0	2.699056	2.214993	0.313485
3	6	0	3.932624	2.638409	1.108894
4	6	0	3.667276	2.472552	2.473467
5	7	0	2.361838	1.950457	2.649455
6	8	0	2.860539	1.332708	-0.665673
7	8	0	0.643738	1.209558	1.310055
8	6	0	1.785833	1.613638	3.939877
9	6	0	5.185513	3.071835	0.703011
10	6	0	4.607036	2.753373	3.457273
11	6	0	5.864378	3.207983	3.033118
12	6	0	6.155401	3.360625	1.675817
13	1	0	1.751285	2.501434	4.579451
14	1	0	0.772815	1.247099	3.773396
15	1	0	2.378992	0.837916	4.435360
16	1	0	4.389517	2.616206	4.511954
17	1	0	6.623706	3.434075	3.776830
18	1	0	7.141654	3.698639	1.369898
19	6	0	1.869654	3.606886	-0.199002
20	6	0	2.560219	4.066796	-1.390432
21	8	0	3.358746	5.102762	-1.221705
22	6	0	4.183275	5.569335	-2.313962
23	6	0	2.560914	3.186551	-2.510626
24	1	0	0.875973	3.226197	-0.439979
25	1	0	1.839552	4.341992	0.605877
26	1	0	4.609856	6.509917	-1.965763
27	1	0	4.980840	4.851637	-2.522423
28	1	0	3.574692	5.736085	-3.206185
29	1	0	1.565841	2.858858	-2.826496
30	1	0	3.211816	3.426764	-3.349387
31	1	0	2.886442	2.185287	-1.868198
32	8	0	-0.854895	-1.595580	2.110525
33	8	0	-2.651070	0.060157	0.700061
34	8	0	-0.991010	-2.528111	-1.049883

35	7	0	-4.336201	0.815167	2.023589
36	1	0	-4.920930	0.643300	2.833397
37	7	0	-2.047135	-2.127201	2.536725
38	7	0	3.251332	-3.028088	-1.026913
39	1	0	3.495786	-3.781276	-1.660281
40	7	0	-0.438681	-3.774148	-0.890695
41	6	0	-4.786910	1.762319	1.075240
42	6	0	-5.836625	1.423592	0.181848
43	6	0	-6.255640	2.373887	-0.767138
44	1	0	-7.043759	2.142312	-1.471337
45	6	0	-5.658678	3.628821	-0.830730
46	1	0	-5.990900	4.346395	-1.570042
47	6	0	-4.627232	3.960733	0.041984
48	1	0	-4.175367	4.940222	-0.043164
49	6	0	-4.172632	3.040075	1.003411
50	6	0	-3.022179	3.426244	1.927983
51	1	0	-2.799567	2.605873	2.641298
52	6	0	-1.736337	3.667472	1.128753
53	1	0	-1.510553	2.780973	0.499483
54	1	0	-0.881943	3.831359	1.819736
55	1	0	-1.828788	4.556414	0.469655
56	6	0	-3.377365	4.649255	2.781707
57	1	0	-2.568014	4.849310	3.516300
58	1	0	-4.314903	4.460555	3.347293
59	1	0	-3.512192	5.556918	2.156689
60	6	0	-6.487947	0.044013	0.202832
61	1	0	-6.081825	-0.570319	1.032880
62	6	0	-7.998916	0.142780	0.445441
63	1	0	-8.199944	0.725430	1.370033
64	1	0	-8.430546	-0.872298	0.578828
65	1	0	-8.517890	0.630446	-0.406502
66	6	0	-6.185223	-0.723657	-1.089177
67	1	0	-6.618325	-0.213349	-1.975315
68	1	0	-6.609686	-1.749036	-1.033306
69	1	0	-5.086670	-0.818106	-1.227514
70	6	0	-3.304273	-0.014401	1.747549
71	6	0	-3.045253	-1.017676	2.871734
72	1	0	-3.994205	-1.516682	3.099162
73	6	0	-2.469729	-0.430694	4.159940
74	1	0	-3.186666	0.227112	4.657222
75	1	0	-1.568683	0.142989	3.927325
76	6	0	-2.150463	-1.693433	4.984201
77	1	0	-3.032898	-1.955211	5.575704
78	6	0	-0.885520	-1.614499	5.867646

79	1	0	-0.689137	-0.593845	6.214994
80	1	0	-1.020902	-2.240410	6.758030
81	6	0	0.243113	-2.186518	4.992512
82	1	0	1.095154	-2.542804	5.581870
83	1	0	0.603888	-1.429329	4.290483
84	6	0	-0.443878	-3.314209	4.204108
85	1	0	0.096563	-3.591027	3.299293
86	1	0	-0.533435	-4.209785	4.832245
87	6	0	-1.868821	-2.810421	3.931989
88	1	0	-2.612231	-3.608618	3.961680
89	6	0	-2.648997	-3.067452	1.505307
90	1	0	-3.628480	-3.362918	1.893926
91	1	0	-2.782409	-2.471901	0.605091
92	6	0	-1.841848	-4.332865	1.206424
93	1	0	-2.490181	-4.965507	0.590198
94	1	0	-1.689855	-4.895980	2.134256
95	6	0	-0.460229	-4.214324	0.559968
96	1	0	0.145244	-3.485146	1.092419
97	1	0	0.028978	-5.192418	0.590318
98	6	0	-1.140047	-4.790161	-1.846248
99	1	0	-1.066854	-5.757674	-1.346471
100	6	0	-2.583310	-4.407828	-2.205987
101	1	0	-3.073614	-3.820444	-1.429086
102	1	0	-3.143863	-5.343570	-2.330654
103	6	0	-2.487733	-3.665847	-3.550992
104	1	0	-2.234180	-2.616970	-3.374354
105	1	0	-3.427081	-3.698330	-4.113872
106	6	0	-1.336583	-4.378876	-4.282520
107	1	0	-0.884121	-3.766275	-5.069947
108	1	0	-1.704131	-5.298668	-4.754390
109	6	0	-0.323136	-4.740625	-3.174474
110	1	0	0.136435	-5.716244	-3.360733
111	6	0	0.800987	-3.712543	-2.927159
112	1	0	0.494911	-2.697499	-3.193519
113	1	0	1.714990	-3.961758	-3.471557
114	6	0	1.001695	-3.813819	-1.414820
115	1	0	1.385866	-4.811280	-1.172898
116	6	0	1.940735	-2.786402	-0.782186
117	6	0	4.225350	-2.028452	-0.781814
118	6	0	4.694512	-1.798385	0.541485
119	6	0	5.648601	-0.787945	0.759981
120	1	0	6.023930	-0.585823	1.754591
121	6	0	6.137392	-0.028420	-0.296856
122	1	0	6.877041	0.739423	-0.111224

123	6	0	5.674693	-0.244189	-1.589924
124	1	0	6.063326	0.378503	-2.384828
125	6	0	4.719947	-1.242080	-1.858389
126	6	0	4.221185	-1.430167	-3.289355
127	1	0	3.504141	-2.271190	-3.351420
128	6	0	5.372797	-1.780616	-4.239615
129	1	0	4.973737	-2.035739	-5.244872
130	1	0	5.928686	-2.663704	-3.857646
131	1	0	6.080431	-0.932617	-4.353089
132	6	0	3.461204	-0.192125	-3.778582
133	1	0	2.589440	0.002490	-3.118747
134	1	0	3.073639	-0.362396	-4.805770
135	1	0	4.114805	0.705378	-3.795886
136	6	0	4.206482	-2.630518	1.724596
137	1	0	3.470071	-3.391193	1.393363
138	6	0	5.361374	-3.410267	2.364152
139	1	0	5.869903	-4.034717	1.598664
140	1	0	4.972657	-4.086182	3.155815
141	1	0	6.107694	-2.728514	2.823974
142	6	0	3.494926	-1.755211	2.765583
143	1	0	4.197917	-1.039654	3.241451
144	1	0	3.057317	-2.393861	3.561897
145	1	0	2.669497	-1.184204	2.291188
146	8	0	1.563912	-1.839136	-0.084588
147	20	0	-0.413642	-0.505838	0.021845
148	8	0	-0.979966	0.847378	-1.851024
149	16	0	-1.257443	1.182182	-3.283920
150	8	0	-0.335629	2.189861	-3.844724
151	8	0	-1.552919	0.017898	-4.137661
152	6	0	-2.875987	2.082398	-3.143913
153	9	0	-2.745920	3.162479	-2.358530
154	9	0	-3.292601	2.489740	-4.352680
155	9	0	-3.820533	1.286813	-2.620121
156	1	0	5.422009	3.169968	-0.352912

L3a-Ca(II)-TS-*re*-1-H

Zero-point correction= 1.29675 a.u.

Thermal correction to Gibbs Free Energy= 1.18379 a.u.

Sum of electronic and zero-point Energies= -4621.03505 a.u.

Sum of electronic and thermal Free Energies= -4621.14801 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.567185	-1.012866	-1.288753
2	6	0	-3.844767	-1.117821	-2.709645
3	8	0	-5.113262	-1.282890	-3.030103
4	6	0	-5.486724	-1.520295	-4.406836
5	6	0	-2.731518	-1.351379	-3.565673
6	1	0	-2.752063	-0.316212	-1.088665
7	1	0	-4.445782	-0.791497	-0.683777
8	1	0	-6.575482	-1.474405	-4.418154
9	1	0	-5.149341	-2.508803	-4.728446
10	1	0	-5.067805	-0.744311	-5.052108
11	1	0	-1.910501	-0.639385	-3.455265
12	1	0	-2.929466	-1.597391	-4.607062
13	1	0	-2.256937	-2.272754	-2.893150
14	6	0	-2.465463	-2.167097	0.633936
15	6	0	-2.924675	-2.509363	-0.816146
16	6	0	-4.077283	-3.473289	-0.543476
17	6	0	-4.248444	-3.588466	0.840991
18	7	0	-3.288250	-2.793813	1.514462
19	8	0	-1.943736	-2.928590	-1.608874
20	8	0	-1.514127	-1.440213	0.943180
21	6	0	-3.150412	-2.747847	2.959807
22	6	0	-4.870558	-4.224304	-1.397640
23	6	0	-5.217376	-4.407591	1.407780
24	1	0	-4.090669	-2.427371	3.418672
25	1	0	-2.361753	-2.038664	3.206827
26	1	0	-2.882735	-3.736074	3.349620
27	6	0	-6.028143	-5.144765	0.532025
28	6	0	-5.855747	-5.062303	-0.851698
29	1	0	-5.340223	-4.487509	2.483356
30	1	0	-6.794812	-5.796341	0.942619
31	1	0	-6.485583	-5.653906	-1.510367
32	8	0	1.014465	-0.444293	2.661983
33	8	0	2.527941	-0.972166	0.322531
34	8	0	1.442735	2.133176	0.683170
35	7	0	4.420771	-2.169475	0.687270
36	1	0	5.105765	-2.489676	1.362284
37	7	0	2.271189	-0.428716	3.210316
38	7	0	-2.576150	3.528448	0.762453
39	1	0	-2.560506	4.536039	0.650022
40	7	0	1.091818	3.151412	1.533621
41	6	0	4.797196	-2.148031	-0.676000

42	6	0	5.726983	-1.178349	-1.136273
43	6	0	6.031174	-1.125847	-2.508750
44	1	0	6.720424	-0.386496	-2.894515
45	6	0	5.445243	-2.015463	-3.403386
46	1	0	5.688595	-1.958720	-4.456631
47	6	0	4.542475	-2.973054	-2.952138
48	1	0	4.098801	-3.644182	-3.675451
49	6	0	4.201521	-3.056804	-1.589946
50	6	0	3.196254	-4.108662	-1.129579
51	1	0	3.071150	-4.074496	-0.027342
52	6	0	1.811331	-3.848819	-1.734942
53	1	0	1.466994	-2.824499	-1.478445
54	1	0	1.073403	-4.569799	-1.322342
55	1	0	1.825415	-3.956516	-2.840128
56	6	0	3.681824	-5.526023	-1.456889
57	1	0	2.995880	-6.276634	-1.008700
58	1	0	4.695085	-5.690832	-1.031699
59	1	0	3.719863	-5.701122	-2.552797
60	6	0	6.368008	-0.171040	-0.185175
61	1	0	6.066734	-0.372518	0.863280
62	6	0	7.898289	-0.267711	-0.215117
63	1	0	8.219365	-1.312053	-0.012700
64	1	0	8.336003	0.383847	0.571441
65	1	0	8.308495	0.050143	-1.196598
66	6	0	5.899811	1.254073	-0.498817
67	1	0	6.214342	1.572199	-1.515398
68	1	0	6.323057	1.967655	0.240033
69	1	0	4.793626	1.307792	-0.431314
70	6	0	3.316660	-1.512145	1.108748
71	6	0	3.148816	-1.543399	2.628261
72	1	0	4.138251	-1.401292	3.075750
73	6	0	2.514749	-2.800500	3.218699
74	1	0	3.153175	-3.675839	3.077054
75	1	0	1.549978	-2.985221	2.738722
76	6	0	2.358100	-2.410524	4.704631
77	1	0	3.273111	-2.693087	5.233603
78	6	0	1.105094	-2.962353	5.420398
79	1	0	0.782923	-3.923365	5.003981
80	1	0	1.332157	-3.126418	6.480933
81	6	0	0.047387	-1.854657	5.274374
82	1	0	-0.744821	-1.922878	6.027963
83	1	0	-0.414112	-1.903202	4.284772
84	6	0	0.858362	-0.552567	5.382579
85	1	0	0.348146	0.304867	4.942235

86	1	0	1.064975	-0.322874	6.435677
87	6	0	2.204379	-0.856893	4.710652
88	1	0	3.043944	-0.355819	5.194770
89	6	0	2.960169	0.906831	3.002072
90	1	0	3.954786	0.810307	3.448178
91	1	0	3.050710	1.020644	1.924408
92	6	0	2.264677	2.132703	3.600075
93	1	0	3.017972	2.928523	3.602333
94	1	0	2.032505	1.955237	4.655954
95	6	0	0.973470	2.658572	2.966495
96	1	0	0.209159	1.884381	2.947345
97	1	0	0.615886	3.505920	3.560437
98	6	0	2.089246	4.350398	1.394275
99	1	0	2.092684	4.834641	2.372256
100	6	0	3.493138	3.949549	0.920537
101	1	0	3.781855	2.944442	1.225395
102	1	0	4.198124	4.653967	1.381589
103	6	0	3.482834	4.144337	-0.605443
104	1	0	3.032137	3.271601	-1.084946
105	1	0	4.489999	4.277389	-1.016159
106	6	0	2.592798	5.383506	-0.804446
107	1	0	2.169069	5.448707	-1.812260
108	1	0	3.177070	6.296471	-0.634429
109	6	0	1.495572	5.263239	0.277960
110	1	0	1.243368	6.241540	0.698241
111	6	0	0.194767	4.567580	-0.168360
112	1	0	0.366839	3.864051	-0.987177
113	1	0	-0.573232	5.283099	-0.472543
114	6	0	-0.219201	3.806782	1.092090
115	1	0	-0.481250	4.524040	1.876699
116	6	0	-1.407947	2.862362	0.918822
117	6	0	-3.774149	2.846823	0.440399
118	6	0	-4.508913	2.183221	1.459676
119	6	0	-5.681821	1.488875	1.111814
120	1	0	-6.256926	0.963296	1.862667
121	6	0	-6.133795	1.466507	-0.203162
122	1	0	-7.039438	0.928585	-0.452390
123	6	0	-5.421202	2.122139	-1.201483
124	1	0	-5.795365	2.075380	-2.215693
125	6	0	-4.235023	2.817530	-0.903190
126	6	0	-3.462796	3.495411	-2.031176
127	1	0	-2.551416	3.992134	-1.641755
128	6	0	-4.301585	4.592347	-2.696279
129	1	0	-3.689038	5.140192	-3.444214

130	1	0	-4.646955	5.323141	-1.933912
131	1	0	-5.187852	4.168670	-3.214290
132	6	0	-2.979892	2.470222	-3.063218
133	1	0	-2.368873	1.694028	-2.559161
134	1	0	-2.344552	2.966678	-3.827333
135	1	0	-3.830548	1.980116	-3.581882
136	6	0	-4.062107	2.214393	2.918732
137	1	0	-3.150343	2.835279	3.038272
138	6	0	-5.128718	2.854896	3.815147
139	1	0	-5.390521	3.865611	3.434870
140	1	0	-4.739368	2.967833	4.849799
141	1	0	-6.050754	2.237600	3.857079
142	6	0	-3.702842	0.808658	3.412314
143	1	0	-4.594912	0.148085	3.431905
144	1	0	-3.279488	0.858435	4.438492
145	1	0	-2.936432	0.358320	2.748068
146	8	0	-1.343976	1.627059	0.944463
147	20	0	0.360886	0.020258	0.437615
148	8	0	0.188142	0.483410	-1.889895
149	16	0	0.609757	1.109131	-3.185225
150	8	0	-0.127561	0.589864	-4.351913
151	8	0	0.787674	2.571486	-3.122160
152	6	0	2.327097	0.432612	-3.392903
153	9	0	2.292794	-0.906259	-3.457336
154	9	0	2.890138	0.896121	-4.517776
155	9	0	3.102139	0.787054	-2.354868
156	1	0	-4.728283	-4.171996	-2.473697

L3a-Ca(II)-TS1-*si*

Zero-point correction= 1.26080 a.u.

Thermal correction to Gibbs Free Energy= 1.15595 a.u.

Sum of electronic and zero-point Energies= -6232.80092 a.u.

Sum of electronic and thermal Free Energies= -6232.90578 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888586	1.229499	-1.832219
2	6	0	-1.072042	2.047323	-0.531317
3	6	0	-2.365128	2.772300	-0.783874
4	6	0	-2.772912	2.474805	-2.099513

5	7	0	-1.861235	1.576183	-2.705659
6	8	0	-0.738958	1.476054	0.565062
7	6	0	-3.182919	3.572539	-0.004555
8	6	0	-3.943387	2.976813	-2.648199
9	8	0	-0.012953	0.368076	-1.981222
10	6	0	-2.012342	1.013742	-4.039967
11	1	0	-1.904120	1.797798	-4.795674
12	1	0	-1.233066	0.264180	-4.179625
13	1	0	-2.994889	0.546119	-4.145500
14	6	0	-4.375259	4.093055	-0.520062
15	6	0	-4.738020	3.795770	-1.833942
16	35	0	-2.715469	3.946980	1.811604
17	1	0	-5.013634	4.713213	0.099179
18	1	0	-5.664688	4.199590	-2.230330
19	1	0	-4.246157	2.736255	-3.661569
20	6	0	0.323212	3.342050	-1.044604
21	6	0	0.331942	4.325416	-0.036293
22	8	0	-0.250902	5.462784	-0.328302
23	6	0	-0.357742	6.543438	0.632702
24	1	0	-0.735509	7.388609	0.058383
25	6	0	0.893915	4.003322	1.300352
26	1	0	-1.072823	6.268584	1.410587
27	1	0	0.472746	3.024410	1.585235
28	1	0	1.135593	2.625242	-0.976777
29	1	0	0.088374	3.686401	-2.049163
30	1	0	1.978455	3.866286	1.219574
31	1	0	0.620677	6.779283	1.055343
32	1	0	0.685940	4.742921	2.072091
33	8	0	2.875958	-0.177827	0.357240
34	8	0	1.648184	-2.352057	-0.885193
35	8	0	0.327271	-1.926491	2.161567
36	8	0	-1.586003	-1.621132	0.112714
37	7	0	5.016091	0.120547	-0.322795
38	1	0	5.805624	-0.255711	-0.836622
39	7	0	2.822626	-2.955737	-0.503125
40	7	0	-3.544839	-2.703278	0.475143
41	1	0	-4.096670	-3.273003	1.107162
42	7	0	-0.280800	-3.151515	2.268928
43	6	0	4.983629	1.517353	-0.091671
44	6	0	5.044341	2.020289	1.236174
45	6	0	4.944931	3.408024	1.444016
46	1	0	4.981779	3.821806	2.443027
47	6	0	4.786638	4.280274	0.372541
48	1	0	4.702430	5.344451	0.552107

49	6	0	4.727190	3.791159	-0.927687
50	1	0	4.592307	4.496825	-1.736774
51	6	0	4.833319	2.412248	-1.185621
52	6	0	4.753755	1.913332	-2.626327
53	1	0	4.910762	0.818092	-2.673795
54	6	0	3.366690	2.171942	-3.224357
55	1	0	2.594865	1.642453	-2.627487
56	1	0	3.317021	1.779648	-4.262679
57	1	0	3.127988	3.256414	-3.246276
58	6	0	5.853419	2.535700	-3.495332
59	1	0	5.856885	2.063811	-4.501413
60	1	0	6.849229	2.363739	-3.033459
61	1	0	5.701038	3.627626	-3.626280
62	6	0	5.213584	1.094342	2.437391
63	1	0	5.294398	0.037166	2.109832
64	6	0	6.509190	1.404058	3.197123
65	1	0	7.378149	1.351120	2.506679
66	1	0	6.666704	0.657017	4.004379
67	1	0	6.479450	2.413517	3.659188
68	6	0	3.998553	1.172524	3.371124
69	1	0	3.914880	2.173910	3.843865
70	1	0	4.085415	0.411777	4.176409
71	1	0	3.063516	0.967813	2.807759
72	6	0	3.894576	-0.622423	-0.190861
73	6	0	4.022991	-2.034186	-0.761775
74	1	0	4.890170	-2.512403	-0.292281
75	6	0	4.171288	-2.094270	-2.283790
76	1	0	5.130592	-1.687067	-2.611965
77	1	0	3.366441	-1.520656	-2.752297
78	6	0	4.049025	-3.599617	-2.577792
79	1	0	5.045027	-4.048530	-2.521607
80	6	0	3.340566	-3.956175	-3.902669
81	1	0	3.514763	-3.202087	-4.678139
82	1	0	3.727550	-4.909972	-4.281337
83	6	0	1.858557	-4.105107	-3.520396
84	1	0	1.290526	-4.695729	-4.247111
85	1	0	1.386501	-3.120819	-3.437416
86	6	0	1.908326	-4.764637	-2.131450
87	1	0	0.990923	-4.626540	-1.560128
88	1	0	2.086331	-5.842448	-2.235632
89	6	0	3.145090	-4.167223	-1.443565
90	1	0	3.670450	-4.886369	-0.814280
91	6	0	2.791612	-3.368968	0.959784
92	1	0	3.788657	-3.756409	1.186351

93	1	0	2.627073	-2.455301	1.526819
94	6	0	1.762280	-4.439115	1.335671
95	1	0	2.017339	-4.752875	2.353744
96	1	0	1.919315	-5.328881	0.715257
97	6	0	0.265281	-4.131865	1.247377
98	1	0	0.020888	-3.708351	0.274890
99	1	0	-0.293185	-5.061467	1.387708
100	6	0	-0.169907	-3.664156	3.740080
101	1	0	-0.175488	-4.752758	3.669104
102	6	0	1.049328	-3.115742	4.495806
103	1	0	1.895178	-2.897725	3.842659
104	1	0	1.361364	-3.891214	5.206916
105	6	0	0.537800	-1.880086	5.257420
106	1	0	0.531704	-1.017065	4.584777
107	1	0	1.160915	-1.633617	6.124081
108	6	0	-0.899719	-2.262980	5.652205
109	1	0	-1.535510	-1.394932	5.858643
110	1	0	-0.886019	-2.879396	6.559070
111	6	0	-1.430842	-3.102264	4.467799
112	1	0	-2.054629	-3.930204	4.817338
113	6	0	-2.214646	-2.321482	3.392219
114	1	0	-1.910399	-1.272421	3.344497
115	1	0	-3.294600	-2.368190	3.549083
116	6	0	-1.802119	-3.036823	2.105587
117	1	0	-2.183753	-4.063729	2.129572
118	6	0	-2.274065	-2.380747	0.806993
119	6	0	-4.224733	-1.999215	-0.547855
120	6	0	-3.990469	-2.324925	-1.910899
121	6	0	-4.638815	-1.577474	-2.910687
122	1	0	-4.479449	-1.798650	-3.957636
123	6	0	-5.496476	-0.534200	-2.578185
124	1	0	-5.980785	0.035321	-3.360960
125	6	0	-5.733138	-0.218393	-1.244837
126	1	0	-6.401380	0.602718	-1.021505
127	6	0	-5.111769	-0.942263	-0.210854
128	6	0	-5.384780	-0.557836	1.240030
129	1	0	-4.846758	-1.232729	1.934695
130	6	0	-6.873579	-0.692763	1.580992
131	1	0	-7.033680	-0.519152	2.666801
132	1	0	-7.228383	-1.718463	1.342178
133	1	0	-7.488951	0.039927	1.017483
134	6	0	-4.876296	0.855568	1.538709
135	1	0	-3.792851	0.921539	1.304612
136	1	0	-5.008107	1.090979	2.616311

137	1	0	-5.424599	1.616239	0.944581
138	6	0	-3.066006	-3.470315	-2.313937
139	1	0	-2.652630	-3.976659	-1.417109
140	6	0	-3.827224	-4.548061	-3.095088
141	1	0	-4.698590	-4.904014	-2.504587
142	1	0	-3.165004	-5.419436	-3.287513
143	1	0	-4.189017	-4.164068	-4.072055
144	6	0	-1.865968	-2.956008	-3.118249
145	1	0	-2.184144	-2.518203	-4.087709
146	1	0	-1.165297	-3.791724	-3.327393
147	1	0	-1.317336	-2.183881	-2.539273
148	20	0	0.543554	-0.588415	0.257644

L3a-Ca(II)-TS2-*si*

Zero-point correction= 1.25926 a.u.

Thermal correction to Gibbs Free Energy= 1.15635 a.u.

Sum of electronic and zero-point Energies= -6232.80262 a.u.

Sum of electronic and thermal Free Energies= -6232.90553 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022913	1.330989	-2.053056
2	6	0	-0.675265	2.327771	-0.920381
3	6	0	-1.890396	3.247265	-0.960528
4	6	0	-2.643722	2.925141	-2.103968
5	7	0	-2.078238	1.799108	-2.754364
6	8	0	-0.406002	1.662822	0.246285
7	6	0	-2.368268	4.240614	-0.124328
8	6	0	-3.804954	3.597882	-2.456059
9	8	0	-0.411212	0.270572	-2.238941
10	6	0	-2.644954	1.152212	-3.929480
11	1	0	-2.528320	1.796411	-4.806388
12	1	0	-2.113182	0.214454	-4.092263
13	1	0	-3.706972	0.947716	-3.773780
14	6	0	-3.540136	4.940407	-0.438979
15	6	0	-4.236949	4.622755	-1.603953
16	35	0	-1.489522	4.636925	1.529746
17	1	0	-3.906046	5.714123	0.226525
18	1	0	-5.143712	5.169698	-1.844058
19	1	0	-4.368823	3.335623	-3.344559

20	6	0	0.653535	3.081326	-1.503001
21	6	0	1.346583	3.763696	-0.393124
22	8	0	1.252274	5.070732	-0.392667
23	6	0	1.880547	5.840805	0.661877
24	1	0	1.813149	6.877266	0.333876
25	6	0	1.811473	2.953322	0.661566
26	1	0	1.333951	5.705631	1.596923
27	1	0	0.662377	2.329344	0.761427
28	1	0	1.287680	2.276197	-1.882807
29	1	0	0.382429	3.761344	-2.311042
30	1	0	2.357845	2.063729	0.342581
31	1	0	2.925056	5.540229	0.774300
32	1	0	2.197835	3.419281	1.563775
33	8	0	2.573176	-0.328388	-0.276715
34	8	0	1.095822	-2.570348	-1.132553
35	8	0	0.148385	-1.940228	1.965015
36	8	0	-1.935216	-1.594951	0.066547
37	7	0	4.822362	-0.614039	-0.326049
38	1	0	5.607679	-1.183801	-0.620758
39	7	0	2.257267	-3.248962	-0.870600
40	7	0	-3.976222	-2.119882	0.900455
41	1	0	-4.503032	-2.487066	1.685596
42	7	0	-0.559012	-3.100795	2.173175
43	6	0	5.086106	0.709926	0.097463
44	6	0	4.969272	1.050017	1.470936
45	6	0	5.156023	2.389164	1.858875
46	1	0	5.062496	2.682948	2.896020
47	6	0	5.456278	3.368466	0.917518
48	1	0	5.591549	4.395025	1.232706
49	6	0	5.584139	3.034474	-0.426701
50	1	0	5.816010	3.820560	-1.133033
51	6	0	5.411288	1.707069	-0.859331
52	6	0	5.553049	1.375489	-2.341731
53	1	0	5.418221	0.288582	-2.515638
54	6	0	4.473913	2.080677	-3.169763
55	1	0	3.467290	1.793363	-2.801284
56	1	0	4.546701	1.773749	-4.235152
57	1	0	4.575167	3.185153	-3.114362
58	6	0	6.955778	1.719663	-2.857297
59	1	0	7.074492	1.367083	-3.904381
60	1	0	7.725471	1.213278	-2.236160
61	1	0	7.140415	2.814500	-2.836541
62	6	0	4.644284	-0.000736	2.528283
63	1	0	4.573170	-1.009339	2.070555

64	6	0	5.754775	-0.091752	3.582023
65	1	0	6.734676	-0.272815	3.090601
66	1	0	5.556632	-0.939711	4.272527
67	1	0	5.821603	0.838174	4.185103
68	6	0	3.287358	0.278206	3.184245
69	1	0	3.286303	1.251534	3.718717
70	1	0	3.052388	-0.521693	3.917135
71	1	0	2.484316	0.289493	2.417076
72	6	0	3.560274	-1.029194	-0.556361
73	6	0	3.488428	-2.401292	-1.223269
74	1	0	4.357138	-2.985079	-0.903954
75	6	0	3.437038	-2.371891	-2.749881
76	1	0	4.371053	-1.997741	-3.175661
77	1	0	2.615459	-1.728484	-3.075715
78	6	0	3.179603	-3.853627	-3.096663
79	1	0	4.144583	-4.357452	-3.204337
80	6	0	2.273389	-4.104070	-4.323194
81	1	0	2.360170	-3.305419	-5.068154
82	1	0	2.570918	-5.039491	-4.812264
83	6	0	0.854496	-4.243779	-3.744924
84	1	0	0.177389	-4.786907	-4.413171
85	1	0	0.422905	-3.257703	-3.548707
86	6	0	1.077932	-4.975373	-2.410253
87	1	0	0.250236	-4.854797	-1.711588
88	1	0	1.213262	-6.049556	-2.590438
89	6	0	2.412634	-4.440679	-1.870234
90	1	0	2.990115	-5.195023	-1.334140
91	6	0	2.329775	-3.674399	0.585644
92	1	0	3.296912	-4.169835	0.714341
93	1	0	2.319639	-2.751533	1.164415
94	6	0	1.227332	-4.621923	1.064968
95	1	0	1.544913	-4.971692	2.053772
96	1	0	1.220355	-5.516543	0.432018
97	6	0	-0.229008	-4.150480	1.125776
98	1	0	-0.532511	-3.721609	0.173702
99	1	0	-0.862175	-5.013135	1.352769
100	6	0	-0.326965	-3.615807	3.632572
101	1	0	-0.407526	-4.701880	3.570816
102	6	0	0.997807	-3.144566	4.248798
103	1	0	1.770677	-2.962588	3.501734
104	1	0	1.348660	-3.943654	4.913948
105	6	0	0.640812	-1.894915	5.073531
106	1	0	0.596525	-1.023152	4.412813
107	1	0	1.371579	-1.687900	5.862642

108	6	0	-0.758151	-2.212589	5.627677
109	1	0	-1.316836	-1.319891	5.930036
110	1	0	-0.673714	-2.858291	6.510140
111	6	0	-1.464627	-2.982853	4.490573
112	1	0	-2.113701	-3.770357	4.884887
113	6	0	-2.282237	-2.118769	3.511130
114	1	0	-1.893987	-1.098430	3.441455
115	1	0	-3.340137	-2.073394	3.781082
116	6	0	-2.071126	-2.840993	2.180049
117	1	0	-2.546428	-3.826920	2.229113
118	6	0	-2.626404	-2.119542	0.951411
119	6	0	-4.663435	-1.320244	-0.044675
120	6	0	-4.817374	-1.775433	-1.382074
121	6	0	-5.465960	-0.944470	-2.313411
122	1	0	-5.594279	-1.259530	-3.340392
123	6	0	-5.951189	0.304197	-1.938766
124	1	0	-6.441684	0.933376	-2.670392
125	6	0	-5.799236	0.752912	-0.631583
126	1	0	-6.177212	1.734398	-0.377371
127	6	0	-5.160131	-0.044608	0.334971
128	6	0	-4.985361	0.494352	1.751701
129	1	0	-4.485889	-0.253222	2.399511
130	6	0	-6.339717	0.791895	2.405668
131	1	0	-6.195045	1.073469	3.470861
132	1	0	-6.985928	-0.111598	2.374704
133	1	0	-6.864346	1.626455	1.894483
134	6	0	-4.087152	1.735867	1.759905
135	1	0	-3.107577	1.497423	1.294437
136	1	0	-3.898137	2.065428	2.803793
137	1	0	-4.556956	2.576349	1.207797
138	6	0	-4.298811	-3.139571	-1.829111
139	1	0	-3.836857	-3.681785	-0.978560
140	6	0	-5.441379	-4.031562	-2.329123
141	1	0	-6.226045	-4.121467	-1.547432
142	1	0	-5.059680	-5.051434	-2.550443
143	1	0	-5.901567	-3.624400	-3.254054
144	6	0	-3.208054	-2.993851	-2.898472
145	1	0	-3.614792	-2.558484	-3.835607
146	1	0	-2.770172	-3.987233	-3.135313
147	1	0	-2.390343	-2.340403	-2.527971
148	20	0	0.237913	-0.696329	-0.029449

L3a-Ca(II)-TS1-*re*

Zero-point correction= 1.26050 a.u.
Thermal correction to Gibbs Free Energy= 1.15561 a.u.
Sum of electronic and zero-point Energies= -6232.79729 a.u.
Sum of electronic and thermal Free Energies= -6232.90219 a.u.
The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.586749	-3.513763	-1.376662
2	6	0	-0.898144	-4.348852	-0.275268
3	8	0	-1.816840	-5.254788	-0.484423
4	6	0	-2.295321	-6.136414	0.565409
5	6	0	-0.275508	-4.081049	1.041875
6	1	0	0.427045	-3.122906	-1.363280
7	1	0	-0.911616	-3.890354	-2.344343
8	1	0	-2.937994	-6.851106	0.052937
9	1	0	-2.874314	-5.558955	1.288152
10	1	0	-1.460192	-6.652356	1.042707
11	1	0	0.804475	-4.259527	0.977881
12	1	0	-0.688259	-4.655332	1.869923
13	1	0	-0.407945	-2.996857	1.213931
14	6	0	-1.008658	-1.251785	-2.418795
15	6	0	-1.476885	-1.863825	-1.073840
16	6	0	-2.925046	-2.174334	-1.359989
17	6	0	-3.152255	-1.950051	-2.731661
18	7	0	-1.982092	-1.433513	-3.343326
19	8	0	-1.041703	-1.303912	-0.000960
20	8	0	0.071204	-0.664038	-2.562551
21	6	0	-1.878237	-1.052111	-4.745158
22	6	0	-3.984223	-2.587042	-0.572298
23	6	0	-4.386756	-2.166637	-3.325729
24	1	0	-1.930416	-1.940438	-5.382524
25	1	0	-0.917860	-0.556141	-4.889544
26	1	0	-2.685892	-0.367593	-5.018226
27	6	0	-5.431886	-2.605488	-2.500157
28	6	0	-5.247685	-2.808694	-1.132496
29	1	0	-4.549929	-1.989665	-4.383196
30	1	0	-6.413265	-2.778168	-2.931395
31	1	0	-6.074815	-3.125973	-0.507203
32	35	0	-3.745350	-2.825912	1.311260
33	8	0	1.248829	2.716463	-0.300531
34	8	0	-1.386492	1.749362	-0.449677

35	8	0	1.152571	0.418201	1.978070
36	7	0	-2.954575	3.233519	0.256412
37	1	0	-3.161989	4.162870	0.602608
38	7	0	0.692487	3.763641	0.385155
39	7	0	4.940134	-1.030517	0.553469
40	1	0	5.555259	-1.229253	1.334292
41	7	0	2.347176	0.702242	2.588484
42	6	0	-3.998086	2.278931	0.254931
43	6	0	-4.343956	1.608129	1.456360
44	6	0	-5.353470	0.629066	1.422526
45	1	0	-5.636954	0.095511	2.320048
46	6	0	-6.006400	0.319569	0.233741
47	1	0	-6.777461	-0.439970	0.224811
48	6	0	-5.674794	0.983049	-0.942981
49	1	0	-6.201356	0.717778	-1.850154
50	6	0	-4.682217	1.979802	-0.952132
51	6	0	-4.367022	2.716581	-2.250128
52	1	0	-3.611894	3.511102	-2.076902
53	6	0	-3.768088	1.763506	-3.288256
54	1	0	-2.855084	1.283629	-2.876991
55	1	0	-3.476153	2.325631	-4.200976
56	1	0	-4.494588	0.975469	-3.578154
57	6	0	-5.607614	3.426639	-2.805798
58	1	0	-5.329232	4.050555	-3.682056
59	1	0	-6.042717	4.096455	-2.033454
60	1	0	-6.382972	2.700841	-3.129814
61	6	0	-3.642751	1.920541	2.774553
62	1	0	-2.885673	2.720663	2.637444
63	6	0	-4.636040	2.443392	3.819442
64	1	0	-5.187721	3.320171	3.417535
65	1	0	-4.093077	2.768654	4.732790
66	1	0	-5.369161	1.661776	4.110850
67	6	0	-2.885928	0.697362	3.302366
68	1	0	-3.578627	-0.133111	3.552590
69	1	0	-2.325829	0.969119	4.221573
70	1	0	-2.158452	0.342300	2.542326
71	6	0	-1.696089	2.896310	-0.099300
72	6	0	-0.729553	4.077776	-0.111241
73	1	0	-1.105413	4.857199	0.558076
74	6	0	-0.469204	4.682931	-1.486613
75	1	0	-1.366493	5.159086	-1.889707
76	1	0	-0.144654	3.898931	-2.176263
77	6	0	0.657432	5.692842	-1.186030
78	1	0	0.201441	6.646449	-0.904259

79	6	0	1.705019	5.877473	-2.305246
80	1	0	1.273714	5.728346	-3.301339
81	1	0	2.101508	6.899550	-2.271419
82	6	0	2.819082	4.871451	-1.969990
83	1	0	3.776019	5.130868	-2.435231
84	1	0	2.538577	3.867808	-2.304504
85	6	0	2.882050	4.898910	-0.432477
86	1	0	3.350397	4.012719	-0.003632
87	1	0	3.449370	5.777047	-0.098585
88	6	0	1.431955	5.096401	0.031558
89	1	0	1.351396	5.716276	0.925676
90	6	0	0.651893	3.481424	1.876787
91	1	0	0.152538	4.337523	2.339633
92	1	0	0.029079	2.595076	1.992037
93	6	0	2.003693	3.274213	2.563198
94	1	0	1.794962	3.266380	3.639169
95	1	0	2.635287	4.155235	2.400743
96	6	0	2.873437	2.071090	2.191861
97	1	0	3.011746	2.028757	1.113524
98	1	0	3.846541	2.180727	2.679729
99	6	0	2.213363	0.516585	4.135088
100	1	0	2.938163	1.204009	4.573424
101	6	0	0.788110	0.727345	4.663113
102	1	0	0.210782	1.426443	4.057220
103	1	0	0.876827	1.146768	5.673255
104	6	0	0.164537	-0.678577	4.730551
105	1	0	-0.212974	-0.954029	3.741708
106	1	0	-0.666128	-0.736806	5.442063
107	6	0	1.344409	-1.583602	5.125501
108	1	0	1.188148	-2.635886	4.862428
109	1	0	1.502156	-1.539980	6.209949
110	6	0	2.568994	-0.980001	4.403326
111	1	0	3.466346	-1.040470	5.025851
112	6	0	2.896708	-1.578245	3.019118
113	1	0	2.006871	-1.976009	2.524476
114	1	0	3.655368	-2.362884	3.070189
115	6	0	3.404673	-0.354111	2.259536
116	1	0	4.323794	-0.003206	2.738276
117	6	0	3.695308	-0.557189	0.771180
118	6	0	5.389925	-1.371843	-0.742308
119	6	0	5.923544	-0.368081	-1.592171
120	6	0	6.341212	-0.724945	-2.887214
121	1	0	6.740158	0.018789	-3.564221
122	6	0	6.257706	-2.043091	-3.324724

123	1	0	6.587873	-2.301324	-4.322819
124	6	0	5.755763	-3.031692	-2.484195
125	1	0	5.709813	-4.047848	-2.853337
126	6	0	5.315002	-2.717907	-1.185644
127	6	0	4.764684	-3.823689	-0.290082
128	1	0	4.441938	-3.413021	0.688946
129	6	0	5.840587	-4.871770	0.014610
130	1	0	5.451146	-5.619315	0.738764
131	1	0	6.730261	-4.384208	0.467936
132	1	0	6.156251	-5.408621	-0.904926
133	6	0	3.524253	-4.475492	-0.911364
134	1	0	2.766386	-3.699852	-1.146611
135	1	0	3.072460	-5.196103	-0.196441
136	1	0	3.776103	-5.022796	-1.843995
137	6	0	6.057460	1.080260	-1.130063
138	1	0	5.731224	1.188277	-0.074532
139	6	0	7.517978	1.546508	-1.171184
140	1	0	8.156134	0.857906	-0.576894
141	1	0	7.606405	2.562009	-0.729058
142	1	0	7.904199	1.586196	-2.211412
143	6	0	5.162244	2.007234	-1.958796
144	1	0	5.466240	2.017462	-3.026776
145	1	0	5.228018	3.044544	-1.568206
146	1	0	4.104517	1.675443	-1.890548
147	8	0	2.892450	-0.334566	-0.148016
148	20	0	0.619530	0.432851	-0.305658

L3a-Ca(II)-TS2-*re*

Zero-point correction= 1.25802 a.u.

Thermal correction to Gibbs Free Energy= 1.15590 a.u.

Sum of electronic and zero-point Energies= -6232.79671 a.u.

Sum of electronic and thermal Free Energies= -6232.89883 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.799178	-3.490653	-1.502607
2	6	0	-0.849300	-4.235253	-0.234926
3	8	0	-1.770646	-5.165427	-0.174000
4	6	0	-1.962536	-5.926935	1.043369
5	6	0	-0.120332	-3.695652	0.846286

6	1	0	0.238104	-3.287969	-1.775963
7	1	0	-1.311991	-4.004644	-2.315250
8	1	0	-2.648963	-6.727538	0.770313
9	1	0	-2.411706	-5.291022	1.807760
10	1	0	-1.009923	-6.337541	1.385240
11	1	0	0.904208	-3.410843	0.603410
12	1	0	-0.232923	-4.132325	1.835278
13	1	0	-0.634526	-2.507440	0.671199
14	6	0	-1.004931	-1.238254	-2.498553
15	6	0	-1.480573	-2.009619	-1.245346
16	6	0	-2.976764	-2.105270	-1.516192
17	6	0	-3.194007	-1.742160	-2.857851
18	7	0	-1.985069	-1.268769	-3.430783
19	8	0	-1.039247	-1.442249	-0.090337
20	8	0	0.103815	-0.693878	-2.591312
21	6	0	-1.853167	-0.762910	-4.790378
22	6	0	-4.069672	-2.467646	-0.751172
23	6	0	-4.443695	-1.794571	-3.457888
24	1	0	-1.992023	-1.579227	-5.506036
25	1	0	-0.851462	-0.347362	-4.901983
26	1	0	-2.595167	0.015179	-4.988128
27	6	0	-5.521679	-2.205522	-2.662003
28	6	0	-5.349933	-2.528489	-1.316768
29	1	0	-4.590844	-1.512989	-4.494832
30	1	0	-6.516072	-2.254897	-3.095247
31	1	0	-6.199979	-2.814204	-0.707339
32	35	0	-3.878214	-2.830493	1.118894
33	8	0	1.278429	2.606212	-0.220908
34	8	0	-1.384400	1.680927	-0.369442
35	8	0	1.135913	0.240464	1.971647
36	7	0	-2.910276	3.188811	0.386349
37	1	0	-3.096355	4.127798	0.718029
38	7	0	0.736782	3.640745	0.496361
39	7	0	4.953580	-1.111592	0.534752
40	1	0	5.624785	-1.155964	1.292813
41	7	0	2.325388	0.487693	2.608910
42	6	0	-3.991944	2.279716	0.340078
43	6	0	-4.352742	1.551196	1.502385
44	6	0	-5.410232	0.626922	1.425022
45	1	0	-5.707817	0.052888	2.292411
46	6	0	-6.094401	0.425502	0.230559
47	1	0	-6.903030	-0.292515	0.187590
48	6	0	-5.745185	1.143720	-0.908529
49	1	0	-6.295090	0.960766	-1.822112

50	6	0	-4.707272	2.092193	-0.870883
51	6	0	-4.374970	2.896400	-2.123356
52	1	0	-3.589609	3.650441	-1.908975
53	6	0	-3.818560	1.987709	-3.221941
54	1	0	-2.926038	1.445588	-2.844312
55	1	0	-3.505261	2.594468	-4.098276
56	1	0	-4.578117	1.250703	-3.557517
57	6	0	-5.591445	3.685204	-2.623198
58	1	0	-5.294782	4.352676	-3.460568
59	1	0	-5.996678	4.320151	-1.806355
60	1	0	-6.395080	3.010705	-2.986532
61	6	0	-3.620547	1.748374	2.825692
62	1	0	-2.827921	2.519184	2.725851
63	6	0	-4.573465	2.250924	3.916997
64	1	0	-5.088000	3.176038	3.579441
65	1	0	-4.002882	2.492864	4.839424
66	1	0	-5.338894	1.487632	4.172028
67	6	0	-2.916789	0.460277	3.264521
68	1	0	-3.644826	-0.353046	3.466245
69	1	0	-2.341310	0.645957	4.195215
70	1	0	-2.209854	0.124531	2.476543
71	6	0	-1.666811	2.828466	0.003140
72	6	0	-0.676696	3.990769	0.005278
73	1	0	-1.036561	4.764941	0.688930
74	6	0	-0.403061	4.617985	-1.357586
75	1	0	-1.289729	5.121600	-1.750262
76	1	0	-0.095185	3.842247	-2.063635
77	6	0	0.745218	5.597993	-1.036174
78	1	0	0.309889	6.559298	-0.747808
79	6	0	1.808066	5.771582	-2.144115
80	1	0	1.385421	5.630326	-3.144964
81	1	0	2.216456	6.788624	-2.103861
82	6	0	2.907161	4.751301	-1.801254
83	1	0	3.873389	5.002611	-2.251715
84	1	0	2.619642	3.753183	-2.145221
85	6	0	2.949404	4.768054	-0.262999
86	1	0	3.406490	3.877352	0.168457
87	1	0	3.517203	5.640310	0.084886
88	6	0	1.495075	4.971772	0.182479
89	1	0	1.405284	5.574021	1.087773
90	6	0	0.682921	3.313926	1.978307
91	1	0	0.192171	4.162777	2.462626
92	1	0	0.046751	2.433769	2.061739
93	6	0	2.024085	3.064154	2.669580

94	1	0	1.804054	3.020726	3.742451
95	1	0	2.671690	3.939632	2.545070
96	6	0	2.875432	1.860291	2.263122
97	1	0	3.019338	1.852869	1.184446
98	1	0	3.847641	1.935282	2.758588
99	6	0	2.169967	0.252685	4.147319
100	1	0	2.893034	0.921392	4.616214
101	6	0	0.739566	0.454832	4.664196
102	1	0	0.172667	1.173464	4.071379
103	1	0	0.817718	0.845477	5.686722
104	6	0	0.110322	-0.950158	4.685203
105	1	0	-0.256703	-1.196890	3.684417
106	1	0	-0.728642	-1.025678	5.385218
107	6	0	1.282099	-1.870098	5.068143
108	1	0	1.123892	-2.915064	4.778314
109	1	0	1.430235	-1.853493	6.154688
110	6	0	2.514873	-1.253970	4.372146
111	1	0	3.408572	-1.339764	4.996845
112	6	0	2.845410	-1.811054	2.971654
113	1	0	1.952558	-2.175283	2.456789
114	1	0	3.591199	-2.609099	2.999923
115	6	0	3.379662	-0.569509	2.261818
116	1	0	4.293220	-0.243064	2.768505
117	6	0	3.683766	-0.720414	0.771748
118	6	0	5.434948	-1.309211	-0.779841
119	6	0	6.083365	-0.246782	-1.462113
120	6	0	6.533193	-0.457477	-2.778291
121	1	0	7.025267	0.333942	-3.328061
122	6	0	6.351575	-1.686036	-3.405357
123	1	0	6.701258	-1.830161	-4.419619
124	6	0	5.720872	-2.729704	-2.735607
125	1	0	5.592117	-3.671144	-3.253104
126	6	0	5.256098	-2.563994	-1.418275
127	6	0	4.559878	-3.725198	-0.715362
128	1	0	4.274645	-3.444536	0.319796
129	6	0	5.487816	-4.939126	-0.587692
130	1	0	4.995578	-5.733815	0.013027
131	1	0	6.426298	-4.649335	-0.068441
132	1	0	5.743997	-5.362908	-1.581533
133	6	0	3.261165	-4.098267	-1.437717
134	1	0	2.624661	-3.196479	-1.553077
135	1	0	2.696943	-4.852746	-0.848706
136	1	0	3.464330	-4.520178	-2.444781
137	6	0	6.287997	1.115445	-0.806087

138	1	0	5.894041	1.115720	0.231663
139	6	0	7.777625	1.462549	-0.698767
140	1	0	8.320012	0.655054	-0.161885
141	1	0	7.909316	2.404556	-0.124222
142	1	0	8.237535	1.598541	-1.700306
143	6	0	5.521743	2.209411	-1.557843
144	1	0	5.913714	2.346465	-2.587560
145	1	0	5.614177	3.176188	-1.018726
146	1	0	4.444675	1.944852	-1.618131
147	8	0	2.854271	-0.552935	-0.134955
148	20	0	0.622644	0.341898	-0.323617

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Zero-point correction= 1.27060 a.u.

Thermal correction to Gibbs Free Energy= 1.17109 a.u.

Sum of electronic and zero-point Energies= -3659.24613 a.u.

Sum of electronic and thermal Free Energies= -3659.34564 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.135407	1.929568	-1.583918
2	6	0	-0.897924	2.528446	-0.172619
3	6	0	-1.975995	3.572505	-0.075692
4	6	0	-2.647927	3.609343	-1.310346
5	7	0	-2.109637	2.638172	-2.196973
6	8	0	-0.619422	1.681780	0.761364
7	6	0	-2.386976	4.392838	0.964816
8	6	0	-3.714941	4.465611	-1.541484
9	8	0	-0.548742	0.925537	-2.011938
10	6	0	-2.613441	2.363906	-3.534601
11	1	0	-2.433467	3.220961	-4.191212
12	1	0	-2.086412	1.491795	-3.922790
13	1	0	-3.686755	2.157957	-3.501411
14	6	0	-3.468854	5.260621	0.753602
15	6	0	-4.115035	5.297021	-0.483897
16	1	0	-3.809001	5.905010	1.558869
17	1	0	-4.951438	5.973483	-0.634724
18	1	0	-4.234929	4.488124	-2.493545
19	6	0	0.666918	3.523108	-0.697622
20	6	0	1.182884	4.036827	0.512257

21	8	0	0.859105	5.270593	0.809169
22	6	0	1.199922	5.861968	2.089956
23	1	0	0.750667	6.853885	2.066009
24	6	0	1.872348	3.133129	1.459024
25	1	0	0.778335	5.274049	2.907619
26	1	0	1.061044	2.510910	1.889477
27	1	0	1.249230	2.707520	-1.116094
28	1	0	0.321234	4.258291	-1.420423
29	1	0	2.518305	2.439550	0.916540
30	1	0	2.285139	5.941985	2.185621
31	1	0	2.422289	3.633656	2.255946
32	8	0	2.500886	-0.102661	-0.228325
33	8	0	0.960423	-2.074695	-1.540164
34	8	0	0.011703	-2.071070	1.651812
35	8	0	-2.042458	-1.285316	-0.102724
36	7	0	4.741187	-0.422506	-0.366257
37	1	0	5.509553	-0.931171	-0.788862
38	7	0	2.102207	-2.823527	-1.424937
39	7	0	-4.104370	-1.816704	0.670850
40	1	0	-4.645169	-2.316708	1.368162
41	7	0	-0.721912	-3.233495	1.609765
42	6	0	5.039657	0.777673	0.321071
43	6	0	4.944168	0.824472	1.736999
44	6	0	5.173518	2.046534	2.394939
45	1	0	5.096177	2.118319	3.471741
46	6	0	5.495538	3.193207	1.675958
47	1	0	5.662434	4.126864	2.197632
48	6	0	5.601153	3.146281	0.289672
49	1	0	5.849184	4.057118	-0.238904
50	6	0	5.382293	1.945645	-0.409968
51	6	0	5.491455	1.932800	-1.931712
52	1	0	5.316196	0.912612	-2.329736
53	6	0	4.425787	2.831359	-2.568397
54	1	0	3.414283	2.506823	-2.245954
55	1	0	4.470939	2.753393	-3.675877
56	1	0	4.568718	3.895515	-2.285107
57	6	0	6.897925	2.335390	-2.391521
58	1	0	6.989438	2.213216	-3.492198
59	1	0	7.657929	1.683230	-1.910193
60	1	0	7.121399	3.393657	-2.140051
61	6	0	4.594908	-0.415421	2.554674
62	1	0	4.494731	-1.303866	1.897166
63	6	0	5.705956	-0.753860	3.556132
64	1	0	6.679299	-0.851518	3.029178

65	1	0	5.487934	-1.722940	4.054254
66	1	0	5.798894	0.026098	4.340894
67	6	0	3.248177	-0.244147	3.266548
68	1	0	3.275545	0.597033	3.991022
69	1	0	2.992821	-1.172326	3.819289
70	1	0	2.443638	-0.052158	2.525439
71	6	0	3.466567	-0.752052	-0.661285
72	6	0	3.356527	-1.954003	-1.597931
73	1	0	4.208087	-2.614787	-1.410513
74	6	0	3.307571	-1.605941	-3.084888
75	1	0	4.252200	-1.176878	-3.427435
76	1	0	2.504682	-0.886348	-3.265016
77	6	0	3.009479	-2.974893	-3.731844
78	1	0	3.960353	-3.469522	-3.950804
79	6	0	2.094288	-2.940067	-4.976825
80	1	0	2.197304	-2.003833	-5.536502
81	1	0	2.369230	-3.756794	-5.655146
82	6	0	0.673600	-3.168049	-4.431634
83	1	0	-0.015761	-3.545374	-5.194641
84	1	0	0.263560	-2.236330	-4.030684
85	6	0	0.882876	-4.167099	-3.280531
86	1	0	0.059350	-4.175594	-2.566616
87	1	0	0.992680	-5.183144	-3.681046
88	6	0	2.230630	-3.786405	-2.649536
89	1	0	2.792029	-4.647482	-2.283464
90	6	0	2.152340	-3.541880	-0.087894
91	1	0	3.102694	-4.083580	-0.063965
92	1	0	2.168296	-2.758603	0.669376
93	6	0	1.017166	-4.532392	0.186095
94	1	0	1.322628	-5.094356	1.075689
95	1	0	0.981047	-5.272672	-0.620976
96	6	0	-0.424078	-4.038318	0.355576
97	1	0	-0.713390	-3.404218	-0.478842
98	1	0	-1.084233	-4.909710	0.392774
99	6	0	-0.488437	-4.063191	2.915372
100	1	0	-0.596187	-5.106626	2.616284
101	6	0	0.853971	-3.770030	3.600567
102	1	0	1.625176	-3.445186	2.901693
103	1	0	1.190079	-4.703961	4.068377
104	6	0	0.536864	-2.725051	4.685118
105	1	0	0.508427	-1.728713	4.232251
106	1	0	1.280428	-2.713137	5.489241
107	6	0	-0.863928	-3.126452	5.177253
108	1	0	-1.397832	-2.310345	5.676565

109	1	0	-0.785970	-3.951727	5.895271
110	6	0	-1.600699	-3.612961	3.909625
111	1	0	-2.263022	-4.454971	4.131380
112	6	0	-2.407865	-2.536972	3.159103
113	1	0	-1.998134	-1.534801	3.315598
114	1	0	-3.461173	-2.533958	3.449380
115	6	0	-2.227863	-2.941530	1.694864
116	1	0	-2.735377	-3.896874	1.519434
117	6	0	-2.756596	-1.933151	0.673414
118	6	0	-4.730463	-0.745008	-0.013053
119	6	0	-4.893751	-0.799190	-1.424686
120	6	0	-5.470693	0.299792	-2.086448
121	1	0	-5.606665	0.289650	-3.159762
122	6	0	-5.875157	1.426638	-1.379756
123	1	0	-6.310273	2.265815	-1.907101
124	6	0	-5.721675	1.481288	0.000848
125	1	0	-6.042633	2.375702	0.518346
126	6	0	-5.155040	0.404799	0.707698
127	6	0	-4.987483	0.513636	2.220876
128	1	0	-4.543365	-0.411623	2.637085
129	6	0	-6.341500	0.689621	2.918259
130	1	0	-6.209637	0.655441	4.021050
131	1	0	-7.029915	-0.133477	2.629740
132	1	0	-6.812233	1.660096	2.654480
133	6	0	-4.028614	1.650055	2.591796
134	1	0	-3.048334	1.495592	2.094430
135	1	0	-3.855428	1.661169	3.689225
136	1	0	-4.437657	2.638071	2.293943
137	6	0	-4.469542	-2.019882	-2.237010
138	1	0	-4.050577	-2.805854	-1.575551
139	6	0	-5.671008	-2.659169	-2.943408
140	1	0	-6.461665	-2.907434	-2.203048
141	1	0	-5.361750	-3.601977	-3.443621
142	1	0	-6.099453	-1.982059	-3.712077
143	6	0	-3.369265	-1.660488	-3.244945
144	1	0	-3.745379	-0.965765	-4.025340
145	1	0	-2.995577	-2.579240	-3.745812
146	1	0	-2.511424	-1.182622	-2.727094
147	20	0	0.160329	-0.460050	-0.055846
148	1	0	-1.890235	4.352831	1.929963

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Zero-point correction= 1.26765 a.u.

Thermal correction to Gibbs Free Energy= 1.16846 a.u.
Sum of electronic and zero-point Energies= -3659.24686 a.u.
Sum of electronic and thermal Free Energies= -3659.34605 a.u.
The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.986439	2.042565	-1.593470
2	6	0	-0.507927	2.786233	-0.322253
3	6	0	-1.596768	3.834602	-0.161255
4	6	0	-2.434178	3.772139	-1.285284
5	7	0	-2.024866	2.711791	-2.138516
6	8	0	-0.312796	1.896796	0.706506
7	6	0	-1.861254	4.750052	0.845873
8	6	0	-3.522737	4.618012	-1.448068
9	8	0	-0.489062	0.979101	-1.993301
10	6	0	-2.694417	2.333808	-3.374051
11	1	0	-2.517377	3.089547	-4.146026
12	1	0	-2.292547	1.375087	-3.702783
13	1	0	-3.770236	2.241694	-3.207648
14	6	0	-2.963058	5.608899	0.708640
15	6	0	-3.774985	5.544538	-0.425490
16	1	0	-3.186909	6.326032	1.492906
17	1	0	-4.623244	6.216514	-0.519728
18	1	0	-4.164067	4.562197	-2.321619
19	6	0	0.896652	3.480945	-0.788783
20	6	0	1.602314	3.913230	0.430195
21	8	0	1.524592	5.194000	0.699004
22	6	0	2.090269	5.713088	1.929389
23	1	0	2.017388	6.796127	1.839370
24	6	0	2.016133	2.897161	1.317604
25	1	0	1.507973	5.364052	2.785357
26	1	0	0.834659	2.357777	1.321628
27	1	0	1.462877	2.689021	-1.284356
28	1	0	0.698647	4.301310	-1.478887
29	1	0	2.511057	2.052472	0.835804
30	1	0	3.135185	5.407007	2.021792
31	1	0	2.422284	3.166169	2.288987
32	8	0	2.464713	-0.233585	-0.255672
33	8	0	0.762179	-2.130716	-1.464981
34	8	0	-0.073958	-1.986179	1.726210
35	8	0	-2.144786	-1.120912	-0.014942

36	7	0	4.674997	-0.707835	-0.443076
37	1	0	5.394508	-1.281551	-0.868547
38	7	0	1.855357	-2.950877	-1.365066
39	7	0	-4.210928	-1.571567	0.801729
40	1	0	-4.755742	-2.013948	1.533872
41	7	0	-0.887177	-3.094720	1.746828
42	6	0	5.074557	0.487606	0.199668
43	6	0	5.010515	0.585521	1.614809
44	6	0	5.331323	1.810551	2.227534
45	1	0	5.280639	1.921396	3.302626
46	6	0	5.713605	2.909745	1.465563
47	1	0	5.951562	3.846549	1.952927
48	6	0	5.793327	2.810354	0.080390
49	1	0	6.094201	3.684211	-0.482174
50	6	0	5.485012	1.604421	-0.574894
51	6	0	5.578047	1.531137	-2.096065
52	1	0	5.328430	0.512451	-2.456163
53	6	0	4.571950	2.478833	-2.757375
54	1	0	3.543649	2.234619	-2.418629
55	1	0	4.603171	2.360781	-3.861660
56	1	0	4.789151	3.539667	-2.511207
57	6	0	7.004766	1.817883	-2.579837
58	1	0	7.076737	1.650515	-3.676020
59	1	0	7.722011	1.131408	-2.080711
60	1	0	7.303749	2.866152	-2.367866
61	6	0	4.602696	-0.603523	2.479555
62	1	0	4.426821	-1.502524	1.852869
63	6	0	5.716854	-0.984551	3.462168
64	1	0	6.666091	-1.164140	2.913393
65	1	0	5.449094	-1.920543	3.998048
66	1	0	5.883711	-0.188043	4.217507
67	6	0	3.290343	-0.323625	3.220507
68	1	0	3.392237	0.533901	3.918557
69	1	0	2.992088	-1.217124	3.807923
70	1	0	2.478817	-0.101665	2.495596
71	6	0	3.373527	-0.956904	-0.696084
72	6	0	3.157768	-2.171395	-1.597370
73	1	0	3.970087	-2.882095	-1.416539
74	6	0	3.087716	-1.858996	-3.091290
75	1	0	4.047643	-1.502283	-3.472094
76	1	0	2.328401	-1.093052	-3.269394
77	6	0	2.682019	-3.221780	-3.691670
78	1	0	3.591702	-3.784937	-3.919937
79	6	0	1.737475	-3.158332	-4.913191

80	1	0	1.889694	-2.248238	-5.503720
81	1	0	1.935810	-4.011687	-5.572913
82	6	0	0.320412	-3.270178	-4.324192
83	1	0	-0.415722	-3.617268	-5.057314
84	1	0	-0.010835	-2.300988	-3.939315
85	6	0	0.492112	-4.250889	-3.151463
86	1	0	-0.309486	-4.183874	-2.416026
87	1	0	0.520019	-5.281904	-3.526794
88	6	0	1.880142	-3.949529	-2.567172
89	1	0	2.390018	-4.839042	-2.194718
90	6	0	1.905502	-3.639060	-0.012120
91	1	0	2.821146	-4.238072	-0.004468
92	1	0	1.992942	-2.840197	0.723213
93	6	0	0.721901	-4.550106	0.323154
94	1	0	1.018034	-5.104057	1.221016
95	1	0	0.616776	-5.308525	-0.460813
96	6	0	-0.679481	-3.961948	0.516660
97	1	0	-0.954067	-3.339392	-0.331551
98	1	0	-1.391249	-4.787794	0.605593
99	6	0	-0.680726	-3.887399	3.080230
100	1	0	-0.867786	-4.931526	2.826346
101	6	0	0.694414	-3.661973	3.724596
102	1	0	1.467907	-3.417324	2.996308
103	1	0	0.977936	-4.598776	4.220731
104	6	0	0.475366	-2.558055	4.774535
105	1	0	0.504658	-1.579340	4.284837
106	1	0	1.236663	-2.568207	5.561908
107	6	0	-0.937952	-2.841500	5.310591
108	1	0	-1.401575	-1.972094	5.789965
109	1	0	-0.901143	-3.643937	6.057268
110	6	0	-1.735945	-3.319804	4.077972
111	1	0	-2.452487	-4.102297	4.345000
112	6	0	-2.480853	-2.217705	3.300427
113	1	0	-1.993607	-1.243567	3.402496
114	1	0	-3.524025	-2.122143	3.611862
115	6	0	-2.365919	-2.700203	1.854117
116	1	0	-2.935507	-3.629312	1.741029
117	6	0	-2.868219	-1.718107	0.794652
118	6	0	-4.833685	-0.560479	0.030568
119	6	0	-5.073149	-0.769304	-1.354528
120	6	0	-5.665098	0.262000	-2.105798
121	1	0	-5.855641	0.136512	-3.163467
122	6	0	-6.013728	1.469433	-1.509521
123	1	0	-6.462994	2.254300	-2.104343

124	6	0	-5.775427	1.678107	-0.155723
125	1	0	-6.046311	2.634033	0.272875
126	6	0	-5.186587	0.675440	0.635842
127	6	0	-4.912550	0.952916	2.110929
128	1	0	-4.459622	0.068103	2.601256
129	6	0	-6.210399	1.248997	2.871843
130	1	0	-6.002646	1.338798	3.959721
131	1	0	-6.935184	0.419054	2.728429
132	1	0	-6.676698	2.196301	2.527987
133	6	0	-3.905673	2.096524	2.277058
134	1	0	-2.970023	1.858899	1.728558
135	1	0	-3.647905	2.228069	3.349768
136	1	0	-4.316171	3.055152	1.896505
137	6	0	-4.705557	-2.081081	-2.042895
138	1	0	-4.277212	-2.800013	-1.314557
139	6	0	-5.944139	-2.765226	-2.634060
140	1	0	-6.713329	-2.910561	-1.845395
141	1	0	-5.671732	-3.764932	-3.035725
142	1	0	-6.385148	-2.167659	-3.459555
143	6	0	-3.634602	-1.859447	-3.119198
144	1	0	-4.020489	-1.234283	-3.952071
145	1	0	-3.305236	-2.834915	-3.537241
146	1	0	-2.745463	-1.359265	-2.680807
147	20	0	0.104475	-0.415869	-0.019490
148	1	0	-1.236576	4.797152	1.733040

L3a-Ca(II)-TS1-*re*-H

Zero-point correction= 1.26919 a.u.

Thermal correction to Gibbs Free Energy= 1.16850 a.u.

Sum of electronic and zero-point Energies= -3659.23958 a.u.

Sum of electronic and thermal Free Energies= -3659.34027 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.279262	3.811296	-1.057830
2	6	0	0.400750	4.631651	0.095901
3	8	0	1.209699	5.650812	-0.008873
4	6	0	1.525257	6.507534	1.121212
5	6	0	-0.222236	4.202145	1.364244
6	1	0	-0.670809	3.288295	-1.132664

7	1	0	0.602854	4.279645	-1.985545
8	1	0	2.184243	7.271419	0.710629
9	1	0	2.042931	5.938766	1.895587
10	1	0	0.612966	6.962859	1.511564
11	1	0	-1.307335	4.119884	1.240400
12	1	0	0.005302	4.827247	2.226525
13	1	0	0.149116	3.166386	1.515260
14	6	0	1.127669	1.685812	-2.122930
15	6	0	1.389002	2.352650	-0.745723
16	6	0	2.786929	2.896113	-0.922128
17	6	0	3.155943	2.710828	-2.265043
18	7	0	2.136816	2.008687	-2.963667
19	8	0	0.993596	1.685000	0.292674
20	8	0	0.162135	0.942903	-2.353128
21	6	0	2.209073	1.616321	-4.363549
22	6	0	3.670961	3.491710	-0.035185
23	6	0	4.382425	3.133834	-2.757584
24	1	0	2.109305	2.494755	-5.009707
25	1	0	1.392586	0.921853	-4.565117
26	1	0	3.163656	1.127308	-4.574097
27	6	0	5.262406	3.748382	-1.853292
28	6	0	4.919740	3.920469	-0.510421
29	1	0	4.663012	2.986407	-3.795454
30	1	0	6.232292	4.085011	-2.208247
31	1	0	5.626773	4.382772	0.172242
32	8	0	-0.552366	-2.658515	-0.343333
33	8	0	1.864266	-1.247457	-0.197350
34	8	0	-1.045869	-0.482616	2.037156
35	7	0	3.646660	-2.495676	0.447180
36	1	0	4.033742	-3.416606	0.617277
37	7	0	0.123940	-3.627378	0.350528
38	7	0	-4.902128	0.365368	0.341702
39	1	0	-5.599672	0.436870	1.074103
40	7	0	-2.212416	-1.010726	2.528791
41	6	0	4.530386	-1.391909	0.455108
42	6	0	4.648292	-0.590844	1.620232
43	6	0	5.481286	0.542388	1.585349
44	1	0	5.583342	1.181584	2.452352
45	6	0	6.190103	0.870027	0.434048
46	1	0	6.828701	1.743760	0.424989
47	6	0	6.076765	0.084286	-0.708155
48	1	0	6.630808	0.375352	-1.590716
49	6	0	5.255548	-1.057706	-0.717874
50	6	0	5.146249	-1.895867	-1.987182

51	1	0	4.507871	-2.786774	-1.815298
52	6	0	4.482080	-1.096513	-3.112033
53	1	0	3.482703	-0.740635	-2.781833
54	1	0	4.337139	-1.739785	-4.006325
55	1	0	5.101157	-0.222015	-3.403912
56	6	0	6.514845	-2.432781	-2.423407
57	1	0	6.394980	-3.133942	-3.277171
58	1	0	6.990344	-2.989117	-1.587177
59	1	0	7.192873	-1.612968	-2.741209
60	6	0	3.886628	-0.927616	2.898205
61	1	0	3.326086	-1.878939	2.782343
62	6	0	4.841523	-1.138992	4.079568
63	1	0	5.604078	-1.905277	3.823364
64	1	0	4.277118	-1.501189	4.965604
65	1	0	5.358296	-0.197318	4.359922
66	6	0	2.849159	0.153249	3.218168
67	1	0	3.329425	1.138817	3.395344
68	1	0	2.279332	-0.127308	4.128636
69	1	0	2.131693	0.250698	2.376568
70	6	0	2.357427	-2.350920	0.070835
71	6	0	1.608929	-3.676039	-0.044695
72	1	0	2.068458	-4.403275	0.631574
73	6	0	1.555038	-4.263185	-1.451969
74	1	0	2.546473	-4.566300	-1.797086
75	1	0	1.151882	-3.518951	-2.144393
76	6	0	0.599533	-5.459196	-1.266359
77	1	0	1.190278	-6.332115	-0.973548
78	6	0	-0.315736	-5.774748	-2.469061
79	1	0	0.156818	-5.519476	-3.424039
80	1	0	-0.535349	-6.849125	-2.490785
81	6	0	-1.605096	-4.981334	-2.198991
82	1	0	-2.467034	-5.379039	-2.745260
83	1	0	-1.474395	-3.933002	-2.485464
84	6	0	-1.776921	-5.076647	-0.672599
85	1	0	-2.419203	-4.297398	-0.261987
86	1	0	-2.211379	-6.048819	-0.406944
87	6	0	-0.352509	-5.048700	-0.099251
88	1	0	-0.235720	-5.682699	0.780709
89	6	0	0.008303	-3.409954	1.849163
90	1	0	0.617023	-4.185862	2.322414
91	1	0	0.453963	-2.434914	2.041656
92	6	0	-1.404837	-3.474382	2.432239
93	1	0	-1.279921	-3.478377	3.521130
94	1	0	-1.854879	-4.444581	2.192631

95	6	0	-2.444937	-2.426661	2.029422
96	1	0	-2.496529	-2.348227	0.945421
97	1	0	-3.419743	-2.735185	2.417447
98	6	0	-2.234452	-0.895759	4.088191
99	1	0	-2.842715	-1.733441	4.431744
100	6	0	-0.837718	-0.863521	4.723906
101	1	0	-0.090577	-1.391907	4.130522
102	1	0	-0.913265	-1.361206	5.698864
103	6	0	-0.511562	0.628486	4.918022
104	1	0	-0.123009	1.038142	3.980870
105	1	0	0.235927	0.797112	5.700664
106	6	0	-1.872947	1.261154	5.254173
107	1	0	-1.906823	2.339907	5.064114
108	1	0	-2.102965	1.110916	6.315852
109	6	0	-2.893654	0.486440	4.392529
110	1	0	-3.834814	0.336690	4.929514
111	6	0	-3.214544	1.100619	3.013956
112	1	0	-2.380138	1.687735	2.621639
113	1	0	-4.110316	1.725889	3.034000
114	6	0	-3.418731	-0.146060	2.153963
115	1	0	-4.293248	-0.687607	2.527759
116	6	0	-3.616427	0.096681	0.657002
117	6	0	-5.270060	0.769489	-0.962704
118	6	0	-5.487455	-0.206496	-1.970526
119	6	0	-5.801604	0.219251	-3.273815
120	1	0	-5.963937	-0.499448	-4.066019
121	6	0	-5.916826	1.573109	-3.572726
122	1	0	-6.161727	1.883103	-4.580509
123	6	0	-5.723027	2.530035	-2.581648
124	1	0	-5.820778	3.574331	-2.847248
125	6	0	-5.398905	2.150254	-1.266409
126	6	0	-5.176127	3.225532	-0.207199
127	1	0	-4.937710	2.766604	0.773759
128	6	0	-6.441636	4.063341	0.008125
129	1	0	-6.291721	4.770236	0.852294
130	1	0	-7.297622	3.402509	0.263254
131	1	0	-6.699699	4.651733	-0.897598
132	6	0	-3.981149	4.115636	-0.566093
133	1	0	-3.076704	3.489882	-0.715155
134	1	0	-3.775101	4.829935	0.259610
135	1	0	-4.170701	4.697592	-1.492728
136	6	0	-5.403480	-1.699711	-1.666734
137	1	0	-5.192032	-1.870920	-0.590775
138	6	0	-6.737284	-2.400970	-1.952499

139	1	0	-7.558789	-1.901789	-1.395162
140	1	0	-6.690694	-3.459544	-1.617819
141	1	0	-6.980246	-2.390128	-3.036065
142	6	0	-4.259854	-2.358726	-2.445094
143	1	0	-4.428618	-2.301283	-3.541053
144	1	0	-4.178245	-3.428867	-2.160925
145	1	0	-3.296736	-1.860132	-2.205183
146	8	0	-2.713317	0.068043	-0.192187
147	20	0	-0.336851	-0.297305	-0.193025
148	1	0	3.406342	3.611387	1.012054

L3a-Ca(II)-TS2-*re*-H

Zero-point correction= 1.26959 a.u.

Thermal correction to Gibbs Free Energy= 1.16930 a.u.

Sum of electronic and zero-point Energies= -3659.23831 a.u.

Sum of electronic and thermal Free Energies= -3659.33861 a.u.

The number of imaginary frequencies 1

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.525215	-3.808416	-1.328762
2	6	0	-0.382426	-4.548048	-0.066881
3	8	0	-1.195064	-5.566757	0.079084
4	6	0	-1.235062	-6.294929	1.332089
5	6	0	0.359205	-3.918757	0.958638
6	1	0	0.445997	-3.449059	-1.672684
7	1	0	-1.019018	-4.386539	-2.109731
8	1	0	-1.847980	-7.172357	1.129095
9	1	0	-1.699803	-5.679606	2.106091
10	1	0	-0.226540	-6.593153	1.627512
11	1	0	1.318199	-3.511104	0.636652
12	1	0	0.379731	-4.364882	1.949588
13	1	0	-0.313977	-2.821549	0.847263
14	6	0	-1.206075	-1.591366	-2.254049
15	6	0	-1.409338	-2.456730	-0.987504
16	6	0	-2.884729	-2.805123	-1.097611
17	6	0	-3.328999	-2.408618	-2.368307
18	7	0	-2.293016	-1.710601	-3.048466
19	8	0	-0.953770	-1.822361	0.131399
20	8	0	-0.202248	-0.889226	-2.456570
21	6	0	-2.409898	-1.134442	-4.380127

22	6	0	-3.756998	-3.436569	-0.225218
23	6	0	-4.620958	-2.656041	-2.811449
24	1	0	-2.338311	-1.920469	-5.139568
25	1	0	-1.598259	-0.419046	-4.518033
26	1	0	-3.369630	-0.624849	-4.489509
27	6	0	-5.490116	-3.309432	-1.924905
28	6	0	-5.072174	-3.686957	-0.647176
29	1	0	-4.954932	-2.351066	-3.797914
30	1	0	-6.509878	-3.512330	-2.239659
31	1	0	-5.770317	-4.173562	0.027558
32	8	0	0.648457	2.546239	-0.181005
33	8	0	-1.831506	1.214626	-0.093729
34	8	0	0.999523	0.191106	2.017225
35	7	0	-3.565362	2.514624	0.594867
36	1	0	-3.906885	3.455378	0.756940
37	7	0	0.002583	3.487140	0.578788
38	7	0	4.878200	-0.596082	0.349324
39	1	0	5.593782	-0.504100	1.060968
40	7	0	2.174372	0.617702	2.581251
41	6	0	-4.523219	1.482281	0.464361
42	6	0	-4.692149	0.538040	1.510148
43	6	0	-5.609949	-0.513720	1.335964
44	1	0	-5.755560	-1.255618	2.109934
45	6	0	-6.353569	-0.623279	0.165655
46	1	0	-7.058228	-1.436627	0.049550
47	6	0	-6.192651	0.304024	-0.858346
48	1	0	-6.776342	0.180518	-1.760862
49	6	0	-5.289729	1.374342	-0.725339
50	6	0	-5.134450	2.373281	-1.867407
51	1	0	-4.440870	3.190327	-1.583427
52	6	0	-4.526508	1.698592	-3.099817
53	1	0	-3.547907	1.244517	-2.834390
54	1	0	-4.349690	2.448013	-3.900822
55	1	0	-5.198129	0.908936	-3.497985
56	6	0	-6.468205	3.049625	-2.208489
57	1	0	-6.305320	3.860101	-2.951084
58	1	0	-6.910212	3.504836	-1.296221
59	1	0	-7.194592	2.327976	-2.637954
60	6	0	-3.912715	0.647890	2.816594
61	1	0	-3.271942	1.554443	2.816715
62	6	0	-4.855937	0.794089	4.016896
63	1	0	-5.545783	1.650873	3.859706
64	1	0	-4.270268	0.992012	4.940245
65	1	0	-5.456218	-0.125894	4.177971

66	6	0	-2.974593	-0.548794	3.000064
67	1	0	-3.537617	-1.504394	3.053206
68	1	0	-2.395178	-0.432961	3.939606
69	1	0	-2.257647	-0.600655	2.154353
70	6	0	-2.280650	2.325993	0.216935
71	6	0	-1.472944	3.621759	0.175970
72	1	0	-1.906021	4.327865	0.890833
73	6	0	-1.378958	4.289738	-1.193216
74	1	0	-2.351518	4.659602	-1.526533
75	1	0	-1.003699	3.571820	-1.927250
76	6	0	-0.371132	5.428160	-0.928698
77	1	0	-0.925949	6.313324	-0.604216
78	6	0	0.585484	5.760548	-2.095657
79	1	0	0.129207	5.559896	-3.071259
80	1	0	0.839497	6.827149	-2.068286
81	6	0	1.842885	4.915203	-1.829510
82	1	0	2.732237	5.309419	-2.332981
83	1	0	1.687643	3.886137	-2.167287
84	6	0	1.973809	4.934297	-0.296296
85	1	0	2.584087	4.121420	0.097411
86	1	0	2.424559	5.881068	0.027467
87	6	0	0.534455	4.917120	0.236016
88	1	0	0.410556	5.496625	1.152148
89	6	0	0.089225	3.155371	2.057914
90	1	0	-0.495852	3.918421	2.578851
91	1	0	-0.397430	2.187603	2.170234
92	6	0	1.492852	3.116886	2.664075
93	1	0	1.348212	3.045592	3.748395
94	1	0	1.990758	4.080082	2.504669
95	6	0	2.490439	2.053422	2.202122
96	1	0	2.566195	2.058815	1.116282
97	1	0	3.469372	2.277977	2.634950
98	6	0	2.146684	0.381949	4.128070
99	1	0	2.778846	1.163625	4.550949
100	6	0	0.732833	0.361124	4.725601
101	1	0	0.022352	0.962375	4.157206
102	1	0	0.802167	0.781925	5.736567
103	6	0	0.344077	-1.126413	4.800257
104	1	0	-0.030827	-1.451014	3.824824
105	1	0	-0.432168	-1.321564	5.547818
106	6	0	1.669581	-1.835884	5.124104
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108	1	0	1.878391	-1.766418	6.198503
109	6	0	2.740126	-1.047102	4.340240

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112	1	0	2.198608	-2.071935	2.471538
113	1	0	3.915179	-2.248220	2.907594
114	6	0	3.352574	-0.275440	2.172634
115	1	0	4.236879	0.193037	2.615561
116	6	0	3.579463	-0.409211	0.666458
117	6	0	5.303157	-0.723277	-0.993290
118	6	0	5.740476	0.422810	-1.707474
119	6	0	6.141151	0.277411	-3.048198
120	1	0	6.473863	1.132346	-3.622071
121	6	0	6.114670	-0.967421	-3.668786
122	1	0	6.423498	-1.061029	-4.702055
123	6	0	5.692000	-2.092439	-2.968090
124	1	0	5.680772	-3.045121	-3.480974
125	6	0	5.284226	-1.994003	-1.625356
126	6	0	4.820248	-3.245937	-0.887552
127	1	0	4.553944	-3.007656	0.163244
128	6	0	5.932616	-4.298790	-0.817867
129	1	0	5.606818	-5.157217	-0.192130
130	1	0	6.842678	-3.862511	-0.353375
131	1	0	6.194113	-4.683055	-1.826338
132	6	0	3.557310	-3.821838	-1.536212
133	1	0	2.783391	-3.030392	-1.614879
134	1	0	3.151020	-4.650998	-0.918127
135	1	0	3.767051	-4.214228	-2.553718
136	6	0	5.771615	1.803561	-1.058822
137	1	0	5.439620	1.749577	-0.001100
138	6	0	7.195098	2.372748	-1.032677
139	1	0	7.881770	1.659715	-0.528261
140	1	0	7.213989	3.327176	-0.464142
141	1	0	7.573587	2.570382	-2.057690
142	6	0	4.808187	2.765500	-1.763084
143	1	0	5.117073	2.955007	-2.812641
144	1	0	4.783427	3.737883	-1.226750
145	1	0	3.781743	2.341246	-1.764074
146	8	0	2.676284	-0.403444	-0.183629
147	20	0	0.348513	0.207797	-0.245799
148	1	0	-3.433383	-3.726930	0.770158
