Electronic Supplementary Information for Dalton Transactions

A hexaaza macrocyclic ligand containing acetohydrazide pendants for Ln(III) complexation in aqueous solution. Solid state and solution structures and DFT calculations

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Electronic Supplementary Information

(λλ)-[La(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.001924	0.000004	0.000034
2	7	-0.001685	2.661487	0.011490
3	7	0.886796	1.227349	-2.285172
4	7	-0.886772	-1.205590	-2.295457
5	7	0.000608	-2.661485	-0.011590
6	7	0.887765	-1.226597	2.285221
7	7	-0.887979	1.204845	2.295417
8	8	2.273709	-0.799131	-1.132089
9	8	-2.270704	0.812345	-1.123140
10	8	2.273039	0.801046	1.132260
11	8	-2.270193	-0.814195	1.122996
12	6	-0.139471	3.339277	1.180109
13	6	-0.163191	4.732896	1.215164
14	1	-0.290745	5.253000	2.156134
15	6	-0.007676	5.443520	0.023638
16	1	-0.009902	6.526542	0.028376
17	6	0.150665	4.744012	-1.174039
18	1	0.275870	5.272827	-2.110461
19	6	0.132924	3.350003	-1.151163
20	6	0.179390	2.549149	-2.439324
21	1	-0.852120	2.319451	-2.725344
22	1	0.638871	3.147484	-3.237741
23	6	0.674810	0.372605	-3.521228
24	1	1.478407	-0.364506	-3.556092
25	1	0.760369	0.990326	-4.426774
26	6	-0.674370	-0.340815	-3.524432
27	1	-1.478114	0.396396	-3.553828
28	1	-0.759413	-0.951153	-4.435007
29	6	-0.180907	-2.526949	-2.461140

30	1	0.851026	-2.295955	-
2.744682				
31	1	-0.640838	-3.117385	-
3.265144				
32	6	-0.136269	-3.339392	-
1.180227				
33	6	-0.158223	-4.733047	-
1.215341				
34	1	-0.285085	-5.253273	-
2.156339				
35	6	-0.001869	-5.443523	-
0.023847				
36	1	-0.002726	-6.526546	-
0.028633				
37	6	0.155511	-4.743865	
1.173879				
38	1	0.281313	-5.272560	
2.110287				
39	6	0.136008	-3.349886	
1.151059				
40	6	0.181409	-2.548981	
2.439228				
41	1	-0.850374	-2.320120	
2.724938				
42	1	0.641160	-3.146910	
3.237791				
43	6	0.674937	-0.372031	
3.521254				
44	1	1.477904	0.365762	
3.556180				
45	1	0.760949	-0.989681	
4.426807				
46	6	-0.674852	0.340246	
3.524388				
47	1	-1.477969	-0.397649	
3.553759				
48	1	-0.760438	0.950509	
4.434963				
49	6	-0.183164	2.526781	
2.461025				
50	1	0.849017	2.296610	
2.744340				
51	1	-0.643423	3.116812	
3.265134				
52	6	2.365885	1.431155	-
2.108695				
53	1	2.527483	2.120484	-
1.271907				
54	1	2.854519	1.839010	-
2.997608				
55	6	2.969096	0.081629	-
1.742378				
56	6	-2.365977	-1.408973	-
2.119588				
57	1	-2.527777	-2.104261	-
1.287811				
58	1	-2.855812	-1.809198	-
3.011274				
59	6	-2.966999	-0.061581	-
1.742132				
60	6	2.367039	-1.429154	
2.108900				
61	1	2.529302	-2.118386	

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1.272163
   62          1                       2.855942   -1.836555
2.997873
   63          6                       2.969138   -0.079127
1.742581
   64          6                      -2.367352    1.406989
2.119562
   65          1                      -2.529736    2.102176
1.287814
   66          1                      -2.857536    1.806759
3.011259
   67          6                      -2.967225    0.059099
1.742047
   68          7                       4.245145    0.152825
2.083202
   69          7                       4.985121   -0.833247
2.818380
   70          1                       5.296391   -0.452937
3.717848
   71          1                       5.766842   -1.191814
2.262286
   72          7                       4.245302   -0.149261   -
2.082979
   73          7                      -4.242355    0.174907   -
2.082239
   74          1                      -4.645138    1.089114   -
1.853845
   75          7                      -4.982870   -0.803688   -
2.826812
   76          1                      -5.765765   -1.165902   -
2.274742
   77          1                      -5.292595   -0.415107   -
3.723275
   78          7                      -4.242376   -0.178502
2.082151
   79          1                      -4.644370   -1.093045
1.853712
   80          7                      -4.983728    0.799402
2.826797
   81          1                      -5.766948    1.160972
2.274763
   82          1                      -5.293104    0.410489
3.723239
   83          1                       4.648682    1.068623
1.862683
   84          7                       4.984485    0.837448   -
2.818098
   85          1                       5.296114    0.457424   -
3.717563
   86          1                       5.765877    1.196659   -
2.261958
   87          1                       4.649599   -1.064723   -
1.862454
 ---------------------------------------------------------------------
 HF = -2103.1525066 Hartree
 Zero-point correction = 0.732786
 Sum of electronic and thermal Enthalpies = -2102.376482
 Sum of electronic and thermal Free Energies = -2102.491071
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$(\lambda\delta)$-[La(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	-0.000034	-0.002583	- 0.063220
2	6	-3.017991	-1.747506	0.909428
3	6	-4.301877	-2.283042	0.855115
4	6	-4.836766	-2.644860	- 0.382861
5	6	-4.068716	-2.453416	- 1.527812
6	6	-2.805331	-1.869272	- 1.412049
7	6	-2.018907	-1.552982	- 2.663531
8	6	0.088689	-0.784835	- 3.652072
9	6	-0.116176	0.729264	- 3.662770
10	6	1.996463	1.515111	- 2.699476
11	6	2.790237	1.852518	- 1.458196
12	6	4.051304	2.438071	- 1.590985
13	6	4.825788	2.649669	- 0.453930
14	6	4.299464	2.305951	0.792861
15	6	3.017515	1.767654	0.863620
16	6	2.340768	1.583843	2.197798
17	6	0.628243	0.476505	3.522925
18	6	-0.606233	-0.425979	3.532246
19	6	-2.332026	-1.545349	2.236138
20	6	0.090427	-2.764385	- 2.192827
21	6	2.383058	-0.880690	2.384913
22	6	-2.363667	0.921745	2.386649
23	7	-2.281469	-1.516724	- 0.212628
24	7	-0.540043	-1.425594	- 2.433953
25	7	0.519488	1.387975	- 2.457913
26	7	2.274731	1.517401	- 0.250164
27	7	1.499356	0.330387	2.292232
28	7	-1.484908	-0.294134	2.305591
29	1	-4.864788	-2.438100	1.766674
30	1	-5.826984	-3.078078	- 0.449336

31	1	-4.444451	-2.743125	-
2.501191				
32	1	-2.365217	-0.582562	-
3.031991				
33	1	-2.231225	-2.303092	-
3.439128				
34	1	1.154503	-1.018142	-
3.641804				
35	1	-0.334125	-1.217380	-
4.570645				
36	1	0.301574	1.147998	-
4.590030				
37	1	-1.181855	0.963114	-
3.650262				
38	1	2.201717	2.253897	-
3.487763				
39	1	2.342541	0.539966	-
3.055648				
40	1	4.420263	2.713375	-
2.571118				
41	1	5.814366	3.084455	-
0.533325				
42	1	4.867530	2.476896	
1.698361				
43	1	1.641994	2.417566	
2.316022				
44	1	3.079461	1.623004	
3.009115				
45	1	0.327001	1.522414	
3.580893				
46	1	1.218347	0.262573	
4.427302				
47	1	-1.190516	-0.201335	
4.437818				
48	1	-0.304742	-1.471136	
3.600027				
49	1	-3.065519	-1.568580	
3.052735				
50	1	-1.635732	-2.379845	
2.363315				
51	1	0.060056	-3.402197	-
3.088263				
52	1	2.889816	-0.934763	
3.358883				
53	1	3.144649	-0.795405	
1.598838				
54	1	-2.865099	0.990706	
3.362385				
55	1	-3.129275	0.828788	
1.605421				
56	6	1.573842	-2.146736	
2.089973				
57	6	1.528785	-2.536676	-
1.706538				
58	6	-1.549842	2.179381	
2.070550				
59	6	-0.111940	2.728719	-
2.230540				
60	1	-0.089343	3.354390	-
3.134729				
61	1	0.446281	3.241205	-
1.437494				
62	6	-1.546182	2.505407	-

1.730418				
63	8	0.622988	-2.108220	
1.256326				
64	8	1.834547	-1.448688	-
1.132296				
65	8	-1.846375	1.424552	-
1.140106				
66	8	-0.612641	2.127302	
1.222481				
67	7	-1.910277	3.291118	
2.730840				
68	1	-2.673367	3.258449	
3.411472				
69	7	-1.237043	4.524754	
2.454363				
70	1	-1.889866	5.207570	
2.059069				
71	1	-0.781070	4.877921	
3.300971				
72	7	-2.407359	3.505609	-
1.956424				
73	1	-2.122942	4.313232	-
2.515740				
74	7	-3.731702	3.434557	-
1.408196				
75	1	-3.948086	4.306948	-
0.917924				
76	1	-4.412956	3.235962	-
2.148241				
77	7	2.386991	-3.540616	-
1.926244				
78	1	2.097035	-4.355419	-
2.472149				
79	7	3.715596	-3.464159	-
1.389065				
80	1	3.934642	-4.330498	-
0.889310				
81	1	4.391266	-3.276303	-
2.137021				
82	7	1.954627	-3.251000	
2.751254				
83	1	2.725567	-3.206436	
3.422270				
84	7	1.292384	-4.493660	
2.488826				
85	1	1.952826	-5.175858	
2.105393				
86	1	0.836281	-4.839539	
3.338434				
87	1	-0.462958	-3.265021	-
1.388890				

HF = -2103.1254227 Hartree
Zero-point correction = 0.731127
Sum of electronic and thermal Enthalpies = -2102.349992
Sum of electronic and thermal Free Energies = -2102.468150

(λλ)-$[Ce(L)]^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	58	0.000242	0.000001	-0.000004
2	7	0.000020	-2.649452	-0.002229
3	7	0.893042	-1.205758	2.279478
4	7	-0.892819	1.201616	2.281625
5	7	0.000220	2.649453	0.002211
6	7	0.893224	1.205690	-2.279470
7	7	-0.892843	-1.201546	-2.281679
8	8	2.250883	0.824288	1.108123
9	8	-2.250277	-0.826518	1.106482
10	8	2.250837	-0.824474	-1.108091
11	8	-2.250202	0.826690	-1.106511
12	6	-0.146100	-3.333467	-1.166157
13	6	-0.168821	-4.727139	-1.196384
14	1	-0.303719	-5.249860	-2.134871
15	6	-0.002360	-5.433923	-0.004387
16	1	-0.003254	-6.516912	-0.005231
17	6	0.165252	-4.729277	1.188688
18	1	0.299259	-5.253670	2.126373
19	6	0.144888	-3.335500	1.160621
20	6	0.199135	-2.532575	2.445380
21	1	-0.830854	-2.311331	2.742915
22	1	0.672902	-3.124329	3.240324
23	6	0.678443	-0.351759	3.515167
24	1	1.474439	0.393707	3.546953
25	1	0.772713	-0.967378	4.421184
26	6	-0.677828	0.345710	3.515916
27	1	-1.473847	-0.399781	3.546838
28	1	-0.771799	0.959928	4.422913
29	6	-0.199213	2.528375	2.449524
30	1	0.830984	2.306883	2.746157
31	1	-0.672776	3.118589	3.245726

32	6	-0.145845	3.333484	1.166135
33	6	-0.168370	4.727160	1.196366
34	1	-0.303228	5.249896	2.134852
35	6	-0.001771	5.433924	0.004380
36	1	-0.002513	6.516914	0.005228
37	6	0.165779	4.729260	-1.188694
38	1	0.299885	5.253637	-2.126373
39	6	0.145217	3.335486	-1.160633
40	6	0.199410	2.532553	-2.445386
41	1	-0.830597	2.311380	-2.742913
42	1	0.673214	3.124269	-3.240336
43	6	0.678594	0.351696	-3.515154
44	1	1.474512	-0.393857	-3.546881
45	1	0.772974	0.967284	-4.421179
46	6	-0.677738	-0.345641	-3.515949
47	1	-1.473677	0.399935	-3.546862
48	1	-0.771761	-0.959827	-4.422962
49	6	-0.199313	-2.528350	-2.449544
50	1	0.830922	-2.306924	-2.746090
51	1	-0.672853	-3.118525	-3.245787
52	6	2.373285	-1.396867	2.098155
53	1	2.537598	-2.085001	1.261158
54	1	2.869121	-1.797232	2.986350
55	6	2.958278	-0.041511	1.726452
56	6	-2.373147	1.392588	2.100777
57	1	-2.537728	2.082085	1.264955
58	1	-2.869046	1.791264	2.989693
59	6	-2.957669	0.037789	1.726898
60	6	2.373476	1.396694	-2.098114
61	1	2.537821	2.084853	-1.261146
62	1	2.869365	1.796986	-2.986315
63	6	2.958333	0.041261	-

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1.726392
   64          6                     -2.373192   -1.392419   -
2.100905
   65          1                     -2.537864   -2.081946   -
1.265125
   66          1                     -2.869080   -1.791017   -
2.989862
   67          6                     -2.957666   -0.037548   -
1.726940
   68          7                      4.229239   -0.212580   -
2.069662
   69          7                      4.981637    0.757162   -
2.813921
   70          1                      5.283160    0.366283   -
3.712189
   71          1                      5.771342    1.106459   -
2.263224
   72          7                      4.229184    0.212230
2.069801
   73          7                     -4.228249   -0.217183
2.070537
   74          1                     -4.618436   -1.137363
1.844016
   75          7                     -4.980619    0.750921
2.816953
   76          1                     -5.770668    1.101007
2.267249
   77          1                     -5.281638    0.358255
3.714607
   78          7                     -4.228230    0.217529   -
2.070560
   79          1                     -4.618344    1.137735   -
1.844016
   80          7                     -4.980677   -0.750495   -
2.816998
   81          1                     -5.770752   -1.100538   -
2.267301
   82          1                     -5.281668   -0.357784   -
3.714643
   83          1                      4.619597   -1.133068   -
1.844690
   84          7                      4.981471   -0.757585
2.814078
   85          1                      5.282984   -0.366744
3.712366
   86          1                      5.771177   -1.106929
2.263410
   87          1                      4.619624    1.132690
1.844861
 ---------------------------------------------------------------------
 HF = -2103.8050032 Hartree
 Zero-point correction = 0.733033
 Sum of electronic and thermal Enthalpies = -2103.028787
 Sum of electronic and thermal Free Energies = -2103.143185
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$(\lambda\delta)$-[Ce(L)]$^{3+}$ (0 imaginary frequencies)

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 Center     Atomic                     Coordinates (Angstroms)
 Number     Number                    X           Y           Z
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1	58	-0.000083	-0.003843	-0.061588
2	6	-3.064913	-1.651834	0.916898
3	6	-4.361801	-2.155138	0.863234
4	6	-4.900710	-2.518392	-0.372294
5	6	-4.122197	-2.360287	-1.515006
6	6	-2.845405	-1.805994	-1.399713
7	6	-2.047687	-1.525690	-2.651169
8	6	0.072132	-0.803651	-3.638600
9	6	-0.107391	0.713010	-3.656414
10	6	2.018776	1.463437	-2.704065
11	6	2.824857	1.778423	-1.466252
12	6	4.099335	2.332848	-1.604965
13	6	4.884962	2.523444	-0.472147
14	6	4.355551	2.191219	0.776243
15	6	3.060808	1.685338	0.852218
16	6	2.387401	1.519457	2.189102
17	6	0.642602	0.472191	3.515671
18	6	-0.616579	-0.391997	3.528774
19	6	-2.380960	-1.456095	2.244173
20	6	0.036655	-2.770461	-2.162034
21	6	2.347996	-0.943668	2.375013
22	6	-2.322734	1.009515	2.371375
23	7	-2.316795	-1.451198	-0.203119
24	7	-0.568494	-1.422496	-2.415580
25	7	0.541978	1.361269	-2.453458
26	7	2.305461	1.453874	-0.257114
27	7	1.504207	0.295839	2.282190
28	7	-1.487879	-0.237646	2.299799
29	1	-4.931779	-2.284930	1.774373
30	1	-5.901246	-2.927238	-0.438321
31	1	-4.499648	-2.652467	-2.486999
32	1	-2.373908	-0.555571	-

3.037880				
33	1	-2.269700	-2.284172	-
3.415828				
34	1	1.133701	-1.055663	-
3.627100				
35	1	-0.358788	-1.235091	-
4.553850				
36	1	0.316936	1.122094	-
4.584921				
37	1	-1.168759	0.965831	-
3.643535				
38	1	2.231780	2.203249	-
3.489322				
39	1	2.345286	0.484959	-
3.069064				
40	1	4.469427	2.600028	-
2.586940				
41	1	5.883783	2.933264	-
0.555774				
42	1	4.931476	2.346491	
1.679622				
43	1	1.719659	2.376998	
2.315148				
44	1	3.131313	1.528878	
2.996481				
45	1	0.373085	1.526934	
3.571479				
46	1	1.228844	0.243532	
4.418946				
47	1	-1.195280	-0.147019	
4.432673				
48	1	-0.346557	-1.445488	
3.600465				
49	1	-3.119173	-1.438743	
3.056633				
50	1	-1.718858	-2.315126	
2.388458				
51	1	-0.002490	-3.415017	-
3.052273				
52	1	2.849501	-1.016270	
3.350476				
53	1	3.113908	-0.881743	
1.590986				
54	1	-2.818505	1.105846	
3.347659				
55	1	-3.092709	0.936080	
1.592378				
56	6	1.499601	-2.182041	
2.075105				
57	6	1.476310	-2.562877	-
1.673242				
58	6	-1.465992	2.233606	
2.040567				
59	6	-0.064667	2.713242	-
2.225331				
60	1	-0.035841	3.336943	-
3.130676				
61	1	0.506181	3.216696	-
1.435470				
62	6	-1.498720	2.514132	-
1.717140				
63	8	0.543931	-2.107508	
1.249111				

64	8	1.797287	-1.475313	-
1.105641				
65	8	-1.812269	1.438520	-
1.123345				
66	8	-0.531611	2.138384	
1.192765				
67	7	-1.787452	3.366119	
2.685697				
68	1	-2.550170	3.368655	
3.367534				
69	7	-1.072540	4.572271	
2.392620				
70	1	-1.703233	5.274047	
1.994591				
71	1	-0.598601	4.917621	
3.232617				
72	7	-2.346663	3.526092	-
1.939389				
73	1	-2.056065	4.326547	-
2.505697				
74	7	-3.666946	3.477666	-
1.377712				
75	1	-3.869670	4.361345	-
0.901807				
76	1	-4.356919	3.274355	-
2.108531				
77	7	2.320586	-3.580512	-
1.882836				
78	1	2.021808	-4.393829	-
2.426131				
79	7	3.647745	-3.520927	-
1.338841				
80	1	3.855178	-4.393288	-
0.844474				
81	1	4.328800	-3.336457	-
2.082898				
82	7	1.850954	-3.303107	
2.724292				
83	1	2.623315	-3.286186	
3.394960				
84	7	1.153110	-4.524246	
2.452583				
85	1	1.796606	-5.226103	
2.075894				
86	1	0.676720	-4.857172	
3.296324				
87	1	-0.527598	-3.254006	-
1.355164				

HF = -2103.7774998 Hartree
Zero-point correction = 0.731427
Sum of electronic and thermal Enthalpies = -2103.001841
Sum of electronic and thermal Free Energies = -2103.119661

(λλ)-[Pr(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	59	-0.000265	0.000000	-

0.000021				
2	7	-0.000460	-2.640067	
0.001882				
3	7	0.896898	-1.192489	
2.274356				
4	7	-0.896906	1.195870	
2.272557				
5	7	0.000840	2.640068	-
0.001896				
6	7	0.897507	1.192047	-
2.274390				
7	7	-0.897563	-1.195427	-
2.272574				
8	8	2.233214	0.840098	
1.090607				
9	8	-2.233599	-0.838166	
1.092079				
10	8	2.232862	-0.841134	-
1.090596				
11	8	-2.233280	0.839188	-
1.092008				
12	6	-0.153196	-3.327280	-
1.159272				
13	6	-0.175509	-4.720997	-
1.187581				
14	1	-0.316314	-5.244544	-
2.124748				
15	6	-0.000667	-5.426456	
0.003749				
16	1	-0.000756	-6.509430	
0.004474				
17	6	0.174306	-4.719428	
1.194120				
18	1	0.315053	-5.241734	
2.131987				
19	6	0.152203	-3.325741	
1.163936				
20	6	0.212720	-2.522920	
2.447116				
21	1	-0.815884	-2.307966	
2.753697				
22	1	0.696845	-3.110980	
3.238567				
23	6	0.680382	-0.340558	
3.510835				
24	1	1.471020	0.410710	
3.541560				
25	1	0.780706	-0.955791	
4.416413				
26	6	-0.680723	0.345497	
3.510166				
27	1	-1.471280	-0.405824	
3.541485				
28	1	-0.781454	0.961842	
4.414944				
29	6	-0.212278	2.526294	
2.443531				
30	1	0.816229	2.311404	
2.750451				
31	1	-0.696248	3.115610	
3.234145				
32	6	-0.151407	3.327358	
1.159266				

33	6	-0.172751	4.721095	1.187605
34	1	-0.313190	5.244717	2.124783
35	6	0.002574	5.426456	-0.003706
36	1	0.003237	6.509430	-0.004408
37	6	0.177043	4.719330	-1.194100
38	1	0.318138	5.241561	-2.131957
39	6	0.153971	3.325664	-1.163946
40	6	0.213939	2.522800	-2.447119
41	1	-0.814802	2.308322	-2.753573
42	1	0.698250	3.110606	-3.238644
43	6	0.680531	0.340199	-3.510844
44	1	1.470769	-0.411491	-3.541542
45	1	0.781181	0.955352	-4.416439
46	6	-0.680946	-0.345136	-3.510160
47	1	-1.471104	0.406608	-3.541434
48	1	-0.782025	-0.961399	-4.414955
49	6	-0.213546	-2.526173	-2.443530
50	1	0.815093	-2.311757	-2.750336
51	1	-0.697714	-3.115237	-3.234208
52	6	2.378037	-1.374043	2.089715
53	1	2.544429	-2.060535	1.251984
54	1	2.878859	-1.769546	2.977202
55	6	2.949245	-0.014106	1.715781
56	6	-2.377971	1.377624	2.087693
57	1	-2.544240	2.063182	1.249172
58	1	-2.878665	1.774354	2.974715
59	6	-2.949602	0.017367	1.715493
60	6	2.378735	1.372892	-2.089820
61	1	2.545497	2.059384	-1.252162
62	1	2.879723	1.768077	-2.977356
63	6	2.949301	0.012710	-1.715794
64	6	-2.378716	-1.376476	-

```
2.087752
   65          1                      -2.545335   -2.062033   -
1.249300
   66          1                      -2.879591   -1.772887   -
2.974814
   67          6                      -2.949694   -0.015976   -
1.715456
   68          7                       4.214812   -0.259951   -
2.063817
   69          7                       4.976931    0.696058   -
2.816023
   70          1                       5.268656    0.296978   -
3.713937
   71          1                       5.774203    1.036595   -
2.270733
   72          7                       4.214869    0.257957
2.063861
   73          7                      -4.215558   -0.253536
2.063238
   74          1                      -4.595394   -1.178173
1.836992
   75          7                      -4.977082    0.704377
2.813634
   76          1                      -5.773801    1.044827
2.267481
   77          1                      -5.269570    0.306969
3.712045
   78          7                      -4.215536    0.255533   -
2.063141
   79          1                      -4.594935    1.180334   -
1.836834
   80          7                      -4.977521   -0.701976   -
2.813584
   81          1                      -5.774377   -1.042104   -
2.267433
   82          1                      -5.269853   -0.304368   -
3.711958
   83          1                       4.593935   -1.184543   -
1.836200
   84          7                       4.976534   -0.698448
2.816025
   85          1                       5.268419   -0.299558
3.713972
   86          1                       5.773664   -1.039311
2.270733
   87          1                       4.594425    1.182384
1.836295
 -------------------------------------------------------------------
 HF = -2104.4403183 Hartree
 Zero-point correction = 0.733095
 Sum of electronic and thermal Enthalpies = -2103.664051
 Sum of electronic and thermal Free Energies = -2103.778391
```

(λδ)-[Pr(L)]$^{3+}$ (0 imaginary frequencies)

```
 -------------------------------------------------------------------
 Center     Atomic                     Coordinates (Angstroms)
 Number     Number                    X           Y           Z
 -------------------------------------------------------------------
    1         59                      -0.000163   -0.004581   -
0.061422
    2          6                      -3.092021   -1.590516
```

0.917424				
3	6	-4.398815	-2.067659	
0.864207				
4	6	-4.946048	-2.418518	-
0.371185				
5	6	-4.164711	-2.274388	-
1.513725				
6	6	-2.877162	-1.745644	-
1.398043				
7	6	-2.074186	-1.481670	-
2.648252				
8	6	0.059367	-0.806336	-
3.632599				
9	6	-0.099137	0.712097	-
3.651489				
10	6	2.041058	1.418112	-
2.703818				
11	6	2.852951	1.719989	-
1.468075				
12	6	4.137290	2.250720	-
1.608414				
13	6	4.926481	2.429940	-
0.476335				
14	6	4.390499	2.110212	
0.772423				
15	6	3.086520	1.628642	
0.849118				
16	6	2.410665	1.476551	
2.185106				
17	6	0.653015	0.458797	
3.512315				
18	6	-0.620280	-0.382386	
3.525619				
19	6	-2.403232	-1.410908	
2.243174				
20	6	-0.016590	-2.768154	-
2.150956				
21	6	2.328503	-0.986168	
2.365038				
22	6	-2.296785	1.052926	
2.366870				
23	7	-2.340026	-1.402057	-
0.202043				
24	7	-0.594168	-1.409343	-
2.408972				
25	7	0.563721	1.346181	-
2.448782				
26	7	2.326146	1.407911	-
0.258923				
27	7	1.507297	0.268418	
2.276127				
28	7	-1.486940	-0.210505	
2.296013				
29	1	-4.970219	-2.187327	
1.775841				
30	1	-5.954500	-2.807476	-
0.437166				
31	1	-4.547765	-2.558118	-
2.486052				
32	1	-2.379853	-0.504954	-
3.034738				
33	1	-2.310678	-2.234971	-
3.413752				

34	1	1.117104	-1.073523	-3.616969
35	1	-0.375344	-1.234336	-4.547709
36	1	0.328790	1.116404	-4.580467
37	1	-1.156679	0.980042	-3.634995
38	1	2.267234	2.151481	-3.491490
39	1	2.347670	0.432509	-3.066487
40	1	4.511750	2.508656	-2.591218
41	1	5.932677	2.821165	-0.560779
42	1	4.968828	2.256525	1.675773
43	1	1.757609	2.345335	2.310797
44	1	3.154240	1.472822	2.992846
45	1	0.402500	1.518151	3.570312
46	1	1.237464	0.218472	4.413772
47	1	-1.195114	-0.128522	4.429598
48	1	-0.368999	-1.440644	3.595883
49	1	-3.139693	-1.378922	3.056817
50	1	-1.757978	-2.282868	2.386262
51	1	-0.066442	-3.414174	-3.039551
52	1	2.829346	-1.070671	3.339835
53	1	3.094270	-0.937506	1.579925
54	1	-2.787346	1.161818	3.344412
55	1	-3.070104	0.993632	1.590000
56	6	1.454001	-2.205452	2.063712
57	6	1.425381	-2.583336	-1.661145
58	6	-1.414937	2.256950	2.030771
59	6	-0.015543	2.709138	-2.217453
60	1	0.021977	3.333162	-3.122209
61	1	0.566729	3.200349	-1.428312
62	6	-1.450855	2.533039	-1.705698
63	8	0.499395	-2.108222	1.238550
64	8	1.762703	-1.498358	-1.097576
65	8	-1.779471	1.460769	-

1.113659				
66	8	-0.483655	2.138131	
1.182340				
67	7	-1.708162	3.397790	
2.674561				
68	1	-2.469002	3.418984	
3.358206				
69	7	-0.965676	4.586417	
2.378194				
70	1	-1.580360	5.302213	
1.980047				
71	1	-0.482464	4.921824	
3.216939				
72	7	-2.284136	3.557688	-
1.924864				
73	1	-1.982606	4.354304	-
2.490926				
74	7	-3.604145	3.528278	-
1.360966				
75	1	-3.792666	4.414183	-
0.883338				
76	1	-4.298283	3.336848	-
2.091080				
77	7	2.254725	-3.613375	-
1.868806				
78	1	1.944135	-4.422816	-
2.411314				
79	7	3.582680	-3.572504	-
1.324749				
80	1	3.777014	-4.446972	-
0.828757				
81	1	4.266384	-3.399804	-
2.069236				
82	7	1.779672	-3.334956	
2.711401				
83	1	2.553037	-3.336376	
3.381154				
84	7	1.053618	-4.539521	
2.439276				
85	1	1.680208	-5.255558	
2.060771				
86	1	0.571141	-4.862370	
3.283454				
87	1	-0.590982	-3.238061	-
1.343248				

HF = -2104.4123342 Hartree
Zero-point correction = 0.731577
Sum of electronic and thermal Enthalpies = -2103.636548
Sum of electronic and thermal Free Energies = -2103.754351

(λλ)-[Eu(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.000000	0.000000	
0.000007				
2	7	0.000004	2.607710	-
0.000021				

3	7	-0.909416	1.162872	2.252291
4	7	0.909397	-1.162848	2.252327
5	7	-0.000007	-2.607710	0.000028
6	7	-0.909357	-1.162873	-2.252310
7	7	0.909422	1.162849	-2.252311
8	8	-2.171149	-0.879102	1.040191
9	8	2.171137	0.879139	1.040182
10	8	-2.171142	0.879089	-1.040203
11	8	2.171150	-0.879125	-1.040156
12	6	0.174698	3.299384	-1.155645
13	6	0.198840	4.693111	-1.185049
14	1	0.359087	5.213862	-2.120697
15	6	-0.000038	5.401345	-0.000040
16	1	-0.000057	6.484279	-0.000048
17	6	-0.198890	4.693121	1.184982
18	1	-0.359146	5.213880	2.120623
19	6	-0.174704	3.299396	1.155597
20	6	-0.258290	2.506125	2.439370
21	1	0.763508	2.315592	2.782368
22	1	-0.779240	3.087510	3.212300
23	6	-0.687801	0.324837	3.497032
24	1	-1.461242	-0.444567	3.528598
25	1	-0.808630	0.944310	4.397090
26	6	0.687774	-0.324790	3.497051
27	1	1.461224	0.444605	3.528621
28	1	0.808577	-0.944250	4.397122
29	6	0.258263	-2.506095	2.439424
30	1	-0.763530	-2.315551	2.782430
31	1	0.779213	-3.087475	3.212358
32	6	0.174683	-3.299383	1.155656
33	6	0.198840	-4.693108	1.185060
34	1	0.359084	-5.213858	

```
2.120709
   35          6                    -0.000017   -5.401345
0.000048
   36          1                    -0.000024   -6.484279
0.000057
   37          6                    -0.198865   -4.693124   -
1.184975
   38          1                    -0.359108   -5.213884   -
2.120618
   39          6                    -0.174695   -3.299397   -
1.155590
   40          6                    -0.258218   -2.506120   -
2.439383
   41          1                     0.763582   -2.315577   -
2.782372
   42          1                    -0.779154   -3.087509   -
3.212320
   43          6                    -0.687732   -0.324833   -
3.497045
   44          1                    -1.461181    0.444560   -
3.528625
   45          1                    -0.808534   -0.944306   -
4.397107
   46          6                     0.687816    0.324795   -
3.497041
   47          1                     1.461267   -0.444599   -
3.528603
   48          1                     0.808631    0.944256   -
4.397109
   49          6                     0.258297    2.506098   -
2.439416
   50          1                    -0.763490    2.315558   -
2.782445
   51          1                     0.779264    3.087479   -
3.212338
   52          6                    -2.393464    1.313055
2.060070
   53          1                    -2.568787    1.995630
1.221777
   54          1                    -2.908209    1.691581
2.946789
   55          6                    -2.918339   -0.061594
1.680055
   56          6                     2.393446   -1.313038
2.060120
   57          1                     2.568774   -1.995622
1.221837
   58          1                     2.908185   -1.691545
2.946851
   59          6                     2.918337    0.061650
1.680060
   60          6                    -2.393407   -1.313072   -
2.060110
   61          1                    -2.568736   -1.995640   -
1.221813
   62          1                    -2.908136   -1.691607   -
2.946835
   63          6                    -2.918318    0.061581   -
1.680084
   64          6                     2.393468    1.313034   -
2.060079
   65          1                     2.568784    1.995604   -
1.221781
```

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    66          1                        2.908223    1.691552   -
2.946796
    67          6                        2.918343   -0.061638   -
1.680042
    68          7                       -4.167014    0.391216   -
2.036915
    69          7                       -4.960747   -0.524153   -
2.807260
    70          1                       -5.225473   -0.103742   -
3.703865
    71          1                       -5.777962   -0.835639   -
2.274154
    72          7                       -4.167044   -0.391227
2.036853
    73          7                        4.167021    0.391307
2.036900
    74          1                        4.510061    1.328460
1.802665
    75          7                        4.960734   -0.524047
2.807286
    76          1                        5.777968   -0.835536
2.274212
    77          1                        5.225423   -0.103622
3.703896
    78          7                        4.167029   -0.391294   -
2.036880
    79          1                        4.510070   -1.328446   -
1.802639
    80          7                        4.960751    0.524060   -
2.807257
    81          1                        5.777979    0.835548   -
2.274174
    82          1                        5.225450    0.103635   -
3.703863
    83          1                       -4.510068    1.328361   -
1.802663
    84          7                       -4.960793    0.524143
2.807183
    85          1                       -5.225538    0.103728
3.703781
    86          1                       -5.777994    0.835632
2.274061
    87          1                       -4.510094   -1.328371
1.802594
 ---------------------------------------------------------------------
 HF = -2106.8825813 Hartree
 Zero-point correction = 0.733228
 Sum of electronic and thermal Enthalpies = -2106.106231
 Sum of electronic and thermal Free Energies = -2106.220318
```

$(\lambda\delta)$-[Eu(L)]$^{3+}$ (0 imaginary frequencies)

```
 ---------------------------------------------------------------------
 Center     Atomic                      Coordinates (Angstroms)
 Number     Number                     X           Y           Z
 ---------------------------------------------------------------------
    1         63                     -0.000380   -0.000263   -
0.075908
    2          6                      3.283332    1.090299
0.829325
    3          6                      4.649451    1.344295
0.746959
```

4	6	5.214424	1.639616	-0.494632
5	6	4.387041	1.662329	-1.612006
6	6	3.033387	1.347964	-1.467318
7	6	2.174546	1.260245	-2.702183
8	6	-0.022980	0.756876	-3.626307
9	6	0.018385	-0.769585	-3.623986
10	6	-2.177978	-1.270608	-2.696022
11	6	-3.035812	-1.352841	-1.460070
12	6	-4.389873	-1.666548	-1.602574
13	6	-5.216456	-1.638694	-0.484748
14	6	-4.650323	-1.339060	0.755296
15	6	-3.283927	-1.086035	0.835705
16	6	-2.615594	-0.989650	2.177116
17	6	-0.702396	-0.288400	3.480192
18	6	0.704855	0.299308	3.478871
19	6	2.616067	0.998195	2.171565
20	6	0.258719	2.711042	-2.149621
21	6	-2.069329	1.416283	2.281026
22	6	2.071805	-1.407867	2.283488
23	7	2.476207	1.060714	-0.267323
24	7	0.701855	1.304874	-2.417608
25	7	-0.705018	-1.313738	-2.412674
26	7	-2.477517	-1.061434	-0.261615
27	7	-1.499137	0.025355	2.230928
28	7	1.500515	-0.017604	2.229760
29	1	5.256293	1.338307	1.643405
30	1	6.271047	1.859022	-0.583202
31	1	4.782079	1.910551	-2.589395
32	1	2.380735	0.298696	-3.181489
33	1	2.456659	2.048894	-3.415268
34	1	-1.056018	1.106359	-3.590749
35	1	0.427104	1.144107	-

```
4.551706
   36          1                     -0.432876   -1.159616   -
4.547633
   37          1                      1.051430   -1.119055   -
3.588711
   38          1                     -2.460611   -2.062493   -
3.405313
   39          1                     -2.384764   -0.311269   -
3.179510
   40          1                     -4.785806   -1.918235   -
2.578716
   41          1                     -6.273341   -1.857471   -
0.571720
   42          1                     -5.256519   -1.329082
1.652143
   43          1                     -2.146617   -1.960078
2.365896
   44          1                     -3.357600   -0.798872
2.963769
   45          1                     -0.655062   -1.374309
3.567795
   46          1                     -1.236268    0.079915
4.369827
   47          1                      1.239451   -0.066793
4.368983
   48          1                      0.657618    1.385426
3.563895
   49          1                      3.358849    0.810784
2.958301
   50          1                      2.146430    1.968917
2.357219
   51          1                      0.338420    3.347436   -
3.042882
   52          1                     -2.574290    1.610589
3.237429
   53          1                     -2.798456    1.503486
1.465370
   54          1                      2.577532   -1.599076
3.240121
   55          1                      2.800602   -1.496861
1.467708
   56          6                     -0.959257    2.424454
1.994585
   57          6                     -1.170067    2.666668   -
1.603608
   58          6                      0.962692   -2.418091
2.000443
   59          6                     -0.261078   -2.718789   -
2.140251
   60          1                     -0.341705   -3.358391   -
3.031140
   61          1                     -0.904642   -3.127567   -
1.351526
   62          6                      1.168422   -2.671925   -
1.596330
   63          8                     -0.079648    2.150318
1.124591
   64          8                     -1.591316    1.612196   -
1.034398
   65          8                      1.589802   -1.615509   -
1.030815
   66          8                      0.080950   -2.146470
1.131810
```

67	7	0.999755	-3.562284	2.700467
68	1	1.742494	-3.718570	3.386541
69	7	0.000759	-4.562509	2.467845
70	1	0.418938	-5.400757	2.053721
71	1	-0.498045	-4.774003	3.337138
72	7	1.902012	-3.780423	-1.741697
73	1	1.553131	-4.562419	-2.300556
74	7	3.190240	-3.859790	-1.106554
75	1	3.289605	-4.775614	-0.658295
76	1	3.933314	-3.697358	-1.795209
77	7	-1.903137	3.775238	-1.751049
78	1	-1.554710	4.555333	-2.312838
79	7	-3.190291	3.857271	-1.114047
80	1	-3.288480	4.774603	-0.668618
81	1	-3.934571	3.692948	-1.800952
82	7	-0.992807	3.569519	2.693395
83	1	-1.734610	3.728612	3.379833
84	7	0.009026	4.566577	2.459203
85	1	-0.406110	5.404122	2.040588
86	1	0.505998	4.780435	3.328962
87	1	0.903473	3.122377	-1.363205

HF = -2106.8537108 Hartree
Zero-point correction = 0.731930
Sum of electronic and thermal Enthalpies = -2106.077656
Sum of electronic and thermal Free Energies = -2106.195955

(λλ)-[Tb(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	65	0.000469	0.000002	-0.000091
2	7	0.000372	2.594377	0.000188
3	7	-0.913201	1.151249	2.245874
4	7	0.913219	-1.151654	

2.245681				
5	7	-0.001088	-2.594373	-
0.000250				
6	7	-0.913844	-1.150709	-
2.245914				
7	7	0.913998	1.151123	-
2.245673				
8	8	-2.142867	-0.891735	
1.020186				
9	8	2.142741	0.891696	
1.020638				
10	8	-2.142386	0.892946	-
1.020287				
11	8	2.142302	-0.892904	-
1.020641				
12	6	0.183363	3.287973	-
1.152997				
13	6	0.208775	4.681778	-
1.182320				
14	1	0.376651	5.201762	-
2.117040				
15	6	0.001176	5.390774	
0.000353				
16	1	0.001425	6.473685	
0.000398				
17	6	-0.206726	4.681763	
1.182946				
18	1	-0.374238	5.201710	
2.117751				
19	6	-0.182058	3.287932	
1.153456				
20	6	-0.274230	2.498560	
2.437553				
21	1	0.744542	2.317570	
2.794745				
22	1	-0.808631	3.077970	
3.202890				
23	6	-0.690185	0.318042	
3.493061				
24	1	-1.457498	-0.457783	
3.524744				
25	1	-0.818371	0.938510	
4.391428				
26	6	0.690138	-0.318648	
3.493061				
27	1	1.457465	0.457149	
3.524971				
28	1	0.818232	-0.939341	
4.391280				
29	6	0.273923	-2.498866	
2.437126				
30	1	-0.744746	-2.317661	
2.794496				
31	1	0.808246	-3.078556	
3.202304				
32	6	0.181342	-3.288073	
1.152949				
33	6	0.205699	-4.681903	
1.182303				
34	1	0.373163	-5.201988	
2.117042				
35	6	-0.002404	-5.390769	-
0.000351				

36	1	-0.002969	-6.473681	-
0.000372				
37	6	-0.209740	-4.681628	-
1.182973				
38	1	-0.377614	-5.201474	-
2.117769				
39	6	-0.184019	-3.287822	-
1.153515				
40	6	-0.275601	-2.498375	-
2.437599				
41	1	0.743305	-2.317932	-
2.794677				
42	1	-0.810252	-3.077450	-
3.203011				
43	6	-0.690304	-0.317612	-
3.493091				
44	1	-1.457147	0.458680	-
3.524778				
45	1	-0.818850	-0.938000	-
4.391462				
46	6	0.690441	0.318236	-
3.493060				
47	1	1.457293	-0.458031	-
3.524946				
48	1	0.818938	0.938856	-
4.391272				
49	6	0.275453	2.498698	-
2.437150				
50	1	-0.743332	2.318052	-
2.794465				
51	1	0.810075	3.078052	-
3.202369				
52	6	-2.398015	1.289242	
2.050573				
53	1	-2.576892	1.972015	
1.213472				
54	1	-2.918407	1.659227	
2.937565				
55	6	-2.903221	-0.090695	
1.666293				
56	6	2.398040	-1.289719	
2.050442				
57	1	2.576949	-1.972562	
1.213423				
58	1	2.918458	-1.659536	
2.937484				
59	6	2.903316	0.090298	
1.666142				
60	6	-2.398744	-1.287887	-
2.050713				
61	1	-2.578062	-1.970666	-
1.213712				
62	1	-2.919285	-1.657492	-
2.937776				
63	6	-2.903213	0.092291	-
1.666315				
64	6	2.398896	1.288351	-
2.050456				
65	1	2.578211	1.971197	-
1.213528				
66	1	2.919515	1.657782	-
2.937543				
67	6	2.903387	-0.091895	-

1.666033				
68	7	-4.144036	0.446936	-
2.025233				
69	7	-4.952319	-0.450424	-
2.801932				
70	1	-5.206597	-0.021074	-
3.697341				
71	1	-5.776869	-0.748824	-
2.272569				
72	7	-4.144162	-0.444744	
2.025399				
73	7	4.144274	0.444295	
2.025135				
74	1	4.471567	1.386144	
1.786948				
75	7	4.952101	-0.453591	
2.801829				
76	1	5.776520	-0.752249	
2.272402				
77	1	5.206579	-0.024417	
3.697269				
78	7	4.144223	-0.446512	-
2.024823				
79	1	4.471016	-1.388522	-
1.786589				
80	7	4.952587	0.450965	-
2.801430				
81	1	5.777075	0.749244	-
2.271897				
82	1	5.206983	0.021646	-
3.696824				
83	1	-4.471103	1.388650	-
1.786206				
84	7	-4.951931	0.453008	
2.802178				
85	1	-5.206291	0.023799	
3.697631				
86	1	-5.776414	0.751771	
2.272913				
87	1	-4.471705	-1.386306	
1.786421				

HF = -2108.0619341 Hartree
Zero-point correction = 0.733351
Sum of electronic and thermal Enthalpies = -2107.285522
Sum of electronic and thermal Free Energies = -2107.399376

$(\lambda\delta)$-[Tb(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	65	-0.000476	-0.000233	-
0.077759				
2	6	3.311203	0.981499	
0.824583				
3	6	4.684961	1.190140	
0.741762				
4	6	5.258914	1.467291	-
0.499687				

5	6	4.431285	1.518108	-1.615686
6	6	3.068213	1.247877	-1.469665
7	6	2.206294	1.191033	-2.702430
8	6	-0.004281	0.755143	-3.621035
9	6	-0.000843	-0.771326	-3.618204
10	6	-2.209957	-1.204817	-2.695282
11	6	-3.070726	-1.254736	-1.461399
12	6	-4.434157	-1.524595	-1.605016
13	6	-5.260921	-1.467360	-0.488714
14	6	-4.685792	-1.184367	0.750891
15	6	-3.311817	-0.976504	0.831618
16	6	-2.641573	-0.901166	2.171670
17	6	-0.711932	-0.260532	3.474061
18	6	0.714028	0.276051	3.472530
19	6	2.642063	0.912118	2.165501
20	6	0.335818	2.694787	-2.137313
21	6	-2.012963	1.485782	2.263371
22	6	2.014975	-1.474745	2.268500
23	7	2.501515	0.977434	-0.270385
24	7	0.737222	1.277908	-2.411729
25	7	-0.740542	-1.289406	-2.405753
26	7	-2.502903	-0.978654	-0.263961
27	7	-1.492113	0.075552	2.220601
28	7	1.493255	-0.065130	2.219934
29	1	5.291277	1.164076	1.638182
30	1	6.322089	1.651866	-0.589047
31	1	4.832664	1.754388	-2.593440
32	1	2.383130	0.226283	-3.186871
33	1	2.509265	1.973999	-3.413320
34	1	-1.028060	1.130607	-3.581747
35	1	0.453507	1.133779	-4.546165
36	1	-0.460154	-1.153312	-

```
4.541198
   37          1                      1.022932   -1.146823   -
3.579269
   38          1                     -2.513355   -1.992036   -
3.401285
   39          1                     -2.387708   -0.242999   -
3.185229
   40          1                     -4.836434   -1.765556   -
2.581259
   41          1                     -6.324315   -1.651499   -
0.576343
   42          1                     -5.291415   -1.153284
1.647619
   43          1                     -2.205352   -1.886560
2.362120
   44          1                     -3.375522   -0.683664
2.958992
   45          1                     -0.703935   -1.347195
3.566644
   46          1                     -1.235558    0.130360
4.360168
   47          1                      1.238222   -0.111304
4.359850
   48          1                      0.706164    1.363060
3.560861
   49          1                      3.376854    0.698695
2.953167
   50          1                      2.205420    1.898166
2.351661
   51          1                      0.425518    3.331560   -
3.029318
   52          1                     -2.509198    1.703966
3.219146
   53          1                     -2.737624    1.596437
1.446549
   54          1                      2.511319   -1.688704
3.225191
   55          1                      2.739936   -1.588224
1.452299
   56          6                     -0.864539    2.447605
1.972250
   57          6                     -1.088904    2.684221   -
1.581468
   58          6                      0.867789   -2.439151
1.980980
   59          6                     -0.337857   -2.704767   -
2.125559
   60          1                     -0.428207   -3.345521   -
3.014650
   61          1                     -0.997543   -3.092143   -
1.339492
   62          6                      1.087554   -2.690819   -
1.571592
   63          8                      0.003735    2.132324
1.104101
   64          8                     -1.532641    1.635249   -
1.017993
   65          8                      1.531049   -1.639396   -
1.012505
   66          8                     -0.002513   -2.127187
1.113658
   67          7                      0.855636   -3.586497
2.676269
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68	1	1.590232	-3.776105	3.362777
69	7	-0.187224	-4.540616	2.441097
70	1	0.193906	-5.397972	2.030334
71	1	-0.698194	-4.727734	3.308962
72	7	1.796066	-3.816984	-1.699611
73	1	1.435234	-4.595342	-2.255989
74	7	3.075488	-3.919531	-1.049111
75	1	3.149901	-4.835266	-0.595614
76	1	3.829203	-3.778047	-1.730920
77	7	-1.796536	3.810588	-1.712456
78	1	-1.435975	4.586571	-2.272312
79	7	-3.074800	3.916633	-1.060183
80	1	-3.147985	4.834467	-0.610740
81	1	-3.829754	3.772438	-1.740060
82	7	-0.848554	3.596012	2.665748
83	1	-1.582492	3.789254	3.351943
84	7	0.197934	4.545906	2.429382
85	1	-0.179037	5.402242	2.012659
86	1	0.706090	4.736062	3.298231
87	1	0.996733	3.085129	-1.353763

HF = -2108.0326242 Hartree
Zero-point correction = 0.731894
Sum of electronic and thermal Enthalpies = -2107.256561
Sum of electronic and thermal Free Energies = -2107.375896

(λλ)-[Tm(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	69	0.000000	0.000000	0.000000
2	7	-0.000004	-2.572915	0.000000
3	7	0.921545	-1.132204	2.231138
4	7	-0.921555	1.132205	2.231136
5	7	0.000004	2.572916	

```
0.000000
     6          7                     0.921558    1.132203   -
2.231135
     7          7                    -0.921550   -1.132202   -
2.231138
     8          8                     2.092749    0.913144
0.988196
     9          8                    -2.092754   -0.913143
0.988188
    10          8                     2.092750   -0.913149   -
0.988188
    11          8                    -2.092747    0.913151   -
0.988197
    12          6                    -0.196856   -3.269881   -
1.148691
    13          6                    -0.223088   -4.663770   -
1.178383
    14          1                    -0.403269   -5.182151   -
2.111721
    15          6                    -0.000011   -5.374184
0.000000
    16          1                    -0.000013   -6.457055
0.000000
    17          6                     0.223071   -4.663771
1.178383
    18          1                     0.403249   -5.182152
2.111722
    19          6                     0.196844   -3.269882
1.148691
    20          6                     0.304022   -2.486310
2.432261
    21          1                    -0.709124   -2.321196
2.812421
    22          1                     0.861226   -3.060953
3.184893
    23          6                     0.694536   -0.305929
3.481687
    24          1                     1.449542    0.482085
3.512327
    25          1                     0.836440   -0.926874
4.377508
    26          6                    -0.694546    0.305931
3.481685
    27          1                    -1.449553   -0.482082
3.512326
    28          1                    -0.836453    0.926878
4.377506
    29          6                    -0.304031    2.486310
2.432260
    30          1                     0.709114    2.321197
2.812423
    31          1                    -0.861239    3.060954
3.184890
    32          6                    -0.196850    3.269883
1.148690
    33          6                    -0.223077    4.663772
1.178382
    34          1                    -0.403261    5.182153
2.111720
    35          6                     0.000008    5.374185
0.000000
    36          1                     0.000010    6.457056
0.000000
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37	6	0.223091	4.663771	-
1.178382				
38	1	0.403276	5.182152	-
2.111720				
39	6	0.196859	3.269882	-
1.148690				
40	6	0.304040	2.486310	-
2.432260				
41	1	-0.709105	2.321201	-
2.812423				
42	1	0.861250	3.060952	-
3.184889				
43	6	0.694547	0.305930	-
3.481685				
44	1	1.449551	-0.482087	-
3.512326				
45	1	0.836456	0.926877	-
4.377506				
46	6	-0.694537	-0.305927	-
3.481686				
47	1	-1.449542	0.482090	-
3.512327				
48	1	-0.836445	-0.926872	-
4.377508				
49	6	-0.304029	-2.486309	-
2.432261				
50	1	0.709117	-2.321197	-
2.812420				
51	1	-0.861235	-3.060950	-
3.184893				
52	6	2.407550	-1.248566	
2.033732				
53	1	2.596613	-1.935187	
1.202610				
54	1	2.935883	-1.599537	
2.923710				
55	6	2.878486	0.138651	
1.637505				
56	6	-2.407560	1.248566	
2.033725				
57	1	-2.596622	1.935190	
1.202606				
58	1	-2.935895	1.599533	
2.923704				
59	6	-2.878495	-0.138649	
1.637489				
60	6	2.407564	1.248559	-
2.033724				
61	1	2.596628	1.935181	-
1.202605				
62	1	2.935901	1.599524	-
2.923702				
63	6	2.878495	-0.138657	-
1.637489				
64	6	-2.407555	-1.248559	-
2.033732				
65	1	-2.596620	-1.935180	-
1.202611				
66	1	-2.935888	-1.599528	-
2.923711				
67	6	-2.878486	0.138659	-
1.637505				
68	7	4.109179	-0.530868	-

1.990097				
69	7	4.942777	0.338606	-
2.772012				
70	1	5.184809	-0.103084	-
3.664834				
71	1	5.775535	0.616399	-
2.244290				
72	7	4.109174	0.530853	
1.990109				
73	7	-4.109179	-0.530856	
1.990100				
74	1	-4.409522	-1.479739	
1.744065				
75	7	-4.942772	0.338620	
2.772016				
76	1	-5.775532	0.616417	
2.244298				
77	1	-5.184802	-0.103068	
3.664840				
78	7	-4.109172	0.530865	-
1.990111				
79	1	-4.409515	1.479747	-
1.744074				
80	7	-4.942768	-0.338615	-
2.772021				
81	1	-5.775524	-0.616411	-
2.244298				
82	1	-5.184804	0.103072	-
3.664843				
83	1	4.409518	-1.479751	-
1.744060				
84	7	4.942771	-0.338627	
2.772018				
85	1	5.184811	0.103060	
3.664839				
86	1	5.775523	-0.616428	
2.244292				
87	1	4.409519	1.479734	
1.744070				

HF = -2110.3939944 Hartree
Zero-point correction = 0.733790
Sum of electronic and thermal Enthalpies = -2109.617282
Sum of electronic and thermal Free Energies = -2109.730672

$(\lambda\delta)$-[Tm(L)]$^{3+}$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	69	0.023485	0.015286	-
0.076884				
2	6	-3.316676	-0.969563	
0.556066				
3	6	-4.683045	-1.173483	
0.379023				
4	6	-5.181374	-1.379677	-
0.907309				
5	6	-4.288488	-1.362689	-
1.973152				
6	6	-2.938470	-1.099000	-

1.729510				
7	6	-2.007915	-0.957097	-
2.903665				
8	6	0.244996	-0.380449	-
3.627461				
9	6	0.165764	1.138677	-
3.496306				
10	6	2.320732	1.597605	-
2.465852				
11	6	3.153296	1.345491	-
1.236620				
12	6	4.539889	1.499554	-
1.339672				
13	6	5.343464	1.182919	-
0.252021				
14	6	4.726188	0.763699	
0.928073				
15	6	3.338550	0.682282	
0.976822				
16	6	2.648760	0.479350	
2.291990				
17	6	0.601648	-0.054630	
3.451088				
18	6	-0.850814	-0.503950	
3.374496				
19	6	-2.736490	-0.983169	
1.938958				
20	6	-0.148946	-2.469624	-
2.374369				
21	6	1.791987	-1.831384	
2.166291				
22	6	-2.035981	1.367914	
2.244280				
23	7	-2.443565	-0.902167	-
0.485190				
24	7	-0.556977	-1.035888	-
2.526358				
25	7	0.841474	1.569569	-
2.214724				
26	7	2.545330	0.936166	-
0.101357				
27	7	1.406589	-0.373437	
2.206753				
28	7	-1.560485	-0.051958	
2.114337				
29	1	-5.341391	-1.198055	
1.238045				
30	1	-6.236441	-1.560302	-
1.070477				
31	1	-4.629658	-1.539942	-
2.985718				
32	1	-2.178755	0.027585	-
3.347485				
33	1	-2.249029	-1.704468	-
3.673867				
34	1	1.281401	-0.710743	-
3.533692				
35	1	-0.123769	-0.700056	-
4.612419				
36	1	0.637747	1.621361	-
4.363511				
37	1	-0.874575	1.465343	-
3.463156				

38	1	2.614022	2.550802	-2.930589
39	1	2.549715	0.811161	-3.191360
40	1	4.974984	1.854892	-2.265914
41	1	6.420780	1.273300	-0.312092
42	1	5.313294	0.533449	1.807994
43	1	2.314980	1.466731	2.625444
44	1	3.345967	0.081298	3.040709
45	1	0.652156	1.024865	3.594520
46	1	1.070612	-0.518649	4.332573
47	1	-1.383837	-0.131139	4.262474
48	1	-0.909455	-1.591983	3.407719
49	1	-3.514087	-0.773579	2.685544
50	1	-2.354957	-1.996370	2.105231
51	1	-0.137989	-3.002104	-3.336354
52	1	2.215365	-2.159135	3.125452
53	1	2.535642	-1.965525	1.370452
54	1	-2.563328	1.532774	3.194190
55	1	-2.719236	1.576653	1.410281
56	6	0.558838	-2.631287	1.770096
57	6	1.207626	-2.510309	-1.676564
58	6	-0.848265	2.308154	2.068111
59	6	0.366230	2.929196	-1.804168
60	1	0.449928	3.663554	-2.618464
61	1	0.985599	3.257437	-0.960122
62	6	-1.064757	2.798575	-1.294020
63	8	-0.190279	-2.189777	0.845829
64	8	1.588758	-1.506000	-0.997390
65	8	-1.476869	1.671925	-0.872308
66	8	0.069779	2.000019	1.246901
67	7	-0.856481	3.436403	2.792116
68	1	-1.607182	3.603399	3.466980
69	7	0.186299	4.402298	

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2.606646
   70          1                      -0.209453    5.303505
2.323801
   71          1                       0.752168    4.484968
3.456820
   72          7                      -1.821974    3.898953   -
1.292798
   73          1                      -1.500147    4.755036   -
1.749375
   74          7                      -3.105675    3.862467   -
0.635435
   75          1                      -3.244976    4.745738   -
0.134081
   76          1                      -3.847604    3.712268   -
1.329296
   77          7                       1.927182   -3.629960   -
1.790245
   78          1                       1.650473   -4.366272   -
2.443069
   79          7                       3.109933   -3.783436   -
0.977850
   80          1                       3.154494   -4.750416   -
0.639967
   81          1                       3.943384   -3.546220   -
1.528789
   82          7                       0.321560   -3.773204
2.433000
   83          1                       0.986561   -4.110857
3.132626
   84          7                      -0.892776   -4.496043
2.172528
   85          1                      -0.710525   -5.313609
1.581538
   86          1                      -1.331659   -4.761289
3.059517
   87          1                      -0.876303   -2.950437   -
1.708974
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 HF = -2110.3650253 Hartree
 Zero-point correction = 0.732504
 Sum of electronic and thermal Enthalpies = -2109.588636
 Sum of electronic and thermal Free Energies = -2109.705946
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