Supporting Information for:

Pyridine and phosphonate containing ligands for stable lanthanide complexation. An experimental and theoretical study to assess the solution structure

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Table S1. Distances (Å) between the Ln^{III} ion and oxygen ($Ln\cdots O_{w2nd}$) and hydrogen ($Ln\cdots H_{w2nd}$) atoms of second sphere water molecules hydrogen bonded to the highly charged phosphonate groups obtained from ab initio calculations at the HF/3-21G* level on $[Gd(L)(H_2O)]^{3-}\cdot 19H_2O$ and $[Lu(L)]^{3-}\cdot 20H_2O$ molecular clusters (L = $\mathbf{L^2}$, $\mathbf{L^3}$).

	(1)[a]		**(2)**[a]	
***tw*-[Gd($\mathbf{L^2}$)($\mathbf{H_2O}$)]$^{3-}$**	**Ln···O_{w2nd}**	**Ln···H_{w2nd}**	**Ln···O_{w2nd}**	**Ln···H_{w2nd}**
	4.12	3.25/4.79	4.09	3.33/4.51
	4.23	4.18/4.36	5.47	4.99/5.28
	5.68	4.98/6.48	5.52	4.80/6.05
	6.00	5.51/5.56	5.95	5.15/6.01
	6.68	6.00/6.28	6.03	5.45/5.65
	7.21	6.40/7.17	6.32	5.39/6.78
			7.01	6.35/6.81
***tw*-[Gd($\mathbf{L^3}$)($\mathbf{H_2O}$)]$^{3-}$**	4.12	3.25/4.79	4.00	3.28/4.42
	4.20	4.16/4.33	5.42	5.24/5.92
	5.69	4.98/6.48	5.73	5.01/6.24
	5.96	5.53/5.48	5.97	5.19/6.02
	6.66	6.26/5.98	6.06	5.47/5.70
	7.21	6.41/7.16	6.42	5.49/6.87
			7.04	6.36/6.85
***tw*-[Lu($\mathbf{L^2}$)]$^{3-}$**	4.03	3.14/4.58	3.91	3.18/4.31
	4.66	4.42/4.57	5.30	4.93/5.29
	5.37	4.65/4.17	5.61	4.88/6.11
	6.11	5.64/5.65	5.85	5.07/5.88
	6.59	5.95/6.15	5.92	5.35/5.53
	6.92	6.10/6.94	6.33	5.39/5.76
			6.91	6.25/6.71
***tw*-[Lu($\mathbf{L^3}$)]$^{3-}$**	4.03	3.13/4.58	3.85	3.16/4.26
	4.64	4.42/4.56	5.09	4.61/5.01
	5.36	4.64/6.15	5.79	5.05/6.24
	6.07	5.62/5.60	5.87	5.11/5.91
	6.57	5.93/6.13	5.95	5.38/5.58
	6.91	6.10/6.93	6.33	5.39/6.76
			6.90	6.23/6.71
***tf*-[Gd($\mathbf{L^2}$)($\mathbf{H_2O}$)]$^{3-}$**	4.35	3.44/4.97	5.62	4.96/6.08
	4.84	4.06/4.79	5.77	5.42/5.63
	5.06	4.85/4.83	6.24	5.37/6.78
	5.89	5.17/6.70	6.36	5.50/6.46
	6.77	6.07/6.41	6.58	5.85/6.40
	7.29	6.45/7.25	7.12	6.45/7.04
***tf*-[Gd($\mathbf{L^3}$)($\mathbf{H_2O}$)]$^{3-}$**	4.36	3.45/4.98	5.69	5.01/6.15
	4.85	4.09/4.79	5.75	5.60/5.41
	5.06	4.84/4.83	6.25	5.38/6.77
	5.90	5.18/5.70	6.38	6.47/5.52
	6.75	6.04/6.39	6.60	5.86/6.43
	7.30	6.46/7.25	7.11	6.43/7.04

[a] Distances corresponding to water molecules hydrogen bonded to phosphonate group (1) and (2) are listed separately.

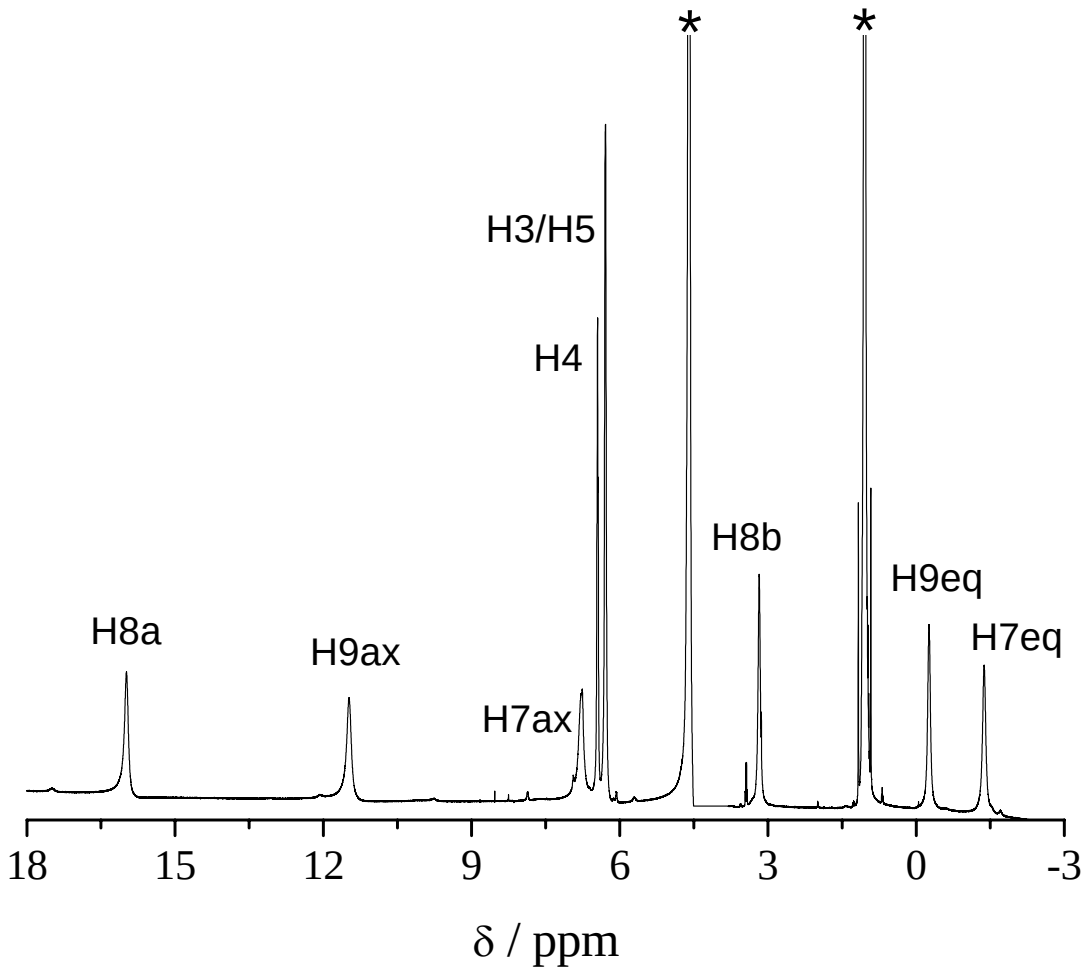

Figure S1. ^{1}H NMR spectra of the Eu^{III} complex of $\mathbf{L^2}$ recorded in D_2O solution (30 mM, pD = 8.0). HOD and ^{t}BuOH signals are denoted with an asterisk.

$[La(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	57	-0.215165	-0.150896	0.471999
2	7	-0.529649	2.566258	0.201002
3	7	0.424785	-2.866013	-0.148587
4	7	-1.275609	-1.532588	-2.026936
5	7	0.327282	1.120072	-2.131508
6	8	-2.528649	0.235030	-0.058139
7	8	2.060189	0.710004	0.253989
8	15	-3.582632	-0.428216	-0.962730
9	15	2.817378	0.696557	-1.077436
10	8	-3.993155	0.526796	-2.066450
11	8	-4.742584	-0.999951	-0.157442
12	8	4.161647	1.404645	-1.002188
13	8	2.923100	-0.716425	-1.647878
14	6	-0.501684	5.292815	0.043356
15	6	0.230610	-4.896174	-1.344421
16	6	0.023934	-3.523498	-1.232025
17	6	-0.550610	-2.764706	-2.397143
18	6	-1.231611	-0.579344	-3.172878
19	6	-2.685880	-1.859403	-1.646215
20	6	1.325543	-4.865447	0.767830
21	6	1.069404	-3.517680	0.822105
22	6	1.520184	-2.727495	2.022377
23	6	0.887043	-5.570900	-0.339639
24	6	-0.522645	4.671258	1.273795
25	6	-0.514749	3.295732	1.305337
26	6	-0.419778	2.564290	2.612213
27	6	-0.498023	4.525997	-1.107427
28	6	-0.538818	3.149166	-0.993905
29	6	-0.637520	2.247158	-2.198899
30	6	0.098561	0.164106	-3.251746
31	6	1.749562	1.632862	-2.203753
32	1	-0.457679	6.361669	-0.027124
33	1	-0.110269	-5.405877	-2.221450
34	1	0.298208	-2.526749	-3.026455
35	1	-1.205012	-3.424435	-2.965418
36	1	-1.365644	-1.128777	-4.106252
37	1	-2.070387	0.087131	-3.083708
38	1	-2.662404	-2.626887	-0.886958
39	1	-3.219774	-2.281197	-2.498025
40	1	1.849079	-5.317173	1.580573
41	1	1.059489	-6.625981	-0.418139
42	1	-0.503156	5.202727	2.199137
43	1	-0.397223	4.978335	-2.068726
44	1	-1.641116	1.846945	-2.218831
45	1	-0.474968	2.829573	-3.103752

46	1	0.130207	0.709321	-4.197329
47	1	0.917022	-0.534119	-3.255474
48	1	1.763655	2.681071	-1.943354
49	1	2.115018	1.547933	-3.224721
50	8	1.226449	-1.498415	2.024450
51	8	2.131289	-3.338124	2.920061
52	8	-0.367787	1.279621	2.516261
53	8	-0.350989	3.216960	3.657218
54	8	3.813730	-0.255111	-4.255955
55	1	3.407809	-0.355358	-3.378841
56	1	4.759448	-0.121338	-4.040390
57	8	6.004076	0.116283	-2.712829
58	1	5.499379	0.752862	-2.164235
59	1	5.985703	-0.720635	-2.214096
60	8	1.055339	-0.052279	4.293420
61	1	1.510694	-0.544714	3.580071
62	8	-0.330850	-2.344635	4.448224
63	1	0.105186	-1.477708	4.616643
64	1	0.378786	-2.965460	4.223285
65	1	0.387193	0.487262	3.798594
66	8	2.141923	2.447516	4.681885
67	1	1.278007	2.879719	4.540966
68	1	1.955060	1.488048	4.721623
69	8	4.694355	-2.065701	2.042067
70	1	4.799232	-2.325890	1.110074
71	1	3.937610	-2.513308	2.447303
72	8	2.483504	2.775495	1.970360
73	1	2.547965	2.662209	2.939419
74	1	2.376006	1.926695	1.495638
75	8	5.752355	0.205859	0.945001
76	1	5.160058	0.800440	0.443526
77	1	5.257324	-0.319905	1.601088
78	8	3.589123	3.953402	-0.124245
79	1	3.982304	3.125312	-0.469294
81	8	5.308744	-1.812629	-0.740520
82	1	5.648584	-1.071632	-0.183301
83	1	4.419620	-1.553275	-1.068074
84	8	2.253881	-2.465732	-3.637116
85	1	2.473501	-2.077515	-2.768333
86	1	2.776482	-1.947143	-4.272758
87	8	2.353990	4.975097	-2.188846
88	1	2.758164	4.681237	-1.322825
89	1	2.918696	4.606218	-2.883173
90	8	-1.677286	-1.576987	2.173482
91	8	-4.025611	-0.518484	2.443777
92	8	-5.034382	2.717366	-0.825247
93	8	-6.891927	0.618128	-0.137138
94	8	-2.494190	-3.966933	1.176392
95	8	-4.899700	-3.837882	-0.285877
96	8	-6.569683	1.493080	-2.678340

97	8	-3.674332	2.038139	1.545364
98	1	-3.984433	0.458973	2.372930
99	1	-4.284659	2.521726	0.962685
100	1	-3.119391	1.477387	0.960914
101	1	-6.343047	1.404404	0.016364
102	1	-6.254468	-0.134979	-0.125275
103	1	-4.426224	2.049879	-1.213243
104	1	-5.759420	2.734627	-1.479331
105	1	-5.689212	1.076606	-2.773685
106	1	-6.952225	1.070284	-1.879962
107	1	-5.036867	-2.874417	-0.261070
108	1	-4.141569	-4.017532	0.297580
109	1	-2.570617	-1.128506	2.347987
110	1	-1.237568	-1.855884	3.013008
111	1	-2.217002	-3.096237	1.539010
112	1	-1.758992	-4.351727	0.689339
113	1	-4.428962	-0.829732	1.603028

HF = -3871.6986394 Hartree
Zero-point correction = 0.964849
Sum of electronic and thermal free energies = -3870.838196

$[Nd(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	60	-0.229668	-0.121304	0.509535
2	7	-0.603462	2.531071	0.189641
3	7	0.528440	-2.780060	-0.098640
4	7	-1.198827	-1.573416	-2.030568
5	7	0.293617	1.110526	-2.135660
6	8	-2.489915	0.157978	-0.071476
7	8	2.003665	0.652056	0.223909
8	15	-3.524820	-0.530821	-0.979255
9	15	2.781827	0.711608	-1.094262
10	8	-3.944068	0.409645	-2.093331
11	8	-4.683587	-1.120646	-0.186219
12	8	4.102098	1.459542	-0.978834
13	8	2.949725	-0.673099	-1.716974
14	6	-0.675598	5.258927	0.024555
15	6	0.485300	-4.831297	-1.276327
16	6	0.190117	-3.473363	-1.181493
17	6	-0.419077	-2.776120	-2.366799
18	6	-1.186845	-0.639506	-3.188989
19	6	-2.592057	-1.945382	-1.642405
20	6	1.536480	-4.714176	0.851845
21	6	1.195363	-3.384411	0.887724
22	6	1.575814	-2.564678	2.091377
23	6	1.164076	-5.455930	-0.254945
24	6	-0.676841	4.640191	1.256610
25	6	-0.621044	3.266343	1.290871
26	6	-0.521167	2.539734	2.597364
27	6	-0.645230	4.488366	-1.123087
28	6	-0.635489	3.111211	-1.006460
29	6	-0.703900	2.206168	-2.210236
30	6	0.111246	0.153982	-3.260556
31	6	1.698418	1.661990	-2.190404
32	1	-0.670818	6.328270	-0.048794
33	1	0.192601	-5.367390	-2.155135
34	1	0.413434	-2.519035	-3.009743
35	1	-1.041960	-3.484705	-2.912839
36	1	-1.289869	-1.206717	-4.116598
37	1	-2.051570	-0.005361	-3.114979
38	1	-2.538673	-2.695602	-0.868327
39	1	-3.115741	-2.401711	-2.483024
40	1	2.071990	-5.122671	1.679384
41	1	1.403711	-6.498929	-0.319686
42	1	-0.682596	5.174320	2.180653
43	1	-0.564764	4.941035	-2.086208
44	1	-1.694695	1.775555	-2.234586
45	1	-0.554266	2.793728	-3.114453

46	1	0.128087	0.704163	-4.204402
47	1	0.956194	-0.511874	-3.261232
48	1	1.687909	2.699167	-1.890109
49	1	2.065155	1.628643	-3.214674
50	8	1.196350	-1.361620	2.090759
51	8	2.218582	-3.135929	2.994277
52	8	-0.440876	1.254361	2.498051
53	8	-0.480317	3.189024	3.643346
54	8	3.847414	-0.160583	-4.307078
55	1	3.413174	-0.258886	-3.442570
56	1	4.782162	-0.009725	-4.055077
57	8	5.991301	0.251510	-2.710484
58	1	5.466942	0.868488	-2.157508
59	1	5.990340	-0.590114	-2.218564
60	8	0.917767	0.007130	4.393884
61	1	1.415688	-0.458958	3.692318
62	8	-0.362010	-2.345502	4.444959
63	1	0.013948	-1.461335	4.661422
64	1	0.394123	-2.921323	4.256126
65	1	0.251077	0.519830	3.871568
66	8	2.027014	2.503201	4.679363
67	1	1.166409	2.941802	4.543425
68	1	1.823408	1.551393	4.775693
69	8	4.764183	-1.957057	2.046007
70	1	4.841344	-2.231924	1.116410
71	1	3.998649	-2.369497	2.472901
72	8	2.373626	2.740673	1.979969
73	1	2.428350	2.650662	2.953985
74	1	2.303499	1.882732	1.520430
75	8	5.772375	0.300151	0.901934
76	1	5.150985	0.883276	0.421150
77	1	5.311415	-0.227159	1.581652
78	8	3.419920	3.983736	-0.101015
79	1	3.009885	3.731249	0.761442
80	1	3.852505	3.175479	-0.444057
81	8	5.348357	-1.720926	-0.773559
82	1	5.669620	-0.975215	-0.209177
83	1	4.455767	-1.480390	-1.105333
84	8	2.369202	-2.436315	-3.709230
85	1	2.561547	-2.045763	-2.834342
86	1	2.870787	-1.879969	-4.329996
87	8	2.211024	5.016237	-2.171724
88	1	2.600142	4.722429	-1.298910
89	1	2.803737	4.668188	-2.853511
90	8	-1.645780	-1.591258	2.125859
91	8	-4.014422	-0.600868	2.412440
92	8	-5.084492	2.572487	-0.897402
93	8	-6.890416	0.424341	-0.256582
94	8	-2.380086	-4.013362	1.142433
95	8	-4.773137	-3.961545	-0.352340

96	8	-6.528248	1.280376	-2.797740
97	8	-3.722850	1.949870	1.496223
98	1	-4.001706	0.377564	2.343698
99	1	-4.339455	2.417059	0.907359
100	1	-3.143219	1.404449	0.923702
101	1	-6.378895	1.231813	-0.084611
102	1	-6.227049	-0.304069	-0.211927
103	1	-4.453587	1.917010	-1.269179
104	1	-5.792321	2.580044	-1.568669
105	1	-5.628901	0.899038	-2.853299
106	1	-6.916925	0.862288	-1.999505
107	1	-4.938549	-3.002625	-0.314338
108	1	-4.014911	-4.124309	0.236174
109	1	-2.551608	-1.163907	2.298806
110	1	-1.211965	-1.861412	2.971196
111	1	-2.143582	-3.129629	1.504315
112	1	-1.606640	-4.387216	0.708589
113	1	-4.410312	-0.923819	1.572926

HF = -3873.6037888 Hartree
Zero-point correction = 0.965335
Sum of electronic and thermal free energies = -3872.742211

[Gd(L^2)(H_2O)]$^{3-}$ 19H_2O (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	64	-0.233859	-0.116898	0.525450
2	7	-0.641611	2.482755	0.168566
3	7	0.566022	-2.729690	-0.108201
4	7	-1.177006	-1.598703	-2.070323
5	7	0.271274	1.087623	-2.165030
6	8	-2.431814	0.096343	-0.068314
7	8	1.929835	0.639137	0.206382
8	15	-3.477330	-0.571512	-0.981209
9	15	2.739782	0.718728	-1.092746
10	8	-3.898936	0.390851	-2.076400
11	8	-4.636693	-1.162776	-0.189816
12	8	4.042867	1.490957	-0.940158
13	8	2.954494	-0.658816	-1.716486
14	6	-0.764833	5.211706	0.007909
15	6	0.603894	-4.789780	-1.274802
16	6	0.258427	-3.442555	-1.188120
17	6	-0.374079	-2.786655	-2.384379
18	6	-1.175890	-0.674019	-3.232306
19	6	-2.560723	-1.980052	-1.671024
20	6	1.640502	-4.625358	0.854258
21	6	1.251527	-3.308825	0.881700
22	6	1.598989	-2.475988	2.083424
23	6	1.300603	-5.386015	-0.249741
24	6	-0.758247	4.590509	1.238667
25	6	-0.677537	3.218322	1.269519
26	6	-0.576222	2.489922	2.572106
27	6	-0.719646	4.442855	-1.139716
28	6	-0.685189	3.065370	-1.026139
29	6	-0.741328	2.166709	-2.234081
30	6	0.109404	0.138412	-3.296741
31	6	1.667298	1.657060	-2.206080
32	1	-0.779164	6.281045	-0.063989
33	1	0.334684	-5.338730	-2.153196
34	1	0.449167	-2.524591	-3.037087
35	1	-0.980788	-3.523878	-2.911300
36	1	-1.265619	-1.245978	-4.158903
37	1	-2.049677	-0.051643	-3.163289
38	1	-2.497824	-2.736238	-0.903674
39	1	-3.096705	-2.428668	-2.508452
40	1	2.186997	-5.009339	1.686226
41	1	1.578812	-6.419697	-0.309104
42	1	-0.777917	5.122140	2.163971
43	1	-0.646859	4.897654	-2.102398
44	1	-1.726084	1.722853	-2.260863
45	1	-0.600684	2.763250	-3.134271

46	1	0.121730	0.694998	-4.237349
47	1	0.964183	-0.515069	-3.299264
48	1	1.641682	2.694460	-1.907364
49	1	2.049934	1.624807	-3.224341
50	8	1.179098	-1.287561	2.081392
51	8	2.256311	-3.024075	2.991993
52	8	-0.473443	1.205596	2.465444
53	8	-0.555638	3.131151	3.623021
54	8	3.856203	-0.098436	-4.291702
55	1	3.423628	-0.225151	-3.429827
56	1	4.784590	0.080050	-4.035095
57	8	5.977630	0.362971	-2.677633
58	1	5.432402	0.958475	-2.121515
59	1	5.997408	-0.483102	-2.193981
60	8	0.876323	0.021649	4.415421
61	1	1.396311	-0.425303	3.718236
62	8	-0.336356	-2.369667	4.418388
63	1	0.006113	-1.478429	4.657125
64	1	0.442645	-2.915115	4.231605
65	1	0.201669	0.510050	3.881524
66	8	1.957522	2.525868	4.683434
67	1	1.093337	2.952406	4.533192
68	1	1.760068	1.573876	4.791737
69	8	4.796380	-1.881038	2.066107
70	1	4.878986	-2.155531	1.136846
71	1	4.020111	-2.282981	2.484642
72	8	2.309567	2.732070	1.982669
73	1	2.363525	2.648422	2.957313
74	1	2.246738	1.872703	1.526597
75	8	5.757277	0.392005	0.922568
76	1	5.113151	0.952715	0.443970
77	1	5.316093	-0.152299	1.602386
78	8	3.312634	4.006094	-0.100953
79	1	2.907721	3.748130	0.761686
80	1	3.760495	3.203089	-0.437443
81	8	5.377150	-1.637920	-0.755091
82	1	5.678756	-0.883500	-0.191523
83	1	4.480125	-1.421324	-1.091527
84	8	2.415504	-2.413033	-3.735502
85	1	2.591941	-2.028650	-2.854453
86	1	2.909684	-1.839247	-4.345966
87	8	2.121240	5.032120	-2.185817
88	1	2.499846	4.739486	-1.308305
89	1	2.724982	4.688177	-2.859914
90	8	-1.594969	-1.601426	2.078328
91	8	-3.978754	-0.659944	2.405466
92	8	-5.060384	2.533399	-0.882819
93	8	-6.852022	0.368548	-0.259875
94	8	-2.305722	-4.039425	1.105889
95	8	-4.723065	-4.007837	-0.349018

96	8	-6.490421	1.240459	-2.795096
97	8	-3.699450	1.889534	1.494098
98	1	-3.975919	0.318781	2.344092
99	1	-4.311393	2.360824	0.903335
100	1	-3.112126	1.349239	0.926194
101	1	-6.346729	1.178502	-0.081314
102	1	-6.183605	-0.355464	-0.217072
103	1	-4.426161	1.882285	-1.258480
104	1	-5.768054	2.542504	-1.553878
105	1	-5.587577	0.867956	-2.849551
106	1	-6.877144	0.815807	-1.999288
107	1	-4.888580	-3.048908	-0.313502
108	1	-3.952326	-4.166362	0.224143
109	1	-2.508138	-1.193281	2.257742
110	1	-1.162504	-1.873015	2.922757
111	1	-2.076976	-3.151485	1.460687
112	1	-1.525081	-4.416744	0.688154
113	1	-4.375121	-0.979707	1.564646

HF = -3876.01405101 Hartree
Zero-point correction = 0.965649
Sum of electronic and thermal free energies = -3875.151867

$[Ho(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	67	-0.234865	-0.114885	0.550371
2	7	-0.674451	2.450420	0.156178
3	7	0.588822	-2.698312	-0.120744
4	7	-1.167575	-1.620173	-2.110465
5	7	0.254836	1.075206	-2.189354
6	8	-2.384390	0.036636	-0.064282
7	8	1.873688	0.642484	0.195491
8	15	-3.442592	-0.601432	-0.985569
9	15	2.705639	0.731148	-1.090225
10	8	-3.861844	0.388541	-2.057402
11	8	-4.604469	-1.191866	-0.197035
12	8	3.998809	1.515209	-0.911837
13	8	2.948006	-0.643282	-1.709862
14	6	-0.829559	5.179801	-0.005502
15	6	0.664130	-4.766268	-1.274645
16	6	0.294556	-3.424275	-1.196372
17	6	-0.348175	-2.797186	-2.403237
18	6	-1.167018	-0.697328	-3.270277
19	6	-2.546354	-2.004058	-1.706947
20	6	1.698621	-4.571788	0.850583
21	6	1.286996	-3.262130	0.870431
22	6	1.624507	-2.421788	2.068363
23	6	1.371242	-5.345454	-0.248021
24	6	-0.820032	4.558649	1.225169
25	6	-0.722608	3.187725	1.255801
26	6	-0.615798	2.462062	2.557850
27	6	-0.772590	4.410568	-1.151926
28	6	-0.723810	3.033061	-1.038798
29	6	-0.771702	2.139059	-2.250029
30	6	0.109159	0.129885	-3.324569
31	6	1.643512	1.659586	-2.218837
32	1	-0.855620	6.248859	-0.078004
33	1	0.404019	-5.324012	-2.150169
34	1	0.472919	-2.533061	-3.057785
35	1	-0.939818	-3.554803	-2.918887
36	1	-1.244497	-1.267598	-4.199470
37	1	-2.046806	-0.082855	-3.204770
38	1	-2.482289	-2.770660	-0.949850
39	1	-3.093678	-2.436809	-2.545858
40	1	2.253458	-4.940610	1.683787
41	1	1.667464	-6.374420	-0.301721
42	1	-0.849186	5.089895	2.150424
43	1	-0.701442	4.865569	-2.114531
44	1	-1.751216	1.683659	-2.275877
45	1	-0.642321	2.743754	-3.146854

46	1	0.120367	0.689331	-4.263883
47	1	0.971223	-0.514131	-3.324934
48	1	1.605287	2.697052	-1.921419
49	1	2.039961	1.627382	-3.231612
50	8	1.179805	-1.242796	2.069851
51	8	2.296717	-2.955471	2.975376
52	8	-0.493210	1.178640	2.449718
53	8	-0.606961	3.100697	3.610057
54	8	3.846383	-0.058121	-4.278274
55	1	3.418923	-0.203044	-3.416432
56	1	4.770016	0.144240	-4.022661
57	8	5.956202	0.445659	-2.663221
58	1	5.399497	1.024358	-2.100910
59	1	5.991472	-0.405049	-2.188723
60	8	0.865264	0.037108	4.422308
61	1	1.396172	-0.397348	3.725707
62	8	-0.293993	-2.383941	4.405776
63	1	0.022844	-1.486763	4.655103
64	1	0.500854	-2.904177	4.212772
65	1	0.181522	0.508982	3.885761
66	8	1.916326	2.553489	4.671921
67	1	1.046832	2.968077	4.519634
68	1	1.729324	1.600146	4.786845
69	8	4.856592	-1.862298	2.066829
70	1	4.935015	-2.120688	1.132334
71	1	4.063570	-2.246323	2.471533
72	8	2.252187	2.744721	1.966606
73	1	2.312216	2.664619	2.941165
74	1	2.199503	1.884041	1.512398
75	8	5.749182	0.446395	0.928425
76	1	5.085783	0.993129	0.459359
77	1	5.329493	-0.116186	1.607105
78	8	3.242482	4.032130	-0.117192
79	1	2.831940	3.771612	0.741821
80	1	3.700863	3.231042	-0.444123
81	8	5.393276	-1.579498	-0.757301
82	1	5.685284	-0.821191	-0.193886
83	1	4.490224	-1.378329	-1.087669
84	8	2.448920	-2.404351	-3.739655
85	1	2.608223	-2.019267	-2.855615
86	1	2.934925	-1.817397	-4.343944
87	8	2.053352	5.048766	-2.210058
88	1	2.430452	4.758006	-1.331436
89	1	2.657650	4.702859	-2.882580
90	8	-1.551742	-1.613818	2.066262
91	8	-3.947579	-0.719882	2.400527
92	8	-5.040062	2.511598	-0.858157
93	8	-6.820827	0.334236	-0.255310
94	8	-2.260905	-4.040043	1.066155
95	8	-4.694251	-4.039721	-0.353379

96	8	-6.460720	1.223502	-2.784090
97	8	-3.678291	1.827184	1.500206
98	1	-3.954159	0.259409	2.350831
99	1	-4.281812	2.312789	0.912301
100	1	-3.088892	1.290647	0.932351
101	1	-6.318425	1.144518	-0.069970
102	1	-6.149671	-0.387779	-0.217215
103	1	-4.403329	1.866039	-1.240989
104	1	-5.748704	2.525782	-1.527587
105	1	-5.555280	0.858494	-2.841269
106	1	-6.843343	0.792276	-1.989673
107	1	-4.860990	-3.080952	-0.320488
108	1	-3.911766	-4.191577	0.205573
109	1	-2.474325	-1.225612	2.247003
110	1	-1.119847	-1.888095	2.909803
111	1	-2.030732	-3.156519	1.430934
112	1	-1.465861	-4.443691	0.703535
113	1	-4.338474	-1.032046	1.553662

HF = -3877.7687759 Hartree
Zero-point correction = 0.965338
Sum of electronic and thermal free energies = -3876.906772

$[Lu(L^2)(H_2O)]^{3-}$ $19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	71	-0.242873	-0.107955	0.589800
2	7	-0.698277	2.419976	0.126061
3	7	0.608234	-2.660842	-0.128586
4	7	-1.154188	-1.648451	-2.161862
5	7	0.238788	1.055006	-2.240654
6	8	-2.328180	-0.018156	-0.065798
7	8	1.800701	0.627397	0.170574
8	15	-3.397289	-0.638817	-0.988205
9	15	2.661183	0.724009	-1.097465
10	8	-3.823478	0.367585	-2.042485
11	8	-4.556574	-1.230437	-0.196069
12	8	3.941657	1.521730	-0.885182
13	8	2.938030	-0.646955	-1.708964
14	6	-0.873264	5.150373	-0.053466
15	6	0.773520	-4.723316	-1.286805
16	6	0.349772	-3.396625	-1.207898
17	6	-0.312907	-2.810080	-2.426263
18	6	-1.161820	-0.731696	-3.321993
19	6	-2.521174	-2.036233	-1.737478
20	6	1.784549	-4.496833	0.843401
21	6	1.323382	-3.204030	0.863821
22	6	1.627875	-2.361026	2.067065
23	6	1.495650	-5.279363	-0.259268
24	6	-0.860121	4.536963	1.180884
25	6	-0.752749	3.167382	1.219400
26	6	-0.644497	2.453422	2.526030
27	6	-0.811266	4.373022	-1.193314
28	6	-0.753064	2.995742	-1.072890
29	6	-0.798795	2.103748	-2.286177
30	6	0.104398	0.111874	-3.375120
31	6	1.621539	1.644905	-2.250753
32	1	-0.906403	6.218673	-0.133462
33	1	0.542138	-5.286306	-2.167010
34	1	0.500842	-2.544823	-3.089298
35	1	-0.886265	-3.596099	-2.921052
36	1	-1.231065	-1.302785	-4.251967
37	1	-2.047493	-0.125440	-3.257577
38	1	-2.444558	-2.806508	-0.985162
39	1	-3.087709	-2.463636	-2.566830
40	1	2.347035	-4.846412	1.679645
41	1	1.832775	-6.295517	-0.314927
42	1	-0.894066	5.073453	2.102975
43	1	-0.742669	4.821761	-2.158924
44	1	-1.772823	1.636895	-2.305105
45	1	-0.687337	2.716765	-3.180521

46	1	0.109314	0.670341	-4.315807
47	1	0.973363	-0.523206	-3.375525
48	1	1.575349	2.683679	-1.958712
49	1	2.039598	1.608582	-3.254644
50	8	1.158152	-1.192045	2.069867
51	8	2.301721	-2.881062	2.981652
52	8	-0.510597	1.169097	2.426210
53	8	-0.645121	3.095214	3.575386
54	8	3.861611	-0.038719	-4.266172
55	1	3.425680	-0.196248	-3.410858
56	1	4.777273	0.181985	-3.997529
57	8	5.939547	0.501933	-2.624094
58	1	5.366324	1.067754	-2.065468
59	1	5.985254	-0.349643	-2.152203
60	8	0.846047	0.073895	4.433696
61	1	1.386731	-0.357606	3.743686
62	8	-0.276077	-2.366595	4.413490
63	1	0.023567	-1.466066	4.669549
64	1	0.528812	-2.869302	4.214949
65	1	0.158378	0.528990	3.888981
66	8	1.881365	2.596582	4.653701
67	1	1.010710	3.004467	4.491319
68	1	1.697067	1.644783	4.784661
69	8	4.859626	-1.806899	2.097931
70	1	4.944047	-2.067985	1.164573
71	1	4.062013	-2.187009	2.497607
72	8	2.212503	2.746990	1.946630
73	1	2.276739	2.676073	2.921587
74	1	2.161095	1.883652	1.499565
75	8	5.715449	0.510076	0.952010
76	1	5.036501	1.036114	0.480483
77	1	5.310893	-0.060869	1.632896
78	8	3.167810	4.042472	-0.151646
79	1	2.761398	3.788681	0.710300
80	1	3.631570	3.238753	-0.465536
81	8	5.390824	-1.531249	-0.724125
82	1	5.667656	-0.763539	-0.166008
83	1	4.487404	-1.347760	-1.064119
84	8	2.486059	-2.405034	-3.757292
85	1	2.627593	-2.020747	-2.869755
86	1	2.972541	-1.810080	-4.353040
87	8	1.996649	5.053286	-2.259144
88	1	2.365252	4.764186	-1.376769
89	1	2.602398	4.699180	-2.925970
90	8	-1.519917	-1.598550	2.063103
91	8	-3.929645	-0.748429	2.397206
92	8	-5.026751	2.475281	-0.863189
93	8	-6.785561	0.275861	-0.259479
94	8	-2.189735	-4.042736	1.066242
95	8	-4.638126	-4.081534	-0.324638

96	8	-6.433148	1.168169	-2.786728
97	8	-3.670828	1.787760	1.479145
98	1	-3.946711	0.230427	2.343060
99	1	-4.271336	2.270754	0.885352
100	1	-3.068900	1.258053	0.920452
101	1	-6.292411	1.091185	-0.071927
102	1	-6.106881	-0.439223	-0.220878
103	1	-4.384329	1.832830	-1.243767
104	1	-5.736801	2.479356	-1.531099
105	1	-5.523309	0.814256	-2.840135
106	1	-6.812978	0.733631	-1.992719
107	1	-4.807857	-3.123029	-0.303420
108	1	-3.847222	-4.221753	0.225449
109	1	-2.450702	-1.228869	2.239500
110	1	-1.092431	-1.871241	2.908826
111	1	-1.974666	-3.153756	1.425051
112	1	-1.393063	-4.423721	0.683490
113	1	-4.311879	-1.067781	1.548568

HF = -3880.0804769 Hartree
Zero-point correction = 0.966038
Sum of electronic and thermal free energies = -3879.217659

$[La(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	57	-0.427682	-0.083001	0.652362
2	7	-1.017458	2.199722	-0.726771
3	7	1.019526	-2.385259	1.106532
4	7	-1.082530	-2.510478	-0.873154
5	7	0.117941	0.017446	-2.212961
6	8	-2.763272	-0.285202	0.028341
7	8	1.889157	0.431880	0.104710
8	15	-3.620837	-1.500659	-0.372461
9	15	2.661649	0.146518	-1.181300
10	8	-4.146845	-1.324479	-1.787397
11	8	-4.702959	-1.818862	0.648999
12	8	3.881665	1.027583	-1.417028
13	8	3.000708	-1.337902	-1.344323
14	6	-1.172876	4.614013	-1.994217
15	6	1.983367	-4.407258	0.360784
16	6	0.974335	-3.443027	0.318389
17	6	-0.121350	-3.634766	-0.707455
18	6	-1.180999	-2.143120	-2.320829
19	6	-2.437559	-2.888550	-0.348278
20	6	3.090176	-3.109300	2.018600
21	6	2.060434	-2.212129	1.933253
22	6	2.085013	-0.966552	2.779320
23	6	3.044237	-4.237583	1.211629
24	6	-1.303520	4.543538	-0.619386
25	6	-1.191269	3.308502	-0.021579
26	6	-1.230362	3.177509	1.477712
27	6	-0.982195	3.454935	-2.723311
28	6	-0.955110	2.242578	-2.054041
29	6	-0.909086	0.920282	-2.782312
30	6	0.023370	-1.348384	-2.802128
31	6	1.488191	0.574509	-2.494363
32	1	-1.196602	5.561581	-2.494737
33	1	1.951827	-5.221606	-0.331640
34	1	0.399635	-3.810674	-1.639212
35	1	-0.668192	-4.539448	-0.455744
36	1	-1.244256	-3.055100	-2.915495
37	1	-2.104551	-1.615295	-2.470903
38	1	-2.343721	-3.226948	0.672244
39	1	-2.838513	-3.718738	-0.932784
40	1	3.916299	-2.899841	2.660674
41	1	3.846804	-4.947589	1.228683
42	1	-1.462249	5.400369	-0.001436
43	1	-0.759849	3.489329	-3.766119
44	1	-1.881593	0.459821	-2.671153
45	1	-0.720475	1.094251	-3.839085

46	1	-0.025102	-1.267064	-3.889373
47	1	0.931870	-1.870818	-2.565138
48	1	1.424132	1.648519	-2.561912
49	1	1.840863	0.205190	-3.454586
50	8	1.001445	-0.286834	2.802811
51	8	3.120971	-0.708446	3.407549
52	8	-1.149958	1.975863	1.927743
53	8	-1.286977	4.209006	2.153245
54	8	3.461402	-1.660205	-4.054144
55	1	3.218069	-1.525054	-3.119499
56	1	4.365634	-1.287613	-4.091462
57	8	5.671093	-0.411203	-3.154119
58	1	5.147897	0.283436	-2.705405
59	1	5.896145	-1.046427	-2.450351
60	8	0.963721	2.137796	3.921019
61	1	1.105343	1.265670	3.482120
62	8	2.659791	0.909420	5.849117
63	1	2.034860	1.517484	5.421501
64	1	2.993031	0.341295	5.135208
65	1	0.019239	2.326660	3.825616
66	8	1.522408	4.357193	2.513542
67	1	0.585720	4.611453	2.533377
68	1	1.592476	3.526120	3.033821
69	8	5.649315	-0.933580	2.176603
70	1	5.558205	-1.457376	1.362315
71	1	4.784214	-0.803044	2.604673
72	8	2.058331	4.740341	-0.029240
73	1	2.040787	4.535026	0.942418
74	1	1.145547	4.819773	-0.328317
75	8	6.126514	0.843432	0.113009
76	1	5.286651	1.124198	-0.311615
77	1	5.968437	0.537720	1.025867
78	8	3.059737	3.516589	-2.181950
79	1	2.793839	3.989912	-1.360407
80	1	3.485325	2.666506	-1.939118
81	8	5.662116	-1.673709	-0.626930
82	1	5.965724	-0.750072	-0.451096
83	1	4.699848	-1.653993	-0.827073
84	8	2.416715	-3.764163	-2.588095
85	1	2.655925	-3.104337	-1.910367
86	1	2.754515	-3.385087	-3.418332
87	8	1.599516	3.474458	-4.350547
88	1	2.138862	3.591268	-3.515012
89	1	2.003698	2.736562	-4.828087
90	8	-3.023965	0.682924	3.522607
91	8	-5.220356	0.464900	2.179759
92	8	-5.733244	0.743669	-2.059721
93	8	-7.135527	-1.097451	-0.353643
94	8	-1.552051	-1.179370	2.770305
95	8	-3.342755	-3.369074	2.614129

96	8	-6.693627	-1.666806	-2.964219
97	8	-4.376236	1.882412	0.057462
98	1	-5.066534	1.124602	1.464475
99	1	-4.958882	1.776699	-0.716878
100	1	-3.674298	1.196214	0.008935
101	1	-6.800649	-0.235004	-0.651256
102	1	-6.375503	-1.527472	0.099270
103	1	-5.011474	0.064255	-1.987227
104	1	-6.371134	0.322045	-2.659716
105	1	-5.739037	-1.788264	-2.799779
106	1	-7.081503	-1.652850	-2.063453
107	1	-4.014785	-2.937675	2.054593
108	1	-2.669185	-2.688246	2.785869
109	1	-3.941427	0.619906	3.120530
110	1	-2.512219	1.375291	3.068902
111	1	-2.214086	-0.481610	3.153448
112	1	-0.750264	-1.213118	3.310559
113	1	-5.145428	-0.420222	1.767444

HF = -3871.6933072 Hartree
Zero-point correction = 0.964000
Sum of electronic and thermal free energies = -3870.833613

$[Nd(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	60	-0.422931	-0.110067	0.635564
2	7	-1.009034	2.146764	-0.697995
3	7	1.018007	-2.362443	1.074199
4	7	-1.086707	-2.516719	-0.885066
5	7	0.098131	-0.003860	-2.214908
6	8	-2.713076	-0.282965	0.048093
7	8	1.834394	0.427029	0.098856
8	15	-3.597087	-1.474911	-0.367199
9	15	2.628144	0.153554	-1.178190
10	8	-4.117820	-1.265686	-1.780108
11	8	-4.687863	-1.783843	0.647660
12	8	3.839960	1.049666	-1.397473
13	8	2.988393	-1.326271	-1.337392
14	6	-1.216995	4.577664	-1.926930
15	6	1.979043	-4.397832	0.361251
16	6	0.970667	-3.433743	0.305172
17	6	-0.127765	-3.640155	-0.712761
18	6	-1.188065	-2.161776	-2.334896
19	6	-2.442397	-2.884446	-0.358941
20	6	3.092219	-3.071800	1.991560
21	6	2.061349	-2.177252	1.895052
22	6	2.079501	-0.922952	2.726436
23	6	3.043614	-4.213690	1.204216
24	6	-1.315079	4.486488	-0.550213
25	6	-1.179280	3.244072	0.025552
26	6	-1.198436	3.078397	1.519271
27	6	-1.033595	3.430589	-2.676282
28	6	-0.979107	2.209148	-2.024789
29	6	-0.937674	0.897174	-2.769223
30	6	0.010926	-1.362937	-2.816742
31	6	1.461854	0.566295	-2.499260
32	1	-1.261850	5.531883	-2.413230
33	1	1.943149	-5.225540	-0.315008
34	1	0.389696	-3.825669	-1.644720
35	1	-0.673575	-4.541912	-0.448446
36	1	-1.246099	-3.078421	-2.923068
37	1	-2.113888	-1.638729	-2.487722
38	1	-2.351106	-3.232974	0.657724
39	1	-2.857049	-3.703241	-0.950056
40	1	3.921217	-2.850986	2.626061
41	1	3.846043	-4.923582	1.230759
42	1	-1.469993	5.332712	0.083300
43	1	-0.838169	3.480196	-3.723892
44	1	-1.907526	0.432059	-2.654908
45	1	-0.756826	1.083608	-3.825282

46	1	-0.041883	-1.272748	-3.903255
47	1	0.921997	-1.884417	-2.587182
48	1	1.387688	1.639070	-2.573212
49	1	1.821003	0.194348	-3.455758
50	8	0.984403	-0.261794	2.753894
51	8	3.116644	-0.646842	3.344127
52	8	-1.115572	1.864855	1.932428
53	8	-1.248662	4.089367	2.226449
54	8	3.455989	-1.643018	-4.045300
55	1	3.214458	-1.513575	-3.109205
56	1	4.353550	-1.255373	-4.086669
57	8	5.648782	-0.361333	-3.151079
58	1	5.119773	0.326270	-2.699083
59	1	5.881114	-0.997054	-2.450010
60	8	1.007297	2.151059	3.910777
61	1	1.087453	1.282460	3.447700
62	8	2.743829	0.952867	5.801725
63	1	2.108717	1.552367	5.375618
64	1	3.058189	0.375562	5.086769
65	1	0.067424	2.378451	3.890407
66	8	1.556912	4.336004	2.449475
67	1	0.616684	4.574040	2.488337
68	1	1.644739	3.509787	2.974245
69	8	5.658047	-0.918620	2.173279
70	1	5.572945	-1.430336	1.350512
71	1	4.785911	-0.774654	2.583290
72	8	2.045554	4.770746	-0.094084
73	1	2.049776	4.546378	0.873492
74	1	1.125587	4.805233	-0.379914
75	8	6.096452	0.886149	0.114242
76	1	5.248450	1.158905	-0.299840
77	1	5.953445	0.575891	1.027642
78	8	3.019883	3.515324	-2.240147
79	1	2.765178	4.008576	-1.426625
80	1	3.441997	2.669195	-1.978079
81	8	5.656079	-1.631979	-0.632788
82	1	5.948897	-0.705045	-0.455664
83	1	4.692171	-1.623818	-0.826893
84	8	2.417923	-3.756644	-2.590629
85	1	2.649935	-3.097927	-1.909489
86	1	2.757485	-3.373018	-3.418025
87	8	1.506442	3.450633	-4.374648
88	1	2.068130	3.572729	-3.554967
89	1	1.896485	2.709160	-4.858294
90	8	-2.973156	0.586218	3.546326
91	8	-5.191584	0.461612	2.225545
92	8	-5.667828	0.835214	-2.020041
93	8	-7.106806	-1.012052	-0.354050
94	8	-1.515876	-1.241372	2.681103
95	8	-3.368309	-3.396258	2.591852

96	8	-6.664305	-1.542304	-2.973068
97	8	-4.306645	1.898110	0.135480
98	1	-5.020615	1.134437	1.526547
99	1	-4.884017	1.822246	-0.646101
100	1	-3.612995	1.204690	0.073816
101	1	-6.757111	-0.149997	-0.635386
102	1	-6.355528	-1.461125	0.094587
103	1	-4.957876	0.142737	-1.957898
104	1	-6.309943	0.436317	-2.630932
105	1	-5.712591	-1.682768	-2.807205
106	1	-7.055389	-1.537786	-2.073625
107	1	-4.030658	-2.941804	2.038992
108	1	-2.668596	-2.739758	2.750256
109	1	-3.897783	0.557213	3.158962
110	1	-2.455693	1.283032	3.106110
111	1	-2.178219	-0.561571	3.094774
112	1	-0.710951	-1.273998	3.216888
113	1	-5.126637	-0.413964	1.791366

HF = -3873.5989517 Hartree
Zero-point correction = 0.964415
Sum of electronic and thermal free energies = -3872.738392

$[Gd(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	64	-0.416193	-0.134451	0.625814
2	7	-1.000278	2.095142	-0.665668
3	7	1.018287	-2.343323	1.030627
4	7	-1.085651	-2.523589	-0.913913
5	7	0.078524	-0.019091	-2.221927
6	8	-2.651920	-0.284844	0.066508
7	8	1.773218	0.423056	0.094086
8	15	-3.563179	-1.448933	-0.369743
9	15	2.590388	0.167028	-1.173587
10	8	-4.077619	-1.197835	-1.778746
11	8	-4.663166	-1.751673	0.636960
12	8	3.792552	1.080794	-1.370495
13	8	2.974222	-1.306745	-1.332961
14	6	-1.261106	4.544357	-1.849978
15	6	1.980367	-4.387377	0.341801
16	6	0.971528	-3.424367	0.275505
17	6	-0.127198	-3.643730	-0.737326
18	6	-1.189834	-2.176602	-2.364257
19	6	-2.440514	-2.881207	-0.384995
20	6	3.095374	-3.042009	1.953259
21	6	2.062909	-2.150515	1.848382
22	6	2.072520	-0.893607	2.673527
23	6	3.047004	-4.192879	1.179376
24	6	-1.325413	4.430073	-0.472659
25	6	-1.166002	3.179716	0.077762
26	6	-1.164020	2.977134	1.564290
27	6	-1.086322	3.410829	-2.621182
28	6	-1.004310	2.179341	-1.990887
29	6	-0.967945	0.880270	-2.755687
30	6	0.002406	-1.368637	-2.841886
31	6	1.434403	0.568136	-2.503793
32	1	-1.327068	5.505669	-2.319677
33	1	1.941914	-5.224459	-0.322779
34	1	0.389289	-3.834176	-1.668991
35	1	-0.669891	-4.545295	-0.465361
36	1	-1.239758	-3.095768	-2.949563
37	1	-2.118938	-1.659647	-2.518549
38	1	-2.349830	-3.242674	0.626521
39	1	-2.871906	-3.685887	-0.983609
40	1	3.925191	-2.812866	2.583700
41	1	3.849825	-4.902050	1.213018
42	1	-1.475727	5.264250	0.177884
43	1	-0.918844	3.477568	-3.672699
44	1	-1.934449	0.408978	-2.638659
45	1	-0.797157	1.083804	-3.810458

46	1	-0.052916	-1.265622	-3.927388
47	1	0.917144	-1.887368	-2.619951
48	1	1.348345	1.639663	-2.579512
49	1	1.803763	0.198534	-3.456999
50	8	0.966055	-0.252203	2.707536
51	8	3.109207	-0.602184	3.284347
52	8	-1.080697	1.752063	1.938568
53	8	-1.203870	3.964958	2.305062
54	8	3.454064	-1.607435	-4.039590
55	1	3.211018	-1.487348	-3.102474
56	1	4.344036	-1.202702	-4.080686
57	8	5.625660	-0.292715	-3.144175
58	1	5.089388	0.385530	-2.687376
59	1	5.865528	-0.930596	-2.447413
60	8	1.035561	2.152324	3.895752
61	1	1.062937	1.287222	3.419282
62	8	2.795060	0.970865	5.759933
63	1	2.152301	1.564226	5.335539
64	1	3.097980	0.389972	5.043112
65	1	0.107838	2.423815	3.919380
66	8	1.590265	4.309474	2.397931
67	1	0.647516	4.532336	2.456918
68	1	1.694595	3.485584	2.922620
69	8	5.661719	-0.901536	2.170892
70	1	5.583681	-1.400530	1.339548
71	1	4.783396	-0.750504	2.565885
72	8	2.024163	4.801077	-0.145393
73	1	2.053410	4.556085	0.816593
74	1	1.098961	4.792477	-0.416360
75	8	6.059408	0.936277	0.124517
76	1	5.203471	1.200815	-0.278990
77	1	5.930707	0.617021	1.036639
78	8	2.969772	3.519990	-2.288496
79	1	2.726632	4.031089	-1.482426
80	1	3.390018	2.678611	-2.008610
81	8	5.649055	-1.579913	-0.640707
82	1	5.928984	-0.650038	-0.457579
83	1	4.683770	-1.584489	-0.828887
84	8	2.429556	-3.741402	-2.609965
85	1	2.649959	-3.088182	-1.920167
86	1	2.770995	-3.345531	-3.430853
87	8	1.407837	3.442765	-4.392253
88	1	1.989286	3.566073	-3.587141
89	1	1.781386	2.696455	-4.881291
90	8	-2.925011	0.478854	3.566040
91	8	-5.163311	0.445476	2.270844
92	8	-5.597392	0.929936	-1.976133
93	8	-7.068613	-0.935726	-0.364252
94	8	-1.477243	-1.303161	2.587497
95	8	-3.387820	-3.431296	2.555466

96	8	-6.619161	-1.412278	-2.993262
97	8	-4.233225	1.904967	0.220248
98	1	-4.974636	1.133129	1.591058
99	1	-4.802525	1.863670	-0.569616
100	1	-3.546628	1.206454	0.143188
101	1	-6.706511	-0.072117	-0.624570
102	1	-6.325580	-1.403227	0.078951
103	1	-4.898112	0.225583	-1.928436
104	1	-6.241373	0.558098	-2.601755
105	1	-5.670221	-1.569082	-2.826604
106	1	-7.014068	-1.422420	-2.095570
107	1	-4.039242	-2.952550	2.010083
108	1	-2.664719	-2.799837	2.705914
109	1	-3.856127	0.482212	3.195776
110	1	-2.403966	1.183598	3.143571
111	1	-2.141822	-0.646005	3.030827
112	1	-0.672832	-1.339138	3.123769
113	1	-5.106063	-0.417994	1.811644

HF = -3876.0097146 Hartree
Zero-point correction = 0.964780
Sum of electronic and thermal free energies = -3875.148507

$[Ho(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	67	-0.415403	-0.156517	0.629282
2	7	-0.991290	2.062929	-0.635108
3	7	1.009529	-2.346138	0.990525
4	7	-1.097426	-2.526484	-0.950063
5	7	0.056178	-0.023531	-2.238373
6	8	-2.612296	-0.286548	0.083081
7	8	1.718851	0.420109	0.080781
8	15	-3.546565	-1.422245	-0.379445
9	15	2.551298	0.177361	-1.180752
10	8	-4.051852	-1.128717	-1.783460
11	8	-4.655660	-1.723321	0.617703
12	8	3.752451	1.096987	-1.354687
13	8	2.943335	-1.293597	-1.344233
14	6	-1.254561	4.531562	-1.780153
15	6	1.959218	-4.398154	0.305403
16	6	0.956565	-3.428475	0.237385
17	6	-0.141689	-3.646168	-0.775204
18	6	-1.204422	-2.178928	-2.399270
19	6	-2.451898	-2.873671	-0.417789
20	6	3.081034	-3.060541	1.916822
21	6	2.054735	-2.162334	1.810234
22	6	2.068044	-0.911285	2.642940
23	6	3.026874	-4.210944	1.142864
24	6	-1.294430	4.398086	-0.403525
25	6	-1.136360	3.138542	0.125336
26	6	-1.121081	2.907685	1.606060
27	6	-1.104111	3.407295	-2.569563
28	6	-1.019481	2.166072	-1.958516
29	6	-1.001924	0.878170	-2.741474
30	6	-0.017705	-1.363332	-2.875124
31	6	1.406882	0.575042	-2.519889
32	1	-1.321788	5.499783	-2.235236
33	1	1.914440	-5.236088	-0.357645
34	1	0.375956	-3.834476	-1.706672
35	1	-0.683798	-4.548931	-0.505302
36	1	-1.250406	-3.097476	-2.986267
37	1	-2.135766	-1.665077	-2.550841
38	1	-2.361354	-3.246561	0.589373
39	1	-2.899124	-3.665548	-1.021982
40	1	3.910208	-2.836976	2.549994
41	1	3.824611	-4.925739	1.177765
42	1	-1.427767	5.224276	0.260833
43	1	-0.958865	3.487803	-3.623328
44	1	-1.966030	0.404855	-2.612075
45	1	-0.851822	1.096551	-3.796751

46	1	-0.079910	-1.248103	-3.959389
47	1	0.900071	-1.881929	-2.664776
48	1	1.313437	1.645683	-2.602094
49	1	1.784435	0.203315	-3.468810
50	8	0.966272	-0.263774	2.671942
51	8	3.101963	-0.634274	3.265674
52	8	-1.051898	1.674068	1.951884
53	8	-1.141073	3.878356	2.370947
54	8	3.434833	-1.585061	-4.047806
55	1	3.189095	-1.469073	-3.110600
56	1	4.320768	-1.171568	-4.087438
57	8	5.595090	-0.257386	-3.146372
58	1	5.058074	0.416554	-2.684648
59	1	5.834472	-0.901260	-2.454821
60	8	1.096003	2.149309	3.850604
61	1	1.087356	1.282041	3.377748
62	8	2.852395	0.974074	5.719364
63	1	2.216980	1.569989	5.287072
64	1	3.131705	0.369781	5.012362
65	1	0.177707	2.447284	3.905234
66	8	1.634614	4.324255	2.375160
67	1	0.687595	4.523832	2.447013
68	1	1.756016	3.488678	2.876796
69	8	5.654702	-0.925277	2.156306
70	1	5.574604	-1.414022	1.318935
71	1	4.776660	-0.777989	2.553572
72	8	2.049795	4.885620	-0.157657
73	1	2.085185	4.622366	0.799478
74	1	1.128004	4.823399	-0.435047
75	8	6.027918	0.939924	0.127432
76	1	5.168384	1.206162	-0.267140
77	1	5.907666	0.610945	1.037192
78	8	2.972739	3.545135	-2.280654
79	1	2.748762	4.077069	-1.483264
80	1	3.370175	2.695632	-1.991669
81	8	5.619502	-1.568730	-0.659196
82	1	5.897744	-0.639916	-0.468209
83	1	4.653083	-1.573856	-0.842650
84	8	2.421018	-3.730119	-2.635087
85	1	2.628938	-3.078993	-1.939566
86	1	2.765762	-3.326088	-3.450672
87	8	1.380046	3.474266	-4.358114
88	1	1.973805	3.592333	-3.560847
89	1	1.753036	2.738987	-4.864025
90	8	-2.889849	0.387383	3.584228
91	8	-5.135061	0.428123	2.309405
92	8	-5.529794	1.035693	-1.952608
93	8	-7.038467	-0.831078	-0.369614
94	8	-1.453461	-1.353084	2.520350
95	8	-3.428304	-3.456239	2.512158

96	8	-6.596667	-1.268082	-3.003822
97	8	-4.175251	1.905988	0.300465
98	1	-4.933296	1.129132	1.646133
99	1	-4.730621	1.905829	-0.499861
100	1	-3.494625	1.203650	0.207842
101	1	-6.658237	0.029941	-0.611683
102	1	-6.306144	-1.323123	0.064811
103	1	-4.837897	0.324677	-1.916546
104	1	-6.181770	0.673957	-2.576333
105	1	-5.651373	-1.447487	-2.838634
106	1	-6.993467	-1.287573	-2.106974
107	1	-4.062953	-2.953442	1.968137
108	1	-2.686860	-2.848992	2.668245
109	1	-3.823428	0.415918	3.218816
110	1	-2.365387	1.108084	3.195016
111	1	-2.115113	-0.708989	2.989369
112	1	-0.655783	-1.417200	3.062568
113	1	-5.088381	-0.423380	1.827097

HF = -3877.7711703 Hartree
Zero-point correction = 0.964938
Sum of electronic and thermal free energies = -3876.909730

$[Lu(L^2)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	71	-0.413596	-0.147515	0.635996
2	7	-0.977543	2.014448	-0.679684
3	7	0.999319	-2.314657	1.006614
4	7	-1.103775	-2.560524	-0.928058
5	7	0.045877	-0.093404	-2.265054
6	8	-2.560256	-0.287267	0.095505
7	8	1.661733	0.404994	0.055648
8	15	-3.518962	-1.408290	-0.353864
9	15	2.518836	0.147913	-1.188182
10	8	-4.024055	-1.114459	-1.758439
11	8	-4.631782	-1.677308	0.648684
12	8	3.713304	1.077774	-1.353008
13	8	2.931308	-1.320733	-1.315778
14	6	-1.253215	4.465995	-1.862039
15	6	1.946915	-4.389277	0.385662
16	6	0.945810	-3.420161	0.287501
17	6	-0.149656	-3.671326	-0.719694
18	6	-1.210730	-2.249688	-2.383655
19	6	-2.456212	-2.880714	-0.381770
20	6	3.072890	-3.004974	1.951706
21	6	2.047121	-2.109914	1.819017
22	6	2.060197	-0.838663	2.618064
23	6	3.016324	-4.178959	1.214561
24	6	-1.276505	4.354809	-0.483139
25	6	-1.114349	3.103494	0.062968
26	6	-1.095808	2.890709	1.544380
27	6	-1.116010	3.328125	-2.633583
28	6	-1.023966	2.096457	-2.004068
29	6	-1.018575	0.797561	-2.767952
30	6	-0.026249	-1.442025	-2.877722
31	6	1.393667	0.505361	-2.553075
32	1	-1.325306	5.426483	-2.332457
33	1	1.898366	-5.248101	-0.249910
34	1	0.371059	-3.885506	-1.643938
35	1	-0.689046	-4.568048	-0.424397
36	1	-1.254818	-3.181864	-2.949484
37	1	-2.142176	-1.739472	-2.546797
38	1	-2.364494	-3.240099	0.629963
39	1	-2.923075	-3.673209	-0.970462
40	1	3.903688	-2.762425	2.575678
41	1	3.812676	-4.893940	1.270888
42	1	-1.403965	5.191443	0.169332
43	1	-0.989096	3.390865	-3.690806
44	1	-1.980725	0.326694	-2.617441
45	1	-0.884309	1.001109	-3.828744

46	1	-0.091224	-1.347844	-3.964259
47	1	0.892390	-1.956217	-2.659524
48	1	1.294922	1.572457	-2.670407
49	1	1.785244	0.106706	-3.485018
50	8	0.953282	-0.199808	2.638886
51	8	3.095030	-0.538176	3.227933
52	8	-1.028797	1.660007	1.900966
53	8	-1.115515	3.866524	2.302768
54	8	3.446086	-1.666825	-4.008619
55	1	3.196179	-1.534762	-3.074497
56	1	4.323958	-1.237730	-4.056916
57	8	5.581019	-0.283931	-3.131078
58	1	5.037724	0.393281	-2.682496
59	1	5.823440	-0.914305	-2.427998
60	8	1.100243	2.225769	3.796070
61	1	1.081054	1.352177	3.335448
62	8	2.864797	1.087342	5.673032
63	1	2.223666	1.673915	5.236104
64	1	3.142948	0.476159	4.971649
65	1	0.186877	2.539550	3.844779
66	8	1.644801	4.376364	2.288846
67	1	0.694425	4.561937	2.353037
68	1	1.772760	3.548133	2.800732
69	8	5.657077	-0.889185	2.177634
70	1	5.583454	-1.381021	1.341323
71	1	4.773824	-0.724354	2.556581
72	8	2.056138	4.922788	-0.248641
73	1	2.093085	4.668647	0.710822
74	1	1.138141	4.829274	-0.530612
75	8	5.992539	0.965871	0.122239
76	1	5.126498	1.215735	-0.269556
77	1	5.884754	0.650006	1.037705
78	8	2.969159	3.510603	-2.333529
79	1	2.755773	4.070767	-1.553543
80	1	3.347140	2.660964	-2.018911
81	8	5.610431	-1.555398	-0.629356
82	1	5.877660	-0.620564	-0.451778
83	1	4.643460	-1.574502	-0.810040
84	8	2.425161	-3.787081	-2.566254
85	1	2.623025	-3.122391	-1.880811
86	1	2.777089	-3.397480	-3.385690
87	8	1.376971	3.390614	-4.405576
88	1	1.968591	3.527156	-3.609361
89	1	1.763581	2.657445	-4.904337
90	8	-2.856489	0.421802	3.577380
91	8	-5.111270	0.480803	2.320739
92	8	-5.492311	1.052440	-1.941828
93	8	-7.012136	-0.792645	-0.355522
94	8	-1.429536	-1.316122	2.494076
95	8	-3.434273	-3.407391	2.560840

96	8	-6.567207	-1.252463	-2.986642
97	8	-4.121688	1.920463	0.298859
98	1	-4.897781	1.173157	1.652285
99	1	-4.675594	1.921547	-0.502540
100	1	-3.444525	1.215088	0.211308
101	1	-6.627728	0.064316	-0.605860
102	1	-6.282600	-1.282030	0.086063
103	1	-4.807211	0.334498	-1.900994
104	1	-6.143220	0.698844	-2.570989
105	1	-5.623109	-1.435368	-2.819610
106	1	-6.964632	-1.262689	-2.089962
107	1	-4.061604	-2.902478	2.010129
108	1	-2.680815	-2.811773	2.699995
109	1	-3.793651	0.458675	3.222769
110	1	-2.330280	1.136505	3.180099
111	1	-2.091401	-0.674508	2.964940
112	1	-0.636603	-1.381866	3.042587
113	1	-5.068441	-0.374576	1.844472

HF = -3880.0752164 Hartree
Zero-point correction = 0.965096
Sum of electronic and thermal free energies = -3879.213582

$[Lu(L^2)]^{3-}\cdot 20H_2O$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	71	-0.413596	-0.147515	0.635996
2	7	-0.977543	2.014448	-0.679684
3	7	0.999319	-2.314657	1.006614
4	7	-1.103775	-2.560524	-0.928058
5	7	0.045877	-0.093404	-2.265054
6	8	-2.560256	-0.287267	0.095505
7	8	1.661733	0.404994	0.055648
8	15	-3.518962	-1.408290	-0.353864
9	15	2.518836	0.147913	-1.188182
10	8	-4.024055	-1.114459	-1.758439
11	8	-4.631782	-1.677308	0.648684
12	8	3.713304	1.077774	-1.353008
13	8	2.931308	-1.320733	-1.315778
14	6	-1.253215	4.465995	-1.862039
15	6	1.946915	-4.389277	0.385662
16	6	0.945810	-3.420161	0.287501
17	6	-0.149656	-3.671326	-0.719694
18	6	-1.210730	-2.249688	-2.383655
19	6	-2.456212	-2.880714	-0.381770
20	6	3.072890	-3.004974	1.951706
21	6	2.047121	-2.109914	1.819017
22	6	2.060197	-0.838663	2.618064
23	6	3.016324	-4.178959	1.214561
24	6	-1.276505	4.354809	-0.483139
25	6	-1.114349	3.103494	0.062968
26	6	-1.095808	2.890709	1.544380
27	6	-1.116010	3.328125	-2.633583
28	6	-1.023966	2.096457	-2.004068
29	6	-1.018575	0.797561	-2.767952
30	6	-0.026249	-1.442025	-2.877722
31	6	1.393667	0.505361	-2.553075
32	1	-1.325306	5.426483	-2.332457
33	1	1.898366	-5.248101	-0.249910
34	1	0.371059	-3.885506	-1.643938
35	1	-0.689046	-4.568048	-0.424397
36	1	-1.254818	-3.181864	-2.949484
37	1	-2.142176	-1.739472	-2.546797
38	1	-2.364494	-3.240099	0.629963
39	1	-2.923075	-3.673209	-0.970462
40	1	3.903688	-2.762425	2.575678
41	1	3.812676	-4.893940	1.270888
42	1	-1.403965	5.191443	0.169332
43	1	-0.989096	3.390865	-3.690806
44	1	-1.980725	0.326694	-2.617441
45	1	-0.884309	1.001109	-3.828744

46	1	-0.091224	-1.347844	-3.964259
47	1	0.892390	-1.956217	-2.659524
48	1	1.294922	1.572457	-2.670407
49	1	1.785244	0.106706	-3.485018
50	8	0.953282	-0.199808	2.638886
51	8	3.095030	-0.538176	3.227933
52	8	-1.028797	1.660007	1.900966
53	8	-1.115515	3.866524	2.302768
54	8	3.446086	-1.666825	-4.008619
55	1	3.196179	-1.534762	-3.074497
56	1	4.323958	-1.237730	-4.056916
57	8	5.581019	-0.283931	-3.131078
58	1	5.037724	0.393281	-2.682496
59	1	5.823440	-0.914305	-2.427998
60	8	1.100243	2.225769	3.796070
61	1	1.081054	1.352177	3.335448
62	8	2.864797	1.087342	5.673032
63	1	2.223666	1.673915	5.236104
64	1	3.142948	0.476159	4.971649
65	1	0.186877	2.539550	3.844779
66	8	1.644801	4.376364	2.288846
67	1	0.694425	4.561937	2.353037
68	1	1.772760	3.548133	2.800732
69	8	5.657077	-0.889185	2.177634
70	1	5.583454	-1.381021	1.341323
71	1	4.773824	-0.724354	2.556581
72	8	2.056138	4.922788	-0.248641
73	1	2.093085	4.668647	0.710822
74	1	1.138141	4.829274	-0.530612
75	8	5.992539	0.965871	0.122239
76	1	5.126498	1.215735	-0.269556
77	1	5.884754	0.650006	1.037705
78	8	2.969159	3.510603	-2.333529
79	1	2.755773	4.070767	-1.553543
80	1	3.347140	2.660964	-2.018911
81	8	5.610431	-1.555398	-0.629356
82	1	5.877660	-0.620564	-0.451778
83	1	4.643460	-1.574502	-0.810040
84	8	2.425161	-3.787081	-2.566254
85	1	2.623025	-3.122391	-1.880811
86	1	2.777089	-3.397480	-3.385690
87	8	1.376971	3.390614	-4.405576
88	1	1.968591	3.527156	-3.609361
89	1	1.763581	2.657445	-4.904337
90	8	-2.856489	0.421802	3.577380
91	8	-5.111270	0.480803	2.320739
92	8	-5.492311	1.052440	-1.941828
93	8	-7.012136	-0.792645	-0.355522
94	8	-1.429536	-1.316122	2.494076
95	8	-3.434273	-3.407391	2.560840

96	8	-6.567207	-1.252463	-2.986642
97	8	-4.121688	1.920463	0.298859
98	1	-4.897781	1.173157	1.652285
99	1	-4.675594	1.921547	-0.502540
100	1	-3.444525	1.215088	0.211308
101	1	-6.627728	0.064316	-0.605860
102	1	-6.282600	-1.282030	0.086063
103	1	-4.807211	0.334498	-1.900994
104	1	-6.143220	0.698844	-2.570989
105	1	-5.623109	-1.435368	-2.819610
106	1	-6.964632	-1.262689	-2.089962
107	1	-4.061604	-2.902478	2.010129
108	1	-2.680815	-2.811773	2.699995
109	1	-3.793651	0.458675	3.222769
110	1	-2.330280	1.136505	3.180099
111	1	-2.091401	-0.674508	2.964940
112	1	-0.636603	-1.381866	3.042587
113	1	-5.068441	-0.374576	1.844472

HF = -3880.0743266 Hartree
Zero-point correction = 0.964286
Sum of electronic and thermal free energies = -3879.217203

$[La(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	57	0.179230	-0.812915	0.314372
2	7	0.447287	-1.258511	-2.357532
3	7	-0.587419	0.473225	2.688579
4	7	1.238974	1.987731	0.996361
5	7	-0.220594	1.528533	-1.638866
6	8	2.507783	-0.428831	-0.164564
7	8	-2.112983	-0.464986	-0.393791
8	15	3.549051	0.585594	0.341745
9	15	-2.764076	0.841142	-0.857561
10	8	4.056887	1.430784	-0.808778
11	8	4.647242	-0.078813	1.163497
12	8	-4.118057	0.625331	-1.521933
13	8	-2.826157	1.884185	0.257460
14	6	0.334112	-1.815875	-5.032251
15	6	-0.607645	2.222446	4.277629
16	6	-0.241997	1.706499	3.033958
17	6	0.457564	2.630855	2.072234
18	6	1.361663	2.903347	-0.198759
19	6	2.582957	1.580679	1.521375
20	6	-1.735156	0.185510	4.751296
21	6	-1.327806	-0.265804	3.521511
22	6	-1.724863	-1.653113	3.086918
23	6	-1.359129	1.460093	5.139531
24	6	0.305917	-2.840745	-4.110561
25	6	0.345236	-2.512587	-2.775918
26	6	0.214948	-3.581455	-1.731936
27	6	0.430345	-0.509992	-4.591436
28	6	0.513601	-0.260497	-3.232828
29	6	0.731692	1.141619	-2.714891
30	6	0.085082	2.890712	-1.063700
31	6	-1.649051	1.485245	-2.127644
32	1	0.253904	-2.021898	-6.080994
33	1	-0.310737	3.217993	4.534751
34	1	-0.318233	3.248025	1.645086
35	1	1.095924	3.285858	2.660108
36	1	2.419993	0.970479	2.397290
37	1	3.152197	2.439297	1.868035
38	1	-2.324352	-0.462891	5.360214
39	1	-1.653666	1.849486	6.093952
40	1	0.216604	-3.869531	-4.380081
41	1	0.369625	0.303992	-5.278294
42	1	1.735316	1.193035	-2.314658
43	1	0.659699	1.811139	-3.562820
44	1	-1.705198	0.864193	-3.009017
45	1	-1.984404	2.473497	-2.422288

46	8	-1.308344	-2.026619	1.953694
47	8	-2.419490	-2.318753	3.876262
48	8	0.239860	-3.161018	-0.513991
49	8	0.054817	-4.749447	-2.093881
50	8	-3.555965	4.219638	-1.104146
51	1	-3.182700	3.408538	-0.719778
52	1	-4.514292	4.014383	-1.129554
53	8	-5.818329	2.769223	-0.871082
54	1	-5.361836	2.010815	-1.294582
55	1	-5.815485	2.564708	0.081211
56	8	-1.121578	-4.596360	1.254460
57	1	-1.545657	-3.753797	1.523883
58	8	0.206314	-4.065996	3.516584
59	1	-0.200574	-4.493810	2.727700
60	1	-0.524228	-3.697655	4.034701
61	1	-0.453573	-4.289346	0.593712
62	8	-2.472642	-5.308897	-1.031603
63	1	-1.647754	-5.372427	-1.548321
64	1	-2.190517	-5.218806	-0.099641
65	8	-4.897442	-1.272495	2.559723
66	1	-4.847020	-0.301743	2.584217
67	1	-4.172897	-1.683019	3.052599
68	8	-2.654344	-2.730039	-1.903531
69	1	-2.765398	-3.642715	-1.563034
70	1	-2.559525	-2.064286	-1.198414
71	8	-5.921314	-0.661942	0.118768
72	1	-5.276372	-0.425940	-0.578845
73	1	-5.509992	-1.222470	0.803627
74	8	-3.581999	-0.998855	-3.684475
75	1	-3.230960	-1.784407	-3.201941
76	1	-3.960562	-0.403852	-3.005498
77	8	-5.227793	1.441944	1.600497
78	1	-5.634982	0.734624	1.043188
79	1	-4.331001	1.628005	1.247850
80	8	-2.053220	4.335313	1.207275
81	1	-2.333647	3.400996	1.139618
82	1	-2.530263	4.772445	0.480748
83	8	-2.325736	0.569049	-5.358145
84	1	-2.746106	-0.142103	-4.797030
85	1	-2.824998	1.377885	-5.175232
86	8	1.578725	-2.092036	2.173035
87	8	3.908788	-2.698498	1.260941
88	8	5.166895	-0.329622	-2.579484
89	8	6.889878	-0.499986	-0.277493
90	8	2.269413	-0.504136	4.260203
91	8	4.677761	0.938938	3.811140
92	8	6.685316	1.757726	-1.754628
93	8	3.669837	-2.453563	-1.451388
94	1	3.896632	-2.871182	0.295049
95	1	4.331273	-2.026818	-2.022027

96	1	3.111873	-1.733612	-1.085729
97	1	6.385035	-0.841484	-1.033652
98	1	6.211814	-0.326578	0.416724
99	1	4.539502	0.220034	-2.061456
100	1	5.909297	0.287414	-2.723412
101	1	5.785171	1.953814	-1.424391
102	1	7.023808	1.075195	-1.136371
103	1	4.869781	0.602347	2.917444
104	1	3.917092	0.422447	4.130385
105	1	2.470389	-2.408804	1.798590
106	1	1.111702	-2.816201	2.656049
107	1	2.065326	-1.095989	3.500506
108	1	1.505468	0.059005	4.420660
109	1	4.329175	-1.816708	1.373768
110	6	1.719907	4.348616	0.255582
111	6	0.197952	3.960557	-2.186689
112	6	0.472504	5.365155	-1.633828
113	6	1.824791	5.339145	-0.911397
114	1	2.655601	4.313130	0.801120
115	1	0.953629	4.728516	0.917323
116	1	2.605380	5.031960	-1.601300
117	1	2.084884	6.323501	-0.530064
118	1	-0.311935	5.643991	-0.937886
119	1	0.476141	6.085917	-2.447423
120	1	1.015289	3.708958	-2.852145
121	1	-0.714629	3.967724	-2.766379
122	1	-0.758784	3.141264	-0.444342
123	1	2.197542	2.539331	-0.769480

HF = -4025.8125052 Hartree
Zero-point correction = 1.065526
Sum of electronic and thermal free energies = -4024.856161

$[Nd(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	60	0.170508	-0.829666	0.268029
2	7	0.494383	-1.075604	-2.383346
3	7	-0.622340	0.305551	2.668332
4	7	1.221198	1.952864	1.131241
5	7	-0.192555	1.663947	-1.531370
6	8	2.447725	-0.423551	-0.129511
7	8	-2.044913	-0.426669	-0.447175
8	15	3.503046	0.562007	0.405680
9	15	-2.724539	0.890719	-0.835054
10	8	4.003391	1.449235	-0.717183
11	8	4.606916	-0.145463	1.182371
12	8	-4.066149	0.683580	-1.527206
13	8	-2.828038	1.856577	0.344563
14	6	0.464312	-1.484092	-5.089563
15	6	-0.662649	1.925711	4.390596
16	6	-0.283715	1.508565	3.114032
17	6	0.421913	2.508440	2.238098
18	6	1.354901	2.952849	0.010558
19	6	2.558495	1.509942	1.636337
20	6	-1.792898	-0.139886	4.692317
21	6	-1.371494	-0.493582	3.435603
22	6	-1.762054	-1.842011	2.893541
23	6	-1.422283	1.099789	5.183559
24	6	0.417899	-2.558642	-4.227180
25	6	0.416804	-2.304337	-2.876428
26	6	0.277386	-3.428455	-1.897009
27	6	0.539945	-0.205432	-4.573054
28	6	0.581960	-0.030964	-3.200545
29	6	0.783024	1.341019	-2.604368
30	6	0.094197	2.988607	-0.873655
31	6	-1.610920	1.639620	-2.045190
32	1	0.416452	-1.631474	-6.150090
33	1	-0.368843	2.898414	4.726600
34	1	-0.353343	3.149375	1.846493
35	1	1.045119	3.122815	2.883897
36	1	2.390965	0.857440	2.480068
37	1	3.138281	2.344570	2.022751
38	1	-2.388191	-0.834309	5.241541
39	1	-1.726791	1.413683	6.162345
40	1	0.347031	-3.571758	-4.555234
41	1	0.498060	0.646085	-5.214415
42	1	1.778263	1.374386	-2.182096
43	1	0.725583	2.054712	-3.417212
44	1	-1.647116	1.083602	-2.970122
45	1	-1.957081	2.642458	-2.269996

46	8	-1.328758	-2.131075	1.743409
47	8	-2.466517	-2.566335	3.622438
48	8	0.269285	-3.071358	-0.657786
49	8	0.143451	-4.578383	-2.320726
50	8	-3.557901	4.262261	-0.879787
51	1	-3.186235	3.433216	-0.533444
52	1	-4.512361	4.049196	-0.946385
53	8	-5.806711	2.773836	-0.799481
54	1	-5.332197	2.045760	-1.254884
55	1	-5.823009	2.514191	0.139140
56	8	-1.095950	-4.673943	0.963504
57	1	-1.545492	-3.853010	1.256128
58	8	0.141574	-4.214898	3.293170
59	1	-0.222539	-4.622164	2.473745
60	1	-0.620033	-3.891750	3.797002
61	1	-0.413050	-4.315901	0.346142
62	8	-2.401454	-5.246282	-1.382961
63	1	-1.566706	-5.260445	-1.887231
64	1	-2.133630	-5.218393	-0.442806
65	8	-4.946137	-1.462108	2.401289
66	1	-4.898311	-0.494285	2.483265
67	1	-4.212196	-1.897836	2.858167
68	8	-2.585817	-2.615175	-2.084391
69	1	-2.697113	-3.546881	-1.800802
70	1	-2.494380	-1.992847	-1.340965
71	8	-5.907212	-0.704834	-0.023831
72	1	-5.241025	-0.425705	-0.684964
73	1	-5.515493	-1.303625	0.640028
74	8	-3.487640	-0.789370	-3.780162
75	1	-3.138728	-1.600230	-3.340004
76	1	-3.879103	-0.240122	-3.070448
77	8	-5.256890	1.306652	1.599037
78	1	-5.646530	0.634367	0.988407
79	1	-4.353527	1.520649	1.280310
80	8	-2.096634	4.250681	1.463747
81	1	-2.364140	3.319300	1.332703
82	1	-2.564666	4.727101	0.756429
83	8	-2.219462	0.889618	-5.330959
84	1	-2.640056	0.140962	-4.820848
85	1	-2.739363	1.677738	-5.117500
86	8	1.508350	-2.154893	2.062224
87	8	3.846796	-2.758112	1.165309
88	8	5.113039	-0.219617	-2.567716
89	8	6.843511	-0.496136	-0.284230
90	8	2.223074	-0.707288	4.250076
91	8	4.655040	0.719299	3.885773
92	8	6.633212	1.829370	-1.651052
93	8	3.615670	-2.380307	-1.529365
94	1	3.840031	-2.888471	0.192899
95	1	4.272482	-1.926544	-2.084365

96	1	3.057360	-1.681621	-1.126828
97	1	6.336376	-0.801813	-1.054088
98	1	6.167344	-0.357037	0.419637
99	1	4.489131	0.306544	-2.021100
100	1	5.854849	0.402599	-2.689168
101	1	5.733548	2.008886	-1.310936
102	1	6.972619	1.117424	-1.067282
103	1	4.840543	0.434252	2.973059
104	1	3.883574	0.200330	4.173482
105	1	2.403326	-2.460558	1.685568
106	1	1.035856	-2.901699	2.502446
107	1	2.007791	-1.245448	3.455170
108	1	1.459074	-0.162847	4.466060
109	1	4.277225	-1.887290	1.318636
110	6	1.685066	4.367524	0.569954
111	6	0.222266	4.125093	-1.927592
112	6	0.477353	5.494806	-1.284369
113	6	1.810774	5.431238	-0.529143
114	1	2.605638	4.306522	1.138927
115	1	0.896260	4.696026	1.233076
116	1	2.611119	5.173353	-1.216710
117	1	2.052786	6.391618	-0.080522
118	1	-0.325910	5.729580	-0.593558
119	1	0.498858	6.263608	-2.052551
120	1	1.053822	3.917703	-2.590822
121	1	-0.678988	4.162823	-2.523935
122	1	-0.760513	3.199595	-0.254014
123	1	2.203899	2.637591	-0.570008

HF = -4027.7181716 Hartree
Zero-point correction = 1.065967
Sum of electronic and thermal free energies = -4026.760301

$[Gd(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	64	-0.165636	-0.865219	-0.232176
2	7	-0.528729	-0.921932	2.388948
3	7	0.646620	0.181220	-2.628165
4	7	-1.216226	1.939114	-1.236336
5	7	0.160701	1.791966	1.437659
6	8	-2.380975	-0.426807	0.083616
7	8	1.960485	-0.378981	0.481892
8	15	-3.456034	0.532837	-0.461519
9	15	2.670940	0.941182	0.805066
10	8	-3.954748	1.440787	0.646425
11	8	-4.561702	-0.210524	-1.201525
12	8	4.002738	0.734720	1.517417
13	8	2.812887	1.837471	-0.424242
14	6	-0.542521	-1.201073	5.115385
15	6	0.739809	1.706015	-4.436380
16	6	0.326755	1.360055	-3.148390
17	6	-0.395447	2.416892	-2.357139
18	6	-1.363186	2.999982	-0.180651
19	6	-2.542340	1.459309	-1.726209
20	6	1.865350	-0.374274	-4.599680
21	6	1.412428	-0.657598	-3.336378
22	6	1.789184	-1.974669	-2.718551
23	6	1.513631	0.837976	-5.166460
24	6	-0.485059	-2.315137	4.305865
25	6	-0.462401	-2.124623	2.945209
26	6	-0.316276	-3.293848	2.024764
27	6	-0.610291	0.049995	4.535692
28	6	-0.631468	0.159958	3.155484
29	6	-0.831351	1.504653	2.500632
30	6	-0.116578	3.080508	0.718324
31	6	1.571387	1.782480	1.963734
32	1	-0.511062	-1.297018	6.182393
33	1	0.459652	2.661222	-4.829284
34	1	0.374508	3.080386	-1.994001
35	1	-1.001002	2.988739	-3.057625
36	1	-2.366062	0.781794	-2.548020
37	1	-3.140465	2.270361	-2.135535
38	1	2.470405	-1.099749	-5.095266
39	1	1.843612	1.098157	-6.152682
40	1	-0.422596	-3.311908	4.682128
41	1	-0.578947	0.931763	5.135327
42	1	-1.818960	1.512542	2.059936
43	1	-0.796454	2.249726	3.287113
44	1	1.595471	1.287188	2.923140
45	1	1.933196	2.792599	2.122833

46	8	1.336443	-2.203713	-1.563147
47	8	2.502936	-2.740328	-3.396338
48	8	-0.285256	-2.994010	0.769689
49	8	-0.198700	-4.424732	2.499867
50	8	3.552324	4.291371	0.691056
51	1	3.179632	3.451472	0.372584
52	1	4.501598	4.070788	0.795324
53	8	5.782807	2.775980	0.742989
54	1	5.290379	2.073718	1.219322
55	1	5.816807	2.473901	-0.182282
56	8	1.087040	-4.726958	-0.717247
57	1	1.550318	-3.921424	-1.028932
58	8	-0.080230	-4.340208	-3.099586
59	1	0.251395	-4.727529	-2.257867
60	1	0.702728	-4.043815	-3.587373
61	1	0.390037	-4.335943	-0.138709
62	8	2.360598	-5.165938	1.672375
63	1	1.518519	-5.141970	2.163701
64	1	2.104320	-5.195543	0.729150
65	8	4.980318	-1.604725	-2.257535
66	1	4.935393	-0.641647	-2.386095
67	1	4.238865	-2.058410	-2.684551
68	8	2.540877	-2.498563	2.223437
69	1	2.655377	-3.443304	1.989017
70	1	2.444977	-1.915940	1.449991
71	8	5.882004	-0.725389	0.148866
72	1	5.193722	-0.413930	0.772494
73	1	5.511718	-1.356429	-0.497273
74	8	3.394745	-0.586823	3.845868
75	1	3.054217	-1.421099	3.445572
76	1	3.793798	-0.079151	3.109523
77	8	5.266479	1.198140	-1.590329
78	1	5.640455	0.560249	-0.934671
79	1	4.357858	1.434555	-1.303463
80	8	2.129551	4.183598	-1.675304
81	1	2.382387	3.256576	-1.493723
82	1	2.588687	4.688878	-0.982578
83	8	2.130704	1.183186	5.295227
84	1	2.545025	0.404187	4.827155
85	1	2.665924	1.951804	5.050857
86	8	-1.440464	-2.217059	-1.960442
87	8	-3.791906	-2.812925	-1.090420
88	8	-5.072423	-0.146863	2.549123
89	8	-6.797428	-0.507934	0.274419
90	8	-2.155867	-0.879706	-4.224617
91	8	-4.620285	0.507441	-3.950811
92	8	-6.593372	1.866859	1.553265
93	8	-3.566596	-2.319761	1.581334
94	1	-3.791720	-2.906634	-0.113928
95	1	-4.219943	-1.843693	2.121911

96	1	-3.005616	-1.642104	1.150156
97	1	-6.291613	-0.785439	1.055743
98	1	-6.119736	-0.394716	-0.432898
99	1	-4.450037	0.362412	1.983658
100	1	-5.816716	0.475678	2.649307
101	1	-5.692392	2.034225	1.211435
102	1	-6.928737	1.131916	0.996065
103	1	-4.799796	0.271844	-3.023008
104	1	-3.833262	-0.004674	-4.206764
105	1	-2.342298	-2.509285	-1.589528
106	1	-0.966594	-2.981749	-2.365667
107	1	-1.937105	-1.374366	-3.403896
108	1	-1.387783	-0.360214	-4.483292
109	1	-4.227956	-1.951517	-1.278320
110	6	-1.674576	4.383966	-0.821520
111	6	-0.262309	4.265079	1.715565
112	6	-0.506548	5.602879	1.003898
113	6	-1.821659	5.502041	0.220173
114	1	-2.581765	4.297424	-1.408878
115	1	-0.868793	4.674336	-1.482620
116	1	-2.638291	5.279499	0.901060
117	1	-2.050991	6.439764	-0.280237
118	1	0.312197	5.809279	0.322037
119	1	-0.548308	6.406812	1.734527
120	1	-1.104610	4.087081	2.374042
121	1	0.629197	4.330177	2.324712
122	1	0.746398	3.265412	0.100945
123	1	-2.221683	2.719655	0.404300

HF = -4030.1292517 Hartree
Zero-point correction = 1.066220
Sum of electronic and thermal free energies = -4029.170596

$[Ho(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	67	-0.161390	-0.903822	-0.220054
2	7	-0.563888	-0.845834	2.377430
3	7	0.660981	0.129456	-2.598672
4	7	-1.216319	1.956485	-1.292070
5	7	0.137846	1.865782	1.389358
6	8	-2.328111	-0.426926	0.025575
7	8	1.895106	-0.356316	0.506834
8	15	-3.421089	0.526081	-0.498076
9	15	2.628962	0.959731	0.798491
10	8	-3.912648	1.424718	0.621195
11	8	-4.531010	-0.229439	-1.219203
12	8	3.954074	0.744186	1.521540
13	8	2.797231	1.817587	-0.454013
14	6	-0.609960	-1.057428	5.112437
15	6	0.775590	1.601565	-4.451079
16	6	0.348173	1.293621	-3.157268
17	6	-0.378050	2.383631	-2.414594
18	6	-1.363381	3.043735	-0.268797
19	6	-2.537983	1.463428	-1.771922
20	6	1.904023	-0.478898	-4.542483
21	6	1.438068	-0.726046	-3.276500
22	6	1.816417	-2.023901	-2.622358
23	6	1.556947	0.715253	-5.148781
24	6	-0.547792	-2.191033	4.331205
25	6	-0.507597	-2.033633	2.966879
26	6	-0.350803	-3.226180	2.080851
27	6	-0.667230	0.178042	4.500116
28	6	-0.674295	0.255034	3.116922
29	6	-0.870385	1.587347	2.435717
30	6	-0.127109	3.137336	0.643246
31	6	1.541571	1.853609	1.926999
32	1	-0.590522	-1.126529	6.181784
33	1	0.499229	2.545173	-4.873288
34	1	0.394060	3.052446	-2.066256
35	1	-0.966237	2.935176	-3.146240
36	1	-2.364732	0.785637	-2.594491
37	1	-3.150983	2.268125	-2.173162
38	1	2.516578	-1.216892	-5.009330
39	1	1.896998	0.947370	-6.138564
40	1	-0.493279	-3.178480	4.732365
41	1	-0.638374	1.074413	5.077607
42	1	-1.850562	1.581068	1.979038
43	1	-0.856064	2.343942	3.212611
44	1	1.553157	1.386807	2.900936
45	1	1.919094	2.862484	2.055340

46	8	1.350719	-2.229410	-1.467788
47	8	2.542980	-2.802682	-3.271746
48	8	-0.296025	-2.957896	0.818445
49	8	-0.243903	-4.345646	2.583665
50	8	3.538575	4.294371	0.608934
51	1	3.167730	3.449293	0.301725
52	1	4.483438	4.070847	0.742334
53	8	5.756690	2.768836	0.746950
54	1	5.253322	2.076340	1.225956
55	1	5.804720	2.451402	-0.172555
56	8	1.101759	-4.743625	-0.583488
57	1	1.571330	-3.944815	-0.902095
58	8	-0.016248	-4.403063	-2.999430
59	1	0.294880	-4.775482	-2.143770
60	1	0.778597	-4.111437	-3.471005
61	1	0.391846	-4.339427	-0.031005
62	8	2.334574	-5.106182	1.838760
63	1	1.484433	-5.068856	2.314837
64	1	2.093615	-5.164977	0.892907
65	8	5.037504	-1.657713	-2.199564
66	1	4.988074	-0.695430	-2.334772
67	1	4.281583	-2.113072	-2.599355
68	8	2.489970	-2.421524	2.315986
69	1	2.614382	-3.370901	2.107126
70	1	2.400930	-1.859287	1.527161
71	8	5.864127	-0.734124	0.223164
72	1	5.157703	-0.416171	0.823284
73	1	5.515745	-1.376245	-0.424288
74	8	3.323267	-0.464508	3.897879
75	1	2.979232	-1.307944	3.521164
76	1	3.731686	0.013111	3.146545
77	8	5.273309	1.152119	-1.561815
78	1	5.637410	0.530742	-0.885010
79	1	4.358480	1.391421	-1.297114
80	8	2.161787	4.134293	-1.782782
81	1	2.399005	3.209758	-1.569631
82	1	2.610729	4.654100	-1.094398
83	8	2.052063	1.346660	5.291897
84	1	2.469567	0.556791	4.845480
85	1	2.583918	2.110589	5.026610
86	8	-1.387186	-2.259857	-1.921112
87	8	-3.755085	-2.829231	-1.091756
88	8	-5.038375	-0.131114	2.538858
89	8	-6.759041	-0.522321	0.262718
90	8	-2.115285	-0.944462	-4.194019
91	8	-4.600522	0.404065	-3.991899
92	8	-6.558890	1.867398	1.510675
93	8	-3.536611	-2.292335	1.563050
94	1	-3.764676	-2.915336	-0.114612
95	1	-4.178376	-1.811724	2.113467

96	1	-2.975600	-1.623039	1.121066
97	1	-6.253167	-0.792376	1.046565
98	1	-6.081105	-0.414610	-0.445717
99	1	-4.413397	0.372166	1.970081
100	1	-5.785489	0.489882	2.625196
101	1	-5.656591	2.030950	1.170944
102	1	-6.891067	1.123985	0.962573
103	1	-4.776993	0.200496	-3.056030
104	1	-3.798860	-0.096467	-4.224297
105	1	-2.300122	-2.540226	-1.565954
106	1	-0.913608	-3.033122	-2.309873
107	1	-1.888130	-1.430116	-3.370437
108	1	-1.330697	-0.481717	-4.505779
109	1	-4.186028	-1.966733	-1.288642
110	6	-1.650577	4.414841	-0.947387
111	6	-0.280540	4.342265	1.614873
112	6	-0.509765	5.667578	0.874996
113	6	-1.809433	5.556735	0.066699
114	1	-2.546435	4.322607	-1.551395
115	1	-0.828997	4.681919	-1.599349
116	1	-2.640639	5.353722	0.736116
117	1	-2.022968	6.485253	-0.457483
118	1	0.322614	5.861559	0.205975
119	1	-0.564427	6.484750	1.590077
120	1	-1.131285	4.179057	2.266525
121	1	0.603873	4.414733	2.233829
122	1	0.743071	3.307526	0.031217
123	1	-2.230623	2.785175	0.313824

HF = -4031.8920973 Hartree
Zero-point correction = 1.066458
Sum of electronic and thermal free energies = -4030.932834

$[Lu(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tw*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	71	-0.158981	-0.952637	-0.209374
2	7	-0.589323	-0.782120	2.361662
3	7	0.674578	0.105939	-2.553596
4	7	-1.226457	1.991785	-1.330960
5	7	0.105419	1.949630	1.354087
6	8	-2.266292	-0.433586	-0.033814
7	8	1.812058	-0.316422	0.512372
8	15	-3.380790	0.505811	-0.539157
9	15	2.571605	0.991294	0.783294
10	8	-3.880330	1.386897	0.591332
11	8	-4.485065	-0.266828	-1.251556
12	8	3.889027	0.756914	1.516029
13	8	2.769912	1.819323	-0.484280
14	6	-0.643754	-0.937403	5.103640
15	6	0.870335	1.569159	-4.409047
16	6	0.389505	1.269379	-3.130901
17	6	-0.363944	2.379246	-2.442282
18	6	-1.386448	3.092503	-0.331196
19	6	-2.532938	1.471356	-1.811339
20	6	1.988313	-0.514971	-4.450678
21	6	1.475556	-0.753618	-3.201739
22	6	1.834843	-2.048602	-2.533669
23	6	1.672046	0.678455	-5.074524
24	6	-0.576727	-2.086321	4.346156
25	6	-0.531902	-1.956087	2.979318
26	6	-0.368298	-3.166933	2.121957
27	6	-0.703101	0.283665	4.464329
28	6	-0.706766	0.333939	3.079202
29	6	-0.912949	1.657268	2.381361
30	6	-0.159229	3.205452	0.591568
31	6	1.504604	1.932170	1.891727
32	1	-0.626952	-0.983510	6.174251
33	1	0.617048	2.514031	-4.842619
34	1	0.397635	3.063235	-2.100800
35	1	-0.932987	2.902159	-3.210490
36	1	-2.347785	0.800952	-2.637477
37	1	-3.169638	2.262207	-2.204627
38	1	2.613462	-1.258306	-4.891375
39	1	2.051605	0.905754	-6.050911
40	1	-0.521300	-3.065386	4.767287
41	1	-0.677917	1.191841	5.023033
42	1	-1.884733	1.628363	1.908899
43	1	-0.929334	2.418243	3.155129
44	1	1.511402	1.491850	2.878134
45	1	1.899752	2.937971	1.990785

46	8	1.353683	-2.245324	-1.383593
47	8	2.565407	-2.838772	-3.165275
48	8	-0.301543	-2.924979	0.853699
49	8	-0.266192	-4.276650	2.645358
50	8	3.532000	4.305718	0.549312
51	1	3.155892	3.461562	0.246101
52	1	4.470430	4.071611	0.707422
53	8	5.726501	2.757779	0.758197
54	1	5.207886	2.074864	1.234676
55	1	5.788767	2.429768	-0.156595
56	8	1.112434	-4.758270	-0.482792
57	1	1.579811	-3.960013	-0.805161
58	8	0.042918	-4.452857	-2.928026
59	1	0.335931	-4.820135	-2.064560
60	1	0.846841	-4.155647	-3.380782
61	1	0.389884	-4.352580	0.049660
62	8	2.324917	-5.051659	1.957931
63	1	1.470403	-5.003152	2.424730
64	1	2.092842	-5.139832	1.012354
65	8	5.059083	-1.701476	-2.129036
66	1	5.010819	-0.740540	-2.276072
67	1	4.299344	-2.159476	-2.518756
68	8	2.459103	-2.356125	2.367056
69	1	2.593925	-3.308075	2.177506
70	1	2.366552	-1.810621	1.568125
71	8	5.827968	-0.739763	0.297953
72	1	5.103047	-0.414022	0.871866
73	1	5.500643	-1.392940	-0.349343
74	8	3.255863	-0.362666	3.926089
75	1	2.918433	-1.216351	3.569080
76	1	3.662750	0.094714	3.161020
77	8	5.263943	1.111498	-1.531699
78	1	5.614768	0.505136	-0.834536
79	1	4.346087	1.361551	-1.287750
80	8	2.180421	4.124301	-1.857166
81	1	2.403325	3.200950	-1.624080
82	1	2.624879	4.651759	-1.172019
83	8	1.989507	1.482318	5.281037
84	1	2.403213	0.682020	4.850286
85	1	2.522862	2.238965	4.998757
86	8	-1.331486	-2.295661	-1.881217
87	8	-3.713325	-2.859420	-1.094114
88	8	-5.021795	-0.136202	2.506686
89	8	-6.721540	-0.550820	0.217972
90	8	-2.029653	-1.000543	-4.178516
91	8	-4.542500	0.293543	-4.042923
92	8	-6.541766	1.849195	1.446992
93	8	-3.508765	-2.276619	1.547958
94	1	-3.731862	-2.931546	-0.116083
95	1	-4.151371	-1.787999	2.091083

96	1	-2.939052	-1.617919	1.104750
97	1	-6.221706	-0.813459	1.008124
98	1	-6.037992	-0.447574	-0.485916
99	1	-4.399074	0.366594	1.932868
100	1	-5.773811	0.479152	2.586353
101	1	-5.636322	2.011242	1.116160
102	1	-6.865771	1.099165	0.902899
103	1	-4.721912	0.113764	-3.102821
104	1	-3.726919	-0.194069	-4.253555
105	1	-2.253790	-2.567997	-1.544174
106	1	-0.857846	-3.074174	-2.258388
107	1	-1.810721	-1.473449	-3.346070
108	1	-1.247541	-0.526791	-4.479189
109	1	-4.142632	-1.999244	-1.305890
110	6	-1.669648	4.451665	-1.034406
111	6	-0.327178	4.422363	1.545399
112	6	-0.557205	5.736995	0.786516
113	6	-1.844611	5.608245	-0.039326
114	1	-2.557834	4.347300	-1.648094
115	1	-0.841107	4.709236	-1.682059
116	1	-2.684136	5.411432	0.621684
117	1	-2.054606	6.528821	-0.578859
118	1	0.282823	5.930112	0.126593
119	1	-0.628120	6.562863	1.490242
120	1	-1.181718	4.261493	2.192958
121	1	0.552418	4.505736	2.170557
122	1	0.715387	3.372855	-0.015956
123	1	-2.257445	2.839241	0.248657

HF = -4034.1976466 Hartree
Zero-point correction = 1.066423
Sum of electronic and thermal free energies = -4033.238341

$[La(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	57	0.359494	0.725621	-0.522229
2	7	0.872020	1.243239	2.108968
3	7	-1.009415	-0.517309	-2.560714
4	7	1.131630	-1.966858	-1.289047
5	7	-0.125100	-1.399199	1.477769
6	8	2.731496	0.248305	-0.227539
7	8	-1.981733	0.528710	0.123640
8	15	3.622106	-0.785266	-0.946514
9	15	-2.699674	-0.649741	0.777171
10	8	4.228406	-1.754041	0.053951
11	8	4.645600	-0.141882	-1.870029
12	8	-3.950200	-0.293037	1.571397
13	8	-2.960396	-1.800546	-0.199786
14	6	1.013058	1.938151	4.751053
15	6	-1.875208	-2.467278	-3.572090
16	6	-0.909180	-1.809130	-2.807883
17	6	0.200825	-2.654360	-2.224222
18	6	1.336213	-2.772016	-0.020497
19	6	2.433976	-1.685852	-1.988937
20	6	-3.062533	-0.413929	-3.750272
21	6	-2.071957	0.167259	-3.006288
22	6	-2.172448	1.623433	-2.637199
23	6	-2.954349	-1.766541	-4.043358
24	6	1.114211	2.910105	3.771847
25	6	1.009991	2.517472	2.457726
26	6	1.010726	3.545238	1.358120
27	6	0.851871	0.616758	4.384151
28	6	0.833074	0.291582	3.035120
29	6	0.827778	-1.153946	2.588930
30	6	0.040085	-2.755197	0.820517
31	6	-1.519337	-1.229694	2.013542
32	1	1.033943	2.207047	5.788646
33	1	-1.796323	-3.525388	-3.709293
34	1	-0.303453	-3.467665	-1.724787
35	1	0.763106	-3.082492	-3.049373
36	1	2.110178	-2.271446	0.526360
37	1	2.238624	-1.091201	-2.868248
38	1	2.880719	-2.613363	-2.339967
39	1	-3.908552	0.166684	-4.042856
40	1	-3.724945	-2.262589	-4.598946
41	1	1.242324	3.948370	3.987438
42	1	0.643630	-0.139384	5.107914
43	1	1.830787	-1.391285	2.262441
44	1	0.586353	-1.761946	3.452006
45	1	-0.808200	-2.848476	0.168600

46	1	-1.495576	-0.489166	2.795348
47	1	-1.869687	-2.146816	2.469922
48	8	-1.119796	2.145691	-2.130206
49	8	-3.237156	2.211348	-2.872162
50	8	0.961051	3.074062	0.164047
51	8	1.007447	4.738788	1.673502
52	8	-3.345788	-4.008169	1.423628
53	1	-3.119660	-3.230403	0.879146
54	1	-4.262108	-3.808732	1.709752
55	8	-5.618347	-2.612890	1.674198
56	1	-5.141689	-1.782970	1.881151
57	1	-5.842629	-2.540307	0.728721
58	8	-1.258224	4.566296	-1.010365
59	1	-1.323339	3.660000	-1.396029
60	8	-2.978213	5.142679	-3.204903
61	1	-2.368912	5.244685	-2.455547
62	1	-3.244323	4.208593	-3.190596
63	1	-0.320561	4.701749	-0.813023
64	8	-1.836732	4.836778	1.595352
65	1	-0.923296	5.110822	1.774653
66	1	-1.898238	4.704717	0.622805
67	8	-5.715325	0.996010	-2.288878
68	1	-5.575210	0.045859	-2.138388
69	1	-4.869277	1.450696	-2.452140
70	8	-2.272443	3.133888	3.544462
71	1	-2.289162	3.731715	2.751140
72	1	-1.356066	3.052540	3.830825
73	8	-6.227048	0.609406	0.396732
74	1	-5.387086	0.526005	0.899114
75	1	-6.084106	1.094343	-0.437648
76	8	-3.165821	0.671136	4.033972
77	1	-2.929302	1.613373	3.865440
78	1	-3.585404	0.309292	3.225058
79	8	-5.632611	-1.602773	-0.968441
80	1	-5.976061	-0.865778	-0.407114
81	1	-4.668238	-1.698109	-0.808623
82	8	-2.261629	-4.353649	-1.108435
83	1	-2.518691	-3.411887	-1.090490
84	1	-2.627389	-4.714670	-0.282478
85	8	-1.577822	-0.921777	5.418598
86	1	-2.172717	-0.258890	4.966416
87	1	-1.875409	-1.794822	5.128459
88	8	2.823174	3.556332	-1.838899
89	8	5.064078	2.510549	-1.097634
90	8	5.745935	-0.524733	1.817956
91	8	7.113503	-0.297689	-0.708014
92	8	1.449574	1.673576	-2.724691
93	8	3.276835	0.234925	-4.332696
94	8	6.849995	-2.686031	0.537836
95	8	4.269182	1.769979	1.364317

96	1	4.916154	2.384856	-0.131743
97	1	4.889789	1.138524	1.772330
98	1	3.589676	1.251868	0.876609
99	1	6.767258	0.007596	0.147060
100	1	6.344035	-0.278319	-1.319907
101	1	5.045393	-0.951444	1.259352
102	1	6.433798	-1.210219	1.864934
103	1	5.893256	-2.705722	0.344266
104	1	7.184160	-1.963093	-0.034520
105	1	3.952171	0.119804	-3.638887
106	1	2.583749	0.782652	-3.926315
107	1	3.755270	3.263018	-1.610160
108	1	2.297126	3.638368	-1.024392
109	1	2.074415	2.453771	-2.460667
110	1	0.620148	2.019140	-3.085475
111	1	5.022987	1.622671	-1.508805
112	6	-0.064347	-3.919224	1.843235
113	1	0.576435	-3.738932	2.698666
114	1	-1.090146	-3.988433	2.173264
115	6	1.920211	-4.171072	-0.360674
116	1	1.418738	-4.591410	-1.223064
117	1	2.961350	-4.013935	-0.608344
118	6	1.801249	-5.186481	0.782126
119	6	0.336879	-5.263820	1.221743
120	1	2.165479	-6.152779	0.442103
121	1	2.418916	-4.880628	1.622053
122	1	-0.302189	-5.462075	0.367793
123	1	0.185779	-6.057071	1.948996

HF = -4025.8103772 Hartree
Zero-point correction = 1.065660
Sum of electronic and thermal free energies = -4024.851446

$[Nd(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	60	-0.349409	-0.681203	-0.530778
2	7	-0.786819	-1.266270	2.047699
3	7	0.958754	0.610728	-2.504949
4	7	-1.219291	1.995942	-1.221726
5	7	0.071730	1.453441	1.501059
6	8	-2.679396	-0.325443	-0.208817
7	8	1.906382	-0.444680	0.158256
8	15	-3.635622	0.689662	-0.868487
9	15	2.634162	0.734093	0.800945
10	8	-4.257083	1.592565	0.183369
11	8	-4.655969	0.034054	-1.786620
12	8	3.906223	0.370472	1.556310
13	8	2.877848	1.888688	-0.175801
14	6	-0.819318	-2.035475	4.672519
15	6	1.732543	2.580085	-3.552784
16	6	0.804972	1.894391	-2.764753
17	6	-0.316737	2.708566	-2.163317
18	6	-1.449537	2.805475	0.039998
19	6	-2.517432	1.673594	-1.909009
20	6	3.001430	0.576249	-3.718789
21	6	2.042629	-0.035126	-2.958476
22	6	2.194485	-1.485002	-2.586991
23	6	2.833939	1.919189	-4.028454
24	6	-0.886240	-2.986411	3.670511
25	6	-0.840352	-2.553951	2.365827
26	6	-0.832028	-3.540887	1.232722
27	6	-0.756650	-0.697947	4.336138
28	6	-0.787817	-0.338147	2.997161
29	6	-0.888727	1.110139	2.579277
30	6	-0.169605	2.822373	0.902955
31	6	1.473418	1.334669	2.045383
32	1	-0.796020	-2.330021	5.702783
33	1	1.606688	3.631388	-3.705035
34	1	0.183418	3.524105	-1.663742
35	1	-0.897150	3.134301	-2.977413
36	1	-2.231783	2.306713	0.577053
37	1	-2.314663	1.110870	-2.806901
38	1	-3.013772	2.586615	-2.229555
39	1	3.867937	0.027563	-4.012953
40	1	3.576001	2.438942	-4.600954
41	1	-0.951689	-4.035500	3.861537
42	1	-0.595431	0.049139	5.079969
43	1	-1.896847	1.268664	2.222757
44	1	-0.730565	1.720867	3.459643
45	1	0.675028	3.038453	0.274711

46	1	1.464570	0.645973	2.875655
47	1	1.812497	2.284168	2.436348
48	8	1.152375	-2.040527	-2.094161
49	8	3.279774	-2.035805	-2.815090
50	8	-0.831245	-3.019955	0.059469
51	8	-0.790438	-4.746044	1.498382
52	8	3.178160	4.099493	1.469553
53	1	2.998852	3.316057	0.915610
54	1	4.096511	3.938397	1.770472
55	8	5.489229	2.763236	1.729307
56	1	5.045989	1.912016	1.921051
57	1	5.718252	2.715662	0.783174
58	8	1.337963	-4.545212	-1.185667
59	1	1.363132	-3.601155	-1.474614
60	8	3.111394	-4.939867	-3.360413
61	1	2.480195	-5.095035	-2.638238
62	1	3.363416	-4.005812	-3.276398
63	1	0.412667	-4.740425	-0.984625
64	8	2.002303	-5.063897	1.360677
65	1	1.068579	-5.256970	1.546682
66	1	2.042338	-4.844330	0.403621
67	8	5.731954	-0.737794	-2.322577
68	1	5.563998	0.202354	-2.139154
69	1	4.895785	-1.219498	-2.458889
70	8	2.504371	-3.439429	3.360440
71	1	2.494676	-4.016438	2.551726
72	1	1.589070	-3.290291	3.623797
73	8	6.229066	-0.407098	0.378530
74	1	5.380042	-0.368802	0.870633
75	1	6.113879	-0.875742	-0.468996
76	8	3.337613	-0.952437	3.867906
77	1	3.152540	-1.897877	3.667069
78	1	3.659495	-0.493891	3.062721
79	8	5.547555	1.811677	-0.931725
80	1	5.919781	1.077073	-0.386448
81	1	4.578769	1.861831	-0.773693
82	8	2.100367	4.396108	-1.061290
83	1	2.390066	3.461663	-1.039966
84	1	2.444463	4.769685	-0.231642
85	8	1.823659	0.560999	5.341597
86	1	2.388246	-0.101223	4.842363
87	1	2.218683	1.427853	5.171638
88	8	-2.701005	-3.544843	-1.913389
89	8	-4.978141	-2.644022	-1.101671
90	8	-5.724071	0.276480	1.918030
91	8	-7.112887	0.088527	-0.593494
92	8	-1.394825	-1.576233	-2.708304
93	8	-3.303887	-0.223432	-4.282575
94	8	-6.897797	2.450602	0.710459
95	8	-4.151572	-1.939975	1.361109

96	1	-4.812521	-2.542580	-0.135875
97	1	-4.787547	-1.344540	1.797938
98	1	-3.494423	-1.386693	0.882558
99	1	-6.748710	-0.228924	0.249812
100	1	-6.349832	0.106504	-1.213359
101	1	-5.043976	0.740683	1.362618
102	1	-6.429564	0.940314	1.998214
103	1	-5.943933	2.500598	0.509192
104	1	-7.218304	1.732876	0.123851
105	1	-3.978478	-0.162201	-3.581608
106	1	-2.573361	-0.729625	-3.888067
107	1	-3.643653	-3.308113	-1.663818
108	1	-2.162401	-3.628846	-1.107387
109	1	-1.996985	-2.385875	-2.476577
110	1	-0.557203	-1.891641	-3.077349
111	1	-4.974841	-1.742181	-1.484275
112	6	-0.178612	3.939479	1.982617
113	1	-0.871827	3.703045	2.781193
114	1	0.818769	4.021965	2.389290
115	6	-2.027019	4.203812	-0.315530
116	1	-1.465640	4.652347	-1.124918
117	1	-3.044816	4.048780	-0.648234
118	6	-2.012532	5.192685	0.856690
119	6	-0.581916	5.297521	1.392497
120	1	-2.381011	6.157661	0.516997
121	1	-2.674187	4.847716	1.646215
122	1	0.099347	5.554075	0.587332
123	1	-0.503459	6.064949	2.158148

HF = -4027.7144096 Hartree
Zero-point correction = 1.065494
Sum of electronic and thermal free energies = -4026.756676

$[Gd(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	64	-0.347463	-0.680495	-0.525165
2	7	-0.841323	-1.169064	2.025772
3	7	0.999152	0.496107	-2.494946
4	7	-1.153242	1.970070	-1.314138
5	7	0.076230	1.475440	1.435110
6	8	-2.614265	-0.289787	-0.234220
7	8	1.860129	-0.492843	0.155071
8	15	-3.571157	0.707500	-0.921214
9	15	2.621461	0.677080	0.780093
10	8	-4.180367	1.644115	0.108110
11	8	-4.602710	0.029666	-1.810203
12	8	3.866981	0.296978	1.570354
13	8	2.911945	1.797334	-0.223540
14	6	-1.049132	-1.893908	4.657774
15	6	1.841597	2.398201	-3.613976
16	6	0.884980	1.770558	-2.813014
17	6	-0.228840	2.631241	-2.269403
18	6	-1.369466	2.822196	-0.081303
19	6	-2.452415	1.650046	-1.995783
20	6	3.055779	0.356021	-3.679045
21	6	2.070206	-0.196089	-2.907466
22	6	2.170467	-1.633128	-2.478570
23	6	2.931319	1.689085	-4.045313
24	6	-1.083798	-2.859560	3.667351
25	6	-0.951995	-2.448812	2.362330
26	6	-0.914608	-3.445168	1.242104
27	6	-0.925654	-0.564906	4.305404
28	6	-0.870648	-0.227025	2.960337
29	6	-0.898732	1.217247	2.519918
30	6	-0.086205	2.822992	0.771947
31	6	1.460136	1.317692	1.997731
32	1	-1.096458	-2.172338	5.691941
33	1	1.744746	3.444898	-3.813767
34	1	0.272076	3.462240	-1.796444
35	1	-0.790407	3.028835	-3.110534
36	1	-2.158503	2.352818	0.471000
37	1	-2.252907	1.058755	-2.874655
38	1	-2.937435	2.560779	-2.339506
39	1	3.909860	-0.228606	-3.938146
40	1	3.695253	2.164051	-4.627908
41	1	-1.189808	-3.903207	3.869659
42	1	-0.776500	0.192755	5.041732
43	1	-1.898805	1.425861	2.166750
44	1	-0.695489	1.832407	3.388431
45	1	0.768627	2.922542	0.129331

46	1	1.422853	0.613267	2.811586
47	1	1.819466	2.250533	2.411563
48	8	1.100148	-2.135543	-1.989725
49	8	3.241904	-2.225177	-2.664675
50	8	-0.871876	-2.930959	0.067618
51	8	-0.889350	-4.650738	1.511197
52	8	3.287192	4.039048	1.362003
53	1	3.067567	3.252887	0.826908
54	1	4.195119	3.838590	1.672870
55	8	5.542860	2.633969	1.686586
56	1	5.066898	1.805869	1.898782
57	1	5.780535	2.548696	0.745173
58	8	1.332864	-4.575243	-0.902607
59	1	1.298246	-3.657098	-1.266720
60	8	3.122668	-5.151663	-3.010411
61	1	2.489060	-5.241813	-2.278606
62	1	3.360273	-4.210077	-3.010474
63	1	0.421312	-4.828732	-0.703300
64	8	1.921400	-4.757260	1.704637
65	1	0.995437	-5.009770	1.847801
66	1	2.008276	-4.632004	0.733793
67	8	5.728688	-1.002561	-2.237705
68	1	5.589594	-0.052278	-2.085566
69	1	4.876375	-1.461777	-2.353644
70	8	2.294720	-3.087201	3.693389
71	1	2.340265	-3.670913	2.890727
72	1	1.362795	-2.954439	3.900946
73	8	6.178700	-0.595241	0.465615
74	1	5.322362	-0.516997	0.941189
75	1	6.067924	-1.090299	-0.367141
76	8	3.110025	-0.577932	4.067632
77	1	2.909844	-1.535720	3.948246
78	1	3.511640	-0.240875	3.239124
79	8	5.597953	1.596427	-0.933816
80	1	5.932366	0.867494	-0.356586
81	1	4.629111	1.687689	-0.797423
82	8	2.233091	4.352450	-1.181840
83	1	2.484890	3.409815	-1.154150
84	1	2.592371	4.718656	-0.355270
85	8	1.466244	0.998085	5.396861
86	1	2.084015	0.342904	4.963878
87	1	1.759633	1.874584	5.112627
88	8	-2.711824	-3.508210	-1.920263
89	8	-4.989438	-2.623921	-1.082434
90	8	-5.617858	0.368971	1.901955
91	8	-7.047458	0.143520	-0.584935
92	8	-1.381596	-1.524068	-2.656938
93	8	-3.331846	-0.273650	-4.331088
94	8	-6.798510	2.526250	0.677311
95	8	-4.103748	-1.881011	1.343320

96	1	-4.801134	-2.510811	-0.121937
97	1	-4.718107	-1.270564	1.790347
98	1	-3.444752	-1.342920	0.850117
99	1	-6.672272	-0.161529	0.258063
100	1	-6.294822	0.142133	-1.216947
101	1	-4.943635	0.817049	1.327390
102	1	-6.317344	1.039444	1.980383
103	1	-5.848060	2.566170	0.457760
104	1	-7.133657	1.801869	0.107524
105	1	-3.981566	-0.189617	-3.608619
106	1	-2.585508	-0.758235	-3.942738
107	1	-3.654575	-3.286465	-1.662909
108	1	-2.170801	-3.599405	-1.117248
109	1	-2.005492	-2.316907	-2.437732
110	1	-0.549872	-1.876342	-3.006383
111	1	-4.974330	-1.726704	-1.475551
112	6	-0.008829	3.995039	1.787679
113	1	-0.671606	3.821268	2.627818
114	1	1.008277	4.067455	2.142946
115	6	-1.927268	4.218906	-0.472865
116	1	-1.389419	4.621802	-1.321245
117	1	-2.960643	4.074070	-0.760218
118	6	-1.843160	5.251409	0.658392
119	6	-0.392729	5.333446	1.141900
120	1	-2.194581	6.213440	0.293447
121	1	-2.487017	4.958057	1.482923
122	1	0.270318	5.523490	0.304237
123	1	-0.263905	6.135066	1.864311

HF = -4030.1261892 Hartree
Zero-point correction = 1.066148
Sum of electronic and thermal free energies = -4028.166682

$[Ho(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	67	-0.340357	-0.680900	-0.552551
2	7	-0.829206	-1.170447	1.975369
3	7	0.990142	0.520948	-2.478436
4	7	-1.177639	1.994004	-1.305767
5	7	0.033328	1.502943	1.432888
6	8	-2.564976	-0.326204	-0.257057
7	8	1.802440	-0.468392	0.171921
8	15	-3.553566	0.671877	-0.896191
9	15	2.568366	0.698570	0.799621
10	8	-4.152939	1.568020	0.173972
11	8	-4.595071	-0.000688	-1.777419
12	8	3.815162	0.310179	1.583495
13	8	2.861305	1.817771	-0.203924
14	6	-1.020397	-1.922185	4.601676
15	6	1.806280	2.425065	-3.615123
16	6	0.860118	1.791644	-2.805481
17	6	-0.256692	2.649098	-2.264881
18	6	-1.400570	2.859401	-0.084547
19	6	-2.475550	1.653609	-1.975637
20	6	3.044059	0.398561	-3.672402
21	6	2.068040	-0.160218	-2.893929
22	6	2.183453	-1.596192	-2.467752
23	6	2.903197	1.727849	-4.046146
24	6	-1.022004	-2.880641	3.603873
25	6	-0.901014	-2.454954	2.302593
26	6	-0.842204	-3.434888	1.170859
27	6	-0.941727	-0.587116	4.258936
28	6	-0.894231	-0.236977	2.916899
29	6	-0.966111	1.207281	2.483386
30	6	-0.130959	2.855174	0.786351
31	6	1.409677	1.348382	2.013783
32	1	-1.060375	-2.209446	5.633690
33	1	1.694440	3.468678	-3.822796
34	1	0.245726	3.480458	-1.794438
35	1	-0.818223	3.045062	-3.107215
36	1	-2.206902	2.407917	0.457965
37	1	-2.274706	1.073153	-2.861323
38	1	-2.986714	2.555308	-2.305317
39	1	3.902713	-0.178852	-3.932337
40	1	3.658664	2.208303	-4.635189
41	1	-1.097338	-3.928505	3.798398
42	1	-0.821040	0.168033	5.002796
43	1	-1.961255	1.378387	2.097236
44	1	-0.817380	1.826220	3.360853
45	1	0.731222	2.973013	0.156531

46	1	1.365375	0.654076	2.836504
47	1	1.771118	2.284990	2.416483
48	8	1.121084	-2.104818	-1.970983
49	8	3.257162	-2.180204	-2.667449
50	8	-0.819316	-2.901683	0.005001
51	8	-0.786519	-4.644612	1.418922
52	8	3.222104	4.063591	1.381036
53	1	3.007923	3.275617	0.846326
54	1	4.128735	3.866278	1.697397
55	8	5.480412	2.664953	1.715980
56	1	5.011137	1.832910	1.926079
57	1	5.719058	2.584194	0.774333
58	8	1.424616	-4.535927	-0.868804
59	1	1.348464	-3.621722	-1.235746
60	8	3.214763	-5.107998	-2.974559
61	1	2.588271	-5.196747	-2.236165
62	1	3.425591	-4.160334	-2.996556
63	1	0.527344	-4.832664	-0.664114
64	8	2.005632	-4.741830	1.738457
65	1	1.075167	-4.990384	1.857238
66	1	2.106323	-4.591733	0.772837
67	8	5.731658	-0.939682	-2.228027
68	1	5.581951	0.007896	-2.068045
69	1	4.884257	-1.406286	-2.350359
70	8	2.353615	-3.127828	3.778557
71	1	2.408778	-3.693066	2.963102
72	1	1.418699	-2.956496	3.942746
73	8	6.143866	-0.549401	0.486287
74	1	5.282630	-0.484757	0.954952
75	1	6.048030	-1.041310	-0.350061
76	8	3.100392	-0.580489	4.080827
77	1	2.939170	-1.547439	3.985833
78	1	3.478667	-0.240680	3.242331
79	8	5.550666	1.640601	-0.906139
80	1	5.888430	0.912746	-0.329277
81	1	4.579896	1.721254	-0.775533
82	8	2.195119	4.371164	-1.172427
83	1	2.444460	3.427913	-1.141564
84	1	2.545951	4.736806	-0.341962
85	8	1.434273	0.954025	5.421108
86	1	2.061534	0.312687	4.980561
87	1	1.711005	1.837225	5.140701
88	8	-2.657293	-3.485089	-1.994090
89	8	-4.942611	-2.673325	-1.117619
90	8	-5.550410	0.249116	1.967339
91	8	-7.015398	0.059961	-0.501287
92	8	-1.347494	-1.464402	-2.657776
93	8	-3.373937	-0.256846	-4.321586
94	8	-6.769062	2.418837	0.802798
95	8	-4.025835	-1.967473	1.295161

96	1	-4.739857	-2.578687	-0.157261
97	1	-4.630445	-1.376905	1.779769
98	1	-3.376771	-1.412523	0.808247
99	1	-6.621995	-0.257071	0.328939
100	1	-6.274605	0.078916	-1.146824
101	1	-4.885915	0.712986	1.394409
102	1	-6.254817	0.912089	2.064164
103	1	-5.822756	2.472474	0.568933
104	1	-7.106470	1.702582	0.224003
105	1	-4.005638	-0.191172	-3.581016
106	1	-2.606644	-0.725783	-3.957472
107	1	-3.601995	-3.285470	-1.721910
108	1	-2.110661	-3.609430	-1.199891
109	1	-1.964860	-2.270003	-2.459640
110	1	-0.522314	-1.803617	-3.032319
111	1	-4.945657	-1.766096	-1.487666
112	6	-0.081546	4.013928	1.819524
113	1	-0.765436	3.827469	2.639880
114	1	0.925983	4.082229	2.201650
115	6	-1.926120	4.264581	-0.492964
116	1	-1.344913	4.670586	-1.310324
117	1	-2.946668	4.139276	-0.832057
118	6	-1.882756	5.285100	0.651555
119	6	-0.448802	5.361471	1.183032
120	1	-2.221298	6.251381	0.285459
121	1	-2.553898	4.982630	1.450598
122	1	0.238616	5.565637	0.368526
123	1	-0.344315	6.152787	1.920605

HF = -4031.887274 Hartree
Zero-point correction = 1.066036
Sum of electronic and thermal free energies = -4030.928243

$[Lu(L^3)(H_2O)]^{3-}\cdot 19H_2O$ (*tf*) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	71	-0.326888	-0.712301	-0.566866
2	7	-0.835721	-1.122865	1.942781
3	7	0.991527	0.494780	-2.457166
4	7	-1.185249	2.029001	-1.334006
5	7	-0.007882	1.576914	1.404563
6	8	-2.497012	-0.357880	-0.300080
7	8	1.731848	-0.441366	0.202425
8	15	-3.511992	0.644577	-0.887588
9	15	2.509790	0.727342	0.816084
10	8	-4.091842	1.502549	0.225266
11	8	-4.571086	-0.020992	-1.753952
12	8	3.748393	0.329932	1.608452
13	8	2.826398	1.822556	-0.206128
14	6	-1.049118	-1.836226	4.579536
15	6	1.799931	2.369012	-3.650201
16	6	0.855568	1.754757	-2.822268
17	6	-0.256134	2.636335	-2.309854
18	6	-1.406682	2.937477	-0.147391
19	6	-2.483218	1.661218	-1.980117
20	6	3.053561	0.354348	-3.641116
21	6	2.078015	-0.188214	-2.851429
22	6	2.201612	-1.612284	-2.392635
23	6	2.903958	1.670042	-4.056639
24	6	-1.016986	-2.810423	3.597966
25	6	-0.887732	-2.402392	2.292049
26	6	-0.810561	-3.395234	1.175018
27	6	-0.998751	-0.506051	4.214233
28	6	-0.938908	-0.175528	2.867519
29	6	-1.042096	1.259830	2.410995
30	6	-0.161580	2.925239	0.756413
31	6	1.356043	1.421042	2.009893
32	1	-1.096475	-2.106580	5.615727
33	1	1.678756	3.404321	-3.891608
34	1	0.260239	3.470609	-1.860836
35	1	-0.807598	3.018936	-3.165570
36	1	-2.244627	2.531371	0.384990
37	1	-2.286760	1.086625	-2.870731
38	1	-3.026360	2.549022	-2.297837
39	1	3.917771	-0.224224	-3.879103
40	1	3.657048	2.138497	-4.658241
41	1	-1.076806	-3.856309	3.808447
42	1	-0.910986	0.262841	4.948270
43	1	-2.023281	1.389134	1.975455
44	1	-0.959797	1.893603	3.287389
45	1	0.714896	3.051376	0.147484

46	1	1.294380	0.754475	2.854664
47	1	1.730464	2.364123	2.384344
48	8	1.136822	-2.117112	-1.898062
49	8	3.280443	-2.194129	-2.568646
50	8	-0.784710	-2.873661	0.003363
51	8	-0.749098	-4.602484	1.432752
52	8	3.173001	4.102542	1.336607
53	1	2.963603	3.303905	0.816010
54	1	4.072363	3.906782	1.673536
55	8	5.417581	2.696883	1.738386
56	1	4.947070	1.867949	1.956047
57	1	5.667652	2.601653	0.800908
58	8	1.452083	-4.549460	-0.798511
59	1	1.365779	-3.636380	-1.165871
60	8	3.251372	-5.120973	-2.888720
61	1	2.619038	-5.209282	-2.154984
62	1	3.463834	-4.173674	-2.906534
63	1	0.559771	-4.853301	-0.582805
64	8	2.030111	-4.732088	1.813485
65	1	1.094264	-4.964281	1.922953
66	1	2.140962	-4.589427	0.848247
67	8	5.749111	-0.941896	-2.164679
68	1	5.595484	0.006114	-2.009884
69	1	4.902841	-1.412539	-2.279313
70	8	2.345862	-3.103360	3.851432
71	1	2.416961	-3.673368	3.041342
72	1	1.409374	-2.911326	3.981345
73	8	6.097875	-0.532635	0.562304
74	1	5.225851	-0.466167	1.010845
75	1	6.023703	-1.032847	-0.270924
76	8	3.060050	-0.536571	4.111307
77	1	2.918294	-1.507319	4.036103
78	1	3.421448	-0.203683	3.262183
79	8	5.523823	1.639155	-0.863674
80	1	5.853423	0.919088	-0.272498
81	1	4.550401	1.718026	-0.750147
82	8	2.197194	4.363825	-1.237733
83	1	2.439493	3.419731	-1.187304
84	1	2.533806	4.740134	-0.406080
85	8	1.379118	0.996057	5.424771
86	1	2.011430	0.353334	4.992800
87	1	1.658373	1.878167	5.143204
88	8	-2.595693	-3.493011	-2.007080
89	8	-4.897175	-2.707881	-1.151283
90	8	-5.482343	0.157474	1.998992
91	8	-6.973840	0.021387	-0.450829
92	8	-1.299946	-1.459885	-2.645664
93	8	-3.363152	-0.282998	-4.305279
94	8	-6.704964	2.356906	0.892066
95	8	-3.954695	-2.024236	1.253623

96	1	-4.689335	-2.623808	-0.191059
97	1	-4.552276	-1.447155	1.762654
98	1	-3.311233	-1.460295	0.771428
99	1	-6.572051	-0.310173	0.369761
100	1	-6.239639	0.049181	-1.103815
101	1	-4.824506	0.632708	1.426759
102	1	-6.182595	0.819653	2.124573
103	1	-5.760935	2.414331	0.651334
104	1	-7.048657	1.650872	0.304395
105	1	-3.991737	-0.218467	-3.562017
106	1	-2.586212	-0.735140	-3.941052
107	1	-3.546574	-3.305114	-1.747926
108	1	-2.058370	-3.614315	-1.206134
109	1	-1.913261	-2.272427	-2.454109
110	1	-0.485616	-1.791712	-3.046785
111	1	-4.908316	-1.794662	-1.506595
112	6	-0.150763	4.079866	1.796409
113	1	-0.873424	3.892478	2.582628
114	1	0.838077	4.136753	2.226205
115	6	-1.855264	4.354590	-0.606003
116	1	-1.191562	4.742564	-1.366836
117	1	-2.844588	4.266567	-1.038032
118	6	-1.877353	5.374335	0.539945
119	6	-0.476485	5.436205	1.155869
120	1	-2.182561	6.344718	0.155599
121	1	-2.598831	5.076779	1.295802
122	1	0.255665	5.647086	0.383010
123	1	-0.410778	6.219370	1.906610-

HF = -4034.1915214 Hartree
Zero-point correction = 1.065899
Sum of electronic and thermal free energies = -4033.232874

$[Lu(L^3)]^{3-}\cdot 20H_2O$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) x	y	z
1	71	0.210899	-0.628604	0.184546
2	7	0.391140	-1.053904	-2.361637
3	7	-0.263774	0.613333	2.494644
4	7	1.078637	2.344393	0.678916
5	7	-0.548752	1.526344	-1.697701
6	8	2.302823	-0.250508	-0.043950
7	8	-1.958672	-0.530080	-0.012758
8	15	3.312400	0.924282	-0.031396
9	15	-2.861956	0.599928	-0.545151
10	8	3.445870	1.494247	-1.435383
11	8	4.628137	0.527015	0.611485
12	8	-4.213262	0.101270	-1.026004
13	8	-2.968522	1.744912	0.453226
14	6	0.488283	-1.801922	-4.998345
15	6	-0.621539	2.386140	4.023359
16	6	-0.182833	1.902009	2.788758
17	6	0.332108	2.913358	1.805664
18	6	0.939546	3.186191	-0.551569
19	6	2.498240	2.097300	1.072013
20	6	-1.220350	0.177972	4.636488
21	6	-0.767978	-0.224071	3.407915
22	6	-0.820270	-1.675638	3.055234
23	6	-1.149296	1.525638	4.950667
24	6	0.545237	-2.758051	-4.004088
25	6	0.497850	-2.334841	-2.699423
26	6	0.563276	-3.302553	-1.559877
27	6	0.396297	-0.470041	-4.646562
28	6	0.355645	-0.122689	-3.306094
29	6	0.333976	1.315734	-2.869794
30	6	-0.455931	2.936049	-1.162658
31	6	-1.971226	1.160606	-2.014923
32	1	0.509478	-2.087046	-6.031442
33	1	-0.550271	3.436103	4.218913
34	1	-0.526402	3.465402	1.455292
35	1	0.952444	3.615166	2.360108
36	1	2.497234	1.641418	2.052100
37	1	3.057664	3.024424	1.165886
38	1	-1.611396	-0.558329	5.302636
39	1	-1.500510	1.887423	5.896566
40	1	0.619036	-3.804894	-4.199228
41	1	0.348805	0.295689	-5.392771
42	1	1.348216	1.571303	-2.596438
43	1	0.030113	1.922922	-3.715377
44	1	-1.982816	0.323241	-2.698610
45	1	-2.493972	1.974489	-2.502524

46	8	-0.311719	-1.981829	1.932737
47	8	-1.348072	-2.454762	3.867456
48	8	0.558592	-2.738925	-0.412110
49	8	0.593644	-4.515037	-1.786863
50	8	-4.120258	3.835161	-0.966756
51	1	-3.591279	3.114774	-0.582113
52	1	-5.034567	3.497479	-0.860481
53	8	-6.103645	2.095147	-0.335718
54	1	-5.617451	1.364614	-0.770624
55	1	-5.971025	1.953383	0.618416
56	8	0.219414	-4.599321	1.534321
57	1	-0.073533	-3.658366	1.600264
58	8	1.026672	-4.137350	4.059032
59	1	0.858550	-4.530240	3.175188
60	1	0.199842	-3.687446	4.299878
61	1	0.858625	-4.585548	0.805984
62	8	-1.604709	-5.408268	-0.361169
63	1	-0.888705	-5.364987	-1.022507
64	1	-1.160592	-5.237564	0.493405
65	8	-4.134901	-1.666696	3.019957
66	1	-4.193435	-0.698020	3.053262
67	1	-3.278416	-1.988652	3.334982
68	8	-2.438132	-3.011727	-1.282370
69	1	-2.283447	-3.902626	-0.895832
70	1	-2.343171	-2.302954	-0.626920
71	8	-5.673108	-1.270522	0.835828
72	1	-5.156002	-0.991881	0.052046
73	1	-5.099618	-1.744435	1.468652
74	8	-3.517988	-1.529503	-3.167884
75	1	-3.091663	-2.226737	-2.612265
76	1	-3.979694	-0.932943	-2.547559
77	8	-5.083496	0.991501	2.134306
78	1	-5.446420	0.202792	1.663066
79	1	-4.282266	1.298462	1.663826
80	8	-2.514449	4.373018	1.213358
81	1	-2.634700	3.406632	1.265766
82	1	-3.112269	4.638604	0.492201
83	8	-4.820243	-2.403005	-5.312998
84	1	-4.262112	-1.984748	-4.607039
85	1	-5.344000	-3.071837	-4.848496
86	8	2.675764	-2.058850	3.290442
87	8	4.433848	-2.196586	1.314068
88	8	4.479040	-0.405665	-3.042639
89	8	6.610571	0.079354	-1.141487
90	8	2.684959	0.382218	3.988517
91	8	4.882839	1.876607	3.148910
92	8	5.821407	1.955030	-2.915957
93	8	3.531350	-2.361802	-1.292615
94	1	4.197393	-2.513608	0.420134
95	1	3.991710	-1.939637	-2.039181

96	1	2.963520	-1.683669	-0.879142
97	1	6.047776	-0.481692	-1.698880
98	1	6.044813	0.301372	-0.363221
99	1	3.904108	0.184332	-2.503001
100	1	5.101324	0.224357	-3.449654
101	1	4.971526	2.112491	-2.460008
102	1	6.349998	1.440606	-2.267383
103	1	5.000470	1.435151	2.290022
104	1	4.162651	1.394501	3.597436
105	1	3.296953	-2.240762	2.539256
106	1	2.158508	-2.834389	3.589144
107	1	2.690281	-0.596546	3.725999
108	1	1.939408	0.552367	4.574801
109	1	4.608347	-1.237715	1.220033
110	6	1.224848	4.683577	-0.247773
111	6	-0.869050	3.998400	-2.220612
112	6	-0.620730	5.429809	-1.722833
113	6	0.871606	5.606078	-1.421123
114	1	2.272352	4.782387	0.013587
115	1	0.639141	5.015962	0.598117
116	1	1.459942	5.351878	-2.298961
117	1	1.099061	6.635877	-1.156542
118	1	-1.197264	5.590270	-0.818422
119	1	-0.959088	6.139026	-2.473496
120	1	-0.319359	3.860963	-3.144302
121	1	-1.925749	3.891194	-2.421739
122	1	-1.187673	2.989043	-0.379370
123	1	1.712068	2.853085	-1.219914

HF = -4034.1884489 Hartree
Zero-point correction = 1.064290
Sum of electronic and thermal free energies = -4033.237802