A NMR and DFT Investigation on the Conformational Properties of Lanthanide(III)-DOTA Analogues Containing Methylenephosphonate Pendant Arms

Mihály Purgel, Zsolt Baranyai, Andrés de Blas, Teresa Rodríguez-Blas, István Bányai, Carlos Platas-Iglesias and Imre Tóth**

Supporting Information

(128 pages including this one)

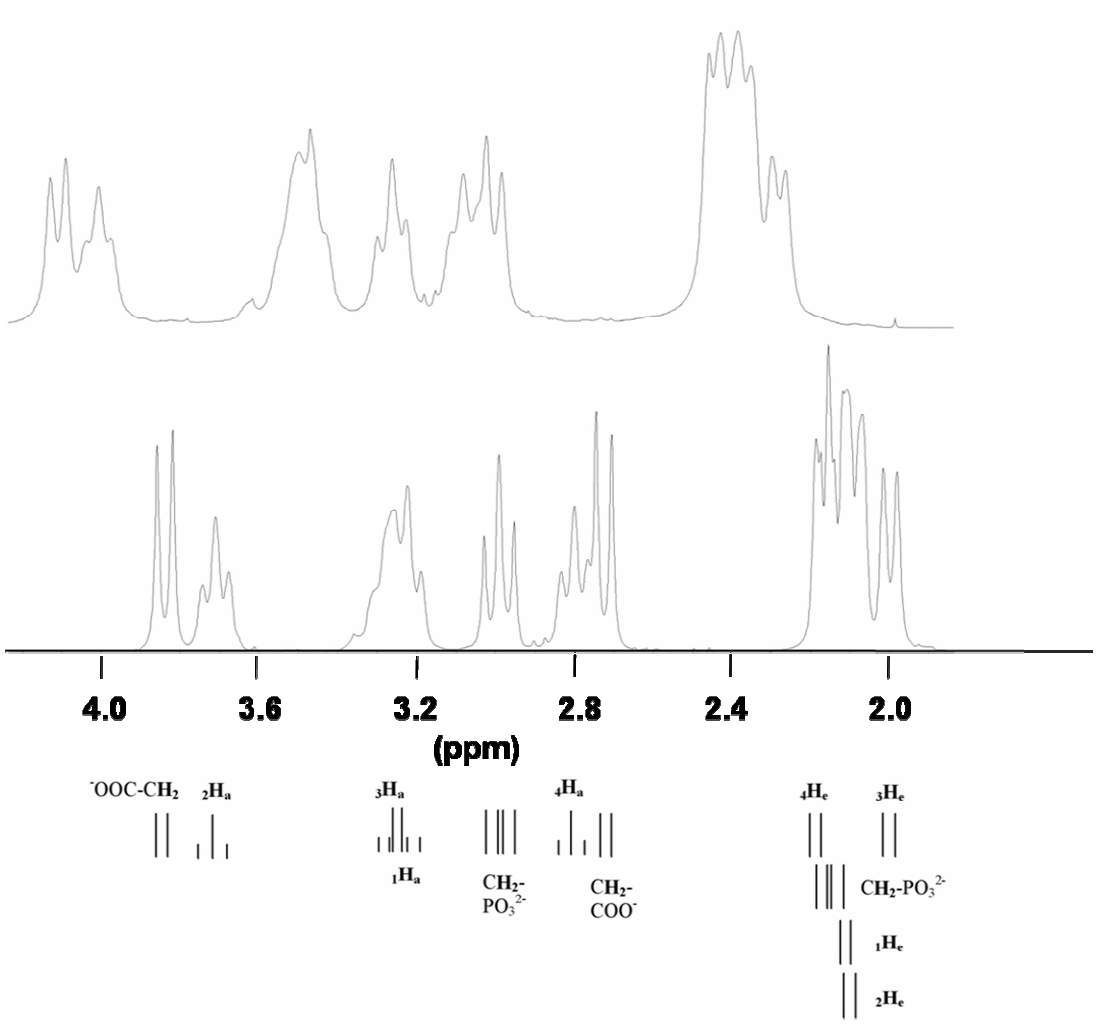

Figure S1. 400 MHz ^{1}H-NMR spectra of $[La(DO2A2P)]^{3-}$ at 273K (A) and 298 K (B) (c_{LaL} = 0.03 M, pD = 9.8).

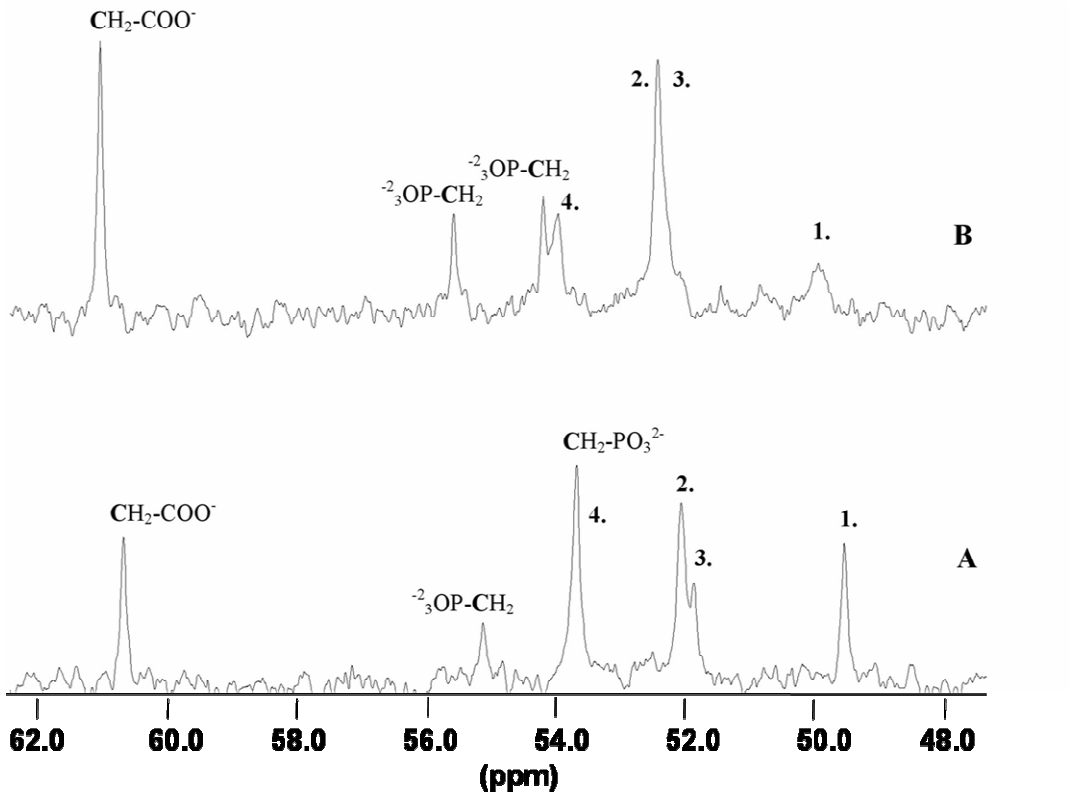

Figure S2. 100 MHz ^{13}C-NMR spectra of $[La(DO2A2P)]^{3-}$ at 273K (A) and 298 K (B) (c_{LaL} = 0.03 M, pD = 9.8).

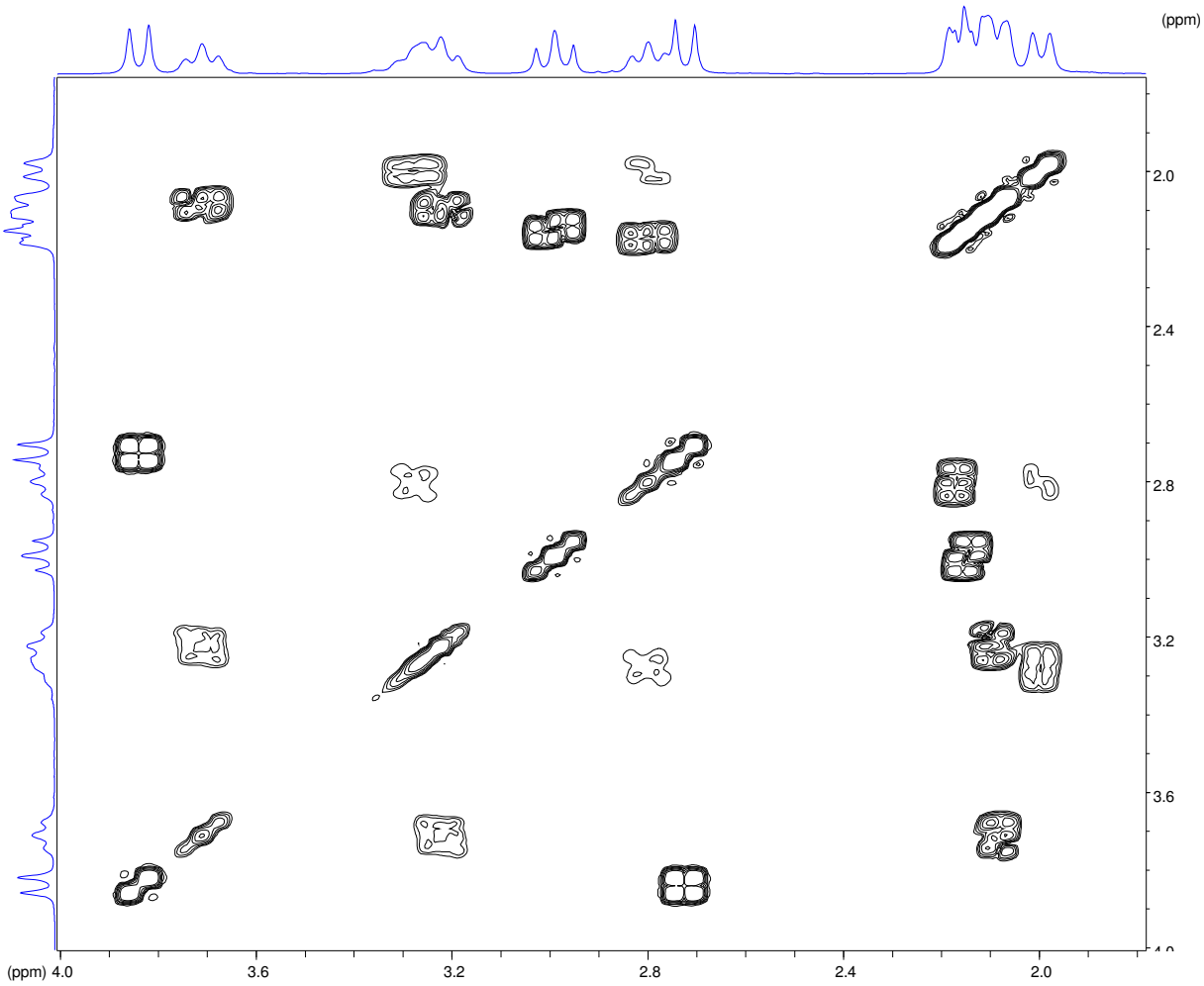

Figure S3. ^{1}H-^{1}H-COSY NMR spectrum of $[La(DO2A2P)]^{3-}$ at 273K (c_{LaL} = 0.03 M, pD = 9.8).

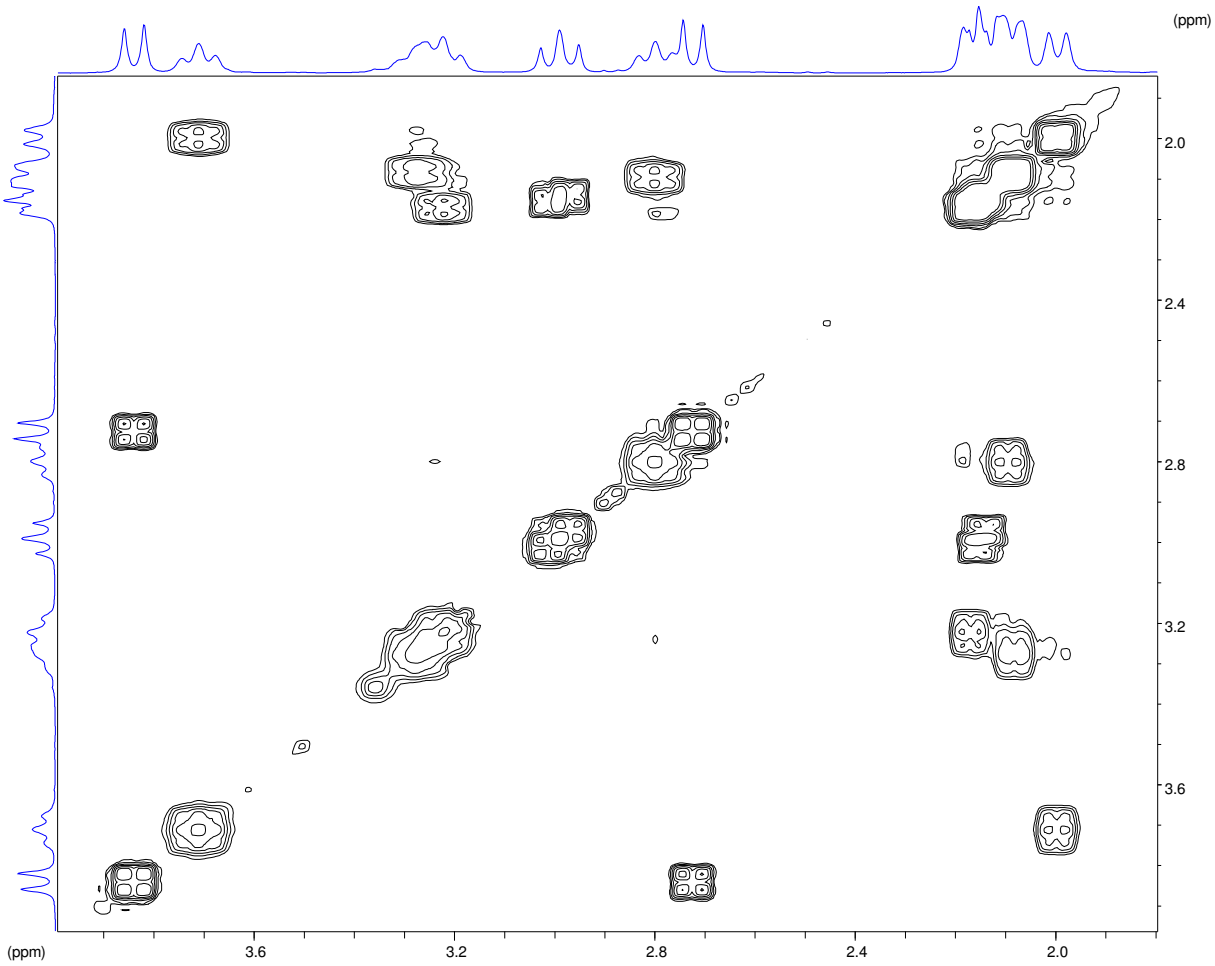

Figure S4. ^{1}H-^{1}H-EXSY NMR spectrum of $[La(DO2A2P)]^{3-}$ at 273K (c_{LaL} = 0.03 M, pD = 9.8, mixing time 300 ms).

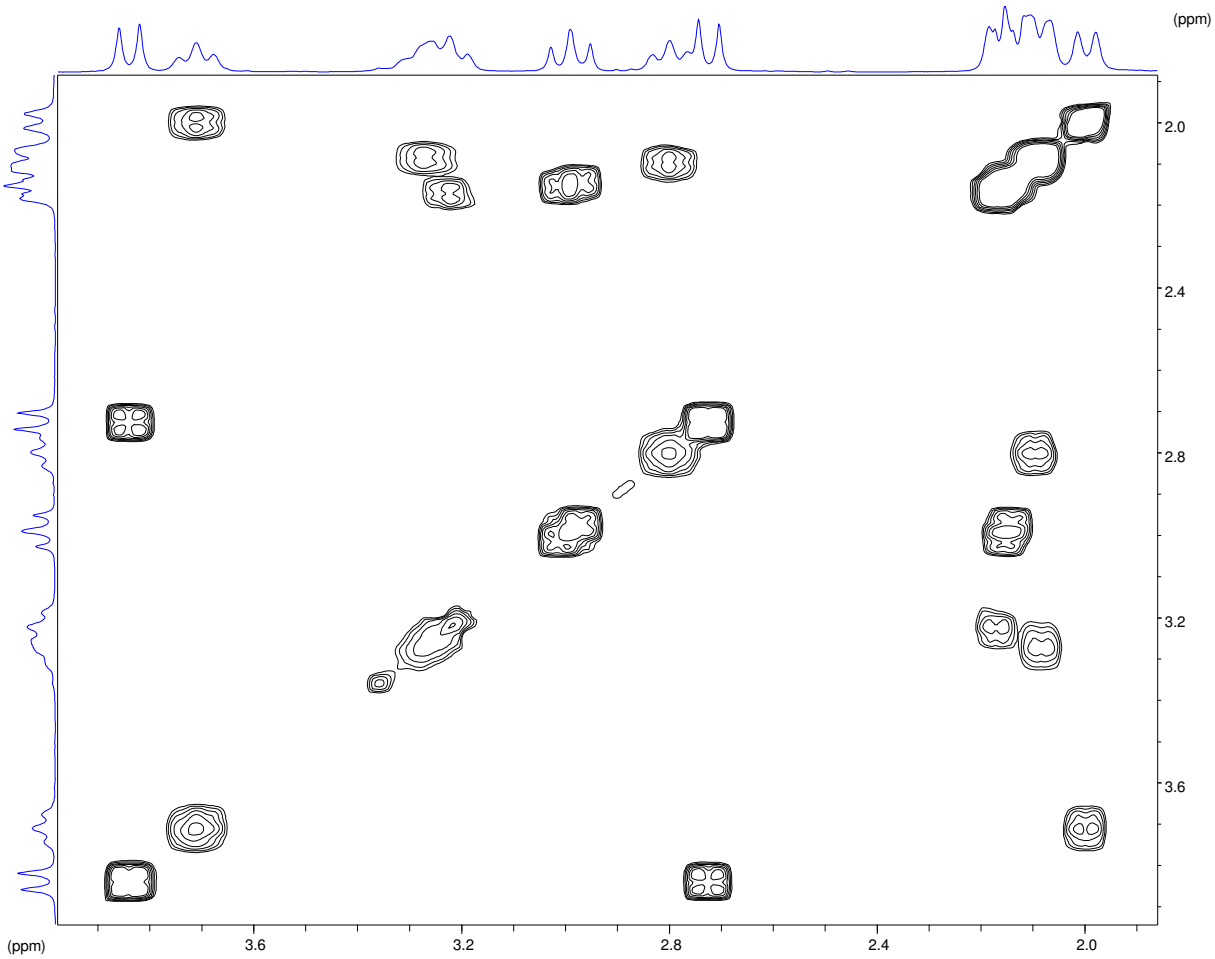

Figure S5. ^{1}H-^{1}H-EXSY NMR spectrum of $[La(DO2A2P)]^{3-}$ at 273K (c_{LaL} = 0.03 M, pD = 9.8, mixing time 500 ms).

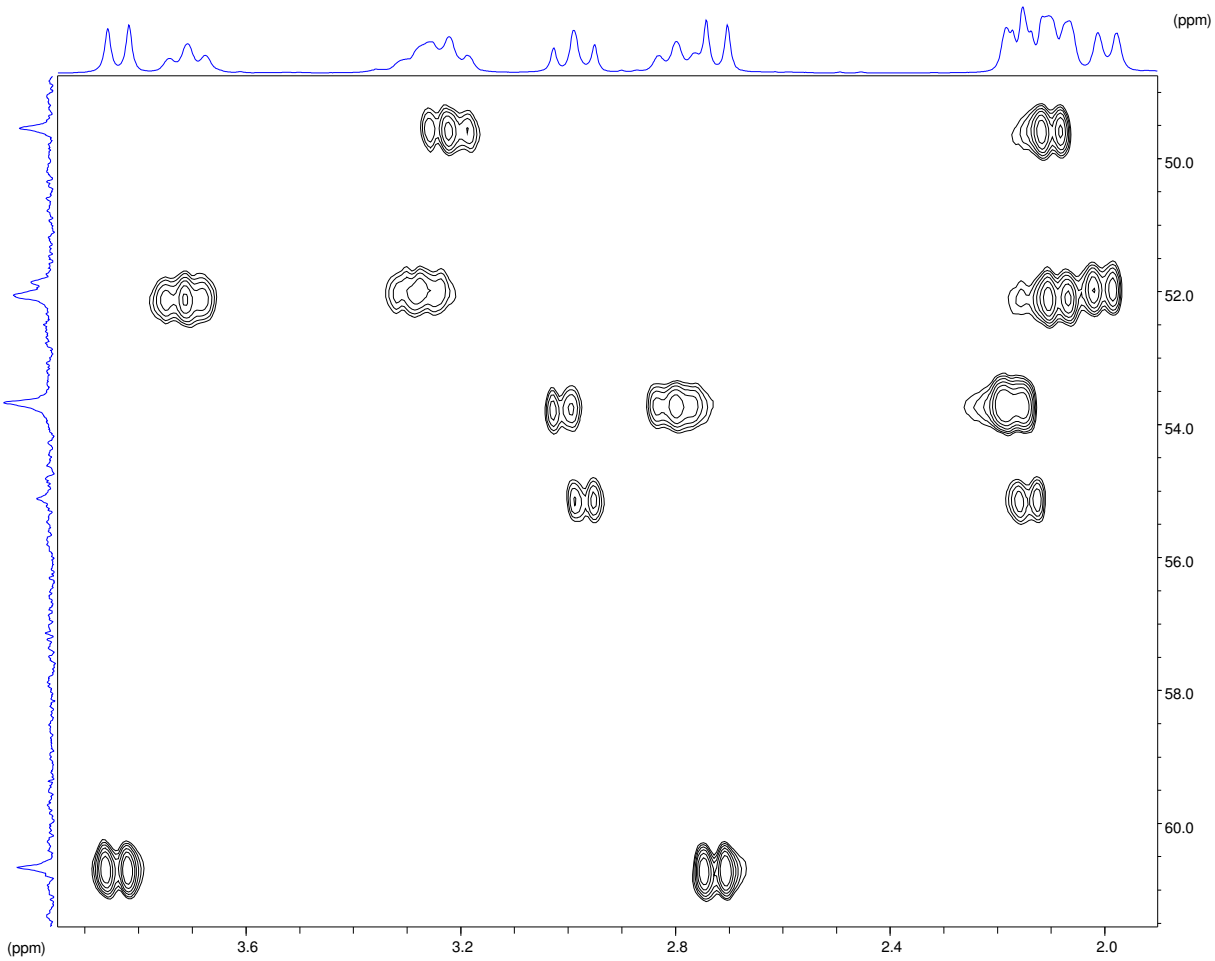

Figure S6. ^{1}H-^{13}C-HSQC NMR spectrum of $[La(DO2A2P)]^{3-}$ at 273K (c_{LaL} = 0.03 M, pD = 9.8).

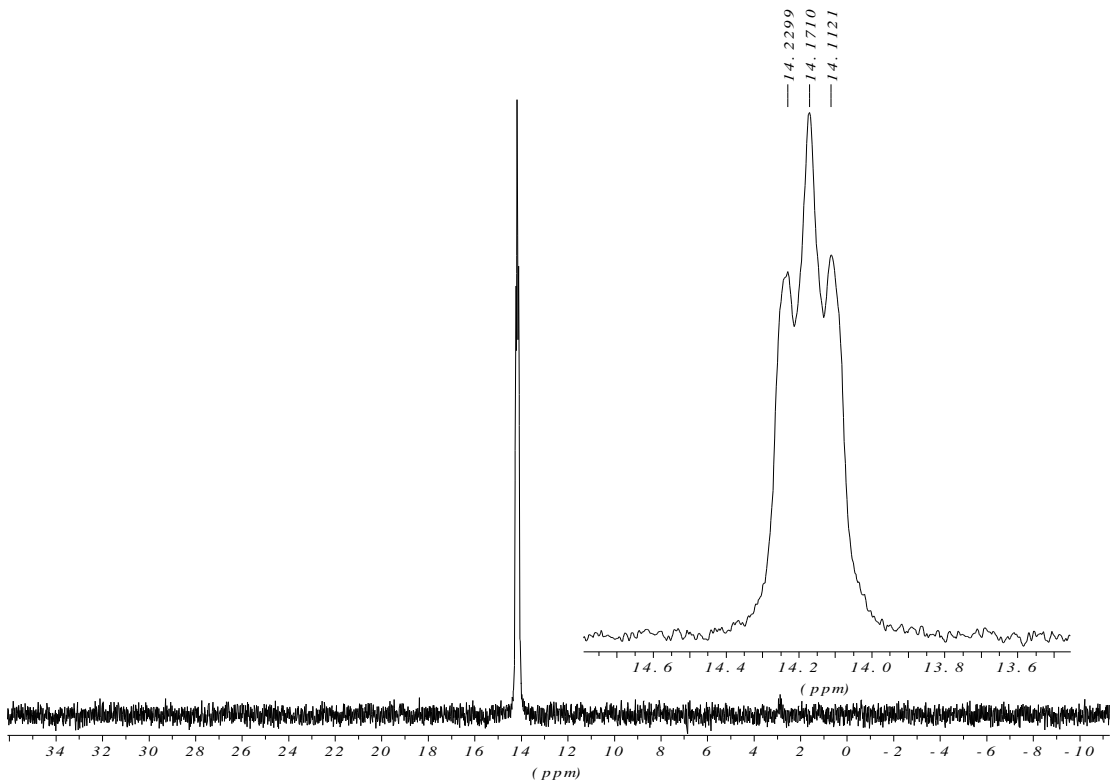

Figure S7. 162 MHz ^{31}P-NMR spectrum of $[La(DO2A2P)]^{3-}$ at 273K (c_{LaL} = 0.03 M, pD = 9.8).

Table S1. ^{1}H NMR spectral data for $[La(DO2A2P)]^{3-}$ as recorded in D_2O solution at 273 K (c_{LaL} = 0.03 M, pD = 9.8, 400 MHz). See Chart 1 for labeling scheme.

	1.		2.		3.		4.		$C\mathbf{H}_2COO^-$		$C\mathbf{H}_2PO_3^{2-}$	
	ax.	eq.	ax.	eq.	ax.	eq.	ax.	eq.	$_5$H	$_6$H	$_7$H	$_8$H
δ (ppm)	3.17	2.04	3.65	2.03	3.20	1.94	2.74	2.12	3.78	2.67	2.93	2.10
$^{2}J_{HH}$ (Hz)	–	13.48	–	15.28	–	14.08	–	12.32	15.84	15.84	15.18	15.24
$^{3}J_{HH}$ (Hz)	13.2	–	13.2	–	12.92	–	13.5	–	–	–	–	–

[Nd(HDO3AP)(H_2O)]$^-$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.120699	2.103627	0.934684
2	6	-2.534375	1.864208	1.303326
3	6	-2.797123	0.445220	1.821014
4	7	-2.444893	-0.636403	0.875914
5	6	-2.222074	-1.906205	1.602758
6	6	-0.846521	-1.983247	2.272184
7	7	0.303599	-1.901368	1.347108
8	6	1.545528	-1.599380	2.100742
9	6	1.675072	-0.135631	2.528109
10	7	1.631484	0.848946	1.423813
11	6	1.203660	2.171312	1.944343
12	6	-0.306957	2.291903	2.152843
13	6	-1.003691	3.269739	0.019696
14	6	0.338454	3.316278	-0.757619
15	8	0.716962	2.176056	-1.235939
16	8	0.920020	4.395202	-0.864806
17	6	-3.491939	-0.794276	-0.165125
18	6	-3.473061	0.344346	-1.216061
19	8	-4.542141	0.814783	-1.597676
20	8	-2.284739	0.683441	-1.601086
21	6	0.471289	-3.172701	0.596054
22	6	-0.543144	-3.379437	-0.553588
23	8	-0.978187	-4.509638	-0.758723
24	8	-0.812383	-2.305536	-1.229489
25	6	2.939695	1.000676	0.734240
26	1	-1.795109	3.171492	-0.729554
27	1	-1.142510	4.214914	0.565717
28	1	-4.492935	-0.862433	0.286814
29	1	-3.278501	-1.722561	-0.703386
30	1	0.430872	-4.038104	1.274588
31	1	1.461272	-3.145569	0.130588
32	1	2.854675	1.888327	0.104724
33	1	3.753740	1.166321	1.459445
34	1	-3.153129	2.055537	0.427302
35	1	-2.861127	2.575195	2.084095
36	1	-3.864420	0.376071	2.096448
37	1	-2.233003	0.284550	2.744585
38	1	-2.989877	-2.052782	2.383671
39	1	-2.336679	-2.729624	0.897808
40	1	-0.799196	-2.922465	2.852742
41	1	-0.753322	-1.168150	2.996814
42	1	1.604705	-2.222080	3.012079
43	1	2.404402	-1.867464	1.483377
44	1	0.870605	0.116542	3.226207
45	1	2.617821	-0.032881	3.093534
46	1	1.535581	2.943200	1.250643
47	1	1.698219	2.386839	2.908591
48	1	-0.630162	1.552933	2.891855
49	1	-0.509518	3.284485	2.595516
50	8	0.299444	-0.773738	-3.153442
51	1	1.222276	-0.948374	-2.871619
52	1	-0.172637	-1.610037	-2.952427
53	15	3.422968	-0.375149	-0.421958
54	8	4.365300	0.444150	-1.493166

55	8	2.111703	-0.746555	-1.157701
56	8	4.224715	-1.440537	0.254091
57	1	3.795986	0.954933	-2.094440
58	60	-0.184390	0.012949	-0.679183

HF = -1934.3865268 Hartree
Zero-point correction = 0.464144
Sum of electronic and thermal Enthalpies = -1933.890492
Sum of electronic and thermal Free Energies = -1933.981111

[Nd(HDO3AP)(H_2O)]$^-$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.668358	1.959986	1.395670
2	6	0.178128	1.827633	2.597473
3	6	1.600978	1.350782	2.300774
4	7	1.673243	0.012714	1.678987
5	6	1.354268	-1.052791	2.646039
6	6	0.979852	-2.372283	1.970126
7	7	-0.222758	-2.268162	1.114191
8	6	-1.441481	-2.353192	1.939410
9	6	-2.687741	-1.770929	1.273989
10	7	-2.549879	-0.355154	0.869008
11	6	-2.662786	0.549829	2.024900
12	6	-2.104368	1.949210	1.756213
13	6	-0.355050	3.212368	0.664197
14	6	-1.039960	3.282793	-0.722281
15	8	-1.245242	2.125933	-1.275457
16	8	-1.295265	4.387272	-1.187767
17	6	3.030646	-0.188284	1.110414
18	6	-0.177545	-3.307715	0.056280
19	6	1.031530	-3.097489	-0.894103
20	8	1.289999	-1.847432	-1.156214
21	8	1.633987	-4.077859	-1.309809
22	6	-3.550726	-0.056671	-0.183662
23	6	-3.256437	-0.848823	-1.488335
24	8	-1.998390	-1.090195	-1.687470
25	8	-4.204469	-1.160133	-2.199546
26	8	0.322729	0.810067	-3.054959
27	1	-0.311899	1.132468	3.286201
28	1	0.241519	2.792069	3.132459
29	1	2.088191	2.049858	1.618540
30	1	2.179257	1.373249	3.243195
31	1	0.521741	-0.718289	3.272614
32	1	2.203325	-1.233195	3.330648
33	1	1.809493	-2.710279	1.347843
34	1	0.840414	-3.145805	2.745911
35	1	-1.246577	-1.825361	2.878917
36	1	-1.654264	-3.401672	2.216899
37	1	-2.920178	-2.348014	0.377635
38	1	-3.543793	-1.898687	1.961058
39	1	-2.125214	0.097503	2.864834
40	1	-3.715394	0.649041	2.347521
41	1	-2.654494	2.405654	0.931918

42	1	-2.287289	2.579838	2.644353
43	1	-0.634488	4.097658	1.255821
44	1	0.723209	3.246176	0.481321
45	1	3.801498	0.114160	1.837591
46	1	3.170517	-1.250574	0.908228
47	1	-0.119048	-4.318293	0.488333
48	1	-1.089095	-3.234630	-0.546299
49	1	-4.572276	-0.281548	0.159689
50	1	-3.495135	1.006689	-0.434327
51	1	-0.331804	1.533466	-2.958734
52	1	1.162723	1.196621	-2.724806
53	15	3.324881	0.726607	-0.505463
54	8	1.904760	1.242941	-0.894149
55	8	3.695759	-0.485157	-1.525431
56	8	4.444917	1.700340	-0.368439
57	1	2.930105	-1.108160	-1.606904
58	60	-0.170935	0.021040	-0.598636

HF = -1934.3886125 Hartree
Zero-point correction = 0.463899
Sum of electronic and thermal Enthalpies = -1933.893136
Sum of electronic and thermal Free Energies = -1933.983000

[Er(HDO3AP)]$^-$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.100689	-0.100609	0.995668
2	15	3.194163	-0.821618	-0.736453
3	8	4.234455	-1.890375	-0.756476
4	7	1.731056	0.198527	1.526818
5	8	1.716931	-1.179343	-1.076084
6	6	1.351358	-0.796239	2.546737
7	6	0.972384	-2.150153	1.945337
8	7	-0.255015	-2.084474	1.117991
9	6	-0.317671	-3.238186	0.178221
10	6	-1.286834	-2.999714	-1.004384
11	8	-1.243699	-1.798543	-1.485691
12	6	-1.460187	-2.036304	1.974801
13	6	-2.710092	-1.499934	1.268663
14	7	-2.509753	-0.151762	0.691289
15	6	-3.457745	0.105645	-0.425843
16	6	-2.982024	1.221255	-1.389322
17	8	-1.711043	1.206289	-1.639460
18	6	-2.621258	0.885149	1.736112
19	6	-2.003801	2.230019	1.342436
20	7	-0.563872	2.124142	1.008171
21	6	-0.144197	3.237895	0.116038
22	6	1.161084	2.955761	-0.658800
23	8	1.977524	3.858082	-0.808598
24	6	0.241421	2.100655	2.247201
25	6	1.666580	1.571901	2.071221
26	8	1.259440	1.739491	-1.110727
27	8	-3.814566	2.006948	-1.835147
28	8	-1.993543	-3.928700	-1.387278

29	8	3.617751	0.451068	-1.649960
30	1	-0.923120	3.359887	-0.641412
31	1	-0.036062	4.177111	0.677848
32	1	-4.460431	0.351412	-0.046323
33	1	-3.513740	-0.808215	-1.022995
34	1	-0.595485	-4.161236	0.707495
35	1	0.677875	-3.356877	-0.257400
36	1	3.695916	0.816334	0.998746
37	1	3.609703	-0.807208	1.663467
38	1	-2.531126	2.634504	0.478443
39	1	-2.163844	2.941973	2.171104
40	1	-3.680620	1.053755	2.000155
41	1	-2.133222	0.509695	2.641651
42	1	-3.542527	-1.501009	1.994454
43	1	-2.995908	-2.177745	0.464615
44	1	-1.688885	-3.041754	2.369234
45	1	-1.237141	-1.408986	2.843545
46	1	0.857726	-2.885938	2.760456
47	1	1.784762	-2.500042	1.305593
48	1	0.509758	-0.401837	3.123788
49	1	2.175002	-0.948686	3.267385
50	1	2.211459	2.228528	1.392333
51	1	2.175609	1.636271	3.050699
52	1	-0.290275	1.490584	2.984206
53	1	0.306716	3.116151	2.676993
54	1	2.866906	1.097419	-1.663556
55	68	-0.135480	-0.034368	-0.573129

HF = -1862.7086863 Hartree
Zero-point correction = 0.439616
Sum of electronic and thermal Enthalpies = -1862.240341
Sum of electronic and thermal Free Energies = -1862.324204

[Er(HDO3AP)]$^{-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.004846	-0.187806	0.934625
2	15	3.202537	0.658202	-0.733136
3	8	4.265583	1.701310	-0.668540
4	7	1.690721	0.095504	1.568695
5	8	1.744617	1.073338	-1.087965
6	6	1.691631	1.469990	2.113664
7	6	0.289583	2.024413	2.373755
8	7	-0.558582	2.059209	1.167936
9	6	-0.208120	3.196685	0.276236
10	6	-0.925483	3.072015	-1.092656
11	8	-1.233503	4.098525	-1.685271
12	6	-1.993256	2.149657	1.528060
13	6	-2.619683	0.800074	1.881692
14	7	-2.494114	-0.192849	0.801518
15	6	-3.431067	0.048156	-0.323744
16	6	-3.057328	-0.825576	-1.552730
17	8	-3.956637	-1.194912	-2.296896
18	6	1.385244	-0.898586	2.611577

19	6	0.949124	-2.240235	2.023008
20	7	-0.259371	-2.132438	1.175812
21	6	-0.258528	-3.218830	0.164794
22	6	0.896980	-3.041855	-0.851442
23	8	1.467887	-4.035566	-1.280147
24	6	-1.471398	-2.141175	2.013657
25	6	-2.697467	-1.567033	1.308193
26	8	-1.132785	1.846626	-1.467197
27	8	1.154391	-1.800269	-1.152066
28	8	-1.787526	-1.080291	-1.656512
29	8	3.607410	-0.582220	-1.701512
30	1	-0.217479	1.411496	3.127469
31	1	0.386966	3.033347	2.812001
32	1	2.218141	2.106070	1.399254
33	1	2.268518	1.515130	3.055327
34	1	0.586358	-0.502398	3.247318
35	1	2.256036	-1.063042	3.271884
36	1	1.754118	-2.649272	1.410353
37	1	0.788480	-2.961340	2.843229
38	1	-1.259727	-1.556486	2.915691
39	1	-1.706536	-3.164547	2.357562
40	1	-2.955504	-2.198890	0.456475
41	1	-3.558206	-1.607108	1.999084
42	1	-2.131077	0.393324	2.774274
43	1	-3.678646	0.961442	2.153084
44	1	-2.523073	2.581900	0.677812
45	1	-2.139770	2.844057	2.373374
46	1	-0.463228	4.159590	0.743477
47	1	0.866543	3.171326	0.079839
48	1	3.828805	0.111943	1.601499
49	1	3.087233	-1.261724	0.767611
50	1	-0.174409	-4.208318	0.638767
51	1	-1.193586	-3.174003	-0.400087
52	1	-4.471826	-0.154963	-0.029293
53	1	-3.349184	1.090949	-0.638389
54	1	2.829275	-1.188736	-1.769987
55	68	-0.148571	0.023229	-0.534582

HF = -1862.7075611 Hartree
Zero-point correction = 0.438747
Sum of electronic and thermal Enthalpies = -1862.239930
Sum of electronic and thermal Free Energies = -1862.324031

[Eu(DOTA)(H_2O)]$^-$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-2.221232	-0.034681	0.989804
2	6	-2.419613	-1.384727	1.562654
3	6	-1.125223	-2.011534	2.090708
4	7	-0.056424	-2.161653	1.081504
5	6	1.255119	-2.332644	1.744298
6	6	1.846042	-1.018033	2.259863

7	7	2.067300	0.002386	1.216406
8	6	2.202886	1.341777	1.828800
9	6	0.862100	1.957650	2.233825
10	7	-0.092889	2.128785	1.121121
11	6	-1.465629	2.292982	1.649553
12	6	-2.114079	0.969689	2.068125
13	6	-3.317393	0.306412	0.045960
14	6	-2.959813	1.483532	-0.896510
15	8	-1.753760	1.437938	-1.360353
16	8	-3.815667	2.335422	-1.128462
17	6	-0.336265	-3.301992	0.171503
18	6	-1.443283	-2.993215	-0.867218
19	8	-2.281654	-3.859136	-1.110810
20	8	-1.355522	-1.815603	-1.392789
21	6	3.263510	-0.319043	0.400412
22	6	3.039489	-1.448413	-0.632917
23	8	3.942898	-2.258618	-0.825727
24	8	1.892936	-1.397661	-1.234625
25	6	0.282422	3.282415	0.264752
26	6	1.473077	3.003228	-0.683643
27	8	2.306330	3.887453	-0.865144
28	8	1.451979	1.828254	-1.231398
29	63	-0.021766	-0.006031	-0.698664
30	1	-3.478655	-0.566888	-0.592819
31	1	-4.248123	0.536105	0.586222
32	1	-0.604141	-4.205676	0.739640
33	1	0.578376	-3.495412	-0.396406
34	1	4.123580	-0.573690	1.038205
35	1	3.508274	0.575387	-0.180177
36	1	-0.573155	3.495786	-0.382546
37	1	0.503064	4.172708	0.872868
38	1	-2.850340	-2.025163	0.793455
39	1	-3.148163	-1.356796	2.393055
40	1	-1.374202	-2.993897	2.531096
41	1	-0.734899	-1.398112	2.908889
42	1	1.177849	-3.031573	2.596782
43	1	1.941657	-2.788395	1.030823
44	1	2.794591	-1.246726	2.779150
45	1	1.177487	-0.592664	3.014761
46	1	2.847623	1.302437	2.725776
47	1	2.704067	1.995709	1.115149
48	1	0.387818	1.328400	2.993476
49	1	1.062434	2.930444	2.718667
50	1	-2.074781	2.773956	0.885057
51	1	-1.471375	2.966504	2.525840
52	1	-1.537735	0.526404	2.886559
53	1	-3.114518	1.194174	2.480115
54	8	0.740359	0.095034	-3.154036
55	1	1.217159	0.929180	-2.955608
56	1	1.396799	-0.609274	-2.968267

HF = -1557.0702277 Hartree
Zero-point correction = 0.453360
Sum of electronic and thermal Enthalpies = -1556.587050
Sum of electronic and thermal Free Energies = -1556.673477

$[Eu(DOTA)(H_2O)]^-$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.016749	-0.003166	-0.649579
2	7	-1.774335	-0.994805	1.354977
3	6	-2.049529	-0.032174	2.434005
4	6	-2.130022	1.413219	1.943281
5	7	-0.894753	1.878176	1.279227
6	6	0.128313	2.233582	2.277467
7	6	1.546000	2.274981	1.708924
8	7	1.977536	0.996154	1.104936
9	6	2.398922	0.041423	2.142920
10	6	2.410027	-1.409376	1.662127
11	7	1.096305	-1.878956	1.172645
12	6	0.208699	-2.220957	2.295419
13	6	-1.266578	-2.270552	1.900005
14	6	-2.979278	-1.258035	0.537595
15	6	-2.656216	-2.041982	-0.757967
16	8	-1.456162	-1.852143	-1.213897
17	8	-3.541768	-2.731169	-1.252522
18	6	-1.215518	3.012853	0.382415
19	6	-2.107491	2.577201	-0.807295
20	8	-1.908766	1.355329	-1.201278
21	8	-2.890322	3.392904	-1.279963
22	6	3.048762	1.260750	0.114048
23	6	2.509855	2.092816	-1.081478
24	8	1.271938	1.847759	-1.375791
25	8	3.270158	2.884572	-1.627108
26	6	1.296562	-3.024419	0.253683
27	6	2.028465	-2.589553	-1.044049
28	8	1.759376	-1.379481	-1.419341
29	8	2.767527	-3.400903	-1.590666
30	8	-0.712910	-0.096407	-3.110046
31	1	-1.257256	-0.122124	3.184601
32	1	-2.993624	-0.280389	2.953417
33	1	-2.949229	1.508002	1.228761
34	1	-2.385524	2.064993	2.798487
35	1	0.082040	1.499146	3.088361
36	1	-0.094514	3.213893	2.737670
37	1	1.605585	3.045420	0.938993
38	1	2.239851	2.583031	2.511853
39	1	1.716648	0.140918	2.994094
40	1	3.405600	0.292616	2.524569
41	1	3.126216	-1.514939	0.845808
42	1	2.774488	-2.052550	2.483407
43	1	0.353758	-1.476266	3.085293
44	1	0.487825	-3.195771	2.735948
45	1	-1.408057	-3.035251	1.134631
46	1	-1.860698	-2.587266	2.776463
47	1	-3.744543	-1.802690	1.112840
48	1	-3.404021	-0.301498	0.220513
49	1	-1.710747	3.830053	0.929813
50	1	-0.284758	3.392971	-0.048247
51	1	3.899835	1.786241	0.574107
52	1	3.400609	0.306414	-0.288392
53	1	1.860066	-3.835628	0.740268
54	1	0.317532	-3.409888	-0.044914
55	1	-1.161119	-0.953867	-2.950154
56	1	-1.402825	0.577566	-2.928906

HF = -1557.0657905 Hartree
Zero-point correction = 0.452357
Sum of electronic and thermal Enthalpies = -1556.583416
Sum of electronic and thermal Free Energies = -1556.670540

[Eu(DO3AP)(H_2O)]$^{2-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.705979	-1.692658	1.005132
2	6	2.934566	-1.004068	1.443509
3	6	2.699881	0.438593	1.899773
4	7	2.120820	1.321693	0.876621
5	6	1.561519	2.533545	1.502209
6	6	0.218977	2.286742	2.193274
7	7	-0.840354	1.760972	1.319640
8	6	-1.899945	1.120979	2.135400
9	6	-1.549279	-0.306990	2.542993
10	7	-1.314207	-1.227716	1.412200
11	6	-0.565527	-2.411237	1.887198
12	6	0.920950	-2.151172	2.166929
13	6	2.037133	-2.814748	0.097658
14	6	0.849677	-3.303250	-0.769897
15	8	0.073039	-2.366147	-1.181364
16	8	0.777579	-4.511778	-1.010557
17	6	3.109124	1.673108	-0.166077
18	6	3.385338	0.524195	-1.170610
19	8	4.559666	0.311629	-1.499986
20	8	2.333735	-0.090184	-1.572449
21	6	-1.422889	2.827531	0.468119
22	6	-0.504258	3.286790	-0.685261
23	8	-0.468406	4.487389	-0.971557
24	8	0.147715	2.336781	-1.277340
25	6	-2.595362	-1.668143	0.757548
26	63	0.078361	-0.040230	-0.674889
27	1	2.788685	-2.449354	-0.608209
28	1	2.456372	-3.667091	0.657753
29	1	4.060275	2.006203	0.282832
30	1	2.680714	2.494425	-0.747579
31	1	-1.697652	3.705732	1.075694
32	1	-2.331265	2.409365	0.019892
33	1	-2.330718	-2.515880	0.122359
34	1	-3.296299	-2.025622	1.533631
35	1	3.647008	-1.009532	0.618276
36	1	3.418226	-1.548380	2.278602
37	1	3.667259	0.844373	2.258363
38	1	2.027702	0.436313	2.763425
39	1	2.263646	2.954532	2.249783
40	1	1.438850	3.289586	0.727306
41	1	-0.104896	3.236900	2.661148
42	1	0.357840	1.576205	3.015479
43	1	-2.084691	1.708176	3.056328
44	1	-2.831924	1.097057	1.550636
45	1	-0.649528	-0.306582	3.171286

46	1	-2.370116	-0.693011	3.177220
47	1	-0.660326	-3.193369	1.134945
48	1	-1.014828	-2.811118	2.818098
49	1	1.015703	-1.398032	2.955575
50	1	1.358398	-3.082585	2.576539
51	8	-0.525711	0.470199	-3.163698
52	1	-1.435532	0.313099	-2.795228
53	1	-0.351470	1.410551	-2.951562
54	15	-3.468089	-0.485472	-0.443904
55	8	-4.297359	-1.393802	-1.319413
56	8	-2.149717	0.095781	-1.168430
57	8	-4.165783	0.623548	0.347568

HF = -1935.5581263 Hartree
Zero-point correction = 0.451274
Sum of electronic and thermal Enthalpies = -1935.075639
Sum of electronic and thermal Free Energies = -1935.164981

$[Eu(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.107598	0.068296	-0.668002
2	7	-0.601221	-1.901551	1.350920
3	6	-1.222122	-1.348386	2.565479
4	6	-2.156623	-0.173340	2.301460
5	7	-1.505685	0.939255	1.574972
6	6	-0.739312	1.775324	2.510087
7	6	0.364738	2.604457	1.853965
8	7	1.408515	1.801351	1.182788
9	6	2.294781	1.148901	2.155729
10	6	3.108027	-0.004692	1.562139
11	7	2.269694	-1.088775	1.030132
12	6	1.792386	-1.970403	2.099918
13	6	0.540254	-2.757646	1.711763
14	6	-1.565503	-2.672680	0.528319
15	6	-0.943214	-3.108791	-0.818573
16	8	-0.043600	-2.300514	-1.293197
17	8	-1.333138	-4.156674	-1.333639
18	6	-2.536750	1.723110	0.827934
19	6	2.168312	2.668161	0.255792
20	6	1.302502	3.164563	-0.933984
21	8	0.354426	2.362396	-1.267667
22	8	1.608034	4.244674	-1.441849
23	6	2.988358	-1.835815	-0.020061
24	6	3.292663	-0.945003	-1.254196
25	8	2.368536	-0.096243	-1.532158
26	8	4.361565	-1.130041	-1.842907
27	8	-0.419175	-0.381335	-3.185263
28	1	-0.415042	-1.044262	3.243784
29	1	-1.791550	-2.133825	3.101566
30	1	-3.016435	-0.489275	1.695368
31	1	-2.551379	0.179109	3.275028
32	1	-0.301068	1.123846	3.276033
33	1	-1.412432	2.469902	3.049884

34	1	-0.080840	3.252271	1.097370
35	1	0.817708	3.265484	2.619300
36	1	1.682004	0.770357	2.979833
37	1	2.996470	1.881394	2.602399
38	1	3.730913	0.369024	0.747695
39	1	3.804064	-0.380107	2.338333
40	1	1.581522	-1.357243	2.982225
41	1	2.581322	-2.686791	2.405490
42	1	0.769273	-3.391694	0.854408
43	1	0.276964	-3.437419	2.546341
44	1	-1.910174	-3.571828	1.067362
45	1	-2.440911	-2.044252	0.310253
46	1	-3.272787	2.143675	1.538426
47	1	-2.035308	2.555776	0.326546
48	1	2.597525	3.535902	0.784963
49	1	2.986485	2.087650	-0.178690
50	1	3.929246	-2.267820	0.362744
51	1	2.342340	-2.648558	-0.365339
52	1	-0.345140	-1.336202	-2.975038
53	1	-1.330617	-0.144526	-2.876919
54	15	-3.405484	0.729649	-0.530936
55	8	-2.078093	0.172157	-1.256422
56	8	-4.176496	1.738288	-1.345321
57	8	-4.144393	-0.428519	0.147484

HF = =-1935.5562396 Hartree
Zero-point correction = 0.450602
Sum of electronic and thermal Enthalpies = -1935.074313
Sum of electronic and thermal Free Energies = -1935.164000

$[Eu(DO2A2P)]^{3-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.273443	1.742733	-1.230857
2	6	2.429108	1.089041	-1.882291
3	6	2.149422	-0.353372	-2.294837
4	7	1.766961	-1.238349	-1.185027
5	6	1.118360	-2.450758	-1.718186
6	6	-0.312066	-2.228004	-2.229561
7	7	-1.273369	-1.742961	-1.230802
8	6	-2.428983	-1.089191	-1.882236
9	6	-2.149171	0.353157	-2.294912
10	7	-1.767007	1.238340	-1.185181
11	6	-1.118266	2.450669	-1.718226
12	6	0.312132	2.227844	-2.229641
13	6	1.747137	2.831158	-0.342743
14	6	0.707165	3.305534	0.697591
15	8	-0.045252	2.383002	1.174413
16	8	0.702778	4.511829	0.993528
17	6	2.927663	-1.609151	-0.308361
18	6	-1.746924	-2.831494	-0.342766
19	6	-0.706938	-3.305337	0.697908
20	8	-0.702222	-4.511641	0.993893
21	8	0.045541	-2.382680	1.174212

22	6	-2.927960	1.609056	-0.308785
23	63	-0.000114	-0.000017	0.666369
24	1	2.607154	2.432717	0.209987
25	1	2.079277	3.700114	-0.940032
26	1	3.777101	-1.929606	-0.943582
27	1	2.595923	-2.472001	0.272493
28	1	-2.078631	-3.700610	-0.940062
29	1	-2.607281	-2.433311	0.209672
30	1	-2.596606	2.472115	0.271969
31	1	-3.777442	1.929016	-0.944153
32	1	3.263958	1.087145	-1.165150
33	1	2.739425	1.654908	-2.786396
34	1	3.057779	-0.746439	-2.799331
35	1	1.348580	-0.381711	-3.044583
36	1	1.712062	-2.880316	-2.554501
37	1	1.104268	-3.197205	-0.925796
38	1	-0.666790	-3.184499	-2.667911
39	1	-0.294342	-1.506559	-3.053912
40	1	-2.739305	-1.655075	-2.786326
41	1	-3.263887	-1.087182	-1.165146
42	1	-1.348206	0.381344	-3.044532
43	1	-3.057415	0.746153	-2.799696
44	1	-1.104127	3.197021	-0.925741
45	1	-1.711931	2.880521	-2.554471
46	1	0.294258	1.506333	-3.053929
47	1	0.666949	3.184253	-2.668031
48	15	-3.505291	0.405252	1.047894
49	8	-4.286895	1.301279	1.990322
50	8	-2.079240	-0.065756	1.583080
51	8	-4.269742	-0.758842	0.392657
52	15	3.505186	-0.405107	1.048008
53	8	4.286458	-1.300995	1.990798
54	8	4.269979	0.758442	0.392278
55	8	2.079056	0.066423	1.582909

HF = -2237.509932 Hartree
Zero-point correction = 0.423264
Sum of electronic and thermal Enthalpies = -2237.056463
Sum of electronic and thermal Free Energies = -2237.143294

$[Eu(DO2A2P)]^{3-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.000167	-0.000179	-0.676233
2	7	-0.935790	-1.877106	1.284578
3	6	-1.701689	-1.307564	2.401646
4	6	-2.653860	-0.186314	1.986326
5	7	-1.966726	0.936073	1.322613
6	6	-1.364907	1.832569	2.312267
7	6	-0.202528	2.670752	1.775499
8	7	0.936631	1.876922	1.284015
9	6	1.702744	1.307872	2.401251
10	6	2.654779	0.186479	1.986302
11	7	1.967443	-0.935911	1.322721

12	6	1.365841	-1.832391	2.312575
13	6	0.203428	-2.670750	1.776225
14	6	-1.791974	-2.712838	0.405830
15	6	-1.025473	-3.185042	-0.855382
16	8	-0.140378	-2.358589	-1.283462
17	8	-1.322137	-4.292364	-1.325599
18	6	-2.893310	1.646500	0.394796
19	6	1.792580	2.712533	0.404861
20	6	1.025098	3.185300	-0.855473
21	8	0.140756	2.358407	-1.284065
22	8	1.320153	4.293656	-1.324387
23	6	2.893685	-1.646263	0.394559
24	1	-0.989125	-0.938242	3.149970
25	1	-2.293800	-2.099474	2.908646
26	1	-3.409036	-0.556617	1.279415
27	1	-3.190555	0.161706	2.895439
28	1	-1.018313	1.228125	3.159908
29	1	-2.127506	2.526773	2.725908
30	1	-0.563060	3.277873	0.944033
31	1	0.124879	3.373430	2.571430
32	1	0.990300	0.938799	3.149824
33	1	2.294803	2.100075	2.907876
34	1	3.410031	0.556452	1.279291
35	1	3.191326	-0.161502	2.895525
36	1	1.019360	-1.227771	3.160147
37	1	2.128581	-2.526441	2.726152
38	1	0.563804	-3.278177	0.944947
39	1	-0.123816	-3.373145	2.572527
40	1	-2.161777	-3.597066	0.957547
41	1	-2.655741	-2.119979	0.071294
42	1	-3.752271	2.054344	0.965449
43	1	-2.347949	2.485601	-0.045275
44	1	2.162977	3.596565	0.956583
45	1	2.655932	2.119416	0.069770
46	1	3.753120	-2.053679	0.964818
47	1	2.348336	-2.485752	-0.044825
48	15	-3.484113	0.586886	-1.063315
49	8	-2.060009	0.110899	-1.601188
50	8	-4.230734	1.547819	-1.966844
51	8	-4.266558	-0.593827	-0.459094
52	15	3.483529	-0.587012	-1.064091
53	8	2.059180	-0.111800	-1.602204
54	8	4.265479	0.594383	-0.460498
55	8	4.230673	-1.547717	-1.967386

HF = -2237.5121571 Hartree
Zero-point correction = 0.422662
Sum of electronic and thermal Enthalpies = -2237.059221
Sum of electronic and thermal Free Energies = -2237.146269

$[Eu(DOA3P)]^{4-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.266834	1.382450	1.425995

2	6	-2.368418	0.583020	2.005284
3	6	-2.013253	-0.874347	2.313529
4	7	-1.623072	-1.686881	1.154379
5	6	-0.885525	-2.879622	1.593400
6	6	0.542880	-2.619097	2.083506
7	7	1.446600	-2.032705	1.100519
8	6	2.594826	-1.389993	1.758818
9	6	2.265294	-0.003542	2.302805
10	7	1.805319	0.962345	1.301401
11	6	1.123951	2.084705	1.980358
12	6	-0.295873	1.762996	2.468094
13	6	-1.857560	2.570384	0.721291
14	6	-2.776660	-2.108257	0.302812
15	6	1.898332	-3.002031	0.085878
16	6	0.847000	-3.382162	-0.988380
17	8	0.868337	-4.565537	-1.393952
18	8	0.083094	-2.439435	-1.374722
19	6	2.912954	1.471582	0.426448
20	63	-0.011910	0.001615	-0.687755
21	1	-2.675686	2.173561	0.115883
22	1	-2.291716	3.253577	1.481507
23	1	-3.559302	-2.562943	0.948156
24	1	-2.386957	-2.887421	-0.355085
25	1	2.260202	-3.932934	0.568752
26	1	2.735229	-2.529584	-0.441864
27	1	2.505208	2.354247	-0.070172
28	1	3.759965	1.797301	1.066591
29	1	-3.210304	0.582508	1.298118
30	1	-2.721386	1.046066	2.955724
31	1	-2.892895	-1.331966	2.820831
32	1	-1.191239	-0.909500	3.039756
33	1	-1.431405	-3.404275	2.413789
34	1	-0.846689	-3.573980	0.754459
35	1	0.948524	-3.588733	2.458760
36	1	0.512722	-1.951191	2.951896
37	1	2.967772	-2.015392	2.604529
38	1	3.404420	-1.286679	1.019584
39	1	1.489037	-0.079035	3.076366
40	1	3.172788	0.384947	2.818641
41	1	1.054100	2.946505	1.304072
42	1	1.713341	2.408233	2.870301
43	1	-0.264849	0.949511	3.206275
44	1	-0.664290	2.657769	3.010968
45	15	3.531405	0.402357	-1.020309
46	8	4.261756	1.389991	-1.920549
47	8	2.134783	-0.125056	-1.565922
48	8	4.398129	-0.752857	-0.466188
49	15	-3.531715	-0.873090	-0.921969
50	8	-4.235116	-1.772513	-1.932779
51	8	-4.428764	0.093606	-0.130764
52	8	-2.188630	-0.198056	-1.434884
53	15	-0.748839	3.510996	-0.484702
54	8	-1.705450	4.248164	-1.411556
55	8	0.214985	4.388166	0.335608
56	8	-0.010721	2.250458	-1.127255

HF = -2615.8046514 Hartree
Zero-point correction = 0.420644
Sum of electronic and thermal Enthalpies = -2615.352153
Sum of electronic and thermal Free Energies = -2615.442492

[Eu(DOA3P)]$^{4-}$ (Δ(δδδδ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.041425	-0.004157	-0.709277
2	7	0.867390	1.590970	1.550131
3	6	1.612133	0.848805	2.575028
4	6	2.549011	-0.239334	2.043086
5	7	1.850343	-1.321529	1.328834
6	6	1.181537	-2.229102	2.257822
7	6	0.039293	-3.033009	1.627821
8	7	-1.075318	-2.209422	1.159310
9	6	-1.884336	-1.723797	2.274966
10	6	-2.787552	-0.544538	1.913994
11	7	-2.046527	0.612832	1.392132
12	6	-1.469260	1.377772	2.501824
13	6	-0.290628	2.285680	2.150032
14	6	1.746034	2.567857	0.830222
15	6	2.769826	-2.058279	0.420221
16	6	-1.881715	-2.932833	0.156473
17	6	-1.066224	-3.284759	-1.117057
18	8	-0.180906	-2.428967	-1.449231
19	8	-1.351047	-4.358719	-1.685223
20	6	-2.908108	1.431001	0.489275
21	1	0.885073	0.402424	3.267562
22	1	2.219173	1.552915	3.187177
23	1	3.294579	0.169464	1.346602
24	1	3.115839	-0.649538	2.912505
25	1	0.792377	-1.647453	3.101990
26	1	1.912038	-2.948876	2.694777
27	1	0.429800	-3.580267	0.768981
28	1	-0.306288	-3.795174	2.366211
29	1	-1.204133	-1.437837	3.087539
30	1	-2.522111	-2.541481	2.687567
31	1	-3.518076	-0.833931	1.145666
32	1	-3.363190	-0.266176	2.827915
33	1	-1.163532	0.657439	3.274458
34	1	-2.250473	2.013084	2.979175
35	1	-0.589036	3.081827	1.453986
36	1	0.020951	2.799219	3.089394
37	1	2.169642	3.283187	1.567158
38	1	2.574400	2.007348	0.386233
39	1	3.566757	-2.549261	1.021167
40	1	2.188547	-2.839627	-0.075562
41	1	-2.290029	-3.869795	0.588933
42	1	-2.722524	-2.297979	-0.154967
43	1	-3.772904	1.828511	1.063420
44	1	-2.313935	2.281151	0.140783
45	15	3.513358	-1.010899	-0.970093
46	8	2.169128	-0.349090	-1.500598
47	8	4.157367	-2.021708	-1.911143
48	8	4.446142	0.002195	-0.287127
49	15	-3.497127	0.495281	-1.056031
50	8	-2.090244	-0.019617	-1.587105
51	8	-4.370941	-0.682261	-0.563039

52	8	-4.195243	1.531218	-1.923196
53	15	0.860043	3.480180	-0.576519
54	8	0.172628	2.205039	-1.242650
55	8	-0.175177	4.410551	0.080270
56	8	1.951030	4.145303	-1.400914

HF = -2615.8070154 Hartree
Zero-point correction = 0.420455
Sum of electronic and thermal Enthalpies = -2615.354725
Sum of electronic and thermal Free Energies = -2615.445257

$[Eu(DOTP)]^{5-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-2.176143	0.258345	1.328907
2	6	-2.459411	-1.059505	1.924772
3	6	-1.220313	-1.835531	2.379880
4	7	-0.257108	-2.173055	1.329626
5	6	1.061056	-2.462426	1.921827
6	6	1.846119	-1.228864	2.377336
7	7	2.175478	-0.259405	1.329997
8	6	2.459013	1.058373	1.925814
9	6	1.220445	1.836494	2.379477
10	7	0.256825	2.172471	1.329189
11	6	-1.061361	2.461603	1.921635
12	6	-1.847789	1.228504	2.376101
13	6	-3.331648	0.672033	0.473239
14	6	-0.679480	-3.329303	0.479199
15	6	3.331309	-0.673779	0.475024
16	6	0.678228	3.328752	0.478509
17	63	0.000013	0.000188	-0.677984
18	1	-3.589354	-0.214668	-0.109625
19	1	-4.196295	0.915417	1.132486
20	1	-0.927442	-4.189757	1.142250
21	1	0.205241	-3.594920	-0.103100
22	1	4.195039	-0.918389	1.135043
23	1	3.590146	0.213027	-0.107114
24	1	-0.206268	3.592637	-0.104864
25	1	0.924528	4.190033	1.141059
26	1	-2.990658	-1.682038	1.191138
27	1	-3.127399	-0.946572	2.816266
28	1	-1.578649	-2.765028	2.883528
29	1	-0.685224	-1.265349	3.151834
30	1	0.946722	-3.131473	2.812432
31	1	1.679959	-2.994934	1.186190
32	1	2.779948	-1.595213	2.866396
33	1	1.288393	-0.697571	3.161175
34	1	3.125545	0.944772	2.818323
35	1	2.992005	1.680311	1.192992
36	1	0.685398	1.269412	3.153896
37	1	1.580251	2.767013	2.880111
38	1	-1.679999	2.995399	1.186806
39	1	-0.946508	3.129451	2.813027
40	1	-1.292583	0.697709	3.162121

41	1	-2.782519	1.596083	2.862364
42	15	2.028152	3.062962	-0.821967
43	8	1.837226	4.217563	-1.807997
44	8	1.588424	1.631906	-1.338385
45	8	3.396602	3.053219	-0.101373
46	15	-2.028386	-3.062399	-0.822318
47	8	-1.840051	-4.218607	-1.806945
48	8	-3.397011	-3.048953	-0.102155
49	8	-1.584794	-1.633183	-1.340523
50	15	-3.065324	2.023979	-0.824566
51	8	-4.215738	1.832899	-1.815326
52	8	-3.060483	3.390999	-0.101162
53	8	-1.631241	1.588066	-1.336609
54	15	3.065961	-2.024145	-0.824838
55	8	4.218770	-1.832913	-1.812886
56	8	1.633605	-1.586216	-1.339242
57	8	3.058755	-3.392249	-0.103311

HF = -2994.0154457 Hartree
Zero-point correction = 0.418604
Sum of electronic and thermal Enthalpies = -2993.563624
Sum of electronic and thermal Free Energies = -2993.656486

$[Eu(DOTP)]^{5-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.001187	-0.004580	-0.742313
2	7	0.977623	-1.945715	1.458234
3	6	-0.011633	-2.200624	2.503154
4	6	-1.471223	-2.233750	2.040618
5	7	-1.947418	-0.971114	1.458636
6	6	-2.202932	0.017592	2.503881
7	6	-2.235513	1.476886	2.040017
8	7	-0.972308	1.952399	1.458714
9	6	0.016077	2.209921	2.503124
10	6	1.475751	2.242239	2.039304
11	7	1.952033	0.978837	1.459978
12	6	2.208377	-0.010211	2.504217
13	6	2.240368	-1.469833	2.040461
14	6	1.190577	-3.133723	0.582813
15	6	-3.134156	-1.182137	0.580610
16	6	-1.182873	3.135596	0.575731
17	6	3.136149	1.190687	0.579836
18	1	0.110164	-1.432331	3.279546
19	1	0.204581	-3.173204	3.011053
20	1	-1.640259	-3.020854	1.292751
21	1	-2.091463	-2.510462	2.931332
22	1	-1.434820	-0.104260	3.280641
23	1	-3.175731	-0.198150	3.011552
24	1	-3.021433	1.644418	1.290694
25	1	-2.514172	2.097738	2.929868
26	1	-0.105566	1.443095	3.281078
27	1	-0.199443	3.183659	3.009624
28	1	1.643284	3.026866	1.288365

29	1	2.096587	2.522759	2.928629
30	1	1.441538	0.111581	3.282043
31	1	3.182114	0.204789	3.010937
32	1	3.027076	-1.638799	1.291988
33	1	2.516718	-2.091206	2.930520
34	1	1.554806	-3.984014	1.205453
35	1	0.220590	-3.414335	0.162204
36	1	-3.988416	-1.539799	1.201600
37	1	-3.407798	-0.212223	0.155421
38	1	-1.540886	3.992265	1.193432
39	1	-0.212726	3.408388	0.150350
40	1	3.989922	1.553660	1.198688
41	1	3.414097	0.220125	0.158617
42	15	-2.819229	-2.353402	-0.878044
43	8	-1.480365	-1.698690	-1.415876
44	8	-4.042280	-2.224844	-1.785775
45	8	-2.596337	-3.756806	-0.270448
46	15	2.814854	2.353422	-0.884854
47	8	1.481251	1.687080	-1.422190
48	8	2.582143	3.758569	-0.285388
49	8	4.038817	2.228146	-1.791336
50	15	2.353697	-2.817458	-0.882231
51	8	1.689171	-1.485446	-1.424198
52	8	3.758280	-2.583911	-0.281090
53	8	2.228361	-4.045268	-1.783977
54	15	-2.353666	2.815971	-0.883050
55	8	-1.696562	1.475910	-1.416667
56	8	-3.757971	2.592772	-0.277999
57	8	-2.226027	4.035503	-1.794993

HF = -2994.01824627 Hartree
Zero-point correction = 0.417956
Sum of electronic and thermal Enthalpies = -2993.566944
Sum of electronic and thermal Free Energies = -2993.660463

$[La(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.792966	-1.670625	0.969843
2	6	2.987746	-0.927697	1.417971
3	6	2.697369	0.503247	1.882279
4	7	2.102892	1.384434	0.864187
5	6	1.492770	2.567590	1.501455
6	6	0.163915	2.270844	2.201790
7	7	-0.896672	1.731042	1.336623
8	6	-1.916944	1.030880	2.155469
9	6	-1.508137	-0.388528	2.540222
10	7	-1.269152	-1.294558	1.398529
11	6	-0.470017	-2.457841	1.844233
12	6	1.010825	-2.156330	2.124409
13	6	2.190572	-2.783698	0.076606
14	6	1.040666	-3.360230	-0.791689
15	8	0.232589	-2.476698	-1.257728
16	8	1.030734	-4.579498	-0.985286
17	6	3.095683	1.796410	-0.154148

18	6	3.464805	0.676064	-1.165464
19	8	4.663496	0.497413	-1.418517
20	8	2.456286	0.051317	-1.653351
21	6	-1.541801	2.801184	0.534543
22	6	-0.665852	3.358738	-0.611984
23	8	-0.672553	4.576041	-0.819199
24	8	-0.007342	2.467848	-1.282813
25	6	-2.550066	-1.769642	0.764361
26	1	2.923766	-2.382986	-0.630296
27	1	2.658969	-3.600705	0.650371
28	1	4.014517	2.177769	0.322553
29	1	2.635973	2.600502	-0.736896
30	1	-1.850197	3.637999	1.182912
31	1	-2.438815	2.358147	0.085827
32	1	-2.271209	-2.606539	0.119768
33	1	-3.220719	-2.158012	1.552253
34	1	3.704269	-0.900200	0.596727
35	1	3.489421	-1.454699	2.253623
36	1	3.646801	0.935606	2.256696
37	1	2.016458	0.469254	2.738023
38	1	2.181772	3.011951	2.247709
39	1	1.335939	3.321418	0.730580
40	1	-0.177835	3.205555	2.687148
41	1	0.331416	1.553492	3.012189
42	1	-2.114785	1.596543	3.087116
43	1	-2.853462	0.977215	1.579394
44	1	-0.596122	-0.363158	3.149668
45	1	-2.302245	-0.805587	3.188873
46	1	-0.542081	-3.226558	1.075621
47	1	-0.898376	-2.892236	2.769631
48	1	1.083951	-1.407129	2.918756
49	1	1.470523	-3.078562	2.529512
50	8	-0.748071	0.668074	-3.259024
51	1	-1.618375	0.420076	-2.844848
52	1	-0.608275	1.594103	-2.970109
53	15	-3.514115	-0.627058	-0.415191
54	8	-4.376454	-1.585633	-1.201536
55	8	-2.262365	-0.040110	-1.241978
56	8	-4.185630	0.488348	0.389964
57	57	0.080798	-0.037407	-0.761295

HF = -1931.8277893 Hartree
Zero-point correction = 0.450837
Sum of electronic and thermal Enthalpies = -1931.345515
Sum of electronic and thermal Free Energies = -1931.435855

[La(DO3AP)(H_2O)]$^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.653283	1.874928	1.375559
2	6	1.226968	1.258515	2.583724
3	6	2.141694	0.070469	2.304235
4	7	1.479337	-1.019396	1.552302
5	6	0.676863	-1.850683	2.464811

6	6	-0.453895	-2.636579	1.796534
7	7	-1.489348	-1.803816	1.147544
8	6	-2.330237	-1.107335	2.131834
9	6	-3.118045	0.070019	1.545961
10	7	-2.261645	1.145688	1.021654
11	6	-1.751272	1.996091	2.104777
12	6	-0.473304	2.751856	1.734410
13	6	1.664457	2.645649	0.608850
14	6	1.103919	3.172104	-0.735224
15	8	0.205928	2.416856	-1.290316
16	8	1.548631	4.232583	-1.175645
17	6	2.511252	-1.818921	0.819831
18	6	-2.306701	-2.653075	0.252951
19	6	-1.514506	-3.199058	-0.968805
20	8	-0.547197	-2.447264	-1.355126
21	8	-1.901500	-4.264831	-1.452411
22	6	-2.985883	1.939014	0.007348
23	6	-3.353853	1.107796	-1.254114
24	8	-2.469865	0.241716	-1.598072
25	8	-4.430039	1.362253	-1.802695
26	8	0.625086	0.570748	-3.280892
27	1	0.394524	0.947017	3.226423
28	1	1.799506	2.008473	3.165308
29	1	3.012383	0.378744	1.709667
30	1	2.520070	-0.306814	3.274920
31	1	0.259706	-1.202325	3.244628
32	1	1.325440	-2.577822	2.990814
33	1	-0.030145	-3.279800	1.022801
34	1	-0.913750	-3.302501	2.553782
35	1	-1.687378	-0.742473	2.938532
36	1	-3.048097	-1.809421	2.600929
37	1	-3.749585	-0.282678	0.728671
38	1	-3.804959	0.452683	2.326729
39	1	-1.564788	1.365492	2.979747
40	1	-2.516497	2.733678	2.418513
41	1	-0.676957	3.398693	0.879897
42	1	-0.202388	3.416655	2.578861
43	1	2.029919	3.503432	1.198988
44	1	2.521908	1.993464	0.384716
45	1	3.225308	-2.251370	1.545246
46	1	2.005759	-2.648152	0.314895
47	1	-2.749700	-3.497290	0.808329
48	1	-3.121360	-2.048448	-0.155750
49	1	-3.903402	2.384812	0.428753
50	1	-2.328451	2.749175	-0.324861
51	1	0.584591	1.507515	-2.991613
52	1	1.498201	0.252059	-2.934828
53	15	3.443802	-0.856636	-0.525430
54	8	2.165329	-0.335401	-1.353259
55	8	4.269842	-1.892881	-1.246962
56	8	4.133485	0.327750	0.161136
57	57	-0.109309	-0.067412	-0.735804

HF = -1931.828071 Hartree
Zero-point correction = 0.449889
Sum of electronic and thermal Enthalpies = -1931.346567
Sum of electronic and thermal Free Energies = -1931.437293

[Ce(DO3AP)(H_2O)]$^{2-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.770181	-1.681204	0.976632
2	6	2.973903	-0.952119	1.422508
3	6	2.697793	0.481506	1.886475
4	7	2.108699	1.365500	0.868052
5	6	1.511753	2.555257	1.504857
6	6	0.178471	2.271111	2.201541
7	7	-0.882077	1.738023	1.332555
8	6	-1.913818	1.051890	2.148373
9	6	-1.521044	-0.370525	2.538438
10	7	-1.282493	-1.279991	1.399347
11	6	-0.496403	-2.449045	1.852138
12	6	0.986109	-2.158981	2.132770
13	6	2.150975	-2.797216	0.080110
14	6	0.992306	-3.350941	-0.790581
15	8	0.191407	-2.453406	-1.241979
16	8	0.968540	-4.567514	-0.998925
17	6	3.102273	1.764629	-0.154245
18	6	3.450750	0.639652	-1.166831
19	8	4.644235	0.457998	-1.441102
20	8	2.432663	0.014303	-1.633644
21	6	-1.510407	2.810341	0.520417
22	6	-0.622963	3.346640	-0.626827
23	8	-0.621969	4.560660	-0.852435
24	8	0.036874	2.442759	-1.278729
25	6	-2.563087	-1.745614	0.758460
26	1	2.890445	-2.405933	-0.625326
27	1	2.605624	-3.623880	0.651037
28	1	4.028526	2.133167	0.318185
29	1	2.651180	2.574647	-0.735274
30	1	-1.810595	3.656049	1.161078
31	1	-2.410437	2.375397	0.070278
32	1	-2.287168	-2.584079	0.114915
33	1	-3.241554	-2.127926	1.542653
34	1	3.689004	-0.932155	0.599833
35	1	3.471521	-1.484330	2.257294
36	1	3.651562	0.906255	2.258676
37	1	2.017922	0.454492	2.743316
38	1	2.204173	2.991120	2.252944
39	1	1.364894	3.311635	0.734557
40	1	-0.157966	3.209246	2.684131
41	1	0.337339	1.553538	3.013584
42	1	-2.109996	1.622201	3.077547
43	1	-2.848526	1.006235	1.568786
44	1	-0.612706	-0.352774	3.153730
45	1	-2.323266	-0.779335	3.182254
46	1	-0.574221	-3.220708	1.087113
47	1	-0.930599	-2.875079	2.778687
48	1	1.064724	-1.408545	2.925479
49	1	1.439248	-3.083823	2.539550
50	8	-0.695843	0.634713	-3.240097
51	1	-1.575924	0.409822	-2.834078
52	1	-0.544055	1.563359	-2.966351
53	15	-3.505845	-0.590636	-0.424222
54	8	-4.358454	-1.536106	-1.236426

55	8	-2.237857	0.000601	-1.223882
56	8	-4.185991	0.518964	0.381504
57	58	0.081205	-0.037735	-0.740470

HF = -1932.4804783 Hartree
Zero-point correction = 0.450893
Sum of electronic and thermal Enthalpies = -1931.998185
Sum of electronic and thermal Free Energies = -1932.088341

$[Ce(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.645184	1.878957	1.370350
2	6	1.229958	1.275501	2.579555
3	6	2.147422	0.089175	2.302636
4	7	1.485938	-1.004325	1.555543
5	6	0.691208	-1.837036	2.472786
6	6	-0.435012	-2.630973	1.807330
7	7	-1.471899	-1.803377	1.154370
8	6	-2.321686	-1.115751	2.136992
9	6	-3.114105	0.057454	1.550040
10	7	-2.260521	1.134189	1.024071
11	6	-1.756531	1.990670	2.104767
12	6	-0.483465	2.752454	1.730993
13	6	1.646130	2.648927	0.589877
14	6	1.069617	3.158681	-0.753519
15	8	0.167302	2.394624	-1.289795
16	8	1.504435	4.216207	-1.210440
17	6	2.516407	-1.800501	0.818091
18	6	-2.278380	-2.655894	0.253099
19	6	-1.471987	-3.190517	-0.963862
20	8	-0.506542	-2.429473	-1.337380
21	8	-1.845030	-4.257434	-1.455513
22	6	-2.982803	1.918621	0.001867
23	6	-3.340298	1.074196	-1.253199
24	8	-2.450780	0.207555	-1.581832
25	8	-4.414193	1.317577	-1.811064
26	8	0.574622	0.534862	-3.263815
27	1	0.403275	0.966316	3.230920
28	1	1.803490	2.032717	3.150643
29	1	3.016029	0.398506	1.705607
30	1	2.528848	-0.283937	3.273743
31	1	0.270648	-1.188183	3.250444
32	1	1.345093	-2.558187	3.000628
33	1	-0.007649	-3.275324	1.036725
34	1	-0.893708	-3.295611	2.566342
35	1	-1.684566	-0.748700	2.947332
36	1	-3.036695	-1.824011	2.601139
37	1	-3.744339	-0.299034	0.733468
38	1	-3.802206	0.439202	2.330189
39	1	-1.565299	1.363187	2.981060
40	1	-2.526412	2.724215	2.416867
41	1	-0.692320	3.397626	0.876612
42	1	-0.213054	3.419190	2.574002

43	1	2.010674	3.514462	1.169194
44	1	2.505830	2.000275	0.364664
45	1	3.235555	-2.231967	1.539097
46	1	2.010646	-2.629433	0.313305
47	1	-2.717768	-3.505551	0.802974
48	1	-3.094681	-2.056273	-0.159379
49	1	-3.903884	2.364346	0.415526
50	1	-2.325924	2.727320	-0.334508
51	1	0.527810	1.475828	-2.990194
52	1	1.456906	0.233227	-2.926618
53	15	3.434742	-0.830543	-0.530088
54	8	2.144603	-0.300106	-1.334663
55	8	4.248592	-1.860798	-1.273496
56	8	4.135872	0.347428	0.155547
57	58	-0.110142	-0.067479	-0.718861

HF = -1932.4803173 Hartree
Zero-point correction = 0.450031
Sum of electronic and thermal Enthalpies = -1931.998731
Sum of electronic and thermal Free Energies = -1932.089232

$[Pr(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.755416	-1.684033	0.982537
2	6	2.964348	-0.963566	1.427608
3	6	2.696539	0.472052	1.889752
4	7	2.110554	1.355931	0.869769
5	6	1.522133	2.550987	1.503868
6	6	0.186321	2.275843	2.198896
7	7	-0.873581	1.743415	1.328962
8	6	-1.911340	1.067141	2.145005
9	6	-1.527011	-0.356365	2.539069
10	7	-1.290156	-1.268501	1.401785
11	6	-0.512597	-2.441262	1.859085
12	6	0.971037	-2.158706	2.139499
13	6	2.125972	-2.800650	0.082645
14	6	0.960415	-3.341146	-0.786425
15	8	0.164164	-2.435378	-1.229513
16	8	0.926090	-4.556427	-1.000735
17	6	3.103949	1.744387	-0.156447
18	6	3.437491	0.613824	-1.167077
19	8	4.627276	0.426085	-1.453086
20	8	2.412333	-0.010175	-1.619854
21	6	-1.492266	2.813908	0.507249
22	6	-0.597245	3.334016	-0.640995
23	8	-0.589605	4.545467	-0.879941
24	8	0.062555	2.420498	-1.279520
25	6	-2.571461	-1.727839	0.758361
26	1	2.866775	-2.413414	-0.623472
27	1	2.574628	-3.632729	0.650407
28	1	4.035419	2.105323	0.311615
29	1	2.658268	2.556930	-0.737949
30	1	-1.788106	3.666799	1.140368

31	1	-2.393581	2.381680	0.057232
32	1	-2.299157	-2.569586	0.117779
33	1	-3.255403	-2.102812	1.541334
34	1	3.679584	-0.949083	0.604941
35	1	3.458273	-1.498435	2.262839
36	1	3.652803	0.892913	2.260072
37	1	2.017281	0.450143	2.747299
38	1	2.216723	2.983011	2.252161
39	1	1.381382	3.307481	0.732545
40	1	-0.147653	3.217263	2.676845
41	1	0.340271	1.560791	3.014197
42	1	-2.105122	1.641286	3.072291
43	1	-2.845501	1.025956	1.564262
44	1	-0.619797	-0.341924	3.156147
45	1	-2.332566	-0.760302	3.181795
46	1	-0.594467	-3.215012	1.096643
47	1	-0.950292	-2.861602	2.786573
48	1	1.053807	-1.408797	2.932353
49	1	1.420385	-3.085780	2.545471
50	8	-0.652707	0.596737	-3.224508
51	1	-1.540294	0.384701	-2.828508
52	1	-0.499477	1.528826	-2.963806
53	15	-3.497949	-0.567011	-0.429806
54	8	-4.346500	-1.504612	-1.255119
55	8	-2.218513	0.021093	-1.213905
56	8	-4.181301	0.543311	0.372262
57	59	0.081379	-0.038215	-0.723981

HF = -1933.115289 Hartree
Zero-point correction = 0.450968
Sum of electronic and thermal Enthalpies = -1932.632963
Sum of electronic and thermal Free Energies = -1932.722928

$[Pr(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.632496	-1.882605	1.368277
2	6	-1.228185	-1.289599	2.577267
3	6	-2.150194	-0.106878	2.300647
4	7	-1.491148	0.990355	1.557221
5	6	-0.704727	1.826015	2.478135
6	6	0.415180	2.629723	1.814583
7	7	1.454426	1.808676	1.157436
8	6	2.315183	1.132272	2.137932
9	6	3.113074	-0.036647	1.550690
10	7	2.263775	-1.117115	1.025916
11	6	1.767247	-1.977363	2.106575
12	6	0.500704	-2.749026	1.731603
13	6	-1.622818	-2.655892	0.577988
14	6	-1.033047	-3.151728	-0.764577
15	8	-0.127970	-2.380192	-1.285710
16	8	-1.459153	-4.207025	-1.234492
17	6	-2.520692	1.781520	0.813653
18	6	2.247327	2.663984	0.246899

19	6	1.422570	3.188411	-0.961679
20	8	0.463704	2.414019	-1.325703
21	8	1.774216	4.261131	-1.456187
22	6	2.986156	-1.894822	-0.001092
23	6	3.331851	-1.041987	-1.253232
24	8	2.435320	-0.178348	-1.571182
25	8	4.404141	-1.274627	-1.818628
26	8	-0.535758	-0.510079	-3.244901
27	1	-0.407250	-0.980181	3.235879
28	1	-1.801223	-2.053243	3.140187
29	1	-3.016564	-0.419117	1.701787
30	1	-2.535609	0.262687	3.271545
31	1	-0.278875	1.177621	3.253378
32	1	-1.364554	2.540169	3.008278
33	1	-0.017261	3.274509	1.047372
34	1	0.871859	3.294034	2.575014
35	1	1.685380	0.763647	2.953357
36	1	3.027130	1.848060	2.595207
37	1	3.740278	0.323244	0.733334
38	1	3.804123	-0.414973	2.329880
39	1	1.569599	-1.350787	2.982169
40	1	2.543134	-2.704235	2.419669
41	1	0.715661	-3.393657	0.878434
42	1	0.233166	-3.416702	2.574705
43	1	-1.983394	-3.528179	1.149612
44	1	-2.486150	-2.013039	0.351527
45	1	-3.243187	2.215053	1.530080
46	1	-2.014551	2.607940	0.305499
47	1	2.686010	3.518480	0.789734
48	1	3.062833	2.068321	-0.172723
49	1	3.911807	-2.336263	0.406936
50	1	2.332136	-2.705302	-0.338232
51	1	-0.478222	-1.453900	-2.983860
52	1	-1.426265	-0.227139	-2.913422
53	15	-3.429814	0.801174	-0.532379
54	8	-2.132072	0.252555	-1.313471
55	8	-4.227671	1.825516	-1.300663
56	8	-4.146250	-0.364173	0.158397
57	59	0.110669	0.065628	-0.704977

HF = -1933.114752 Hartree
Zero-point correction = 0.450165
Sum of electronic and thermal Enthalpies = -1932.633088
Sum of electronic and thermal Free Energies = -1932.723391

$[Nd(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.738738	-1.689692	0.988461
2	6	2.954503	-0.980127	1.431463
3	6	2.698484	0.457839	1.892479
4	7	2.115539	1.342831	0.872086
5	6	1.536594	2.542967	1.504633
6	6	0.198349	2.276882	2.198095

7	7	-0.862002	1.748741	1.326434
8	6	-1.907451	1.083884	2.141635
9	6	-1.535374	-0.341780	2.539290
10	7	-1.299274	-1.256436	1.403799
11	6	-0.531271	-2.433093	1.866467
12	6	0.953417	-2.158279	2.146894
13	6	2.096346	-2.808736	0.086559
14	6	0.923990	-3.332486	-0.782835
15	8	0.134555	-2.416464	-1.216852
16	8	0.877699	-4.545804	-1.005583
17	6	3.108315	1.720523	-0.158360
18	6	3.424908	0.585144	-1.168282
19	8	4.610352	0.390785	-1.467513
20	8	2.391818	-0.035919	-1.606789
21	6	-1.468746	2.819798	0.496825
22	6	-0.565818	3.323007	-0.652149
23	8	-0.548872	4.531899	-0.903221
24	8	0.090919	2.398896	-1.278544
25	6	-2.580492	-1.709022	0.756131
26	1	2.841298	-2.429066	-0.619164
27	1	2.535011	-3.647411	0.652401
28	1	4.045659	2.072389	0.304910
29	1	2.668538	2.536582	-0.739260
30	1	-1.758501	3.679491	1.123557
31	1	-2.372082	2.392738	0.046205
32	1	-2.310277	-2.551671	0.116023
33	1	-3.269706	-2.079911	1.536426
34	1	3.668643	-0.972088	0.607750
35	1	3.444991	-1.518667	2.266358
36	1	3.658753	0.872801	2.259158
37	1	2.021526	0.442406	2.752033
38	1	2.233679	2.970456	2.253208
39	1	1.401992	3.300084	0.732812
40	1	-0.131538	3.220710	2.674255
41	1	0.346935	1.561884	3.014520
42	1	-2.098287	1.661724	3.067237
43	1	-2.840816	1.049123	1.559310
44	1	-0.630940	-0.333195	3.160615
45	1	-2.346766	-0.739483	3.178502
46	1	-0.617461	-3.209331	1.107045
47	1	-0.972888	-2.846967	2.794982
48	1	1.040024	-1.406937	2.938024
49	1	1.398419	-3.086756	2.554633
50	8	-0.616137	0.565508	-3.208929
51	1	-1.510296	0.370641	-2.819363
52	1	-0.454625	1.499543	-2.960706
53	15	-3.490882	-0.539877	-0.434668
54	8	-4.334564	-1.467672	-1.275737
55	8	-2.199611	0.046879	-1.200987
56	8	-4.177757	0.569336	0.365869
57	60	0.080987	-0.038462	-0.709728

HF = -1933.7381574 Hartree
Zero-point correction = 0.451043
Sum of electronic and thermal Enthalpies = -1933.255796
Sum of electronic and thermal Free Energies = -1933.345579

$[Nd(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.617804	-1.888372	1.363660
2	6	-1.227812	-1.309844	2.572588
3	6	-2.154781	-0.130725	2.297588
4	7	-1.498847	0.972025	1.559958
5	6	-0.721963	1.810196	2.485621
6	6	0.388876	2.627596	1.824244
7	7	1.432671	1.816701	1.162065
8	6	2.306627	1.154085	2.139953
9	6	3.112411	-0.008635	1.552206
10	7	2.270234	-1.094594	1.028119
11	6	1.779668	-1.957923	2.108410
12	6	0.523113	-2.743606	1.729322
13	6	-1.593714	-2.668284	0.562306
14	6	-0.987964	-3.147298	-0.779221
15	8	-0.085819	-2.362935	-1.286004
16	8	-1.399198	-4.202999	-1.261258
17	6	-2.527226	1.758570	0.810180
18	6	2.209039	2.677873	0.243044
19	6	1.367356	3.186809	-0.960174
20	8	0.415348	2.398754	-1.313342
21	8	1.699857	4.262586	-1.461031
22	6	2.997209	-1.864991	-0.000718
23	6	3.327106	-1.005545	-1.252159
24	8	2.418252	-0.152509	-1.563396
25	8	4.400920	-1.220787	-1.821615
26	8	-0.498134	-0.472739	-3.222986
27	1	-0.414673	-1.001682	3.241469
28	1	-1.801000	-2.082013	3.123544
29	1	-3.018768	-0.445528	1.696568
30	1	-2.544858	0.233298	3.268766
31	1	-0.288324	1.161856	3.256683
32	1	-1.388737	2.514749	3.020097
33	1	-0.050699	3.272113	1.061013
34	1	0.841953	3.292049	2.586625
35	1	1.685801	0.782922	2.961184
36	1	3.014091	1.879207	2.589409
37	1	3.735656	0.356266	0.734056
38	1	3.807448	-0.382038	2.330252
39	1	1.570461	-1.331080	2.981189
40	1	2.562252	-2.675280	2.427055
41	1	0.747460	-3.385300	0.876408
42	1	0.260308	-3.414855	2.570984
43	1	-1.947306	-3.548788	1.125599
44	1	-2.462738	-2.034507	0.333944
45	1	-3.252366	2.195292	1.522032
46	1	-2.020209	2.581842	0.298134
47	1	2.640984	3.540133	0.778926
48	1	3.028396	2.090628	-0.180800
49	1	3.929415	-2.295866	0.403775
50	1	2.351051	-2.681975	-0.336771
51	1	-0.429599	-1.421563	-2.984936
52	1	-1.398025	-0.212553	-2.898056
53	15	-3.426841	0.768154	-0.534064
54	8	-2.121299	0.200378	-1.289074

55	8	-4.206597	1.786351	-1.328546
56	8	-4.160431	-0.383445	0.160995
57	60	0.110833	0.062652	-0.691365

HF = -1933.7372539 Hartree
Zero-point correction = 0.450300
Sum of electronic and thermal Enthalpies = -1933.255511
Sum of electronic and thermal Free Energies = -1933.345614

$[Sm(DO3AP)(H_2O)]^{2-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.716718	-1.690656	1.000834
2	6	2.940261	-0.993979	1.441413
3	6	2.697185	0.447289	1.898181
4	7	2.117077	1.330175	0.874999
5	6	1.550550	2.538384	1.501992
6	6	0.209328	2.285229	2.193667
7	7	-0.849891	1.757228	1.320992
8	6	-1.904343	1.108849	2.137210
9	6	-1.545118	-0.317920	2.541788
10	7	-1.309962	-1.236757	1.409510
11	6	-0.554787	-2.418062	1.880354
12	6	0.931032	-2.153066	2.161024
13	6	2.058369	-2.811709	0.095661
14	6	0.876736	-3.313722	-0.772652
15	8	0.095136	-2.384475	-1.192464
16	8	0.814452	-4.524213	-1.006492
17	6	3.107580	1.690469	-0.163017
18	6	3.399032	0.545810	-1.168697
19	8	4.577455	0.341047	-1.488174
20	8	2.354257	-0.072499	-1.582346
21	6	-1.441124	2.824248	0.475687
22	6	-0.526780	3.298531	-0.675459
23	8	-0.496330	4.502168	-0.949439
24	8	0.126992	2.356926	-1.278814
25	6	-2.591524	-1.681019	0.757745
26	1	2.807636	-2.440754	-0.609849
27	1	2.484840	-3.658961	0.658019
28	1	4.053591	2.030846	0.291223
29	1	2.675277	2.509561	-0.744932
30	1	-1.722117	3.696517	1.088941
31	1	-2.347312	2.401927	0.026615
32	1	-2.325978	-2.528533	0.122491
33	1	-3.289101	-2.040903	1.535739
34	1	3.654004	-0.995093	0.617273
35	1	3.425926	-1.535508	2.277150
36	1	3.661617	0.856955	2.260112
37	1	2.022684	0.440646	2.759949
38	1	2.250665	2.962263	2.249805
39	1	1.423977	3.294372	0.727675
40	1	-0.117073	3.233639	2.663248
41	1	0.351521	1.574205	3.014842
42	1	-2.091190	1.693195	3.059524

43	1	-2.836861	1.080788	1.553279
44	1	-0.643204	-0.313727	3.166918
45	1	-2.361778	-0.708401	3.178742
46	1	-0.646276	-3.198012	1.125397
47	1	-1.001847	-2.823074	2.810135
48	1	1.022803	-1.400945	2.950971
49	1	1.370807	-3.083662	2.569823
50	8	-0.547985	0.497943	-3.176674
51	1	-1.453532	0.328038	-2.802784
52	1	-0.379432	1.436698	-2.952711
53	15	-3.475516	-0.504499	-0.442872
54	8	-4.311933	-1.420123	-1.303800
55	8	-2.165037	0.074119	-1.183210
56	8	-4.167593	0.607868	0.348925
57	62	0.079868	-0.040171	-0.685941

HF = -1934.9599227 Hartree
Zero-point correction = 0.451188
Sum of electronic and thermal Enthalpies = -1934.477486
Sum of electronic and thermal Free Energies = -1934.566974

$[Sm(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.609324	-1.897674	1.354106
2	6	-1.225718	-1.336062	2.567297
3	6	-2.157245	-0.159245	2.300098
4	7	-1.504168	0.950016	1.570110
5	6	-0.733699	1.785997	2.502467
6	6	0.373738	2.610250	1.845296
7	7	1.417622	1.804161	1.177538
8	6	2.298168	1.146233	2.152339
9	6	3.107904	-0.010721	1.559863
10	7	2.267221	-1.094144	1.029353
11	6	1.785345	-1.970682	2.101898
12	6	0.530680	-2.755328	1.716346
13	6	-1.578611	-2.670512	0.538558
14	6	-0.961555	-3.122022	-0.806057
15	8	-0.063508	-2.319818	-1.293346
16	8	-1.355293	-4.175028	-1.307755
17	6	-2.534872	1.735538	0.823780
18	6	2.185246	2.669921	0.255775
19	6	1.330061	3.172872	-0.939342
20	8	0.381423	2.375832	-1.282720
21	8	1.644972	4.253033	-1.441660
22	6	2.987965	-1.848871	-0.014462
23	6	3.303801	-0.967252	-1.252812
24	8	2.385329	-0.116632	-1.542976
25	8	4.375453	-1.162303	-1.833364
26	8	-0.441531	-0.410031	-3.197884
27	1	-0.416194	-1.031067	3.242238
28	1	-1.796426	-2.116962	3.108576
29	1	-3.018156	-0.474426	1.695064
30	1	-2.550461	0.197050	3.272879

31	1	-0.298190	1.135055	3.270397
32	1	-1.404175	2.484555	3.040335
33	1	-0.068913	3.257377	1.086253
34	1	0.826604	3.272258	2.609878
35	1	1.681670	0.770012	2.974685
36	1	3.002265	1.874925	2.601335
37	1	3.731557	0.360059	0.744639
38	1	3.803046	-0.386937	2.336447
39	1	1.576622	-1.354145	2.982293
40	1	2.571606	-2.688828	2.409949
41	1	0.757406	-3.392012	0.860322
42	1	0.266399	-3.432299	2.552902
43	1	-1.927098	-3.563264	1.085681
44	1	-2.451450	-2.039335	0.317343
45	1	-3.268068	2.158733	1.535623
46	1	-2.032412	2.567118	0.321355
47	1	2.614580	3.535033	0.789153
48	1	3.004704	2.087493	-0.173915
49	1	3.924881	-2.282992	0.375528
50	1	2.340474	-2.661327	-0.358025
51	1	-0.370933	-1.362571	-2.975730
52	1	-1.348688	-0.163261	-2.883971
53	15	-3.412152	0.745585	-0.533036
54	8	-2.090321	0.193197	-1.272151
55	8	-4.191424	1.757604	-1.335250
56	8	-4.144164	-0.416106	0.146987
57	62	0.108991	0.067916	-0.676915

HF = -1934.9582817 Hartree
Zero-point correction = 0.450483
Sum of electronic and thermal Enthalpies = -1934.476428
Sum of electronic and thermal Free Energies = -1934.566283

$[Eu(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.705979	-1.692658	1.005132
2	6	2.934566	-1.004068	1.443509
3	6	2.699881	0.438593	1.899773
4	7	2.120820	1.321693	0.876621
5	6	1.561519	2.533545	1.502209
6	6	0.218977	2.286742	2.193274
7	7	-0.840354	1.760972	1.319640
8	6	-1.899945	1.120979	2.135400
9	6	-1.549279	-0.306990	2.542993
10	7	-1.314207	-1.227716	1.412200
11	6	-0.565527	-2.411237	1.887198
12	6	0.920950	-2.151172	2.166929
13	6	2.037133	-2.814748	0.097658
14	6	0.849677	-3.303250	-0.769897
15	8	0.073039	-2.366147	-1.181364
16	8	0.777579	-4.511778	-1.010557
17	6	3.109124	1.673108	-0.166077
18	6	3.385338	0.524195	-1.170610

19	8	4.559666	0.311629	-1.499986
20	8	2.333735	-0.090184	-1.572449
21	6	-1.422889	2.827531	0.468119
22	6	-0.504258	3.286790	-0.685261
23	8	-0.468406	4.487389	-0.971557
24	8	0.147715	2.336781	-1.277340
25	6	-2.595362	-1.668143	0.757548
26	63	0.078361	-0.040230	-0.674889
27	1	2.788685	-2.449354	-0.608209
28	1	2.456372	-3.667091	0.657753
29	1	4.060275	2.006203	0.282832
30	1	2.680714	2.494425	-0.747579
31	1	-1.697652	3.705732	1.075694
32	1	-2.331265	2.409365	0.019892
33	1	-2.330718	-2.515880	0.122359
34	1	-3.296299	-2.025622	1.533631
35	1	3.647008	-1.009532	0.618276
36	1	3.418226	-1.548380	2.278602
37	1	3.667259	0.844373	2.258363
38	1	2.027702	0.436313	2.763425
39	1	2.263646	2.954532	2.249783
40	1	1.438850	3.289586	0.727306
41	1	-0.104896	3.236900	2.661148
42	1	0.357840	1.576205	3.015479
43	1	-2.084691	1.708176	3.056328
44	1	-2.831924	1.097057	1.550636
45	1	-0.649528	-0.306582	3.171286
46	1	-2.370116	-0.693011	3.177220
47	1	-0.660326	-3.193369	1.134945
48	1	-1.014828	-2.811118	2.818098
49	1	1.015703	-1.398032	2.955575
50	1	1.358398	-3.082585	2.576539
51	8	-0.525711	0.470199	-3.163698
52	1	-1.435532	0.313099	-2.795228
53	1	-0.351470	1.410551	-2.951562
54	15	-3.468089	-0.485472	-0.443904
55	8	-4.297359	-1.393802	-1.319413
56	8	-2.149717	0.095781	-1.168430
57	8	-4.165783	0.623548	0.347568

HF = -1935.5581263 Hartree
Zero-point correction = 0.451274
Sum of electronic and thermal Enthalpies = -1935.075639
Sum of electronic and thermal Free Energies = -1935.164981

$[Eu(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.107598	0.068296	-0.668002
2	7	-0.601221	-1.901551	1.350920
3	6	-1.222122	-1.348386	2.565479
4	6	-2.156623	-0.173340	2.301460
5	7	-1.505685	0.939255	1.574972
6	6	-0.739312	1.775324	2.510087

7	6	0.364738	2.604457	1.853965
8	7	1.408515	1.801351	1.182788
9	6	2.294781	1.148901	2.155729
10	6	3.108027	-0.004692	1.562139
11	7	2.269694	-1.088775	1.030132
12	6	1.792386	-1.970403	2.099918
13	6	0.540254	-2.757646	1.711763
14	6	-1.565503	-2.672680	0.528319
15	6	-0.943214	-3.108791	-0.818573
16	8	-0.043600	-2.300514	-1.293197
17	8	-1.333138	-4.156674	-1.333639
18	6	-2.536750	1.723110	0.827934
19	6	2.168312	2.668161	0.255792
20	6	1.302502	3.164563	-0.933984
21	8	0.354426	2.362396	-1.267667
22	8	1.608034	4.244674	-1.441849
23	6	2.988358	-1.835815	-0.020061
24	6	3.292663	-0.945003	-1.254196
25	8	2.368536	-0.096243	-1.532158
26	8	4.361565	-1.130041	-1.842907
27	8	-0.419175	-0.381335	-3.185263
28	1	-0.415042	-1.044262	3.243784
29	1	-1.791550	-2.133825	3.101566
30	1	-3.016435	-0.489275	1.695368
31	1	-2.551379	0.179109	3.275028
32	1	-0.301068	1.123846	3.276033
33	1	-1.412432	2.469902	3.049884
34	1	-0.080840	3.252271	1.097370
35	1	0.817708	3.265484	2.619300
36	1	1.682004	0.770357	2.979833
37	1	2.996470	1.881394	2.602399
38	1	3.730913	0.369024	0.747695
39	1	3.804064	-0.380107	2.338333
40	1	1.581522	-1.357243	2.982225
41	1	2.581322	-2.686791	2.405490
42	1	0.769273	-3.391694	0.854408
43	1	0.276964	-3.437419	2.546341
44	1	-1.910174	-3.571828	1.067362
45	1	-2.440911	-2.044252	0.310253
46	1	-3.272787	2.143675	1.538426
47	1	-2.035308	2.555776	0.326546
48	1	2.597525	3.535902	0.784963
49	1	2.986485	2.087650	-0.178690
50	1	3.929246	-2.267820	0.362744
51	1	2.342340	-2.648558	-0.365339
52	1	-0.345140	-1.336202	-2.975038
53	1	-1.330617	-0.144526	-2.876919
54	15	-3.405484	0.729649	-0.530936
55	8	-2.078093	0.172157	-1.256422
56	8	-4.176496	1.738288	-1.345321
57	8	-4.144393	-0.428519	0.147484

HF = =-1935.5562396 Hartree
Zero-point correction = 0.450602
Sum of electronic and thermal Enthalpies = -1935.074313
Sum of electronic and thermal Free Energies = -1935.164000

$[Gd(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.697606	-1.693624	1.009462
2	6	2.929699	-1.010912	1.446338
3	6	2.700762	0.432794	1.902029
4	7	2.123096	1.315811	0.878442
5	6	1.569001	2.530742	1.502015
6	6	0.225497	2.289112	2.192740
7	7	-0.833713	1.763825	1.318962
8	6	-1.896509	1.130069	2.135139
9	6	-1.550924	-0.298331	2.545084
10	7	-1.317022	-1.220557	1.415365
11	6	-0.573659	-2.406073	1.893114
12	6	0.913433	-2.150304	2.172203
13	6	2.020773	-2.815769	0.099377
14	6	0.828669	-3.293089	-0.767648
15	8	0.056395	-2.349615	-1.172424
16	8	0.748222	-4.499996	-1.013642
17	6	3.110016	1.659848	-0.167531
18	6	3.373374	0.508022	-1.171727
19	8	4.543745	0.291058	-1.511892
20	8	2.316300	-0.104448	-1.561708
21	6	-1.410428	2.829040	0.462072
22	6	-0.489197	3.275581	-0.693880
23	8	-0.450011	4.473318	-0.991476
24	8	0.161768	2.318819	-1.275942
25	6	-2.598629	-1.657254	0.759428
26	1	2.773815	-2.454066	-0.606701
27	1	2.434614	-3.672254	0.657162
28	1	4.065337	1.986376	0.277387
29	1	2.685683	2.483538	-0.748576
30	1	-1.679972	3.712249	1.064709
31	1	-2.320923	2.413694	0.015654
32	1	-2.336183	-2.506782	0.125832
33	1	-3.302618	-2.010227	1.534795
34	1	3.641307	-1.019553	0.620422
35	1	3.411801	-1.557082	2.281125
36	1	3.669976	0.835849	2.258894
37	1	2.029601	0.433490	2.766493
38	1	2.272500	2.950369	2.249084
39	1	1.449027	3.286038	0.725943
40	1	-0.096670	3.241061	2.658235
41	1	0.362031	1.580000	3.016573
42	1	-2.079492	1.719689	3.054849
43	1	-2.828135	1.108689	1.549835
44	1	-0.651881	-0.299848	3.174375
45	1	-2.373684	-0.681323	3.178680
46	1	-0.671058	-3.189475	1.142532
47	1	-1.024801	-2.802294	2.824673
48	1	1.010813	-1.397335	2.960692
49	1	1.348992	-3.082897	2.581259
50	8	-0.503973	0.443979	-3.152725
51	1	-1.417711	0.295357	-2.791438
52	1	-0.328497	1.386341	-2.951203
53	15	-3.460871	-0.471004	-0.445283
54	8	-4.286519	-1.374285	-1.329469

55	8	-2.136016	0.108200	-1.159268
56	8	-4.161039	0.638332	0.343567
57	64	0.077456	-0.039945	-0.664849

HF = -1936.148901 Hartree
Zero-point correction = 0.451337
Sum of electronic and thermal Enthalpies = -1935.666372
Sum of electronic and thermal Free Energies = -1935.755641

$[Gd(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.593513	-1.905470	1.347902
2	6	-1.218521	-1.360244	2.563758
3	6	-2.156159	-0.187060	2.302957
4	7	-1.507728	0.929001	1.579834
5	6	-0.745087	1.765187	2.517404
6	6	0.355725	2.598827	1.862093
7	7	1.399874	1.798670	1.188177
8	6	2.290937	1.151054	2.159661
9	6	3.107862	0.000842	1.565035
10	7	2.272229	-1.084097	1.031418
11	6	1.799030	-1.970575	2.098401
12	6	0.549327	-2.760133	1.707461
13	6	-1.553101	-2.675120	0.518837
14	6	-0.926265	-3.096698	-0.830228
15	8	-0.026373	-2.282345	-1.294013
16	8	-1.312126	-4.140174	-1.357146
17	6	-2.539776	1.711176	0.832733
18	6	2.152968	2.666924	0.257275
19	6	1.278978	3.157082	-0.928727
20	8	0.331430	2.350769	-1.254393
21	8	1.576908	4.236905	-1.441488
22	6	2.989476	-1.823707	-0.024404
23	6	3.282336	-0.925230	-1.255347
24	8	2.354048	-0.077019	-1.521096
25	8	4.347270	-1.103181	-1.853274
26	8	-0.400220	-0.354104	-3.174500
27	1	-0.413652	-1.056753	3.245003
28	1	-1.786475	-2.150013	3.095069
29	1	-3.014917	-0.503805	1.695887
30	1	-2.552240	0.161528	3.277387
31	1	-0.304279	1.113282	3.281525
32	1	-1.420601	2.456118	3.058949
33	1	-0.092677	3.246772	1.107388
34	1	0.808474	3.259446	2.627877
35	1	1.681253	0.770012	2.984937
36	1	2.990090	1.886981	2.604687
37	1	3.729947	0.377585	0.751392
38	1	3.804736	-0.373674	2.340945
39	1	1.586133	-1.360745	2.982586
40	1	2.590370	-2.685428	2.401624
41	1	0.780607	-3.391554	0.848763
42	1	0.286827	-3.442640	2.540027

43	1	-1.893870	-3.580177	1.050452
44	1	-2.431139	-2.049527	0.303878
45	1	-3.278611	2.128148	1.542462
46	1	-2.039931	2.545736	0.333102
47	1	2.581009	3.537170	0.783260
48	1	2.970805	2.088684	-0.180643
49	1	3.934392	-2.252751	0.351835
50	1	2.345715	-2.637641	-0.370850
51	1	-0.323016	-1.311145	-2.976287
52	1	-1.315437	-0.126502	-2.871134
53	15	-3.400056	0.715031	-0.528928
54	8	-2.067599	0.155194	-1.243152
55	8	-4.165047	1.720595	-1.352843
56	8	-4.143739	-0.441349	0.147225
57	64	0.106539	0.069100	-0.659868

HF = -1936.1468235 Hartree
Zero-point correction = 0.450691
Sum of electronic and thermal Enthalpies = -1935.664842
Sum of electronic and thermal Free Energies = -1935.754412

$[Tb(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.685653	-1.695243	1.018029
2	6	2.921520	-1.018903	1.453479
3	6	2.699924	0.426766	1.906271
4	7	2.125300	1.309241	0.880879
5	6	1.577193	2.528157	1.501213
6	6	0.231687	2.293767	2.190242
7	7	-0.827311	1.769593	1.315744
8	6	-1.895247	1.145250	2.132181
9	6	-1.557865	-0.283888	2.546277
10	7	-1.324549	-1.209241	1.418990
11	6	-0.587822	-2.396661	1.901685
12	6	0.899693	-2.145837	2.181705
13	6	2.001155	-2.820477	0.109369
14	6	0.807452	-3.286544	-0.761037
15	8	0.039358	-2.337052	-1.159935
16	8	0.721440	-4.491541	-1.014336
17	6	3.112219	1.644163	-0.167494
18	6	3.363200	0.489599	-1.171215
19	8	4.529544	0.270833	-1.523911
20	8	2.301457	-0.123219	-1.547689
21	6	-1.395104	2.833329	0.451417
22	6	-0.468059	3.264661	-0.705136
23	8	-0.418898	4.459678	-1.012159
24	8	0.178340	2.298604	-1.277102
25	6	-2.606450	-1.641684	0.761427
26	1	2.760278	-2.466721	-0.594099
27	1	2.404502	-3.681285	0.668223
28	1	4.071935	1.962552	0.273953
29	1	2.694031	2.471182	-0.748149
30	1	-1.658426	3.723093	1.047211

31	1	-2.307989	2.421961	0.006340
32	1	-2.347426	-2.494847	0.131500
33	1	-3.314941	-1.987465	1.535950
34	1	3.632872	-1.032959	0.627322
35	1	3.401179	-1.566090	2.289016
36	1	3.671346	0.826128	2.261471
37	1	2.029619	0.432736	2.771507
38	1	2.281656	2.945879	2.248489
39	1	1.462222	3.283006	0.723853
40	1	-0.087958	3.248134	2.652636
41	1	0.364232	1.586484	3.016413
42	1	-2.075954	1.738360	3.050127
43	1	-2.826289	1.128003	1.545790
44	1	-0.660779	-0.288256	3.178469
45	1	-2.384122	-0.661969	3.178282
46	1	-0.687707	-3.182239	1.153615
47	1	-1.041977	-2.788154	2.833783
48	1	0.999161	-1.390815	2.968078
49	1	1.331645	-3.078732	2.594046
50	8	-0.474731	0.410763	-3.134611
51	1	-1.392810	0.276947	-2.778597
52	1	-0.291804	1.354208	-2.945948
53	15	-3.454950	-0.453078	-0.449330
54	8	-4.278020	-1.350987	-1.340882
55	8	-2.120530	0.119232	-1.151673
56	8	-4.155904	0.659992	0.333644
57	65	0.076718	-0.041908	-0.657506

HF = -1936.7379894 Hartree
Zero-point correction = 0.451403
Sum of electronic and thermal Enthalpies = -1936.255432
Sum of electronic and thermal Free Energies = -1936.344556

$[Tb(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.585509	-1.912053	1.344475
2	6	-1.216539	-1.376473	2.561267
3	6	-2.158492	-0.206179	2.303597
4	7	-1.513758	0.914746	1.584996
5	6	-0.756459	1.751223	2.525961
6	6	0.339772	2.592397	1.873060
7	7	1.387116	1.799039	1.196021
8	6	2.283571	1.156512	2.165821
9	6	3.105600	0.011242	1.569195
10	7	2.274749	-1.076157	1.033820
11	6	1.805684	-1.967151	2.098388
12	6	0.560766	-2.762093	1.703592
13	6	-1.537863	-2.683249	0.508960
14	6	-0.903052	-3.091169	-0.840115
15	8	-0.013644	-2.261937	-1.298358
16	8	-1.270877	-4.138783	-1.371540
17	6	-2.547931	1.694229	0.838888
18	6	2.132975	2.673368	0.265319

19	6	1.252698	3.157468	-0.918052
20	8	0.314820	2.340449	-1.245705
21	8	1.535370	4.243495	-1.426215
22	6	2.994465	-1.808988	-0.024400
23	6	3.276531	-0.905606	-1.253794
24	8	2.340119	-0.064648	-1.514450
25	8	4.341646	-1.071836	-1.854784
26	8	-0.377162	-0.322412	-3.158707
27	1	-0.415065	-1.073210	3.246739
28	1	-1.782369	-2.171561	3.087012
29	1	-3.014981	-0.524762	1.694327
30	1	-2.557477	0.137381	3.278703
31	1	-0.312089	1.098885	3.287753
32	1	-1.435435	2.436662	3.070333
33	1	-0.112183	3.241087	1.121089
34	1	0.789975	3.252764	2.640560
35	1	1.677605	0.771919	2.992275
36	1	2.979263	1.896179	2.610070
37	1	3.725679	0.392332	0.755951
38	1	3.804728	-0.361352	2.344063
39	1	1.587978	-1.360121	2.983412
40	1	2.600414	-2.678311	2.401714
41	1	0.796612	-3.390760	0.844016
42	1	0.300462	-3.448245	2.533873
43	1	-1.872069	-3.595010	1.033392
44	1	-2.420580	-2.063539	0.296390
45	1	-3.290993	2.104608	1.548166
46	1	-2.051775	2.533166	0.343228
47	1	2.554247	3.547186	0.790899
48	1	2.955179	2.102011	-0.173255
49	1	3.944203	-2.230868	0.347973
50	1	2.356549	-2.627658	-0.370004
51	1	-0.293868	-1.281206	-2.972273
52	1	-1.296250	-0.106568	-2.858423
53	15	-3.396579	0.697022	-0.528042
54	8	-2.055668	0.144191	-1.232870
55	8	-4.160546	1.698841	-1.356944
56	8	-4.139600	-0.463681	0.141246
57	65	0.105950	0.071108	-0.658339

HF = -1936.735469 Hartree
Zero-point correction = 0.450743
Sum of electronic and thermal Enthalpies = -1936.253462
Sum of electronic and thermal Free Energies = -1936.342958

$[Dy(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.678890	-1.694495	1.023110
2	6	2.917503	-1.022536	1.457011
3	6	2.699955	0.423794	1.909300
4	7	2.126716	1.305827	0.883138
5	6	1.582510	2.527183	1.501285
6	6	0.236132	2.296791	2.189637

7	7	-0.822170	1.772581	1.314593
8	6	-1.893088	1.153680	2.131030
9	6	-1.559803	-0.275487	2.547935
10	7	-1.326553	-1.202590	1.422096
11	6	-0.594067	-2.391063	1.908185
12	6	0.893725	-2.143105	2.187823
13	6	1.987958	-2.820170	0.112972
14	6	0.791575	-3.276368	-0.758501
15	8	0.025355	-2.322131	-1.149740
16	8	0.700499	-4.479544	-1.018610
17	6	3.112431	1.634206	-0.167903
18	6	3.351229	0.478043	-1.172208
19	8	4.513558	0.256944	-1.536593
20	8	2.285001	-0.134155	-1.536634
21	6	-1.384159	2.835109	0.445294
22	6	-0.456805	3.252448	-0.715811
23	8	-0.407932	4.443667	-1.037339
24	8	0.190536	2.280057	-1.275811
25	6	-2.608052	-1.632907	0.762788
26	1	2.749879	-2.470663	-0.589482
27	1	2.384824	-3.684733	0.670621
28	1	4.076186	1.945163	0.270069
29	1	2.698802	2.464278	-0.747343
30	1	-1.639214	3.730653	1.036036
31	1	-2.300926	2.428310	0.004185
32	1	-2.349521	-2.486659	0.133573
33	1	-3.319011	-1.976491	1.536025
34	1	3.627708	-1.038795	0.629901
35	1	3.396629	-1.571093	2.291948
36	1	3.672506	0.821197	2.263857
37	1	2.029918	0.432043	2.774757
38	1	2.287752	2.944061	2.248346
39	1	1.469886	3.281341	0.722809
40	1	-0.082662	3.252684	2.649527
41	1	0.366671	1.591082	3.017506
42	1	-2.073086	1.749011	3.047688
43	1	-2.823573	1.138055	1.543825
44	1	-0.663499	-0.280838	3.181264
45	1	-2.387646	-0.650983	3.179412
46	1	-0.695822	-3.178298	1.162082
47	1	-1.049842	-2.778957	2.840993
48	1	0.995012	-1.387679	2.973588
49	1	1.324390	-3.076524	2.600431
50	8	-0.453434	0.379505	-3.119822
51	1	-1.375577	0.257407	-2.770697
52	1	-0.266617	1.324902	-2.946124
53	15	-3.447732	-0.441464	-0.450368
54	8	-4.265699	-1.335062	-1.350921
55	8	-2.107388	0.130697	-1.141431
56	8	-4.152724	0.670842	0.330141
57	66	0.075458	-0.042274	-0.648618

HF = -1937.3248613 Hartree
Zero-point correction = 0.451462
Sum of electronic and thermal Enthalpies = -1936.842271
Sum of electronic and thermal Free Energies = -1936.931314

$[Dy(DO3AP)(H_2O)]^{2-}$ (Δ(δδδδ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.578308	-1.916978	1.341219
2	6	-1.212245	-1.389069	2.559584
3	6	-2.157550	-0.220727	2.305748
4	7	-1.515810	0.904074	1.590838
5	6	-0.761718	1.740041	2.534339
6	6	0.331712	2.585491	1.882738
7	7	1.379391	1.795400	1.202565
8	6	2.279936	1.156343	2.170637
9	6	3.105600	0.014812	1.572272
10	7	2.277622	-1.073255	1.034723
11	6	1.812252	-1.969405	2.095961
12	6	0.569342	-2.765879	1.698167
13	6	-1.526762	-2.686379	0.500045
14	6	-0.888116	-3.080601	-0.850887
15	8	-0.001617	-2.243477	-1.300640
16	8	-1.248999	-4.125863	-1.391573
17	6	-2.551626	1.682316	0.846253
18	6	2.119364	2.672159	0.269760
19	6	1.232100	3.151611	-0.909866
20	8	0.296728	2.329674	-1.232995
21	8	1.506114	4.239054	-1.419554
22	6	2.996056	-1.798374	-0.029025
23	6	3.267446	-0.886890	-1.254409
24	8	2.324760	-0.050007	-1.505843
25	8	4.331016	-1.042067	-1.861004
26	8	-0.360563	-0.294814	-3.147112
27	1	-0.412370	-1.086217	3.247146
28	1	-1.776024	-2.188231	3.081456
29	1	-3.012888	-0.540073	1.695383
30	1	-2.557808	0.118454	3.281902
31	1	-0.315168	1.087027	3.294299
32	1	-1.442664	2.422060	3.080630
33	1	-0.122643	3.235190	1.133136
34	1	0.781786	3.244757	2.651254
35	1	1.676593	0.768622	2.997583
36	1	2.973042	1.898689	2.614533
37	1	3.724886	0.399276	0.759978
38	1	3.805748	-0.357095	2.346611
39	1	1.592992	-1.366165	2.983244
40	1	2.608969	-2.679627	2.396598
41	1	0.807000	-3.391515	0.836828
42	1	0.310074	-3.455354	2.526032
43	1	-1.856899	-3.603746	1.017308
44	1	-2.412165	-2.069445	0.290950
45	1	-3.297574	2.087373	1.555612
46	1	-2.058050	2.524526	0.353754
47	1	2.538768	3.547993	0.793478
48	1	2.941951	2.103774	-0.171746
49	1	3.949636	-2.217334	0.336894
50	1	2.360474	-2.618161	-0.376026
51	1	-0.274820	-1.255494	-2.972396
52	1	-1.282874	-0.086867	-2.851802
53	15	-3.391581	0.684545	-0.524771
54	8	-2.045238	0.134148	-1.221265

55	8	-4.152397	1.683961	-1.359420
56	8	-4.136275	-0.477735	0.139838
57	66	0.104250	0.072561	-0.654058

HF = -1937.3221025 Hartree
Zero-point correction = 0.450820
Sum of electronic and thermal Enthalpies = -1936.840047
Sum of electronic and thermal Free Energies = -1936.929459

$[Ho(DO3AP)(H_2O)]^{2-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.671012	-1.695376	1.027922
2	6	2.913438	-1.029913	1.459901
3	6	2.703251	0.417973	1.910621
4	7	2.130424	1.299532	0.884330
5	6	1.591613	2.523966	1.500335
6	6	0.244694	2.298750	2.189098
7	7	-0.814571	1.776033	1.314556
8	6	-1.888460	1.164128	2.131955
9	6	-1.561244	-0.265719	2.551068
10	7	-1.329411	-1.194456	1.426379
11	6	-0.602037	-2.384680	1.915217
12	6	0.886468	-2.141040	2.193763
13	6	1.971473	-2.821432	0.115737
14	6	0.770113	-3.267424	-0.753778
15	8	0.009570	-2.306943	-1.140629
16	8	0.669658	-4.469185	-1.016715
17	6	3.113532	1.620077	-0.171065
18	6	3.339902	0.459999	-1.173313
19	8	4.498574	0.231008	-1.544361
20	8	2.268142	-0.147544	-1.529015
21	6	-1.370814	2.837362	0.440523
22	6	-0.440097	3.242828	-0.721593
23	8	-0.383185	4.431733	-1.050286
24	8	0.202344	2.263256	-1.274681
25	6	-2.611762	-1.621119	0.766744
26	1	2.734231	-2.475935	-0.587719
27	1	2.363587	-3.689771	0.670973
28	1	4.081343	1.925934	0.261622
29	1	2.702598	2.451202	-0.750841
30	1	-1.621677	3.737270	1.026437
31	1	-2.289057	2.432973	0.000366
32	1	-2.356557	-2.477671	0.140078
33	1	-3.325641	-1.958801	1.539889
34	1	3.623021	-1.050701	0.632320
35	1	3.390395	-1.579973	2.295122
36	1	3.678557	0.812109	2.261402
37	1	2.035926	0.430473	2.778197
38	1	2.298456	2.940020	2.246380
39	1	1.481198	3.277155	0.720605
40	1	-0.071451	3.256090	2.647949
41	1	0.373327	1.593580	3.017746
42	1	-2.065566	1.761894	3.047593

43	1	-2.818910	1.151818	1.544761
44	1	-0.666074	-0.273668	3.185976
45	1	-2.391548	-0.637667	3.181435
46	1	-0.706762	-3.173491	1.171177
47	1	-1.059206	-2.768668	2.848945
48	1	0.990573	-1.385211	2.978823
49	1	1.314992	-3.075399	2.606672
50	8	-0.437916	0.358145	-3.108984
51	1	-1.362504	0.244530	-2.764001
52	1	-0.247545	1.304280	-2.944047
53	15	-3.441261	-0.427245	-0.450125
54	8	-4.256734	-1.316278	-1.357314
55	8	-2.094511	0.140895	-1.132264
56	8	-4.146961	0.687120	0.326785
57	67	0.073713	-0.042448	-0.643132

HF = -1937.909419 Hartree
Zero-point correction = 0.451544
Sum of electronic and thermal Enthalpies = -1937.426778
Sum of electronic and thermal Free Energies = -1937.515702

$[Ho(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.570335	-1.922491	1.338280
2	6	-1.207181	-1.402124	2.558056
3	6	-2.156571	-0.236410	2.307804
4	7	-1.518384	0.892704	1.596852
5	6	-0.767751	1.728187	2.543007
6	6	0.322605	2.578438	1.892958
7	7	1.371071	1.792273	1.209551
8	6	2.275860	1.156659	2.175730
9	6	3.105471	0.019268	1.575295
10	7	2.280817	-1.069813	1.035622
11	6	1.819839	-1.971406	2.093532
12	6	0.578949	-2.769758	1.693268
13	6	-1.514518	-2.690430	0.491506
14	6	-0.871564	-3.071171	-0.860848
15	8	0.010633	-2.225212	-1.302764
16	8	-1.223880	-4.114971	-1.409874
17	6	-2.556125	1.669400	0.853917
18	6	2.104987	2.672207	0.275273
19	6	1.211089	3.146807	-0.900897
20	8	0.278512	2.319888	-1.219917
21	8	1.476319	4.235799	-1.411768
22	6	2.998123	-1.786852	-0.033688
23	6	3.258381	-0.867578	-1.255240
24	8	2.310019	-0.034095	-1.496660
25	8	4.319661	-1.012660	-1.868277
26	8	-0.344887	-0.268867	-3.135964
27	1	-0.408834	-1.098837	3.247254
28	1	-1.768242	-2.205395	3.076688
29	1	-3.010367	-0.557000	1.696072
30	1	-2.558666	0.098072	3.284875

31	1	-0.318835	1.074511	3.301012
32	1	-1.450865	2.406450	3.091368
33	1	-0.134376	3.229097	1.145830
34	1	0.772146	3.236682	2.662657
35	1	1.675355	0.765550	3.003192
36	1	2.966246	1.901765	2.619309
37	1	3.723663	0.407551	0.763955
38	1	3.806866	-0.351744	2.348994
39	1	1.599424	-1.372294	2.983403
40	1	2.618887	-2.680575	2.390786
41	1	0.818422	-3.393059	0.830660
42	1	0.320932	-3.461992	2.519244
43	1	-1.840481	-3.613327	1.001615
44	1	-2.402679	-2.076605	0.285375
45	1	-3.305119	2.068712	1.563378
46	1	-2.065484	2.515191	0.364769
47	1	2.521591	3.550238	0.797572
48	1	2.928666	2.107586	-0.168815
49	1	3.955762	-2.202434	0.325600
50	1	2.365330	-2.608168	-0.381945
51	1	-0.257251	-1.231140	-2.971822
52	1	-1.270097	-0.067764	-2.845665
53	15	-3.386984	0.671333	-0.521635
54	8	-2.035053	0.124916	-1.210638
55	8	-4.145776	1.668454	-1.360812
56	8	-4.132106	-0.493625	0.137645
57	67	0.102440	0.074504	-0.650728

HF = -1937.9064159 Hartree
Zero-point correction = 0.450897
Sum of electronic and thermal Enthalpies = -1937.424316
Sum of electronic and thermal Free Energies = -1937.513619

$[Er(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.666703	-1.693120	1.033066
2	6	2.911175	-1.030825	1.463596
3	6	2.704195	0.417912	1.912841
4	7	2.131304	1.298057	0.885784
5	6	1.595259	2.524573	1.499256
6	6	0.248259	2.302181	2.188464
7	7	-0.810827	1.778407	1.314525
8	6	-1.886127	1.170887	2.132986
9	6	-1.561086	-0.258686	2.554284
10	7	-1.329839	-1.188641	1.430566
11	6	-0.605355	-2.379488	1.921832
12	6	0.883287	-2.137618	2.199829
13	6	1.961922	-2.819083	0.119346
14	6	0.758272	-3.257264	-0.750294
15	8	-0.000516	-2.292886	-1.131329
16	8	0.652335	-4.457717	-1.017050
17	6	3.112027	1.612610	-0.173016
18	6	3.328051	0.449814	-1.173795

19	8	4.483266	0.216652	-1.553125
20	8	2.252185	-0.155952	-1.520013
21	6	-1.363537	2.837451	0.435981
22	6	-0.432436	3.231810	-0.729143
23	8	-0.374165	4.417638	-1.068611
24	8	0.209490	2.246892	-1.273373
25	6	-2.612462	-1.613790	0.771002
26	1	2.726281	-2.476476	-0.583695
27	1	2.349278	-3.690493	0.673046
28	1	4.083332	1.913664	0.255185
29	1	2.703370	2.444840	-0.752745
30	1	-1.609406	3.741929	1.017007
31	1	-2.284048	2.435065	-0.001213
32	1	-2.359204	-2.472543	0.146678
33	1	-3.328363	-1.947094	1.544192
34	1	3.620170	-1.054093	0.635511
35	1	3.387435	-1.581263	2.298960
36	1	3.680655	0.811035	2.261802
37	1	2.037989	0.432769	2.781287
38	1	2.302839	2.941263	2.244313
39	1	1.485745	3.276399	0.717990
40	1	-0.067310	3.260724	2.645264
41	1	0.376276	1.598570	3.018568
42	1	-2.061978	1.770641	3.047591
43	1	-2.816518	1.159483	1.545787
44	1	-0.666053	-0.266793	3.189413
45	1	-2.391920	-0.629095	3.184898
46	1	-0.711404	-3.169665	1.179379
47	1	-1.063530	-2.760907	2.856155
48	1	0.988857	-1.381494	2.984434
49	1	1.311148	-3.072336	2.612745
50	8	-0.421752	0.333649	-3.097389
51	1	-1.349090	0.227233	-2.758327
52	1	-0.229571	1.280993	-2.942390
53	15	-3.434138	-0.419422	-0.449676
54	8	-4.246145	-1.306035	-1.362378
55	8	-2.082499	0.146482	-1.124000
56	8	-4.142136	0.696398	0.323116
57	68	0.072155	-0.043056	-0.637501

HF = -1938.4930595 Hartree
Zero-point correction = 0.451616
Sum of electronic and thermal Enthalpies = -1938.010378
Sum of electronic and thermal Free Energies = -1938.099191

$[Er(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.563539	-1.927238	1.336576
2	6	-1.203772	-1.414260	2.557339
3	6	-2.156075	-0.250173	2.310516
4	7	-1.520796	0.882379	1.602874
5	6	-0.773036	1.717314	2.551219
6	6	0.314106	2.572172	1.902245

7	7	1.363711	1.789881	1.216373
8	6	2.272136	1.157537	2.180978
9	6	3.105400	0.023783	1.578995
10	7	2.284003	-1.066462	1.037746
11	6	1.825951	-1.972087	2.092866
12	6	0.587466	-2.772658	1.689668
13	6	-1.503509	-2.693481	0.484147
14	6	-0.856665	-3.061301	-0.869501
15	8	0.022219	-2.207666	-1.303492
16	8	-1.201720	-4.103002	-1.427017
17	6	-2.559976	1.657642	0.861160
18	6	2.092109	2.672698	0.280907
19	6	1.192955	3.141668	-0.893151
20	8	0.263476	2.309564	-1.208490
21	8	1.449995	4.231703	-1.405693
22	6	3.000581	-1.776577	-0.035921
23	6	3.249198	-0.851957	-1.255514
24	8	2.295720	-0.021506	-1.487965
25	8	4.307084	-0.989499	-1.875957
26	8	-0.331900	-0.245438	-3.125433
27	1	-0.407442	-1.111753	3.249254
28	1	-1.763503	-2.221338	3.071619
29	1	-3.009005	-0.571433	1.698063
30	1	-2.558925	0.080354	3.288681
31	1	-0.321439	1.062856	3.306982
32	1	-1.457844	2.391922	3.102105
33	1	-0.145570	3.222972	1.156935
34	1	0.762672	3.230254	2.672676
35	1	1.674121	0.763417	3.008836
36	1	2.960053	1.905080	2.624394
37	1	3.722429	0.415318	0.768287
38	1	3.808098	-0.346027	2.352176
39	1	1.603058	-1.375775	2.984048
40	1	2.626814	-2.679791	2.389118
41	1	0.829081	-3.392923	0.825416
42	1	0.330964	-3.468247	2.513338
43	1	-1.825928	-3.621491	0.987280
44	1	-2.394046	-2.082301	0.280797
45	1	-3.312082	2.051598	1.570393
46	1	-2.071979	2.506785	0.375350
47	1	2.505291	3.553194	0.801835
48	1	2.917505	2.111902	-0.164656
49	1	3.962600	-2.187257	0.317397
50	1	2.371423	-2.600667	-0.383959
51	1	-0.238154	-1.208774	-2.971701
52	1	-1.260164	-0.054466	-2.838624
53	15	-3.382238	0.659281	-0.518545
54	8	-2.025124	0.115125	-1.199477
55	8	-4.137614	1.654267	-1.363272
56	8	-4.129060	-0.507220	0.135946
57	68	0.100825	0.076396	-0.648408

HF = -1938.4898459 Hartree
Zero-point correction = 0.450962
Sum of electronic and thermal Enthalpies = -1938.007708
Sum of electronic and thermal Free Energies = -1938.096936

$[Tm(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.658164	-1.695494	1.038883
2	6	2.906265	-1.039374	1.467366
3	6	2.706642	0.410724	1.915611
4	7	2.135510	1.291393	0.888512
5	6	1.605009	2.520780	1.500319
6	6	0.256683	2.304204	2.188654
7	7	-0.802816	1.782370	1.314367
8	6	-1.881871	1.182023	2.132854
9	6	-1.563732	-0.248274	2.556852
10	7	-1.333865	-1.180359	1.434730
11	6	-0.614879	-2.372983	1.929056
12	6	0.874504	-2.135949	2.206595
13	6	1.945143	-2.822544	0.124260
14	6	0.738337	-3.250105	-0.746102
15	8	-0.016478	-2.280290	-1.120851
16	8	0.626538	-4.448412	-1.019848
17	6	3.114524	1.598523	-0.173525
18	6	3.318119	0.434196	-1.174825
19	8	4.468989	0.198610	-1.565581
20	8	2.238055	-0.170279	-1.509778
21	6	-1.348752	2.840717	0.431069
22	6	-0.414921	3.222225	-0.735790
23	8	-0.349512	4.405346	-1.083424
24	8	0.222673	2.230308	-1.272215
25	6	-2.616885	-1.601536	0.773716
26	1	2.712264	-2.485474	-0.578385
27	1	2.325665	-3.697812	0.676718
28	1	4.089917	1.892443	0.250448
29	1	2.710412	2.433592	-0.752309
30	1	-1.588412	3.749975	1.007231
31	1	-2.271753	2.442341	-0.004430
32	1	-2.366023	-2.462160	0.151061
33	1	-3.335858	-1.930454	1.545925
34	1	3.614095	-1.066607	0.638390
35	1	3.381055	-1.591486	2.302514
36	1	3.685610	0.799873	2.262218
37	1	2.042238	0.429495	2.785433
38	1	2.313810	2.935433	2.245395
39	1	1.498952	3.272457	0.718385
40	1	-0.056237	3.264469	2.643804
41	1	0.381734	1.601374	3.019892
42	1	-2.055743	1.784208	3.046250
43	1	-2.811700	1.173951	1.544835
44	1	-0.669979	-0.259232	3.193760
45	1	-2.397329	-0.614436	3.186318
46	1	-0.723830	-3.164512	1.188447
47	1	-1.074782	-2.750447	2.864105
48	1	0.982736	-1.379048	2.990137
49	1	1.299464	-3.071552	2.620707
50	8	-0.407953	0.312618	-3.086252
51	1	-1.337549	0.217874	-2.750241
52	1	-0.209097	1.260055	-2.941581
53	15	-3.428853	-0.404271	-0.449932
54	8	-4.238706	-1.286353	-1.368794

55	8	-2.071389	0.158219	-1.115540
56	8	-4.137468	0.713074	0.320092
57	69	0.070595	-0.043828	-0.632473

HF = -1939.0728823 Hartree
Zero-point correction = 0.451682
Sum of electronic and thermal Enthalpies = -1938.590162
Sum of electronic and thermal Free Energies = -1938.678882

$[Tm(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.555686	-1.932588	1.334959
2	6	-1.198957	-1.426317	2.556639
3	6	-2.155587	-0.265255	2.312515
4	7	-1.523859	0.871351	1.608475
5	6	-0.779598	1.706159	2.559160
6	6	0.304247	2.566051	1.911709
7	7	1.355416	1.788385	1.223118
8	6	2.267725	1.159379	2.185976
9	6	3.104883	0.029689	1.581979
10	7	2.287133	-1.062173	1.039223
11	6	1.833567	-1.972556	2.091639
12	6	0.597307	-2.775671	1.686647
13	6	-1.491111	-2.698188	0.477442
14	6	-0.839890	-3.053978	-0.876910
15	8	0.034002	-2.191887	-1.304263
16	8	-1.175408	-4.095421	-1.440737
17	6	-2.564679	1.644689	0.867683
18	6	2.077659	2.675135	0.286944
19	6	1.172700	3.138655	-0.884460
20	8	0.247029	2.300842	-1.196382
21	8	1.420353	4.230480	-1.397695
22	6	3.003374	-1.764775	-0.038980
23	6	3.240716	-0.834571	-1.256232
24	8	2.283256	-0.005770	-1.478581
25	8	4.294941	-0.965346	-1.884271
26	8	-0.318953	-0.224707	-3.115649
27	1	-0.404185	-1.122532	3.249828
28	1	-1.755668	-2.237124	3.068477
29	1	-3.006836	-0.588020	1.698613
30	1	-2.560565	0.060914	3.291310
31	1	-0.325434	1.051360	3.313110
32	1	-1.466640	2.376993	3.111983
33	1	-0.158175	3.217385	1.168556
34	1	0.751574	3.223589	2.683331
35	1	1.672267	0.761888	3.014115
36	1	2.952963	1.909400	2.629443
37	1	3.720073	0.424931	0.771632
38	1	3.809388	-0.338682	2.354269
39	1	1.609271	-1.379753	2.984858
40	1	2.636916	-2.678693	2.385220
41	1	0.840745	-3.394047	0.821452
42	1	0.342530	-3.473544	2.508950

43	1	-1.809169	-3.631187	0.974167
44	1	-2.384410	-2.090511	0.276187
45	1	-3.320039	2.033307	1.576456
46	1	-2.079411	2.497167	0.385078
47	1	2.486378	3.558281	0.806916
48	1	2.905446	2.119268	-0.160185
49	1	3.969749	-2.170396	0.308363
50	1	2.378286	-2.591815	-0.387200
51	1	-0.220435	-1.188827	-2.970580
52	1	-1.249761	-0.042454	-2.832004
53	15	-3.378291	0.646027	-0.516269
54	8	-2.016263	0.105432	-1.190451
55	8	-4.132162	1.639009	-1.364663
56	8	-4.125260	-0.522974	0.133504
57	69	0.099595	0.078550	-0.646170

HF = -1939.0694212 Hartree
Zero-point correction = 0.451013
Sum of electronic and thermal Enthalpies = -1938.587255
Sum of electronic and thermal Free Energies = -1938.676410

$[Yb(DO3AP)(H_2O)]^{2-}$ ($\Delta(\lambda\lambda\lambda\lambda)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.652549	-1.695549	1.043931
2	6	2.903475	-1.043936	1.470228
3	6	2.709179	0.407158	1.917550
4	7	2.138871	1.287594	0.890330
5	6	1.612389	2.519217	1.500148
6	6	0.263622	2.306705	2.188722
7	7	-0.796397	1.785687	1.314868
8	6	-1.877690	1.190780	2.133962
9	6	-1.563698	-0.239628	2.560292
10	7	-1.335514	-1.173443	1.439398
11	6	-0.620250	-2.367152	1.935991
12	6	0.869545	-2.133067	2.212776
13	6	1.932713	-2.823113	0.128251
14	6	0.722907	-3.241692	-0.741876
15	8	-0.028340	-2.267206	-1.111743
16	8	0.604846	-4.438337	-1.020111
17	6	3.115357	1.588146	-0.175253
18	6	3.307290	0.421679	-1.175945
19	8	4.454303	0.180814	-1.574761
20	8	2.222863	-0.180097	-1.501374
21	6	-1.337420	2.842713	0.427461
22	6	-0.402503	3.212132	-0.742033
23	8	-0.332863	4.392192	-1.099157
24	8	0.232061	2.214064	-1.270555
25	6	-2.619263	-1.592017	0.778591
26	1	2.701500	-2.490193	-0.574480
27	1	2.307863	-3.701560	0.679371
28	1	4.094514	1.876336	0.244054
29	1	2.714259	2.424890	-0.753651
30	1	-1.571088	3.756500	0.998927

31	1	-2.262982	2.447631	-0.005493
32	1	-2.371033	-2.454969	0.158170
33	1	-3.340390	-1.916114	1.550823
34	1	3.610133	-1.074112	0.640335
35	1	3.377556	-1.597167	2.305071
36	1	3.690052	0.793641	2.262038
37	1	2.046373	0.428944	2.788572
38	1	2.322266	2.933382	2.244548
39	1	1.508067	3.270117	0.717171
40	1	-0.047476	3.268299	2.642434
41	1	0.387212	1.604833	3.021000
42	1	-2.049928	1.795056	3.046303
43	1	-2.807333	1.184650	1.545780
44	1	-0.670280	-0.251905	3.197624
45	1	-2.398513	-0.602873	3.189860
46	1	-0.731253	-3.159867	1.196944
47	1	-1.081237	-2.741682	2.871689
48	1	0.979829	-1.375305	2.995203
49	1	1.292958	-3.069043	2.627816
50	8	-0.396662	0.291781	-3.075858
51	1	-1.328598	0.204999	-2.744656
52	1	-0.194698	1.239989	-2.941765
53	15	-3.423030	-0.393368	-0.448418
54	8	-4.230380	-1.272093	-1.372710
55	8	-2.060717	0.165952	-1.106772
56	8	-4.132572	0.725705	0.318215
57	70	0.068527	-0.044482	-0.628453

HF = -1939.6572617 Hartree
Zero-point correction = 0.451746
Sum of electronic and thermal Enthalpies = -1939.174500
Sum of electronic and thermal Free Energies = -1939.263156

$[Yb(DO3AP)(H_2O)]^{2-}$ ($\Delta(\delta\delta\delta\delta)$) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.547595	-1.938325	1.333449
2	6	-1.192800	-1.438683	2.556446
3	6	-2.153425	-0.280150	2.315905
4	7	-1.525532	0.860597	1.615552
5	6	-0.783969	1.694601	2.568540
6	6	0.297140	2.558819	1.922621
7	7	1.348879	1.785003	1.230758
8	6	2.264887	1.158244	2.191363
9	6	3.105789	0.032749	1.584851
10	7	2.291415	-1.060188	1.040299
11	6	1.841816	-1.975663	2.089335
12	6	0.606964	-2.780079	1.682379
13	6	-1.479720	-2.701490	0.470814
14	6	-0.825459	-3.045000	-0.884831
15	8	0.043846	-2.174946	-1.305665
16	8	-1.153816	-4.084506	-1.456377
17	6	-2.568305	1.632685	0.876826
18	6	2.065638	2.674898	0.293806

19	6	1.155349	3.134198	-0.874721
20	8	0.232275	2.292198	-1.183790
21	8	1.395779	4.227015	-1.389107
22	6	3.005569	-1.754652	-0.043769
23	6	3.231565	-0.817446	-1.257424
24	8	2.268959	0.008110	-1.470187
25	8	4.282840	-0.938963	-1.892147
26	8	-0.309850	-0.202905	-3.107087
27	1	-0.399090	-1.134338	3.250637
28	1	-1.746803	-2.253009	3.065815
29	1	-3.003352	-0.604068	1.700974
30	1	-2.559762	0.041410	3.295728
31	1	-0.327604	1.038993	3.320437
32	1	-1.472671	2.361969	3.123607
33	1	-0.167667	3.211229	1.181934
34	1	0.744057	3.215197	2.695490
35	1	1.671989	0.756977	3.019533
36	1	2.947602	1.910351	2.635311
37	1	3.719445	0.431875	0.775213
38	1	3.811970	-0.334507	2.356235
39	1	1.616841	-1.386831	2.985066
40	1	2.647064	-2.681176	2.379636
41	1	0.851446	-3.395909	0.815582
42	1	0.353856	-3.480899	2.502747
43	1	-1.794787	-3.639204	0.960607
44	1	-2.374918	-2.095769	0.272388
45	1	-3.326181	2.015951	1.585874
46	1	-2.085780	2.488494	0.397459
47	1	2.471574	3.559881	0.812877
48	1	2.894565	2.122751	-0.155632
49	1	3.975913	-2.157100	0.296297
50	1	2.382841	-2.582933	-0.393097
51	1	-0.209861	-1.168217	-2.971830
52	1	-1.242825	-0.026070	-2.827578
53	15	-3.374304	0.634868	-0.511476
54	8	-2.007777	0.099431	-1.180946
55	8	-4.127501	1.626375	-1.362224
56	8	-4.120294	-0.537748	0.132713
57	70	0.097209	0.080880	-0.645484

HF = -1939.6536578 Hartree
Zero-point correction = 0.451060
Sum of electronic and thermal Enthalpies = -1939.171461
Sum of electronic and thermal Free Energies = -1939.260584

$[Lu(DO3AP)(H_2O)]^{2-}$ (Δ(λλλλ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.651643	-1.692274	1.046832
2	6	2.904281	-1.043047	1.471026
3	6	2.712456	0.408434	1.918130
4	7	2.140540	1.287714	0.891393
5	6	1.615633	2.520349	1.499458
6	6	0.267578	2.308619	2.189438

7	7	-0.792635	1.786938	1.316604
8	6	-1.874228	1.194576	2.136655
9	6	-1.560977	-0.235503	2.564167
10	7	-1.332841	-1.169810	1.443792
11	6	-0.618924	-2.363509	1.941935
12	6	0.871097	-2.129914	2.216874
13	6	1.926845	-2.818742	0.128723
14	6	0.713228	-3.231456	-0.738603
15	8	-0.036230	-2.253661	-1.103682
16	8	0.589795	-4.426888	-1.019209
17	6	3.113152	1.583753	-0.178330
18	6	3.295242	0.414577	-1.177366
19	8	4.438996	0.167258	-1.581480
20	8	2.206607	-0.183479	-1.495329
21	6	-1.331357	2.842357	0.426476
22	6	-0.398512	3.201018	-0.747759
23	8	-0.329872	4.377588	-1.116177
24	8	0.235801	2.198459	-1.268025
25	6	-2.616557	-1.588144	0.783253
26	1	2.694706	-2.486870	-0.575426
27	1	2.300512	-3.699454	0.677300
28	1	4.095481	1.868657	0.235904
29	1	2.712562	2.420828	-0.756472
30	1	-1.558515	3.760139	0.994219
31	1	-2.260162	2.450403	-0.002190
32	1	-2.368794	-2.451544	0.163378
33	1	-3.338450	-1.910790	1.555396
34	1	3.609796	-1.074437	0.640202
35	1	3.378722	-1.596858	2.305303
36	1	3.694564	0.794220	2.260193
37	1	2.051640	0.431403	2.790660
38	1	2.326166	2.935981	2.242505
39	1	1.510476	3.269918	0.715264
40	1	-0.043230	3.270578	2.642725
41	1	0.391934	1.607340	3.022096
42	1	-2.045510	1.799946	3.048483
43	1	-2.804107	1.188792	1.549063
44	1	-0.667612	-0.247544	3.201545
45	1	-2.395940	-0.598125	3.193928
46	1	-0.731312	-3.157653	1.204638
47	1	-1.079652	-2.735853	2.878657
48	1	0.982676	-1.372176	2.999144
49	1	1.295059	-3.066037	2.631200
50	8	-0.388723	0.272924	-3.067370
51	1	-1.322387	0.190237	-2.741497
52	1	-0.186059	1.221807	-2.939616
53	15	-3.415869	-0.388354	-0.444900
54	8	-4.218078	-1.264910	-1.375807
55	8	-2.050553	0.172181	-1.096004
56	8	-4.129266	0.729580	0.319715
57	71	0.065732	-0.044622	-0.624380

HF = -1940.2130118 Hartree
Zero-point correction = 0.451825
Sum of electronic and thermal Enthalpies = -1939.730193
Sum of electronic and thermal Free Energies = -1939.818788

$[Lu(DO3AP)(H_2O)]^{2-}$ (Δ(δδδδ)) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.543231	1.942451	1.331864
2	6	1.188644	1.448262	2.556486
3	6	2.150653	0.289934	2.320225
4	7	1.524596	-0.853390	1.623000
5	6	0.783482	-1.685361	2.577559
6	6	-0.296687	-2.550890	1.932172
7	7	-1.346944	-1.777824	1.237489
8	6	-2.264824	-1.151593	2.196428
9	6	-3.107498	-0.028398	1.588262
10	7	-2.294609	1.063849	1.041549
11	6	-1.846494	1.983794	2.086519
12	6	-0.610951	2.785903	1.676837
13	6	1.474350	2.700484	0.464403
14	6	0.821008	3.029466	-0.895007
15	8	-0.051262	2.157000	-1.305182
16	8	1.151903	4.060771	-1.479569
17	6	2.568020	-1.625983	0.886411
18	6	-2.060770	-2.668520	0.299485
19	6	-1.146895	-3.125319	-0.866981
20	8	-0.221406	-2.283396	-1.169946
21	8	-1.385905	-4.216245	-1.385571
22	6	-3.005054	1.750913	-0.048750
23	6	-3.220035	0.806978	-1.258963
24	8	-2.254166	-0.017835	-1.460247
25	8	-4.266641	0.922368	-1.902261
26	8	0.302800	0.181828	-3.099622
27	1	0.395187	1.145501	3.251701
28	1	1.741852	2.264896	3.063202
29	1	3.000739	0.613159	1.705348
30	1	2.556536	-0.027991	3.301482
31	1	0.326169	-1.028282	3.327590
32	1	1.472006	-2.351225	3.134772
33	1	0.169167	-3.204708	1.193484
34	1	-0.744943	-3.205750	2.705602
35	1	-1.673177	-0.747950	3.024350
36	1	-2.946317	-1.904443	2.641142
37	1	-3.721043	-0.429948	0.779712
38	1	-3.814088	0.338999	2.359333
39	1	-1.622361	1.398924	2.985116
40	1	-2.651585	2.691128	2.373292
41	1	-0.854917	3.398254	0.807399
42	1	-0.358038	3.490241	2.494329
43	1	1.786582	3.643340	0.946215
44	1	2.371267	2.095667	0.271686
45	1	3.327712	-2.005036	1.595840
46	1	2.087043	-2.484374	0.410243
47	1	-2.466301	-3.554369	0.817487
48	1	-2.889319	-2.117630	-0.151941
49	1	-3.979000	2.151391	0.283495
50	1	-2.383496	2.579622	-0.398890
51	1	0.200830	1.147816	-2.971192
52	1	1.237427	0.009534	-2.824160
53	15	3.368516	-0.629335	-0.505308
54	8	1.999039	-0.093344	-1.168473

55	8	4.116488	-1.620445	-1.361167
56	8	4.117854	0.543256	0.134765
57	71	-0.094520	-0.083409	-0.643615

HF = -1940.2092927 Hartree
Zero-point correction = 0.451109
Sum of electronic and thermal Enthalpies = -1939.727058
Sum of electronic and thermal Free Energies = -1939.816169

[Lu(DO2A2P)]$^{3-}$ TSAP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.917814	-1.861989	-1.301579
2	6	1.699534	-1.316877	-2.417872
3	6	2.654814	-0.198370	-2.004894
4	7	1.966394	0.924550	-1.347056
5	6	1.375806	1.824087	-2.337423
6	6	0.215558	2.660431	-1.796721
7	7	-0.917651	1.861714	-1.301276
8	6	-1.699598	1.316769	-2.417614
9	6	-2.654895	0.198282	-2.004724
10	7	-1.966495	-0.924703	-1.346994
11	6	-1.375879	-1.824167	-2.337361
12	6	-0.215588	-2.660502	-1.796740
13	6	1.750289	-2.686450	-0.392402
14	6	0.952247	-3.096374	0.868278
15	8	0.068568	-2.240447	1.240396
16	8	1.214213	-4.189726	1.387968
17	6	2.879468	1.624274	-0.401585
18	6	-1.750222	2.686193	-0.392038
19	6	-0.951720	3.096868	0.868098
20	8	-0.068769	2.240681	1.241164
21	8	-1.212736	4.191100	1.386569
22	6	-2.879543	-1.624460	-0.401532
23	1	0.996703	-0.951070	-3.177701
24	1	2.289778	-2.119978	-2.909677
25	1	3.404620	-0.570749	-1.293659
26	1	3.196889	0.145089	-2.912864
27	1	1.028280	1.222627	-3.187256
28	1	2.141369	2.517288	-2.748701
29	1	0.579483	3.266905	-0.966515
30	1	-0.117921	3.364376	-2.589044
31	1	-0.996895	0.950963	-3.177574
32	1	-2.289733	2.120063	-2.909184
33	1	-3.404701	0.570635	-1.293484
34	1	-3.196824	-0.144987	-2.912877
35	1	-1.028449	-1.222641	-3.187187
36	1	-2.141363	-2.517482	-2.748591
37	1	-0.579488	-3.266784	-0.966384
38	1	0.117622	-3.364689	-2.589023
39	1	2.103880	-3.597424	-0.910675
40	1	2.623545	-2.104246	-0.064914

41	1	3.757492	2.022289	-0.950121
42	1	2.334545	2.466654	0.031014
43	1	-2.104261	3.596851	-0.910586
44	1	-2.623190	2.103732	-0.064289
45	1	-3.757322	-2.022883	-0.950242
46	1	-2.334555	-2.466721	0.031268
47	15	3.410155	0.541804	1.058572
48	8	1.963219	0.042997	1.509417
49	8	4.106305	1.478940	2.023939
50	8	4.227543	-0.622492	0.467928
51	15	-3.410431	-0.541916	1.058631
52	8	-1.963428	-0.043224	1.509415
53	8	-4.227807	0.622285	0.467940
54	8	-4.106542	-1.479024	2.024003
55	71	-0.000027	-0.000001	0.625293

HF = -2242.1652599 Hartree
Zero-point correction = 0.423251
Sum of electronic and thermal Enthalpies = -2241.711976
Sum of electronic and thermal Free Energies = -2241.798347

$[Lu(DO2A2P)]^{3-}$ TS_1 (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.627172	2.292097	0.897745
2	6	-0.631036	3.008979	1.149553
3	6	-1.630929	2.198656	1.977240
4	7	-2.080114	0.984261	1.294522
5	6	-2.327304	-0.120955	2.231406
6	6	-1.036497	-0.839246	2.635998
7	7	-0.308888	-1.468322	1.514691
8	6	1.045417	-1.934713	1.930787
9	6	2.008504	-0.889411	2.527803
10	7	2.557495	0.056508	1.580317
11	6	2.713080	1.413203	2.049537
12	6	1.414671	2.222888	2.130446
13	6	1.382767	2.915220	-0.206345
14	6	0.575569	2.975130	-1.529245
15	8	-0.170520	1.953825	-1.748361
16	8	0.722859	3.974542	-2.244331
17	6	-3.257016	1.249860	0.427424
18	6	-1.079474	-2.656924	1.033073
19	6	-0.557765	-3.240200	-0.301035
20	8	-0.683551	-4.457599	-0.479652
21	8	-0.097973	-2.358283	-1.109021
22	6	3.705502	-0.445868	0.791812
23	1	1.715555	3.936420	0.058470
24	1	2.253774	2.288333	-0.418952
25	1	-3.022424	2.125171	-0.186563
26	1	-4.136420	1.505542	1.054126
27	1	-2.115777	-2.352233	0.830575
28	1	-1.076866	-3.438735	1.812162
29	1	4.513694	0.296740	0.840624
30	1	4.091912	-1.362870	1.263300

31	1	-1.087237	3.230688	0.183356
32	1	-0.440048	3.980674	1.656467
33	1	-2.493237	2.851743	2.221448
34	1	-1.184828	1.926448	2.941737
35	1	-2.812509	0.243027	3.163611
36	1	-3.032995	-0.800456	1.735596
37	1	-1.279889	-1.602960	3.402987
38	1	-0.368505	-0.120046	3.117910
39	1	0.921824	-2.736825	2.686675
40	1	1.525023	-2.377596	1.049681
41	1	1.521297	-0.339828	3.343310
42	1	2.819610	-1.477209	3.013096
43	1	3.393975	1.920220	1.362645
44	1	3.192377	1.483294	3.058838
45	1	0.784074	1.795670	2.916539
46	1	1.685059	3.247086	2.478061
47	15	3.386410	-0.846546	-1.048494
48	8	4.464103	-0.082923	-1.805481
49	8	1.935403	-0.180359	-1.237387
50	8	3.362027	-2.366545	-1.091515
51	15	-3.647198	-0.158227	-0.766397
52	8	-4.015786	-1.365644	0.114386
53	8	-4.703603	0.392874	-1.704691
54	8	-2.196295	-0.317502	-1.401696
55	71	-0.139599	-0.125089	-0.743690

HF = -2242.1318645 Hartree
Zero-point correction = 0.421595
Sum of electronic and thermal Enthalpies = -2241.680209
Sum of electronic and thermal Free Energies = -2241.767534

$[Lu(DO2A2P)]^{3-}$ I_1 (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.480227	2.563718	0.748562
2	6	-0.838912	3.169616	0.928328
3	6	-1.765545	2.345902	1.825884
4	7	-2.113839	1.047208	1.251382
5	6	-2.223697	-0.001566	2.272554
6	6	-0.856809	-0.574412	2.665309
7	7	-0.150173	-1.290313	1.581256
8	6	1.257109	-1.619238	1.961962
9	6	2.191763	-0.467159	2.379762
10	7	2.529610	0.544278	1.378097
11	6	2.609789	1.890210	1.920546
12	6	1.263088	2.626495	1.978412
13	6	1.178559	3.140591	-0.404307
14	6	0.452472	2.906429	-1.759197
15	8	-0.145324	1.779349	-1.869814
16	8	0.538084	3.809051	-2.602755
17	6	-3.324142	1.143157	0.398297
18	6	-0.864362	-2.578425	1.307877
19	6	-0.429354	-3.297431	0.009429
20	8	-0.503707	-4.531487	-0.010735

21	8	-0.113062	-2.503311	-0.946176
22	6	3.676180	0.202689	0.507297
23	1	1.350129	4.227915	-0.281141
24	1	2.150909	2.648614	-0.500148
25	1	-3.177732	1.987344	-0.283686
26	1	-4.211859	1.372358	1.024400
27	1	-1.930596	-2.364362	1.158424
28	1	-0.743692	-3.254399	2.171016
29	1	3.981095	1.124618	0.001500
30	1	4.539373	-0.139448	1.116403
31	1	-1.302471	3.254092	-0.057221
32	1	-0.755763	4.201458	1.341306
33	1	-2.678983	2.942754	2.024508
34	1	-1.295179	2.193386	2.804817
35	1	-2.702464	0.385559	3.199299
36	1	-2.884772	-0.773029	1.858523
37	1	-0.991921	-1.254575	3.531055
38	1	-0.213667	0.240049	3.010400
39	1	1.225493	-2.313952	2.826570
40	1	1.740028	-2.144382	1.123974
41	1	1.782982	0.050345	3.259021
42	1	3.115826	-0.971676	2.729014
43	1	3.295222	2.465752	1.293283
44	1	3.046334	1.926553	2.945763
45	1	0.664255	2.195856	2.786552
46	1	1.467329	3.682615	2.278458
47	15	3.347628	-1.027870	-0.882877
48	8	4.471110	-0.774545	-1.874161
49	8	1.929505	-0.451468	-1.364113
50	8	3.247741	-2.395464	-0.210412
51	15	-3.632413	-0.370101	-0.681958
52	8	-3.870124	-1.536865	0.290746
53	8	-4.757922	0.030324	-1.616979
54	8	-2.195875	-0.453579	-1.369053
55	71	-0.129283	-0.251624	-0.788309

HF = -2242.1362418 Hartree
Zero-point correction = 0.421564
Sum of electronic and thermal Enthalpies = -2241.683827
Sum of electronic and thermal Free Energies = -2241.773207

$[Lu(DO2A2P)]^{3-}$ TS_2 (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.696921	2.889096	0.748788
2	6	-2.106823	3.029291	1.070884
3	6	-2.708019	1.852093	1.847490
4	7	-2.588111	0.581889	1.162599
5	6	-2.515507	-0.550404	2.080206
6	6	-1.092508	-0.769194	2.610711
7	7	-0.129203	-1.314996	1.627816
8	6	1.263996	-1.237286	2.143319
9	6	1.822788	0.174719	2.378211
10	7	1.861487	1.076711	1.198705

11	6	1.620379	2.473413	1.610696
12	6	0.180176	2.909008	1.901290
13	6	-0.285623	3.738791	-0.368517
14	6	0.077483	3.025084	-1.711911
15	8	0.209789	1.759784	-1.678203
16	8	0.221982	3.794478	-2.674116
17	6	-3.566308	0.417578	0.072098
18	6	-0.478095	-2.746799	1.383525
19	6	0.221910	-3.400303	0.174431
20	8	0.384516	-4.626602	0.208239
21	8	0.484208	-2.588608	-0.779874
22	6	3.205388	1.057613	0.524608
23	1	-1.075126	4.465385	-0.606723
24	1	0.586074	4.349797	-0.091919
25	1	-3.541711	1.323074	-0.542608
26	1	-4.596408	0.330475	0.481396
27	1	-1.542095	-2.799906	1.127523
28	1	-0.284094	-3.335492	2.296429
29	1	3.195886	1.872808	-0.204197
30	1	3.986785	1.285722	1.277108
31	1	-2.646021	3.120582	0.123982
32	1	-2.316728	3.964994	1.646577
33	1	-3.772020	2.107590	2.066686
34	1	-2.220420	1.776502	2.828192
35	1	-3.182410	-0.409002	2.961804
36	1	-2.877302	-1.426610	1.529311
37	1	-1.133806	-1.450588	3.485415
38	1	-0.702613	0.183210	2.982006
39	1	1.327396	-1.776279	3.111223
40	1	1.946600	-1.737687	1.441624
41	1	1.255984	0.678121	3.172106
42	1	2.846088	0.029826	2.760814
43	1	2.006478	3.107609	0.810792
44	1	2.226776	2.718921	2.508595
45	1	-0.246022	2.267111	2.677993
46	1	0.248270	3.930111	2.356883
47	15	3.649798	-0.462191	-0.483081
48	8	4.885197	-0.042590	-1.260781
49	8	2.313300	-0.504903	-1.359984
50	8	3.764501	-1.622684	0.505927
51	15	-3.230498	-1.016428	-1.108292
52	8	-3.297094	-2.285823	-0.246784
53	8	-4.246397	-0.838741	-2.221295
54	8	-1.731299	-0.659124	-1.537491
55	71	0.244298	-0.337310	-0.780889

HF = -2242.132116 Hartree
Zero-point correction = 0.421220
Sum of electronic and thermal Enthalpies = -2241.680743
Sum of electronic and thermal Free Energies = -2241.768319

$[Lu(DO2A2P)]^{3-}$ I_2 (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	7	-0.971162	2.842904	0.670282
2	6	-2.358877	2.980300	1.077922
3	6	-2.911295	1.754919	1.822311
4	7	-2.713112	0.513729	1.110711
5	6	-2.621416	-0.642615	1.991275
6	6	-1.210343	-0.809018	2.574614
7	7	-0.190175	-1.319577	1.630125
8	6	1.177526	-1.178159	2.194952
9	6	1.681133	0.262099	2.385051
10	7	1.726303	1.104345	1.159119
11	6	1.398194	2.511757	1.477346
12	6	-0.054050	2.882357	1.792298
13	6	-0.588442	3.695795	-0.447690
14	6	0.300104	3.064945	-1.568492
15	8	0.386450	1.795680	-1.591736
16	8	0.787059	3.889065	-2.357930
17	6	-3.602401	0.346935	-0.049776
18	6	-0.477147	-2.764186	1.388334
19	6	0.267384	-3.405126	0.200148
20	8	0.454704	-4.627702	0.244113
21	8	0.534146	-2.592689	-0.751541
22	6	3.108336	1.130418	0.557124
23	1	-1.502012	4.011027	-0.965552
24	1	-0.094315	4.628680	-0.113869
25	1	-3.570340	1.271302	-0.635143
26	1	-4.656040	0.207132	0.277354
27	1	-1.531498	-2.855526	1.107875
28	1	-0.285950	-3.340158	2.309956
29	1	3.095052	1.907353	-0.211184
30	1	3.829255	1.437016	1.340574
31	1	-2.954237	3.126115	0.172605
32	1	-2.531807	3.880411	1.718315
33	1	-3.989272	1.954988	2.038730
34	1	-2.427088	1.680350	2.805028
35	1	-3.330396	-0.567928	2.848472
36	1	-2.913156	-1.515865	1.395478
37	1	-1.257677	-1.492963	3.447260
38	1	-0.869596	0.156169	2.961153
39	1	1.222997	-1.675499	3.185961
40	1	1.903571	-1.682187	1.540969
41	1	1.071801	0.781677	3.135545
42	1	2.695953	0.170723	2.801456
43	1	1.726033	3.115757	0.629648
44	1	2.009849	2.845040	2.341690
45	1	-0.437855	2.229841	2.582013
46	1	-0.017302	3.909531	2.237406
47	15	3.676759	-0.414887	-0.343315
48	8	4.944668	0.010529	-1.062566
49	8	2.399784	-0.553204	-1.295619
50	8	3.768065	-1.523253	0.707589
51	15	-3.140531	-1.034066	-1.252755
52	8	-3.195990	-2.330396	-0.433112
53	8	-4.107938	-0.858647	-2.409305
54	8	-1.637902	-0.605753	-1.605933
55	71	0.316775	-0.341550	-0.773613

HF = -2242.1327646 Hartree
Zero-point correction = 0.421278
Sum of electronic and thermal Enthalpies = -2241.680492
Sum of electronic and thermal Free Energies = -2241.770327

$[Lu(DO2A2P)]^{3-}$ TS_3 (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.807316	2.825315	0.809906
2	6	-2.084216	2.802950	1.506107
3	6	-2.353557	1.463355	2.207001
4	7	-2.290892	0.319257	1.305995
5	6	-2.150329	-0.949351	2.031989
6	6	-0.760634	-1.118095	2.660088
7	7	0.337456	-1.436924	1.718586
8	6	1.654469	-1.007567	2.267587
9	6	1.887915	0.502726	2.322994
10	7	1.890335	1.189132	1.021097
11	6	1.677578	2.636538	1.209504
12	6	0.301792	3.092277	1.705507
13	6	-0.778693	3.612019	-0.416190
14	6	0.140290	3.084797	-1.562893
15	8	0.319352	1.825192	-1.606599
16	8	0.559216	3.951688	-2.346289
17	6	-3.455092	0.315597	0.386096
18	6	0.388011	-2.917325	1.468879
19	6	0.113795	-3.427010	0.030477
20	8	0.115557	-4.660109	-0.088529
21	8	-0.055379	-2.534400	-0.859519
22	6	3.196829	1.029896	0.296696
23	1	-1.788593	3.605952	-0.842189
24	1	-0.508561	4.670010	-0.227585
25	1	-3.559762	1.320802	-0.028899
26	1	-4.382098	0.099022	0.957696
27	1	-0.320904	-3.426606	2.133477
28	1	1.388100	-3.279156	1.726177
29	1	3.201452	1.791100	-0.486801
30	1	4.024237	1.266368	0.996097
31	1	-2.873911	2.982177	0.773708
32	1	-2.172591	3.616749	2.262711
33	1	-3.346754	1.529482	2.708602
34	1	-1.619660	1.337729	3.011900
35	1	-2.901731	-1.022532	2.852390
36	1	-2.383254	-1.749640	1.313686
37	1	-0.819158	-1.903597	3.436984
38	1	-0.489006	-0.201106	3.190792
39	1	1.770958	-1.396775	3.300985
40	1	2.447355	-1.445288	1.638685
41	1	1.132629	0.978046	2.959597
42	1	2.859919	0.657194	2.836294
43	1	1.876193	3.120736	0.251906
44	1	2.428691	3.041712	1.923306
45	1	0.079579	2.625279	2.671105
46	1	0.389626	4.186573	1.913812
47	15	3.540681	-0.559410	-0.663012
48	8	4.663892	-0.166939	-1.605410
49	8	2.110976	-0.699263	-1.355512
50	8	3.814548	-1.679523	0.347883
51	15	-3.319228	-0.831401	-1.102309

52	8	-3.354970	-2.241902	-0.520716
53	8	-4.437014	-0.380562	-2.028307
54	8	-1.864314	-0.379142	-1.606908
55	71	0.094289	-0.293305	-0.733909

HF = -2242.127026 Hartree
Zero-point correction = 0.421389
Sum of electronic and thermal Enthalpies = -2241.675410
Sum of electronic and thermal Free Energies = -2241.763862

$[Lu(DO2A2P)]^{3-}$ I_3 (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.885979	2.732708	1.000776
2	6	-1.985362	2.448179	1.907247
3	6	-1.935807	1.009141	2.442527
4	7	-1.956050	-0.018311	1.395279
5	6	-1.705636	-1.360785	1.957165
6	6	-0.294167	-1.543978	2.543819
7	7	0.845497	-1.440710	1.599135
8	6	2.029051	-0.788984	2.214328
9	6	1.980286	0.736108	2.233461
10	7	1.901395	1.356284	0.909046
11	6	1.636967	2.797946	1.030932
12	6	0.307507	3.210910	1.673251
13	6	-1.211496	3.454428	-0.221682
14	6	-0.327390	3.103436	-1.459393
15	8	0.045066	1.887577	-1.545565
16	8	-0.103612	4.034596	-2.248709
17	6	-3.272395	0.021626	0.688973
18	6	1.263114	-2.789057	1.121485
19	6	0.349393	-3.396404	0.045102
20	8	0.312865	-4.632002	-0.042263
21	8	-0.229668	-2.530310	-0.700028
22	6	3.157395	1.194267	0.107673
23	1	-2.234893	3.189598	-0.510256
24	1	-1.171171	4.552933	-0.080173
25	1	-3.483844	1.061094	0.437960
26	1	-4.066141	-0.317739	1.384258
27	1	1.356869	-3.484597	1.974087
28	1	2.246895	-2.666747	0.648343
29	1	3.131121	1.977517	-0.653138
30	1	4.033296	1.398714	0.756478
31	1	-2.927315	2.612267	1.380948
32	1	-2.001902	3.135198	2.781091
33	1	-2.788000	0.866427	3.144070
34	1	-1.022755	0.906600	3.037902
35	1	-2.426952	-1.571266	2.777749
36	1	-1.918550	-2.081393	1.159433
37	1	-0.271386	-2.532675	3.034903
38	1	-0.134574	-0.811912	3.344988
39	1	2.163119	-1.139721	3.258330
40	1	2.904393	-1.096408	1.626756
41	1	1.119989	1.068877	2.824750

42	1	2.886158	1.089421	2.778083
43	1	1.681541	3.220203	0.026184
44	1	2.444375	3.291773	1.618896
45	1	0.274534	2.867036	2.713414
46	1	0.314250	4.324647	1.725545
47	15	3.447311	-0.363911	-0.932521
48	8	4.425230	0.106323	-1.992868
49	8	1.960327	-0.603284	-1.454971
50	8	3.915829	-1.487484	0.007603
51	15	-3.402417	-0.877856	-0.968673
52	8	-3.497317	-2.358828	-0.641131
53	8	-4.578990	-0.189774	-1.645933
54	8	-1.986067	-0.417679	-1.572476
55	71	-0.030628	-0.263341	-0.704520

HF = -2242.1327274 Hartree
Zero-point correction = 0.422143
Sum of electronic and thermal Enthalpies = -2241.679757
Sum of electronic and thermal Free Energies = -2241.769266

$[Lu(DO2A2P)]^{3-}$ TS_4 (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.899236	2.632485	1.017615
2	6	-2.005433	2.351068	1.921413
3	6	-1.952216	0.917166	2.468707
4	7	-1.972004	-0.108829	1.421202
5	6	-1.680389	-1.448928	1.962596
6	6	-0.260187	-1.607114	2.534396
7	7	0.865212	-1.472997	1.579797
8	6	2.053004	-0.835086	2.199401
9	6	1.999586	0.689314	2.245307
10	7	1.904079	1.330218	0.931010
11	6	1.621563	2.766014	1.079517
12	6	0.274958	3.139596	1.708818
13	6	-1.243244	3.375287	-0.191182
14	6	-0.301041	3.125303	-1.407283
15	8	0.112173	1.926509	-1.543288
16	8	-0.070352	4.104109	-2.134778
17	6	-3.305004	-0.102242	0.743702
18	6	1.274928	-2.804290	1.052391
19	6	0.339835	-3.376096	-0.025312
20	8	0.299149	-4.608196	-0.150517
21	8	-0.257275	-2.486899	-0.728408
22	6	3.156481	1.193037	0.118410
23	1	-2.234640	3.042777	-0.517984
24	1	-1.284557	4.467585	-0.009777
25	1	-3.609316	0.935755	0.612306
26	1	-4.050399	-0.575353	1.412599
27	1	1.381336	-3.527392	1.880588
28	1	2.251726	-2.667776	0.568792
29	1	3.116372	1.986339	-0.631086
30	1	4.034679	1.395744	0.764311
31	1	-2.943335	2.505160	1.385414

32	1	-2.031241	3.048964	2.785616
33	1	-2.801215	0.776053	3.174506
34	1	-1.036116	0.819574	3.060407
35	1	-2.389786	-1.692340	2.784895
36	1	-1.873580	-2.160427	1.153493
37	1	-0.211776	-2.598416	3.019692
38	1	-0.109096	-0.876616	3.338299
39	1	2.194908	-1.204889	3.235799
40	1	2.925008	-1.129973	1.600100
41	1	1.144182	1.009801	2.851109
42	1	2.909582	1.038522	2.784709
43	1	1.676458	3.211519	0.085919
44	1	2.411757	3.257021	1.692219
45	1	0.239462	2.782791	2.744616
46	1	0.247745	4.251595	1.772823
47	15	3.447700	-0.349355	-0.945097
48	8	4.411694	0.140661	-2.009094
49	8	1.956903	-0.593370	-1.452398
50	8	3.934413	-1.481554	-0.024202
51	15	-3.413295	-0.825435	-1.004002
52	8	-3.517777	-2.330937	-0.838809
53	8	-4.579803	-0.061646	-1.616499
54	8	-1.991200	-0.307616	-1.547599
55	71	-0.027902	-0.223197	-0.690998

HF = -2242.1327053 Hartree
Zero-point correction = 0.422208
Sum of electronic and thermal Enthalpies = -2241.680543
Sum of electronic and thermal Free Energies = -2241.767497

[Lu(DO2A2P)]$^{3-}$ SAP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.256838	1.729972	-1.251758
2	6	2.424262	1.095897	-1.897665
3	6	2.157456	-0.347188	-2.313931
4	7	1.760819	-1.226496	-1.205858
5	6	1.124693	-2.441759	-1.743654
6	6	-0.304863	-2.220366	-2.254293
7	7	-1.256718	-1.729874	-1.251904
8	6	-2.424240	-1.095776	-1.897834
9	6	-2.157275	0.347269	-2.313993
10	7	-1.760794	1.226492	-1.205816
11	6	-1.124686	2.441805	-1.743467
12	6	0.304909	2.220436	-2.254059
13	6	1.701290	2.805902	-0.336394
14	6	0.643837	3.214579	0.710744
15	8	-0.098920	2.258888	1.134095
16	8	0.608972	4.406678	1.057858
17	6	2.908412	-1.586229	-0.310238
18	6	-1.701289	-2.805890	-0.336634
19	6	-0.643986	-3.214415	0.710822
20	8	-0.609215	-4.406486	1.057997
21	8	0.098825	-2.258752	1.134052

22	6	-2.908503	1.586048	-0.310277
23	1	2.570951	2.417551	0.208266
24	1	2.007311	3.702013	-0.907334
25	1	3.777167	-1.888536	-0.927979
26	1	2.578842	-2.454506	0.262592
27	1	-2.006964	-3.702114	-0.907608
28	1	-2.571134	-2.417615	0.207761
29	1	-2.579128	2.454396	0.262551
30	1	-3.777289	1.888177	-0.928073
31	1	3.252722	1.100223	-1.173578
32	1	2.735414	1.668069	-2.797695
33	1	3.073616	-0.739378	-2.805261
34	1	1.366847	-0.379256	-3.074568
35	1	1.722246	-2.865926	-2.580142
36	1	1.113034	-3.192336	-0.954932
37	1	-0.663314	-3.177478	-2.689494
38	1	-0.287896	-1.500603	-3.080423
39	1	-2.735358	-1.667895	-2.797896
40	1	-3.252675	-1.100145	-1.173729
41	1	-1.366470	0.379281	-3.074439
42	1	-3.073221	0.739676	-2.805603
43	1	-1.113106	3.192345	-0.954716
44	1	-1.722146	2.865966	-2.580010
45	1	0.287949	1.500686	-3.080204
46	1	0.663315	3.177581	-2.689273
47	15	-3.419042	0.367974	1.054934
48	8	-4.154384	1.239603	2.054458
49	8	-1.965358	-0.108859	1.503599
50	8	-4.213367	-0.788886	0.421098
51	15	3.419030	-0.368199	1.054943
52	8	4.154281	-1.239843	2.054521
53	8	4.213466	0.788615	0.421129
54	8	1.965360	0.108716	1.503553
55	71	0.000015	0.000046	0.602920

HF = -2242.1646697 Hartree
Zero-point correction = 0.423767
Sum of electronic and thermal Enthalpies = -2241.710914
Sum of electronic and thermal Free Energies = -2241.797048

$[Lu(DO2A2P)]^{3-}$ TSAP $\Delta(\delta_{1a}\delta_{1b}\delta_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.917814	-1.861989	-1.301579
2	6	1.699534	-1.316877	-2.417872
3	6	2.654814	-0.198370	-2.004894
4	7	1.966394	0.924550	-1.347056
5	6	1.375806	1.824087	-2.337423
6	6	0.215558	2.660431	-1.796721
7	7	-0.917651	1.861714	-1.301276
8	6	-1.699598	1.316769	-2.417614
9	6	-2.654895	0.198282	-2.004724

10	7	-1.966495	-0.924703	-1.346994
11	6	-1.375879	-1.824167	-2.337361
12	6	-0.215588	-2.660502	-1.796740
13	6	1.750289	-2.686450	-0.392402
14	6	0.952247	-3.096374	0.868278
15	8	0.068568	-2.240447	1.240396
16	8	1.214213	-4.189726	1.387968
17	6	2.879468	1.624274	-0.401585
18	6	-1.750222	2.686193	-0.392038
19	6	-0.951720	3.096868	0.868098
20	8	-0.068769	2.240681	1.241164
21	8	-1.212736	4.191100	1.386569
22	6	-2.879543	-1.624460	-0.401532
23	1	0.996703	-0.951070	-3.177701
24	1	2.289778	-2.119978	-2.909677
25	1	3.404620	-0.570749	-1.293659
26	1	3.196889	0.145089	-2.912864
27	1	1.028280	1.222627	-3.187256
28	1	2.141369	2.517288	-2.748701
29	1	0.579483	3.266905	-0.966515
30	1	-0.117921	3.364376	-2.589044
31	1	-0.996895	0.950963	-3.177574
32	1	-2.289733	2.120063	-2.909184
33	1	-3.404701	0.570635	-1.293484
34	1	-3.196824	-0.144987	-2.912877
35	1	-1.028449	-1.222641	-3.187187
36	1	-2.141363	-2.517482	-2.748591
37	1	-0.579488	-3.266784	-0.966384
38	1	0.117622	-3.364689	-2.589023
39	1	2.103880	-3.597424	-0.910675
40	1	2.623545	-2.104246	-0.064914
41	1	3.757492	2.022289	-0.950121
42	1	2.334545	2.466654	0.031014
43	1	-2.104261	3.596851	-0.910586
44	1	-2.623190	2.103732	-0.064289
45	1	-3.757322	-2.022883	-0.950242
46	1	-2.334555	-2.466721	0.031268
47	15	3.410155	0.541804	1.058572
48	8	1.963219	0.042997	1.509417
49	8	4.106305	1.478940	2.023939
50	8	4.227543	-0.622492	0.467928
51	15	-3.410431	-0.541916	1.058631
52	8	-1.963428	-0.043224	1.509415
53	8	-4.227807	0.622285	0.467940
54	8	-4.106542	-1.479024	2.024003
55	71	-0.000027	-0.000001	0.625293

HF = -2242.1652599 Hartree
Zero-point correction = 0.423251
Sum of electronic and thermal Enthalpies = -2241.711976
Sum of electronic and thermal Free Energies = -2241.798347

$[Lu(DO2A2P)]^{3-}$ $TS_{TSAP\text{-}1a}$ $\Delta(\delta_{1a}\delta_{1b}X_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	7	0.962502	-2.051787	1.055885
2	6	1.615004	-1.612287	2.293084
3	6	2.442597	-0.343682	2.123585
4	7	1.683689	0.774916	1.528691
5	6	0.872888	1.449209	2.549295
6	6	-0.178618	2.397105	1.975200
7	7	-1.255417	1.730301	1.222502
8	6	-2.329812	1.215493	2.109203
9	6	-2.638103	-0.316509	2.178100
10	7	-1.909601	-1.239002	1.284496
11	6	-1.321693	-2.349101	2.040091
12	6	-0.125092	-2.994393	1.343786
13	6	1.906403	-2.656379	0.089081
14	6	1.220100	-2.891979	-1.280718
15	8	0.291595	-2.048883	-1.570413
16	8	1.599103	-3.857275	-1.956922
17	6	2.633782	1.683623	0.818390
18	6	-1.851725	2.698601	0.259606
19	6	-0.880930	3.137509	-0.848296
20	8	-1.064738	4.250109	-1.362492
21	8	0.040873	2.288214	-1.139401
22	6	-2.789702	-1.760904	0.200697
23	1	2.755899	-1.977274	-0.066620
24	1	2.289209	-3.621878	0.470277
25	1	3.384582	2.074925	1.533789
26	1	2.069477	2.524021	0.410994
27	1	-2.209928	3.599197	0.792009
28	1	-2.710723	2.193197	-0.199493
29	1	-2.213699	-2.487300	-0.378407
30	1	-3.653097	-2.290110	0.654298
31	1	2.271709	-2.410484	2.700780
32	1	0.836605	-1.446993	3.046087
33	1	3.302096	-0.530476	1.464582
34	1	2.840698	-0.053282	3.119485
35	1	0.368294	0.683305	3.154594
36	1	1.524187	2.023810	3.243794
37	1	0.317276	3.094809	1.299301
38	1	-0.595519	3.003100	2.806103
39	1	-2.123410	1.558592	3.138004
40	1	-3.261815	1.678889	1.783907
41	1	-2.465299	-0.640510	3.215899
42	1	-3.709904	-0.411314	1.973803
43	1	-2.072388	-3.144406	2.239191
44	1	-1.009792	-1.977202	3.022891
45	1	0.236214	-3.836993	1.973482
46	1	-0.448592	-3.423792	0.394686
47	15	-3.361412	-0.464404	-1.030698
48	8	-4.124711	-1.231005	-2.093898
49	8	-1.926616	0.064605	-1.482901
50	8	-4.125715	0.598690	-0.222793
51	15	3.444582	0.843631	-0.681314
52	8	4.114674	1.959236	-1.456513
53	8	4.339590	-0.284666	-0.133020
54	8	2.120284	0.239426	-1.329312
55	71	0.071787	0.054413	-0.632107

HF = -2242.1445617 Hartree
Zero-point correction = 0.423512
Sum of electronic and thermal Enthalpies = -2241.691533

Sum of electronic and thermal Free Energies = -2241.776829

$[Lu(DO2A2P)]^{3-}$ $TS_{TSAP\text{-}1b}$ $\Delta(\delta_{1a}X_{1b}\delta_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.710856	-1.530232	1.578896
2	6	1.357372	-0.689051	2.598002
3	6	2.438092	0.240630	2.041409
4	7	1.938914	1.250646	1.087814
5	6	1.509538	2.498050	1.749321
6	6	-0.006754	2.898081	1.828420
7	7	-1.022071	2.019805	1.215813
8	6	-1.993281	1.588519	2.227809
9	6	-2.919203	0.472241	1.758801
10	7	-2.175326	-0.709672	1.310795
11	6	-1.670344	-1.460789	2.456792
12	6	-0.424660	-2.284912	2.149389
13	6	1.633437	-2.523147	0.961292
14	6	0.931926	-3.210526	-0.236714
15	8	0.079942	-2.464405	-0.844311
16	8	1.225502	-4.388231	-0.485320
17	6	2.984622	1.567230	0.056618
18	6	-1.689654	2.717925	0.088616
19	6	-0.663145	3.062411	-1.011280
20	8	-0.669321	4.207914	-1.489373
21	8	0.129836	2.097696	-1.306884
22	6	-2.975241	-1.527050	0.362289
23	1	2.541448	-2.029464	0.583796
24	1	1.925820	-3.286958	1.704788
25	1	3.877530	2.000509	0.549322
26	1	2.545439	2.321643	-0.598978
27	1	-2.167736	3.649933	0.444421
28	1	-2.463567	2.069744	-0.344589
29	1	-2.391459	-2.415460	0.106985
30	1	-3.917849	-1.857434	0.845685
31	1	1.818357	-1.323865	3.385499
32	1	0.576483	-0.095138	3.091004
33	1	3.204381	-0.342883	1.514007
34	1	2.930800	0.728315	2.908813
35	1	1.904336	2.507036	2.781222
36	1	2.014856	3.321043	1.234527
37	1	-0.098533	3.893485	1.374826
38	1	-0.258053	3.035180	2.891221
39	1	-1.420289	1.262602	3.107308
40	1	-2.620064	2.441930	2.570013
41	1	-3.604010	0.220050	2.599898
42	1	-3.542795	0.795558	0.914502
43	1	-2.445259	-2.149775	2.858286
44	1	-1.449831	-0.756898	3.268096
45	1	-0.103972	-2.806324	3.075687
46	1	-0.691874	-3.056603	1.427784
47	15	-3.322120	-0.639033	-1.275806
48	8	-3.956940	-1.681115	-2.173514
49	8	-1.818811	-0.243862	-1.653001

50	8	-4.140495	0.618881	-0.935201
51	15	3.473895	0.135327	-1.055089
52	8	4.304510	0.747116	-2.164784
53	8	4.142772	-0.917592	-0.150994
54	8	2.007187	-0.330941	-1.485995
55	71	0.054689	-0.127406	-0.624697

HF = -2242.1439125 Hartree
Zero-point correction = 0.423216
Sum of electronic and thermal Enthalpies = -2241.691137
Sum of electronic and thermal Free Energies = -2241.776833

$[Lu(DO2A2P)]^{3-}$ I_{1a} $\Delta(\delta_{1a}\delta_{1b}\lambda_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.661292	-1.328723	1.685772
2	6	1.230125	-0.356247	2.633566
3	6	2.296687	0.579119	2.037805
4	7	1.850058	1.405142	0.900905
5	6	1.328558	2.722313	1.287915
6	6	-0.042493	2.761827	1.973063
7	7	-1.125147	2.102317	1.247070
8	6	-2.230841	1.751009	2.138766
9	6	-3.072479	0.583965	1.621529
10	7	-2.263876	-0.591568	1.282268
11	6	-1.764368	-1.245063	2.487930
12	6	-0.484957	-2.053356	2.281970
13	6	1.645551	-2.356998	1.244556
14	6	1.036527	-3.213376	0.107491
15	8	0.192338	-2.581604	-0.629272
16	8	1.384951	-4.398538	0.017583
17	6	2.964209	1.618231	-0.077355
18	6	-1.616282	2.870750	0.088285
19	6	-0.598173	3.019445	-1.067470
20	8	-0.473338	4.141475	-1.584681
21	8	0.016208	1.944055	-1.388464
22	6	-3.011010	-1.490372	0.366228
23	1	2.557950	-1.874629	0.858288
24	1	1.918256	-3.010004	2.093528
25	1	3.820887	2.109781	0.425319
26	1	2.579320	2.297031	-0.841175
27	1	-1.940064	3.881304	0.406414
28	1	-2.477688	2.335161	-0.333477
29	1	-2.418814	-2.397972	0.219192
30	1	-3.978241	-1.782637	0.825733
31	1	1.693430	-0.887079	3.492931
32	1	0.399238	0.227973	3.038901
33	1	3.139327	-0.021687	1.671984
34	1	2.670424	1.218541	2.866311
35	1	2.041670	3.229228	1.976334
36	1	1.284858	3.334241	0.386990
37	1	-0.274497	3.833503	2.168516
38	1	0.037847	2.287355	2.958468
39	1	-1.802273	1.503858	3.119872

40	1	-2.904895	2.616821	2.319288
41	1	-3.829926	0.338553	2.401741
42	1	-3.616059	0.857358	0.707294
43	1	-2.525811	-1.931138	2.920869
44	1	-1.587891	-0.479858	3.252552
45	1	-0.184059	-2.487403	3.258247
46	1	-0.708025	-2.888592	1.618550
47	15	-3.268010	-0.752425	-1.362665
48	8	-3.961338	-1.840875	-2.158345
49	8	-1.733913	-0.519813	-1.748839
50	8	-4.000100	0.587587	-1.177640
51	15	3.513894	0.075823	-0.990000
52	8	4.409790	0.556605	-2.113578
53	8	4.122554	-0.860616	0.070403
54	8	2.072299	-0.439518	-1.459259
55	71	0.087867	-0.241245	-0.671883

HF = -2242.157696 Hartree
Zero-point correction = 0.423174
Sum of electronic and thermal Enthalpies = -2241.704302
Sum of electronic and thermal Free Energies = -2241.791503

$[Lu(DO2A2P)]^{3-}$ I_{1b} $\Delta(\delta_{1a}\lambda_{1b}\delta_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.871261	-2.082729	0.995092
2	6	1.482712	-1.670240	2.264062
3	6	2.340533	-0.414176	2.145378
4	7	1.620265	0.734338	1.553568
5	6	0.805428	1.406769	2.573050
6	6	-0.248353	2.367587	2.013861
7	7	-1.275487	1.764018	1.152026
8	6	-2.432180	1.202307	1.880401
9	6	-2.288726	-0.227445	2.404960
10	7	-1.941359	-1.222451	1.390681
11	6	-1.410049	-2.446161	2.000128
12	6	-0.236210	-3.027198	1.208770
13	6	1.853909	-2.682875	0.061111
14	6	1.241907	-2.884005	-1.348954
15	8	0.345466	-2.020207	-1.672642
16	8	1.648927	-3.839799	-2.022351
17	6	2.606303	1.644831	0.893786
18	6	-1.779592	2.785671	0.197310
19	6	-0.745427	3.186464	-0.869307
20	8	-0.817205	4.331665	-1.337682
21	8	0.092974	2.265301	-1.190916
22	6	-3.037841	-1.556767	0.439074
23	1	2.716148	-2.010895	-0.041686
24	1	2.206503	-3.658277	0.445142
25	1	3.329818	2.017431	1.646129
26	1	2.062050	2.497170	0.482810
27	1	-2.111956	3.693936	0.732645
28	1	-2.643406	2.346749	-0.317777
29	1	-2.740470	-2.487490	-0.052682

30	1	-3.964426	-1.772289	1.011445
31	1	2.108403	-2.484927	2.686768
32	1	0.680478	-1.497594	2.988377
33	1	3.219347	-0.600834	1.511980
34	1	2.712070	-0.153775	3.159206
35	1	0.313063	0.639144	3.179477
36	1	1.456876	1.982145	3.266222
37	1	0.268657	3.130286	1.425974
38	1	-0.719397	2.896031	2.869919
39	1	-2.690910	1.848218	2.747637
40	1	-3.277649	1.201738	1.179572
41	1	-1.523152	-0.271805	3.189437
42	1	-3.254390	-0.477853	2.901817
43	1	-2.189667	-3.227725	2.082650
44	1	-1.097963	-2.237242	3.030721
45	1	0.121581	-3.944605	1.725317
46	1	-0.592902	-3.327271	0.220813
47	15	-3.414012	-0.410402	-1.023341
48	8	-4.136651	-1.321924	-1.997352
49	8	-1.925939	-0.025144	-1.432439
50	8	-4.192777	0.803964	-0.487842
51	15	3.475468	0.819647	-0.580878
52	8	4.168872	1.942203	-1.324442
53	8	4.353587	-0.307759	-0.004741
54	8	2.178331	0.212583	-1.278176
55	71	0.100388	0.041876	-0.659737

HF = -2242.1545728 Hartree
Zero-point correction = 0.423175
Sum of electronic and thermal Enthalpies = -2241.701185
Sum of electronic and thermal Free Energies = -2241.788035

$[Lu(DO2A2P)]^{3-}$ TS_{1a-2a} $\Delta(X_{1a}\delta_{1b}\lambda_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.752917	-1.498029	1.618680
2	6	1.542033	-0.684043	2.559480
3	6	2.579133	0.241455	1.910777
4	7	2.048731	1.201667	0.931491
5	6	1.580847	2.455966	1.525707
6	6	0.243554	2.379870	2.274219
7	7	-0.866158	1.786085	1.514325
8	6	-1.865254	1.225485	2.431530
9	6	-2.855268	0.294899	1.745832
10	7	-2.202683	-0.864401	1.118915
11	6	-1.824581	-1.870113	2.125603
12	6	-0.315381	-2.231327	2.350985
13	6	1.589102	-2.509329	0.906963
14	6	0.706486	-3.230313	-0.134734
15	8	-0.119014	-2.452201	-0.736519
16	8	0.832375	-4.457313	-0.274746
17	6	3.060123	1.493169	-0.129316
18	6	-1.475560	2.766298	0.584540
19	6	-0.522068	3.165300	-0.565366

20	8	-0.434662	4.368002	-0.863657
21	8	0.095219	2.180500	-1.100581
22	6	-3.089998	-1.430285	0.055319
23	1	2.436301	-2.027131	0.395959
24	1	1.989403	-3.245738	1.626953
25	1	3.991831	1.884657	0.325778
26	1	2.629523	2.270878	-0.763005
27	1	-1.785247	3.673095	1.137651
28	1	-2.358168	2.312109	0.112145
29	1	-2.597109	-2.327785	-0.324694
30	1	-4.066396	-1.719381	0.493826
31	1	2.089935	-1.341353	3.269269
32	1	0.828743	-0.112843	3.162192
33	1	3.321023	-0.366546	1.376265
34	1	3.106746	0.769543	2.735877
35	1	2.331257	2.853154	2.246603
36	1	1.497345	3.191573	0.726714
37	1	-0.014935	3.407569	2.604931
38	1	0.378458	1.795061	3.189813
39	1	-1.325650	0.673374	3.215220
40	1	-2.431242	2.028985	2.952343
41	1	-3.593763	-0.034702	2.510036
42	1	-3.413372	0.810210	0.952542
43	1	-2.332491	-2.808207	1.869400
44	1	-2.240769	-1.566018	3.101009
45	1	-0.109670	-2.159438	3.431883
46	1	-0.204192	-3.290425	2.103174
47	15	-3.322804	-0.285370	-1.426969
48	8	-4.106920	-1.092755	-2.442568
49	8	-1.780406	-0.069479	-1.786682
50	8	-3.952488	1.017830	-0.900051
51	15	3.412000	0.035676	-1.260733
52	8	4.199093	0.592480	-2.429536
53	8	4.077101	-1.045737	-0.388949
54	8	1.896394	-0.358009	-1.599021
55	71	0.008906	-0.101003	-0.621000

HF = -2242.1465217 Hartree
Zero-point correction = 0.423716
Sum of electronic and thermal Enthalpies = -2241.693403
Sum of electronic and thermal Free Energies = -2241.778454

$[Lu(DO2A2P)]^{3-}$ TS_{1b-2b} $\Delta(\lambda_{1a}\delta_{1b}\delta_{2a}X_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.388218	1.856386	0.963590
2	6	-2.442516	1.276572	1.815884
3	6	-2.104806	-0.062728	2.475378
4	7	-1.619194	-1.098219	1.553575
5	6	-0.862787	-2.120216	2.288972
6	6	0.180222	-2.819603	1.422872
7	7	1.244216	-1.916991	0.957879
8	6	2.115008	-1.480188	2.074984
9	6	2.314294	0.048412	2.322492

10	7	1.517988	1.014809	1.518895
11	6	0.688677	1.843897	2.407996
12	6	-0.396128	2.651691	1.693397
13	6	-2.011022	2.683885	-0.096808
14	6	-1.043822	3.010200	-1.252303
15	8	-0.127513	2.131709	-1.465005
16	8	-1.233829	4.061301	-1.880698
17	6	-2.717686	-1.731125	0.762568
18	6	2.048725	-2.605078	-0.085721
19	6	1.259231	-2.864679	-1.384325
20	8	1.626542	-3.808872	-2.097029
21	8	0.277325	-2.060087	-1.600924
22	6	2.449782	1.860021	0.704302
23	1	-2.845316	2.105680	-0.509213
24	1	-2.406132	3.630280	0.316296
25	1	-3.530785	-2.031236	1.454864
26	1	-2.307476	-2.646319	0.328265
27	1	2.428532	-3.570977	0.297175
28	1	2.900320	-1.954070	-0.315116
29	1	1.857378	2.588319	0.147004
30	1	3.134075	2.407424	1.382307
31	1	-3.321212	1.106267	1.178380
32	1	-2.721625	1.986065	2.625487
33	1	-3.023104	-0.405639	2.998574
34	1	-1.345209	0.071575	3.253281
35	1	-0.350394	-1.640316	3.132476
36	1	-1.537981	-2.883824	2.727666
37	1	-0.304671	-3.236703	0.537868
38	1	0.605528	-3.670302	1.997269
39	1	1.745209	-1.939796	3.004181
40	1	3.116712	-1.882679	1.897485
41	1	2.129989	0.244305	3.391693
42	1	3.366593	0.240323	2.105497
43	1	1.322969	2.560100	2.974202
44	1	0.225381	1.190589	3.153092
45	1	-0.892136	3.298983	2.449299
46	1	0.084968	3.322399	0.977802
47	15	3.382695	0.862136	-0.597700
48	8	4.131989	1.881747	-1.433093
49	8	2.114603	0.196628	-1.290907
50	8	4.213102	-0.191160	0.160497
51	15	-3.406389	-0.806524	-0.745529
52	8	-4.040377	-1.909326	-1.572037
53	8	-4.335001	0.312565	-0.241927
54	8	-2.038793	-0.223309	-1.304822
55	71	0.030603	0.000106	-0.639515

HF = -2242.143046 Hartree
Zero-point correction = 0.423167
Sum of electronic and thermal Enthalpies = -2241.690238
Sum of electronic and thermal Free Energies = -2241.775906

$[Lu(DO2A2P)]^{3-}$ TS_{1a-2c} $\Delta(\delta_{1a}X_{1b}\lambda_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	7	0.677027	-1.898492	1.254708
2	6	1.224531	-1.277687	2.468003
3	6	2.235323	-0.172781	2.181395
4	7	1.669112	0.962414	1.411096
5	6	1.041511	1.963812	2.306598
6	6	-0.455392	2.420703	2.130606
7	7	-1.304096	1.887896	1.047712
8	6	-2.620290	1.454389	1.566321
9	6	-2.595678	0.103991	2.264023
10	7	-2.141177	-0.988008	1.409623
11	6	-1.662166	-2.121904	2.198522
12	6	-0.449165	-2.798698	1.564316
13	6	1.676327	-2.680488	0.479003
14	6	1.090321	-3.079494	-0.901192
15	8	0.234414	-2.244800	-1.375689
16	8	1.471525	-4.144293	-1.405193
17	6	2.768803	1.596319	0.597988
18	6	-1.556708	2.909292	0.002911
19	6	-0.340615	3.213797	-0.884997
20	8	-0.144824	4.389798	-1.228700
21	8	0.339989	2.179201	-1.221999
22	6	-3.117481	-1.420016	0.371930
23	1	2.577823	-2.078483	0.300297
24	1	1.962336	-3.593385	1.033003
25	1	3.547005	1.984325	1.283783
26	1	2.324295	2.433915	0.059389
27	1	-1.919611	3.849391	0.457412
28	1	-2.341610	2.506886	-0.647883
29	1	-2.756477	-2.379715	-0.008971
30	1	-4.101277	-1.608321	0.851636
31	1	1.706439	-2.038582	3.119402
32	1	0.386932	-0.859890	3.039707
33	1	3.084522	-0.561678	1.602190
34	1	2.637827	0.180123	3.152292
35	1	1.122420	1.588615	3.337798
36	1	1.661906	2.869816	2.273692
37	1	-0.452599	3.520503	2.060603
38	1	-0.955585	2.189102	3.080509
39	1	-3.020390	2.203588	2.283622
40	1	-3.316995	1.388183	0.718225
41	1	-1.924573	0.147796	3.135319
42	1	-3.617775	-0.084914	2.664930
43	1	-2.449660	-2.890808	2.335728
44	1	-1.407562	-1.778200	3.208820
45	1	-0.110357	-3.617995	2.233916
46	1	-0.754768	-3.255102	0.621319
47	15	-3.361396	-0.400921	-1.219071
48	8	-3.991496	-1.404626	-2.165165
49	8	-1.843500	-0.030413	-1.534981
50	8	-4.179101	0.853775	-0.873069
51	15	3.526302	0.451120	-0.699814
52	8	4.356291	1.341623	-1.601021
53	8	4.257313	-0.665174	0.073684
54	8	2.173001	-0.107889	-1.330105
55	71	0.119905	-0.036899	-0.648593

HF = -2242.1348337 Hartree
Zero-point correction = 0.422950
Sum of electronic and thermal Enthalpies = -2241.682165

Sum of electronic and thermal Free Energies = -2241.768398

$[Lu(DO2A2P)]^{3-}$ TS_{1b-2d} $\Delta(X_{1a}\lambda_{1b}\delta_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.153303	-1.542782	1.368922
2	6	2.148607	-0.738879	2.113013
3	6	1.820712	0.746424	2.289599
4	7	1.737914	1.540613	1.054392
5	6	1.294719	2.902718	1.405479
6	6	-0.231480	3.229923	1.348378
7	7	-1.152284	2.139523	0.998790
8	6	-1.886884	1.693637	2.183195
9	6	-2.644889	0.388537	1.980008
10	7	-1.790894	-0.714870	1.506318
11	6	-1.047094	-1.287062	2.630222
12	6	0.124702	-2.172270	2.216229
13	6	1.835198	-2.634592	0.614531
14	6	0.937195	-3.213899	-0.492762
15	8	0.079297	-2.388300	-0.978569
16	8	1.117890	-4.395303	-0.823851
17	6	3.035413	1.627901	0.309589
18	6	-2.030584	2.564615	-0.117413
19	6	-1.178285	2.835300	-1.382617
20	8	-1.448882	3.835095	-2.065326
21	8	-0.229188	1.990895	-1.585310
22	6	-2.622098	-1.708474	0.764328
23	1	2.738499	-2.214299	0.152626
24	1	2.136796	-3.445986	1.300938
25	1	3.862715	1.838005	1.017086
26	1	2.943316	2.489795	-0.353519
27	1	-2.578880	3.488220	0.147379
28	1	-2.762587	1.778316	-0.344305
29	1	-1.980402	-2.538479	0.464035
30	1	-3.420499	-2.098465	1.427133
31	1	3.094506	-0.810587	1.558512
32	1	2.304307	-1.164170	3.126017
33	1	2.611215	1.166528	2.953594
34	1	0.873414	0.875633	2.824599
35	1	1.689221	3.177626	2.405276
36	1	1.777221	3.582809	0.702672
37	1	-0.355478	4.018216	0.600171
38	1	-0.538577	3.683333	2.308074
39	1	-1.157284	1.595742	3.000095
40	1	-2.615281	2.464942	2.520388
41	1	-3.130989	0.117548	2.942711
42	1	-3.442490	0.515633	1.234208
43	1	-1.718796	-1.893554	3.277629
44	1	-0.680491	-0.465858	3.257514
45	1	0.590401	-2.587063	3.134432
46	1	-0.273502	-3.022974	1.659137
47	15	-3.332098	-1.000587	-0.849178
48	8	-3.901203	-2.186292	-1.599666
49	8	-1.982996	-0.384897	-1.437785

50	8	-4.303493	0.126420	-0.448587
51	15	3.511607	0.260388	-0.907898
52	8	4.340408	0.983275	-1.952806
53	8	4.212204	-0.850807	-0.105289
54	8	2.054305	-0.170611	-1.382992
55	71	0.012206	-0.102597	-0.642091

HF = -2242.1399293 Hartree
Zero-point correction = 0.423360
Sum of electronic and thermal Enthalpies = -2241.687033
Sum of electronic and thermal Free Energies = -2241.772433

$[Lu(DO2A2P)]^{3-}$ TS_{1a-2d} $\Delta(\delta_{1a}\delta_{1b}\lambda_{2a}X_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.976024	-1.348882	1.567203
2	6	1.861313	-0.518770	2.433904
3	6	2.214790	0.968336	2.061906
4	7	1.759980	1.567832	0.787208
5	6	1.222160	2.924523	1.001211
6	6	-0.122640	3.005402	1.723513
7	7	-1.183329	2.200187	1.131712
8	6	-2.192622	1.827870	2.120513
9	6	-2.921904	0.538760	1.757811
10	7	-2.015387	-0.564426	1.404208
11	6	-1.335179	-1.057518	2.601506
12	6	-0.141265	-1.962100	2.324803
13	6	1.762841	-2.483769	0.984300
14	6	0.973151	-3.237978	-0.097301
15	8	0.065340	-2.541991	-0.686898
16	8	1.261768	-4.426774	-0.298703
17	6	2.876477	1.702850	-0.200493
18	6	-1.793639	2.796780	-0.069386
19	6	-0.833543	2.931597	-1.278787
20	8	-0.847960	4.002998	-1.905585
21	8	-0.105828	1.904708	-1.519890
22	6	-2.781073	-1.587936	0.637807
23	1	2.682434	-2.063054	0.554900
24	1	2.038752	-3.191166	1.787398
25	1	3.704269	2.281762	0.255707
26	1	2.478067	2.275946	-1.040692
27	1	-2.202254	3.799674	0.163917
28	1	-2.617030	2.145169	-0.393286
29	1	-2.129560	-2.443126	0.448404
30	1	-3.652467	-1.932150	1.231307
31	1	2.817721	-1.041156	2.511201
32	1	1.414614	-0.494479	3.440104
33	1	3.309289	1.032152	2.098805
34	1	1.824282	1.592929	2.877308
35	1	1.942751	3.542733	1.580811
36	1	1.131852	3.394424	0.023512
37	1	-0.401657	4.081297	1.787415
38	1	0.011666	2.664902	2.758312
39	1	-1.685920	1.720776	3.089312

40	1	-2.950034	2.629258	2.265515
41	1	-3.564398	0.251848	2.621311
42	1	-3.582907	0.687952	0.892512
43	1	-2.038670	-1.615030	3.260806
44	1	-0.990191	-0.192314	3.182107
45	1	0.229642	-2.358396	3.291002
46	1	-0.485953	-2.819404	1.746402
47	15	-3.303484	-0.957640	-1.081992
48	8	-3.897467	-2.162448	-1.783893
49	8	-1.864192	-0.502218	-1.603992
50	8	-4.212502	0.265646	-0.864288
51	15	3.483300	0.097461	-0.920697
52	8	4.411793	0.467577	-2.061297
53	8	4.068013	-0.703033	0.255801
54	8	2.061108	-0.475960	-1.384397
55	71	0.042305	-0.221791	-0.645194

HF = -2242.1381479 Hartree
Zero-point correction = 0.423358
Sum of electronic and thermal Enthalpies = -2241.685200
Sum of electronic and thermal Free Energies = -2241.770971

$[Lu(DO2A2P)]^{3-}$ TS_{1b-2c} $\Delta(\delta_{1a}\lambda_{1b}X_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.655304	-1.631697	1.519998
2	6	1.252010	-0.860996	2.620194
3	6	2.259818	0.199294	2.166888
4	7	1.762225	1.164893	1.164384
5	6	1.126434	2.352600	1.756378
6	6	-0.340067	2.222914	2.186479
7	7	-1.317369	1.932116	1.131381
8	6	-2.641071	1.687629	1.749982
9	6	-3.169282	0.223933	1.781790
10	7	-2.267790	-0.810976	1.259894
11	6	-1.743396	-1.623475	2.349398
12	6	-0.494402	-2.424386	1.998502
13	6	1.617096	-2.572508	0.882802
14	6	0.989091	-3.189509	-0.391095
15	8	0.151697	-2.420406	-0.993698
16	8	1.316682	-4.342713	-0.701489
17	6	2.903128	1.589680	0.282781
18	6	-1.451561	3.015512	0.135375
19	6	-0.275860	3.194398	-0.848026
20	8	0.005549	4.356094	-1.188331
21	8	0.273932	2.112792	-1.250221
22	6	-2.930396	-1.577276	0.172698
23	1	2.539200	-2.043216	0.595299
24	1	1.879490	-3.381806	1.588906
25	1	3.715631	2.015176	0.903279
26	1	2.520034	2.368679	-0.377422
27	1	-1.650154	3.987716	0.625771
28	1	-2.315263	2.742816	-0.481923
29	1	-2.258902	-2.374483	-0.155898

30	1	-3.865300	-2.043167	0.548001
31	1	1.771805	-1.539797	3.329797
32	1	0.436414	-0.396887	3.183792
33	1	3.122614	-0.300115	1.706591
34	1	2.616622	0.732195	3.073586
35	1	1.693337	2.679600	2.654376
36	1	1.204940	3.167996	1.035474
37	1	-0.599459	3.177418	2.701374
38	1	-0.434772	1.437818	2.944983
39	1	-2.645967	2.112334	2.771280
40	1	-3.379067	2.246332	1.173080
41	1	-3.474884	-0.030059	2.814291
42	1	-4.054882	0.229537	1.144090
43	1	-2.503001	-2.346667	2.729102
44	1	-1.525391	-0.953972	3.192295
45	1	-0.198507	-3.019784	2.888105
46	1	-0.744808	-3.136388	1.212205
47	15	-3.263289	-0.516681	-1.364807
48	8	-3.935396	-1.449981	-2.353802
49	8	-1.749886	-0.144495	-1.726809
50	8	-4.039179	0.727727	-0.901113
51	15	3.535817	0.217169	-0.837412
52	8	4.437222	0.889157	-1.853016
53	8	4.161009	-0.847231	0.086193
54	8	2.125713	-0.279023	-1.403709
55	71	0.107715	-0.107904	-0.663010

HF = -2242.142027 Hartree
Zero-point correction = 0.423415
Sum of electronic and thermal Enthalpies = -2241.689014
Sum of electronic and thermal Free Energies = -2241.774901

$[Lu(DO2A2P)]^{3-}$ I_{2a} $\Delta(\lambda_{1a}\delta_{1b}\lambda_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.829528	-1.558061	1.638051
2	6	1.775810	-0.875087	2.536000
3	6	2.743456	0.081907	1.833215
4	7	2.121752	1.086795	0.958230
5	6	1.628495	2.274504	1.661314
6	6	0.297943	2.108679	2.416997
7	7	-0.829138	1.557816	1.638066
8	6	-1.775312	0.874763	2.536130
9	6	-2.743070	-0.082124	1.833392
10	7	-2.121412	-1.086847	0.958181
11	6	-1.628106	-2.274577	1.661236
12	6	-0.297570	-2.108769	2.417005
13	6	1.512318	-2.620211	0.856362
14	6	0.605199	-3.201332	-0.249916
15	8	-0.073488	-2.321019	-0.887695
16	8	0.597862	-4.431181	-0.420052
17	6	3.083898	1.474491	-0.118344
18	6	-1.512143	2.619920	0.856495
19	6	-0.605034	3.201363	-0.249653

20	8	-0.597856	4.431293	-0.419360
21	8	0.073777	2.321366	-0.887711
22	6	-3.083730	-1.474468	-0.118275
23	1	2.397344	-2.189504	0.360493
24	1	1.835050	-3.434703	1.531699
25	1	4.037706	1.821346	0.327118
26	1	2.632192	2.305752	-0.663134
27	1	-1.835036	3.434246	1.531949
28	1	-2.397147	2.189115	0.360662
29	1	-2.632068	-2.305657	-0.663224
30	1	-4.037446	-1.821401	0.327296
31	1	2.386371	-1.613379	3.099066
32	1	1.187343	-0.339597	3.287180
33	1	3.423349	-0.495327	1.193208
34	1	3.353287	0.572971	2.624564
35	1	2.373879	2.627835	2.409892
36	1	1.519761	3.070689	0.926739
37	1	0.028729	3.101398	2.831356
38	1	0.459514	1.456924	3.280083
39	1	-1.186700	0.339197	3.287139
40	1	-2.385743	1.613035	3.099345
41	1	-3.352778	-0.573352	2.624720
42	1	-3.423028	0.495140	1.193500
43	1	-1.519273	-3.070704	0.926612
44	1	-2.373533	-2.627952	2.409729
45	1	-0.459070	-1.456943	3.280063
46	1	-0.028487	-3.101519	2.831366
47	15	-3.359293	-0.110149	-1.385442
48	8	-4.173764	-0.736386	-2.500237
49	8	-1.824385	0.159811	-1.748001
50	8	-3.968349	1.086802	-0.630522
51	15	3.359043	0.110362	-1.385795
52	8	4.173357	0.736650	-2.500664
53	8	3.968169	-1.086736	-0.631154
54	8	1.823993	-0.159243	-1.747939
55	71	-0.000183	-0.000055	-0.640023

HF = -2242.1615748 Hartree
Zero-point correction = 0.424239
Sum of electronic and thermal Enthalpies = -2241.707419
Sum of electronic and thermal Free Energies = -2241.793524

$[Lu(DO2A2P)]^{3-}$ I_{2b} $\Delta(\delta_{1a}\lambda_{1b}\delta_{2a}\lambda_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.316189	1.900391	0.870845
2	6	-2.297961	1.344386	1.825941
3	6	-1.920369	0.023147	2.512162
4	7	-1.494982	-1.060379	1.612872
5	6	-0.718069	-2.071415	2.351482
6	6	0.314119	-2.782893	1.478024
7	7	1.315857	-1.900058	0.871276
8	6	2.297440	-1.343992	1.826554
9	6	1.920140	-0.022365	2.512227

10	7	1.494555	1.060846	1.612625
11	6	0.717773	2.072106	2.351078
12	6	-0.314654	2.783408	1.477686
13	6	-2.027836	2.647496	-0.197505
14	6	-1.156951	2.904634	-1.445018
15	8	-0.232491	2.034088	-1.657770
16	8	-1.426852	3.895126	-2.138348
17	6	-2.640222	-1.724091	0.915447
18	6	2.027759	-2.647518	-0.196684
19	6	1.157471	-2.904651	-1.444584
20	8	1.428159	-3.894760	-2.138158
21	8	0.232571	-2.034575	-1.657292
22	6	2.639685	1.724476	0.914895
23	1	-2.881903	2.036440	-0.508360
24	1	-2.403345	3.615261	0.182252
25	1	-3.398306	-2.013215	1.671746
26	1	-2.247192	-2.646380	0.479382
27	1	2.402937	-3.615266	0.183437
28	1	2.882097	-2.036698	-0.507270
29	1	2.246341	2.646276	0.478096
30	1	3.397568	2.014463	1.671066
31	1	-3.222262	1.151147	1.264084
32	1	-2.516691	2.080890	2.628803
33	1	-2.808438	-0.288133	3.102341
34	1	-1.115172	0.180079	3.236731
35	1	-0.204521	-1.594856	3.191516
36	1	-1.386880	-2.835578	2.795688
37	1	-0.205306	-3.295695	0.663338
38	1	0.806239	-3.567923	2.093024
39	1	2.515652	-2.080321	2.629712
40	1	3.221974	-1.151198	1.264920
41	1	1.115229	-0.178864	3.237249
42	1	2.808468	0.289126	3.101902
43	1	1.386672	2.836373	2.794957
44	1	0.204369	1.595796	3.191333
45	1	-0.806940	3.568226	2.092848
46	1	0.204618	3.296567	0.663114
47	15	3.434151	0.843498	-0.562548
48	8	4.109469	1.966726	-1.326145
49	8	2.107545	0.262796	-1.211462
50	8	4.339702	-0.278178	-0.022166
51	15	-3.434130	-0.843830	-0.562801
52	8	-4.108984	-1.967516	-1.326157
53	8	-4.339940	0.278032	-0.023314
54	8	-2.107318	-0.263265	-1.211451
55	71	0.000070	-0.000159	-0.663199

HF = -2242.1535176 Hartree
Zero-point correction = 0.423266
Sum of electronic and thermal Enthalpies = -2241.699962
Sum of electronic and thermal Free Energies = -2241.787051

$[Lu(DO2A2P)]^{3-}$ I_{2c} $\Delta(\delta_{1a}\lambda_{1b}\lambda_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	7	0.558286	-1.758664	1.379351
2	6	1.081252	-1.045533	2.553534
3	6	2.122294	0.033866	2.230046
4	7	1.699280	1.075595	1.265048
5	6	1.055290	2.243643	1.893105
6	6	-0.443218	2.121946	2.194166
7	7	-1.299290	1.899044	1.028496
8	6	-2.686105	1.604105	1.435369
9	6	-2.883611	0.256508	2.124087
10	7	-2.304935	-0.864049	1.391369
11	6	-1.827423	-1.921870	2.272190
12	6	-0.584096	-2.627499	1.734070
13	6	1.565853	-2.630655	0.711697
14	6	1.016459	-3.134705	-0.647817
15	8	0.193260	-2.326779	-1.220121
16	8	1.386809	-4.246120	-1.047617
17	6	2.897499	1.533873	0.478493
18	6	-1.338850	3.057647	0.116683
19	6	-0.123072	3.234212	-0.818946
20	8	0.222514	4.397308	-1.085525
21	8	0.384884	2.149198	-1.267959
22	6	-3.153530	-1.382983	0.287704
23	1	2.497093	-2.074844	0.522625
24	1	1.799841	-3.498798	1.354478
25	1	3.673749	1.911404	1.171687
26	1	2.564278	2.355803	-0.156489
27	1	-1.500543	3.998644	0.675879
28	1	-2.197371	2.896441	-0.543950
29	1	-2.700234	-2.319994	-0.047335
30	1	-4.160902	-1.628826	0.686096
31	1	1.550139	-1.757008	3.266995
32	1	0.229112	-0.601139	3.076569
33	1	3.010376	-0.442048	1.793025
34	1	2.423967	0.501146	3.190603
35	1	1.565997	2.495786	2.846230
36	1	1.205225	3.098954	1.230941
37	1	-0.745911	3.052212	2.728445
38	1	-0.606103	1.299340	2.897031
39	1	-3.063837	2.396057	2.122229
40	1	-3.306828	1.593041	0.528211
41	1	-2.438897	0.271894	3.129148
42	1	-3.976722	0.128181	2.274094
43	1	-2.598962	-2.702538	2.450773
44	1	-1.606718	-1.493350	3.258075
45	1	-0.262217	-3.382642	2.481952
46	1	-0.853992	-3.168059	0.825897
47	15	-3.338498	-0.386275	-1.321485
48	8	-3.953674	-1.395089	-2.272731
49	8	-1.803449	-0.048850	-1.604397
50	8	-4.145382	0.884420	-1.016649
51	15	3.581196	0.220791	-0.681268
52	8	4.530855	0.941024	-1.616680
53	8	4.162653	-0.888969	0.217764
54	8	2.198567	-0.241028	-1.332223
55	71	0.136294	-0.067143	-0.684351

HF = -2242.1516415 Hartree
Zero-point correction = 0.423290
Sum of electronic and thermal Enthalpies = -2241.698081

Sum of electronic and thermal Free Energies = -2241.785798

$[Lu(DO2A2P)]^{3-}$ I_{2d} $\Delta(\delta_{1a}\delta_{1b}\lambda_{2a}\lambda_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.091883	-1.399668	1.501400
2	6	2.052955	-0.523354	2.216411
3	6	1.712946	0.972609	2.225540
4	7	1.646225	1.593274	0.898916
5	6	1.127424	2.971541	0.973960
6	6	-0.263452	3.144299	1.596911
7	7	-1.268455	2.214334	1.091553
8	6	-2.201508	1.783573	2.127851
9	6	-2.862667	0.446467	1.809364
10	7	-1.911620	-0.614319	1.431905
11	6	-1.199193	-1.085804	2.621158
12	6	0.018224	-1.966230	2.344138
13	6	1.823053	-2.553736	0.896030
14	6	0.979336	-3.263881	-0.176577
15	8	0.133427	-2.506723	-0.780452
16	8	1.185439	-4.471244	-0.370498
17	6	2.965686	1.661535	0.194802
18	6	-1.952263	2.697438	-0.121126
19	6	-1.000934	2.889346	-1.329775
20	8	-1.105904	3.936937	-1.986086
21	8	-0.176059	1.927857	-1.534683
22	6	-2.653002	-1.670520	0.681088
23	1	2.737885	-2.165091	0.428059
24	1	2.106564	-3.279282	1.679016
25	1	3.754832	1.949256	0.917290
26	1	2.879576	2.475507	-0.528120
27	1	-2.456649	3.662794	0.080492
28	1	-2.708774	1.957769	-0.418206
29	1	-1.968961	-2.494162	0.469882
30	1	-3.489575	-2.054302	1.299242
31	1	3.021853	-0.645220	1.714870
32	1	2.156779	-0.850578	3.270869
33	1	2.481155	1.475996	2.856610
34	1	0.749854	1.130231	2.719288
35	1	1.825706	3.616231	1.553450
36	1	1.109994	3.351447	-0.046363
37	1	-0.564842	4.200340	1.438596
38	1	-0.189352	3.014382	2.683736
39	1	-1.641264	1.717123	3.071108
40	1	-3.006729	2.530774	2.307234
41	1	-3.453486	0.134993	2.699957
42	1	-3.565430	0.548538	0.970753
43	1	-1.879320	-1.666571	3.284821
44	1	-0.884707	-0.210516	3.201729
45	1	0.437498	-2.285449	3.320364
46	1	-0.329860	-2.873284	1.845742
47	15	-3.258851	-1.060451	-1.019069
48	8	-3.800524	-2.291696	-1.716036
49	8	-1.866293	-0.510455	-1.575254

50	8	-4.232931	0.104476	-0.763484
51	15	3.522403	0.208879	-0.878053
52	8	4.394276	0.846889	-1.942625
53	8	4.188220	-0.818315	0.054793
54	8	2.095650	-0.288754	-1.392043
55	71	0.059376	-0.189777	-0.663911

HF = -2242.1504393 Hartree
Zero-point correction = 0.423272
Sum of electronic and thermal Enthalpies = -2241.696905
Sum of electronic and thermal Free Energies = -2241.784031

$[Lu(DO2A2P)]^{3-}$ TS_{2a-3a} $\Delta(\lambda_{1a}\delta_{1b}\lambda_{2a}X_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.048790	-1.456604	1.523096
2	6	2.246592	-0.920413	2.234700
3	6	2.796000	0.495186	1.871207
4	7	2.122605	1.287294	0.826010
5	6	1.593711	2.544794	1.358016
6	6	0.337709	2.351996	2.211113
7	7	-0.805893	1.733106	1.521910
8	6	-1.728397	1.155906	2.511906
9	6	-2.673102	0.100513	1.936700
10	7	-2.028307	-0.959586	1.144996
11	6	-1.425213	-2.021193	1.958391
12	6	-0.019912	-1.724103	2.509894
13	6	1.457784	-2.705503	0.815891
14	6	0.418383	-3.258093	-0.172513
15	8	-0.239512	-2.367186	-0.814709
16	8	0.315876	-4.492692	-0.274118
17	6	3.036507	1.528795	-0.326688
18	6	-1.515388	2.700213	0.645813
19	6	-0.679084	3.147515	-0.574984
20	8	-0.728978	4.342616	-0.906778
21	8	0.002911	2.214014	-1.128987
22	6	-3.026309	-1.498677	0.166792
23	1	2.360686	-2.445405	0.243993
24	1	1.705180	-3.490507	1.553787
25	1	3.980609	1.993888	0.021915
26	1	2.530311	2.227100	-0.996485
27	1	-1.806784	3.592912	1.230517
28	1	-2.423490	2.218120	0.249410
29	1	-2.571513	-2.367177	-0.310911
30	1	-3.943911	-1.819975	0.697990
31	1	3.071189	-1.611417	2.051997
32	1	2.042291	-0.943017	3.317300
33	1	3.822299	0.325782	1.537907
34	1	2.831902	1.091981	2.799510
35	1	2.344113	3.058387	2.000619
36	1	1.387315	3.212499	0.524918
37	1	0.050414	3.333796	2.643218
38	1	0.603805	1.705591	3.057911
39	1	-1.126000	0.731399	3.322405

40	1	-2.349694	1.947607	2.982409
41	1	-3.241105	-0.338688	2.786898
42	1	-3.392199	0.583320	1.261902
43	1	-1.387817	-2.930091	1.358087
44	1	-2.064315	-2.251694	2.839790
45	1	-0.071108	-0.858406	3.173798
46	1	0.266583	-2.587708	3.147490
47	15	-3.408901	-0.273968	-1.216402
48	8	-4.244904	-1.034659	-2.227006
49	8	-1.906199	0.025626	-1.670699
50	8	-4.038895	0.967432	-0.552697
51	15	3.349200	-0.032902	-1.316195
52	8	4.202003	0.376499	-2.502192
53	8	3.922494	-1.070510	-0.333599
54	8	1.824599	-0.361793	-1.677998
55	71	-0.026401	-0.058888	-0.630798

HF = -2242.1471144 Hartree
Zero-point correction = 0.424227
Sum of electronic and thermal Enthalpies = -2241.693540
Sum of electronic and thermal Free Energies = -2241.778464

$[Lu(DO2A2P)]^{3-}$ TS_{2c-3a} $\Delta(\delta_{1a}\lambda_{1b}X_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.280294	1.676609	1.269822
2	6	-2.567799	1.172721	1.783220
3	6	-2.510715	-0.280682	2.218611
4	7	-2.132527	-1.223381	1.162406
5	6	-1.739241	-2.490789	1.793498
6	6	-0.221045	-2.848006	1.776094
7	7	0.762766	-1.832515	1.334799
8	6	1.316875	-1.113528	2.490403
9	6	2.279588	0.028863	2.140709
10	7	1.750299	1.088274	1.256515
11	6	1.094613	2.189377	1.979122
12	6	-0.363590	1.952392	2.380422
13	6	-1.534881	2.872517	0.435529
14	6	-0.395077	3.238809	-0.535170
15	8	0.210111	2.240505	-1.059976
16	8	-0.182464	4.445608	-0.743963
17	6	-3.190630	-1.419262	0.125605
18	6	1.779757	-2.558822	0.519194
19	6	1.093450	-3.071807	-0.772808
20	8	1.423136	-4.185108	-1.209215
21	8	0.193658	-2.282893	-1.245903
22	6	2.860005	1.643866	0.408818
23	1	-2.409984	2.633330	-0.182772
24	1	-1.767870	3.748316	1.069534
25	1	-4.171732	-1.584354	0.617705
26	1	-2.926642	-2.337862	-0.403300
27	1	2.179947	-3.419230	1.085389
28	1	2.621264	-1.904030	0.250297
29	1	2.438414	2.480074	-0.149777

30	1	3.673610	2.020653	1.058619
31	1	-3.307899	1.266534	0.975621
32	1	-2.906291	1.781620	2.650524
33	1	-3.507018	-0.546173	2.640211
34	1	-1.794016	-0.403895	3.041910
35	1	-2.108241	-2.525191	2.834498
36	1	-2.255251	-3.307480	1.278694
37	1	-0.109156	-3.697504	1.101889
38	1	0.071551	-3.222815	2.775992
39	1	0.466180	-0.748122	3.079706
40	1	1.873068	-1.812038	3.153899
41	1	2.631794	0.466653	3.098611
42	1	3.152983	-0.391444	1.623306
43	1	1.138423	3.076781	1.345628
44	1	1.659017	2.436566	2.903823
45	1	-0.416199	1.114489	3.082218
46	1	-0.704079	2.849593	2.944128
47	15	3.501990	0.431066	-0.873290
48	8	4.332098	1.241462	-1.847786
49	8	2.091884	-0.072814	-1.431292
50	8	4.210878	-0.688646	-0.084597
51	15	-3.371018	-0.182752	-1.305087
52	8	-4.142828	-0.979937	-2.340091
53	8	-4.029502	1.103553	-0.777379
54	8	-1.829215	0.039032	-1.642187
55	71	0.072985	-0.034396	-0.644590

HF = -2242.1418622 Hartree
Zero-point correction = 0.423539
Sum of electronic and thermal Enthalpies = -2241.688859
Sum of electronic and thermal Free Energies = -2241.774080

$[Lu(DO2A2P)]^{3-}$ TS_{2d-3b} $\Delta(\delta_{1a}X_{1b}\lambda_{2a}\lambda_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.133490	-1.543612	1.379900
2	6	2.046797	-0.714124	2.201605
3	6	1.628908	0.751378	2.362414
4	7	1.502014	1.493387	1.100419
5	6	0.863024	2.803191	1.329627
6	6	-0.582576	2.773199	1.827828
7	7	-1.522082	2.009111	1.009123
8	6	-2.695585	1.601815	1.806021
9	6	-2.935297	0.073716	1.975411
10	7	-1.904004	-0.837789	1.440305
11	6	-1.144108	-1.415202	2.548902
12	6	0.080185	-2.233808	2.147696
13	6	1.910282	-2.589813	0.652593
14	6	1.108077	-3.191400	-0.516210
15	8	0.239183	-2.399290	-1.037905
16	8	1.365168	-4.356399	-0.854318
17	6	2.818015	1.745981	0.424620
18	6	-1.960977	2.721522	-0.209572
19	6	-0.873476	2.974820	-1.276971

20	8	-0.909967	4.061124	-1.876464
21	8	-0.034183	2.021515	-1.462677
22	6	-2.560212	-1.822878	0.531799
23	1	2.817886	-2.119118	0.253596
24	1	2.207276	-3.398420	1.344088
25	1	3.558418	2.074771	1.180022
26	1	2.648122	2.582387	-0.255974
27	1	-2.410970	3.698824	0.053034
28	1	-2.727382	2.085531	-0.671476
29	1	-1.816718	-2.541881	0.183195
30	1	-3.355916	-2.372975	1.073596
31	1	3.027397	-0.732828	1.706205
32	1	2.152394	-1.148431	3.216702
33	1	2.380512	1.239068	3.022217
34	1	0.670409	0.809082	2.885715
35	1	1.450229	3.392282	2.068531
36	1	0.905028	3.345796	0.386731
37	1	-0.907368	3.832801	1.936334
38	1	-0.603979	2.350493	2.838725
39	1	-2.638581	2.078208	2.798724
40	1	-3.595782	1.994825	1.323724
41	1	-3.100398	-0.146890	3.047110
42	1	-3.854399	-0.134174	1.425610
43	1	-1.785113	-2.083100	3.170698
44	1	-0.839202	-0.592408	3.209207
45	1	0.514682	-2.669118	3.071493
46	1	-0.260721	-3.074902	1.540091
47	15	-3.222306	-0.984163	-1.041195
48	8	-3.788115	-2.106653	-1.888702
49	8	-1.846101	-0.362770	-1.561992
50	8	-4.182697	0.135442	-0.598888
51	15	3.534605	0.423383	-0.722088
52	8	4.391511	1.207283	-1.697484
53	8	4.248797	-0.622528	0.153805
54	8	2.169300	-0.140003	-1.319691
55	71	0.098201	-0.116591	-0.655591

HF = -2242.1387355 Hartree
Zero-point correction = 0.423343
Sum of electronic and thermal Enthalpies = -2241.685798
Sum of electronic and thermal Free Energies = -2241.771444

$[Lu(DO2A2P)]^{3-}$ TS_{2c-3b} $\Delta(\delta_{1a}\lambda_{1b}\lambda_{2a}X_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.859460	-1.731994	1.313785
2	6	1.677946	-1.115081	2.388689
3	6	2.111308	0.391130	2.296800
4	7	1.667186	1.254127	1.167807
5	6	1.032555	2.495008	1.653417
6	6	-0.437040	2.347569	2.036517
7	7	-1.314133	1.986255	0.924016
8	6	-2.655923	1.621819	1.404314
9	6	-2.706190	0.305711	2.175004

10	7	-2.024663	-0.802067	1.495195
11	6	-1.398040	-1.698358	2.463488
12	6	-0.258820	-2.519226	1.876180
13	6	1.672983	-2.684167	0.497077
14	6	0.930492	-3.122176	-0.779526
15	8	0.041171	-2.292295	-1.206418
16	8	1.230919	-4.218665	-1.271734
17	6	2.839375	1.634063	0.307808
18	6	-1.447260	3.058460	-0.077776
19	6	-0.288465	3.192296	-1.093077
20	8	-0.029094	4.335206	-1.504568
21	8	0.265262	2.093412	-1.445185
22	6	-2.905846	-1.521981	0.532591
23	1	2.614970	-2.186442	0.233280
24	1	1.906806	-3.581166	1.099970
25	1	3.610664	2.122177	0.934411
26	1	2.473457	2.352959	-0.426586
27	1	-1.615984	4.040052	0.403631
28	1	-2.330455	2.812442	-0.675777
29	1	-2.358625	-2.399865	0.182884
30	1	-3.813937	-1.876308	1.063389
31	1	2.604860	-1.691459	2.480483
32	1	1.128550	-1.234102	3.333088
33	1	3.204209	0.380457	2.281498
34	1	1.783198	0.869515	3.233304
35	1	1.580046	2.899915	2.529319
36	1	1.121636	3.246516	0.867722
37	1	-0.770164	3.301057	2.506625
38	1	-0.526420	1.573061	2.807112
39	1	-3.065442	2.420903	2.064221
40	1	-3.321521	1.504309	0.538414
41	1	-2.252992	0.426715	3.169205
42	1	-3.773484	0.069484	2.346704
43	1	-2.130722	-2.403680	2.916983
44	1	-1.004054	-1.091755	3.290492
45	1	0.115798	-3.208822	2.660675
46	1	-0.647605	-3.141929	1.069876
47	15	-3.386170	-0.625381	-1.073302
48	8	-3.920244	-1.736288	-1.956410
49	8	-1.947385	-0.061342	-1.475999
50	8	-4.352198	0.513892	-0.712492
51	15	3.521810	0.198487	-0.668803
52	8	4.504994	0.781919	-1.665300
53	8	4.062936	-0.803007	0.369788
54	8	2.137821	-0.295542	-1.292506
55	71	0.058616	-0.064699	-0.646302

HF = -2242.1382345 Hartree
Zero-point correction = 0.423405
Sum of electronic and thermal Enthalpies = -2241.685199
Sum of electronic and thermal Free Energies = -2241.770988

$[Lu(DO2A2P)]^{3-}$ TS_{2d-3a} $\Delta(X_{1a}\delta_{1b}\lambda_{2a}\lambda_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	7	1.126803	-1.522492	1.458716
2	6	2.287705	-0.802991	2.038911
3	6	2.060311	0.694612	2.208096
4	7	1.874316	1.408800	0.942689
5	6	1.417521	2.784805	1.179276
6	6	0.055121	2.904517	1.873974
7	7	-0.995982	2.059216	1.295581
8	6	-1.876785	1.525529	2.334785
9	6	-2.723890	0.359428	1.854195
10	7	-1.924994	-0.768180	1.325006
11	6	-1.365298	-1.554272	2.444614
12	6	0.151900	-1.973578	2.484320
13	6	1.633699	-2.711101	0.711028
14	6	0.557097	-3.309305	-0.202767
15	8	-0.179099	-2.429907	-0.778576
16	8	0.497492	-4.544006	-0.322056
17	6	3.105017	1.454387	0.093190
18	6	-1.729078	2.759909	0.219073
19	6	-0.812676	3.074593	-0.989529
20	8	-0.882170	4.205589	-1.495940
21	8	-0.043979	2.109887	-1.340419
22	6	-2.816296	-1.581685	0.429113
23	1	2.478601	-2.378810	0.093826
24	1	1.994095	-3.480596	1.416236
25	1	3.989517	1.655090	0.729889
26	1	2.981621	2.312182	-0.571118
27	1	-2.158374	3.705914	0.601064
28	1	-2.545980	2.121009	-0.145322
29	1	-2.249000	-2.454590	0.106822
30	1	-3.701598	-1.916376	1.005315
31	1	3.140205	-0.956801	1.362513
32	1	2.550803	-1.227183	3.028815
33	1	2.925413	1.113013	2.771793
34	1	1.173012	0.856021	2.832194
35	1	2.154723	3.346807	1.796971
36	1	1.367724	3.274496	0.208471
37	1	-0.238375	3.971918	1.853363
38	1	0.162519	2.644626	2.933876
39	1	-1.237887	1.203734	3.171188
40	1	-2.555782	2.305936	2.745877
41	1	-3.355792	0.020839	2.702897
42	1	-3.406888	0.669023	1.050291
43	1	-1.956702	-2.477569	2.547822
44	1	-1.546097	-0.986862	3.367909
45	1	0.531100	-1.658870	3.468317
46	1	0.177196	-3.070778	2.492330
47	15	-3.336491	-0.659698	-1.143496
48	8	-4.015794	-1.692803	-2.019087
49	8	-1.888288	-0.191908	-1.630099
50	8	-4.168886	0.559110	-0.698208
51	15	3.450412	0.036875	-1.118196
52	8	4.261616	0.689561	-2.220701
53	8	4.119306	-1.103721	-0.331385
54	8	1.948611	-0.331123	-1.516194
55	71	0.002811	-0.104306	-0.620398

HF = -2242.1376044 Hartree
Zero-point correction = 0.423455
Sum of electronic and thermal Enthalpies = -2241.684531

Sum of electronic and thermal Free Energies = -2241.770444

$[Lu(DO2A2P)]^{3-}$ TS_{2b-3b} $\Delta(\delta_{1a}\lambda_{1b}X_{2a}\lambda_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.196636	-1.767775	1.117696
2	6	2.072519	-1.040252	2.060294
3	6	1.600488	0.362140	2.459388
4	7	1.399367	1.336631	1.364884
5	6	0.761339	2.548219	1.946878
6	6	-0.740368	2.876984	1.637776
7	7	-1.545647	1.959363	0.820579
8	6	-2.654634	1.349341	1.569580
9	6	-2.224508	0.151954	2.404685
10	7	-1.657182	-0.948237	1.617190
11	6	-0.921562	-1.868217	2.494794
12	6	0.187255	-2.616895	1.764198
13	6	1.994657	-2.635261	0.208400
14	6	1.212066	-3.024883	-1.062799
15	8	0.296148	-2.192505	-1.415103
16	8	1.531590	-4.078278	-1.632595
17	6	2.685658	1.755757	0.700683
18	6	-2.060561	2.643046	-0.387124
19	6	-0.948368	2.975667	-1.401525
20	8	-1.018991	4.052563	-2.013129
21	8	-0.043347	2.069487	-1.531520
22	6	-2.686065	-1.693263	0.825992
23	1	2.887344	-2.075242	-0.091402
24	1	2.314277	-3.554351	0.731904
25	1	3.406050	2.075876	1.479482
26	1	2.428139	2.629949	0.099579
27	1	-2.590882	3.576236	-0.122629
28	1	-2.766645	1.958429	-0.868222
29	1	-2.220544	-2.630354	0.512196
30	1	-3.531960	-1.953679	1.494692
31	1	3.055917	-0.937331	1.579094
32	1	2.198432	-1.619145	2.999196
33	1	2.356078	0.756859	3.173087
34	1	0.656288	0.311221	3.008587
35	1	0.887639	2.526126	3.042979
36	1	1.342820	3.409430	1.609675
37	1	-0.746289	3.855282	1.140072
38	1	-1.250272	3.033076	2.603475
39	1	-3.120351	2.088933	2.257477
40	1	-3.423426	1.021521	0.853681
41	1	-1.467315	0.466773	3.137885
42	1	-3.103700	-0.194164	2.991086
43	1	-1.602646	-2.613630	2.955797
44	1	-0.487076	-1.302904	3.327092
45	1	0.673870	-3.309381	2.484001
46	1	-0.259631	-3.233708	0.980400
47	15	-3.326380	-0.969484	-0.817211
48	8	-3.814752	-2.194198	-1.565207
49	8	-1.971394	-0.324655	-1.344913

50	8	-4.367304	0.115994	-0.495716
51	15	3.502084	0.627870	-0.577812
52	8	4.303863	1.587185	-1.436615
53	8	4.293508	-0.462309	0.168493
54	8	2.180498	0.047938	-1.241011
55	71	0.073099	-0.040807	-0.650212

HF = -2242.1356603 Hartree
Zero-point correction = 0.422927
Sum of electronic and thermal Enthalpies = -2241.682922
Sum of electronic and thermal Free Energies = -2241.769544

$[Lu(DO2A2P)]^{3-}$ I_{3a} $\Delta(\lambda_{1a}\delta_{1b}\lambda_{2a}\lambda_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.141380	-1.500585	1.445713
2	6	2.404209	-0.926130	1.963955
3	6	2.356639	0.584286	2.159670
4	7	2.027500	1.325137	0.941182
5	6	1.544037	2.670905	1.266661
6	6	0.204577	2.692943	2.021040
7	7	-0.865192	1.875349	1.419469
8	6	-1.702103	1.268639	2.463002
9	6	-2.601647	0.138842	1.964626
10	7	-1.928637	-0.938353	1.215033
11	6	-1.291490	-1.947439	2.075487
12	6	0.148428	-1.636337	2.522186
13	6	1.448392	-2.802692	0.805927
14	6	0.365845	-3.298304	-0.170651
15	8	-0.212500	-2.372278	-0.837678
16	8	0.167869	-4.523323	-0.243471
17	6	3.159353	1.397118	-0.030146
18	6	-1.656059	2.681125	0.455436
19	6	-0.797213	3.113978	-0.755938
20	8	-0.905452	4.280081	-1.165800
21	8	-0.021381	2.198121	-1.212751
22	6	-2.929270	-1.557626	0.282523
23	1	2.361186	-2.649107	0.215323
24	1	1.638220	-3.577153	1.571601
25	1	4.100758	1.626492	0.508927
26	1	2.943697	2.242694	-0.687317
27	1	-2.053632	3.583681	0.956431
28	1	-2.502169	2.085932	0.076518
29	1	-2.454414	-2.428933	-0.168549
30	1	-3.820568	-1.886497	0.851566
31	1	3.187376	-1.148836	1.225900
32	1	2.674119	-1.399161	2.932350
33	1	3.342718	0.906263	2.561500
34	1	1.619768	0.837074	2.930060
35	1	2.280564	3.228969	1.889971
36	1	1.437564	3.211428	0.328384
37	1	-0.115347	3.748517	2.105234
38	1	0.362163	2.346912	3.049479
39	1	-1.031851	0.903650	3.250987

40	1	-2.357792	2.026108	2.946315
41	1	-3.130151	-0.278880	2.849357
42	1	-3.359821	0.550467	1.284708
43	1	-1.292955	-2.899095	1.541187
44	1	-1.889300	-2.106165	2.998732
45	1	0.157954	-0.709753	3.102603
46	1	0.459514	-2.444777	3.219284
47	15	-3.398970	-0.415230	-1.143836
48	8	-4.187358	-1.266562	-2.118807
49	8	-1.923718	-0.025052	-1.620622
50	8	-4.107604	0.804321	-0.520260
51	15	3.405366	-0.031295	-1.253601
52	8	4.241837	0.587372	-2.357856
53	8	4.008468	-1.230519	-0.501211
54	8	1.876176	-0.286204	-1.635295
55	71	-0.009744	-0.056426	-0.636076

HF = -2242.1595998 Hartree
Zero-point correction = 0.423607
Sum of electronic and thermal Enthalpies = -2241.705857
Sum of electronic and thermal Free Energies = -2241.792683

$[Lu(DO2A2P)]^{3-}$ I_{3b} $\Delta(\delta_{1a}\lambda_{1b}\lambda_{2a}\lambda_{2b})$ (0 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.074208	-1.715089	1.246119
2	6	1.954078	-0.953218	2.163373
3	6	1.528736	0.500602	2.424095
4	7	1.459260	1.354999	1.227267
5	6	0.820167	2.648063	1.548738
6	6	-0.670455	2.594160	1.888514
7	7	-1.509987	1.976435	0.866209
8	6	-2.760810	1.463553	1.440508
9	6	-2.569333	0.185916	2.254417
10	7	-1.832737	-0.872739	1.550625
11	6	-1.129681	-1.720676	2.517554
12	6	0.029525	-2.505901	1.916359
13	6	1.859934	-2.666333	0.408431
14	6	1.076475	-3.108733	-0.844165
15	8	0.192788	-2.268777	-1.259415
16	8	1.358710	-4.208663	-1.340099
17	6	2.805879	1.648381	0.631826
18	6	-1.805324	2.875946	-0.260668
19	6	-0.636470	3.112424	-1.245230
20	8	-0.541544	4.239590	-1.756004
21	8	0.110747	2.093748	-1.468911
22	6	-2.705712	-1.671623	0.638006
23	1	2.781063	-2.162507	0.092037
24	1	2.134319	-3.560589	0.996367
25	1	3.515653	1.901661	1.443307
26	1	2.674451	2.540203	0.016451
27	1	-2.169328	3.858512	0.096073
28	1	-2.600116	2.394300	-0.839745
29	1	-2.114808	-2.521309	0.289893

30	1	-3.564339	-2.070505	1.216495
31	1	2.954765	-0.934315	1.708295
32	1	2.021211	-1.461243	3.147028
33	1	2.252615	0.926823	3.153268
34	1	0.547564	0.524785	2.906660
35	1	1.345540	3.136694	2.398056
36	1	0.956384	3.293479	0.681255
37	1	-0.999336	3.636037	2.098364
38	1	-0.813463	2.043475	2.823968
39	1	-3.236565	2.221646	2.103784
40	1	-3.457305	1.229454	0.622629
41	1	-2.027156	0.407483	3.185258
42	1	-3.573704	-0.168377	2.561302
43	1	-1.818155	-2.449086	3.000618
44	1	-0.743404	-1.086093	3.325018
45	1	0.479950	-3.121635	2.723521
46	1	-0.365246	-3.203124	1.174231
47	15	-3.309100	-0.873638	-0.982812
48	8	-3.766395	-2.060924	-1.806763
49	8	-1.939032	-0.198172	-1.443178
50	8	-4.364845	0.189979	-0.640682
51	15	3.544660	0.409717	-0.592008
52	8	4.427823	1.254968	-1.489468
53	8	4.237083	-0.697293	0.225783
54	8	2.189464	-0.101989	-1.250316
55	71	0.083526	-0.056018	-0.656218

HF = -2242.1523985 Hartree
Zero-point correction = 0.423472
Sum of electronic and thermal Enthalpies = -2241.698695
Sum of electronic and thermal Free Energies = -2241.785988

$[Lu(DO2A2P)]^{3-}$ $TS_{3a\text{-}SAP}$ $\Delta(\lambda_{1a}X_{1b}\lambda_{2a}\lambda_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.163701	1.601912	1.352580
2	6	-2.377502	1.017016	1.963981
3	6	-2.243601	-0.467481	2.275894
4	7	-1.880498	-1.282691	1.112001
5	6	-1.291798	-2.554487	1.551813
6	6	0.097300	-2.403381	2.181715
7	7	1.116502	-1.739787	1.345712
8	6	2.208199	-1.212579	2.204810
9	6	2.638199	0.281620	2.060699
10	7	1.914100	1.175312	1.128990
11	6	1.231398	2.270317	1.832680
12	6	-0.149303	1.888921	2.377280
13	6	-1.552800	2.813905	0.590769
14	6	-0.539898	3.255297	-0.485132
15	8	0.094904	2.301293	-1.056423
16	8	-0.442898	4.472695	-0.715542
17	6	-3.029196	-1.524899	0.185501
18	6	1.688104	-2.699894	0.356921
19	6	0.710007	-3.134404	-0.749978

20	8	0.777209	-4.308307	-1.149168
21	8	-0.096292	-2.223408	-1.161387
22	6	2.864702	1.692804	0.092188
23	1	-2.480198	2.560400	0.061469
24	1	-1.749402	3.659211	1.275361
25	1	-3.922297	-1.821795	0.771201
26	1	-2.738494	-2.372504	-0.438192
27	1	2.044704	-3.603890	0.884729
28	1	2.548905	-2.197598	-0.108881
29	1	2.331203	2.442999	-0.492319
30	1	3.736501	2.168809	0.581986
31	1	-3.200100	1.137410	1.244579
32	1	-2.635404	1.554023	2.901877
33	1	-3.206202	-0.815079	2.708394
34	1	-1.488703	-0.618875	3.055697
35	1	-1.939300	-3.059081	2.304316
36	1	-1.236596	-3.213094	0.687919
37	1	0.441400	-3.414478	2.483024
38	1	0.002697	-1.828673	3.108910
39	1	1.927397	-1.382671	3.254711
40	1	3.108900	-1.806580	2.019017
41	1	2.613396	0.730928	3.069195
42	1	3.674499	0.247218	1.720702
43	1	1.132899	3.114512	1.150373
44	1	1.838096	2.633525	2.689078
45	1	-0.043604	0.999626	3.011887
46	1	-0.502105	2.710626	3.038072
47	15	3.380906	0.347695	-1.110000
48	8	4.202808	1.027787	-2.188103
49	8	1.918107	-0.110410	-1.566699
50	8	4.062405	-0.752798	-0.272889
51	15	-3.453194	-0.194010	-1.098411
52	8	-4.262791	-0.946419	-2.137707
53	8	-4.146996	0.983796	-0.389322
54	8	-1.968693	0.185288	-1.539711
55	71	-0.023995	0.017097	-0.614805

HF = -2242.1467507 Hartree
Zero-point correction = 0.423978
Sum of electronic and thermal Enthalpies = -2241.693365
Sum of electronic and thermal Free Energies = -2241.778389

$[Lu(DO2A2P)]^{3-}$ $TS_{3b\text{-}SAP}$ $\Delta(X_{1a}\lambda_{1b}\lambda_{2a}\lambda_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.238882	-1.795417	1.212873
2	6	2.240788	-1.042428	1.995675
3	6	1.790997	0.365872	2.387386
4	7	1.578099	1.274981	1.249892
5	6	0.947007	2.528381	1.705202
6	6	-0.517392	2.400787	2.125906
7	7	-1.400098	1.836798	1.102905
8	6	-2.588100	1.223601	1.716904
9	6	-2.282106	-0.136705	2.320895

10	7	-1.740014	-1.134602	1.378787
11	6	-1.185718	-2.252210	2.177178
12	6	0.326980	-2.626217	2.025771
13	6	1.896174	-2.681914	0.210865
14	6	0.884668	-3.142502	-0.854335
15	8	0.006172	-2.258795	-1.174826
16	8	0.989860	-4.294499	-1.304542
17	6	2.847999	1.621079	0.525191
18	6	-1.799196	2.831407	0.087113
19	6	-0.686597	3.186108	-0.924089
20	8	-0.646592	4.353710	-1.345681
21	8	0.085297	2.214805	-1.246397
22	6	-2.777020	-1.652389	0.414886
23	1	2.705075	-2.119716	-0.267633
24	1	2.332870	-3.569020	0.702858
25	1	3.644002	1.836269	1.264390
26	1	2.639302	2.543283	-0.018603
27	1	-2.158389	3.761306	0.566620
28	1	-2.621800	2.384216	-0.481888
29	1	-2.311726	-2.509089	-0.075921
30	1	-3.651420	-2.013888	0.992687
31	1	3.151587	-0.965029	1.383773
32	1	2.495088	-1.582835	2.930471
33	1	2.555802	0.789664	3.075286
34	1	0.855199	0.304174	2.957588
35	1	1.513412	2.962973	2.557803
36	1	1.014609	3.240886	0.884107
37	1	-0.869386	3.408787	2.432514
38	1	-0.588193	1.773781	3.021102
39	1	-2.998094	1.870998	2.523510
40	1	-3.360603	1.101810	0.941506
41	1	-1.547703	-0.027314	3.131393
42	1	-3.211806	-0.518503	2.794295
43	1	-1.762824	-3.157305	1.950173
44	1	-1.373514	-2.052716	3.242779
45	1	0.746482	-2.724126	3.042469
46	1	0.352273	-3.633015	1.597164
47	15	-3.351919	-0.595577	-1.059205
48	8	-3.953827	-1.619767	-2.000810
49	8	-1.941217	0.000718	-1.499605
50	8	-4.287811	0.515425	-0.550795
51	15	3.466588	0.469684	-0.849019
52	8	4.220890	1.389186	-1.789215
53	8	4.269084	-0.665525	-0.188429
54	8	2.058084	-0.050905	-1.383018
55	71	0.028186	-0.012698	-0.602212

HF = -2242.1382828 Hartree
Zero-point correction = 0.423482
Sum of electronic and thermal Enthalpies = -2241.685217
Sum of electronic and thermal Free Energies = -2241.770873

$[Lu(DO2A2P)]^{3-}$ SAP $\Delta(\lambda_{1a}\lambda_{1b}\lambda_{2a}\lambda_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	7	1.256838	1.729972	-1.251758
2	6	2.424262	1.095897	-1.897665
3	6	2.157456	-0.347188	-2.313931
4	7	1.760819	-1.226496	-1.205858
5	6	1.124693	-2.441759	-1.743654
6	6	-0.304863	-2.220366	-2.254293
7	7	-1.256718	-1.729874	-1.251904
8	6	-2.424240	-1.095776	-1.897834
9	6	-2.157275	0.347269	-2.313993
10	7	-1.760794	1.226492	-1.205816
11	6	-1.124686	2.441805	-1.743467
12	6	0.304909	2.220436	-2.254059
13	6	1.701290	2.805902	-0.336394
14	6	0.643837	3.214579	0.710744
15	8	-0.098920	2.258888	1.134095
16	8	0.608972	4.406678	1.057858
17	6	2.908412	-1.586229	-0.310238
18	6	-1.701289	-2.805890	-0.336634
19	6	-0.643986	-3.214415	0.710822
20	8	-0.609215	-4.406486	1.057997
21	8	0.098825	-2.258752	1.134052
22	6	-2.908503	1.586048	-0.310277
23	1	2.570951	2.417551	0.208266
24	1	2.007311	3.702013	-0.907334
25	1	3.777167	-1.888536	-0.927979
26	1	2.578842	-2.454506	0.262592
27	1	-2.006964	-3.702114	-0.907608
28	1	-2.571134	-2.417615	0.207761
29	1	-2.579128	2.454396	0.262551
30	1	-3.777289	1.888177	-0.928073
31	1	3.252722	1.100223	-1.173578
32	1	2.735414	1.668069	-2.797695
33	1	3.073616	-0.739378	-2.805261
34	1	1.366847	-0.379256	-3.074568
35	1	1.722246	-2.865926	-2.580142
36	1	1.113034	-3.192336	-0.954932
37	1	-0.663314	-3.177478	-2.689494
38	1	-0.287896	-1.500603	-3.080423
39	1	-2.735358	-1.667895	-2.797896
40	1	-3.252675	-1.100145	-1.173729
41	1	-1.366470	0.379281	-3.074439
42	1	-3.073221	0.739676	-2.805603
43	1	-1.113106	3.192345	-0.954716
44	1	-1.722146	2.865966	-2.580010
45	1	0.287949	1.500686	-3.080204
46	1	0.663315	3.177581	-2.689273
47	15	-3.419042	0.367974	1.054934
48	8	-4.154384	1.239603	2.054458
49	8	-1.965358	-0.108859	1.503599
50	8	-4.213367	-0.788886	0.421098
51	15	3.419030	-0.368199	1.054943
52	8	4.154281	-1.239843	2.054521
53	8	4.213466	0.788615	0.421129
54	8	1.965360	0.108716	1.503553
55	71	0.000015	0.000046	0.602920

HF = -2242.1646697 Hartree
Zero-point correction = 0.423767
Sum of electronic and thermal Enthalpies = -2241.710914

Sum of electronic and thermal Free Energies = -2241.797048

[La(DO2A2P)]$^{3-}$ TSAP $\Delta(\delta_{1a}\delta_{1b}\delta_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.953043	1.892628	-1.276878
2	6	-1.692273	1.292018	-2.396698
3	6	-2.652430	0.175981	-1.981613
4	7	-1.978195	-0.951089	-1.311567
5	6	-1.361737	-1.846831	-2.295065
6	6	-0.195642	-2.681021	-1.756047
7	7	0.953020	-1.892607	-1.276923
8	6	1.692247	-1.291986	-2.396739
9	6	2.652405	-0.175953	-1.981649
10	7	1.978179	0.951102	-1.311570
11	6	1.361706	1.846860	-2.295045
12	6	0.195619	2.681045	-1.756000
13	6	-1.838598	2.744604	-0.442641
14	6	-1.122078	3.276744	0.826198
15	8	-0.251012	2.477597	1.326492
16	8	-1.451958	4.398177	1.238245
17	6	-2.925711	-1.667272	-0.407518
18	6	1.838571	-2.744587	-0.442692
19	6	1.122042	-3.276774	0.826123
20	8	0.250996	-2.477634	1.326467
21	8	1.452122	-4.398104	1.238291
22	6	2.925708	1.667271	-0.407524
23	1	-0.962431	0.906273	-3.118601
24	1	-2.274828	2.069840	-2.935559
25	1	-3.410389	0.549405	-1.279367
26	1	-3.184509	-0.170908	-2.893898
27	1	-1.017632	-1.243636	-3.144071
28	1	-2.118049	-2.547448	-2.708280
29	1	-0.552234	-3.278766	-0.915664
30	1	0.122705	-3.391575	-2.548882
31	1	0.962401	-0.906233	-3.118635
32	1	2.274800	-2.069801	-2.935613
33	1	3.410377	-0.549388	-1.279422
34	1	3.184469	0.170954	-2.893936
35	1	1.017588	1.243679	-3.144055
36	1	2.118013	2.547482	-2.708259
37	1	0.552222	3.278781	-0.915615
38	1	-0.122734	3.391610	-2.548823
39	1	-2.210117	3.602220	-1.033537
40	1	-2.701037	2.148111	-0.109880
41	1	-3.773669	-2.064492	-1.001564
42	1	-2.393766	-2.518797	0.027200
43	1	2.210112	-3.602186	-1.033600
44	1	2.701000	-2.148090	-0.109906
45	1	3.773663	2.064492	-1.001574
46	1	2.393773	2.518796	0.027205
47	15	-3.561165	-0.640655	1.059220

48	8	-2.162571	-0.228983	1.703901
49	8	-4.382666	-1.620246	1.875260
50	8	-4.276796	0.582204	0.456867
51	15	3.561169	0.640644	1.059207
52	8	2.162578	0.228973	1.703897
53	8	4.276795	-0.582216	0.456850
54	8	4.382677	1.620228	1.875249
55	57	0.000003	-0.000017	0.765190

HF = -2233.7848412 Hartree
Zero-point correction = 0.421784
Sum of electronic and thermal Enthalpies = -2233.332407
Sum of electronic and thermal Free Energies = -2233.420707

$[La(DO2A2P)]^{3-}$ $TS_{TSAP\text{-}1a}$ $\Delta(\delta_{1a}\delta_{1b}X_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.771136	-1.622979	1.514437
2	6	1.382957	-0.756521	2.535472
3	6	2.457832	0.198509	2.000693
4	7	1.972601	1.238918	1.068121
5	6	1.529370	2.469694	1.754753
6	6	0.009789	2.852814	1.865874
7	7	-1.014768	1.994182	1.231696
8	6	-1.933906	1.479388	2.258882
9	6	-2.874333	0.381962	1.775418
10	7	-2.153491	-0.794290	1.268667
11	6	-1.619280	-1.579418	2.385531
12	6	-0.369478	-2.390823	2.051662
13	6	1.731836	-2.592279	0.918616
14	6	1.090578	-3.348184	-0.276624
15	8	0.234902	-2.660889	-0.943651
16	8	1.448973	-4.518194	-0.474599
17	6	3.047775	1.591278	0.073248
18	6	-1.757565	2.764355	0.196759
19	6	-0.799580	3.276263	-0.907064
20	8	-0.872229	4.472752	-1.233348
21	8	-0.001628	2.384838	-1.367640
22	6	-3.013219	-1.590118	0.346829
23	1	2.619684	-2.064543	0.536188
24	1	2.055780	-3.323039	1.682040
25	1	3.920771	2.013616	0.608363
26	1	2.626341	2.372828	-0.564083
27	1	-2.266916	3.628834	0.660619
28	1	-2.520016	2.118809	-0.261887
29	1	-2.446811	-2.475763	0.042209
30	1	-3.918245	-1.934413	0.887746
31	1	1.847328	-1.375262	3.334190
32	1	0.583024	-0.177328	3.013358
33	1	3.231800	-0.365712	1.463532
34	1	2.939922	0.667505	2.883743
35	1	1.944158	2.474699	2.779283
36	1	2.009670	3.304801	1.237521
37	1	-0.091243	3.860813	1.446292

38	1	-0.232291	2.952733	2.934926
39	1	-1.316223	1.113267	3.090006
40	1	-2.551807	2.303629	2.677212
41	1	-3.534925	0.104009	2.626760
42	1	-3.522966	0.732797	0.960628
43	1	-2.386247	-2.284807	2.769342
44	1	-1.398251	-0.900377	3.216901
45	1	-0.059221	-2.945794	2.962619
46	1	-0.632428	-3.133790	1.298320
47	15	-3.506857	-0.692713	-1.256805
48	8	-4.283167	-1.729209	-2.045830
49	8	-2.053029	-0.362078	-1.829304
50	8	-4.233347	0.596230	-0.833616
51	15	3.611984	0.219720	-1.090150
52	8	4.548103	0.910775	-2.063448
53	8	4.188179	-0.896495	-0.199065
54	8	2.195970	-0.193075	-1.699894
55	57	0.031849	-0.102846	-0.754721

HF = -2233.7623651 Hartree
Zero-point correction = 0.422399
Sum of electronic and thermal Enthalpies = -2233.310058
Sum of electronic and thermal Free Energies = -2233.396698

$[La(DO2A2P)]^{3-}$ I_{1a} $\Delta(\delta_{1a}\delta_{1b}\lambda_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.703980	-1.482414	1.615249
2	6	1.294055	-0.528791	2.568766
3	6	2.370621	0.411168	1.987670
4	7	1.946620	1.307223	0.890885
5	6	1.452717	2.617163	1.338067
6	6	0.089498	2.650603	2.036024
7	7	-1.028030	2.068571	1.282174
8	6	-2.108949	1.657013	2.189857
9	6	-2.988999	0.539193	1.635376
10	7	-2.225735	-0.653110	1.236586
11	6	-1.720350	-1.357602	2.418703
12	6	-0.459945	-2.192566	2.187548
13	6	1.673336	-2.507275	1.138805
14	6	1.060096	-3.368282	0.002419
15	8	0.222104	-2.743679	-0.745651
16	8	1.417992	-4.551909	-0.080157
17	6	3.082087	1.546495	-0.061503
18	6	-1.563436	2.980502	0.247215
19	6	-0.590849	3.297615	-0.919932
20	8	-0.484278	4.486179	-1.264377
21	8	-0.007108	2.279507	-1.428170
22	6	-3.050080	-1.511811	0.338339
23	1	2.575652	-2.017568	0.736298
24	1	1.969905	-3.164617	1.976703
25	1	3.938685	1.987872	0.485351
26	1	2.727870	2.284655	-0.785416
27	1	-1.880543	3.933673	0.711602

28	1	-2.442547	2.497639	-0.199013
29	1	-2.474290	-2.415269	0.112505
30	1	-3.973275	-1.822796	0.869090
31	1	1.765312	-1.076385	3.414005
32	1	0.473891	0.054319	2.996597
33	1	3.192728	-0.193522	1.583403
34	1	2.769841	1.004573	2.837611
35	1	2.179793	3.078779	2.043057
36	1	1.414709	3.266177	0.463564
37	1	-0.116674	3.710424	2.298975
38	1	0.168053	2.112952	2.987280
39	1	-1.647398	1.340837	3.134132
40	1	-2.761018	2.516876	2.451104
41	1	-3.738433	0.283636	2.418549
42	1	-3.549264	0.860800	0.745734
43	1	-2.496143	-2.036452	2.832527
44	1	-1.521283	-0.621593	3.205310
45	1	-0.177983	-2.664178	3.152812
46	1	-0.703171	-3.000302	1.497046
47	15	-3.491211	-0.725457	-1.341739
48	8	-4.269794	-1.808338	-2.064890
49	8	-2.016969	-0.475518	-1.906360
50	8	-4.200575	0.604975	-1.040357
51	15	3.633839	0.057261	-1.069945
52	8	4.621735	0.611728	-2.078867
53	8	4.141069	-0.981051	-0.051934
54	8	2.218490	-0.361032	-1.683631
55	57	0.035231	-0.183630	-0.786961

HF = -2233.7754196 Hartree
Zero-point correction = 0.422531
Sum of electronic and thermal Enthalpies = -2233.322376
Sum of electronic and thermal Free Energies = -2233.410356

$[La(DO2A2P)]^{3-}$ TS_{1a-2a} $\Delta(X_{1a}\delta_{1b}\lambda_{2a}\delta_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.770289	-1.572092	1.571195
2	6	1.532994	-0.728191	2.509490
3	6	2.579995	0.205204	1.880483
4	7	2.085395	1.188502	0.900881
5	6	1.605799	2.438505	1.499878
6	6	0.272601	2.359411	2.256382
7	7	-0.855102	1.784311	1.499987
8	6	-1.819301	1.165517	2.424392
9	6	-2.830906	0.252817	1.744498
10	7	-2.214010	-0.911987	1.087800
11	6	-1.816410	-1.933684	2.076003
12	6	-0.304110	-2.304287	2.292800
13	6	1.638685	-2.575397	0.885996
14	6	0.800480	-3.376399	-0.140599
15	8	-0.017320	-2.660399	-0.822499
16	8	0.964477	-4.606399	-0.198695
17	6	3.146293	1.498296	-0.109223

18	6	-1.518602	2.809710	0.654585
19	6	-0.606904	3.355104	-0.474719
20	8	-0.552101	4.586103	-0.631824
21	8	0.001192	2.450500	-1.145818
22	6	-3.154914	-1.462688	0.056905
23	1	2.469885	-2.073101	0.365192
24	1	2.068585	-3.271295	1.628897
25	1	4.053995	1.875695	0.402473
26	1	2.753893	2.301694	-0.737625
27	1	-1.859498	3.651313	1.285783
28	1	-2.390305	2.353310	0.164989
29	1	-2.685518	-2.361891	-0.351793
30	1	-4.105014	-1.759484	0.544208
31	1	2.077894	-1.369190	3.236690
32	1	0.801697	-0.160887	3.092289
33	1	3.329792	-0.398799	1.352384
34	1	3.093298	0.720906	2.721780
35	1	2.356902	2.838406	2.218175
36	1	1.514499	3.171403	0.699376
37	1	0.023805	3.383613	2.599079
38	1	0.413002	1.763814	3.163684
39	1	-1.247901	0.588118	3.164292
40	1	-2.373098	1.942021	2.995291
41	1	-3.553404	-0.078778	2.522501
42	1	-3.405506	0.782516	0.972298
43	1	-2.321013	-2.868084	1.803408
44	1	-2.229807	-1.649380	3.058603
45	1	-0.098307	-2.250084	3.375199
46	1	-0.201314	-3.359688	2.027804
47	15	-3.510716	-0.321992	-1.416098
48	8	-4.428620	-1.135493	-2.309393
49	8	-2.023217	-0.146898	-1.970303
50	8	-4.043011	1.001311	-0.836102
51	15	3.577186	0.081991	-1.276419
52	8	4.500285	0.692485	-2.313724
53	8	4.123985	-1.054708	-0.393216
54	8	2.106384	-0.255108	-1.807314
55	57	-0.003513	-0.083999	-0.758709

HF = -2233.7643163 Hartree
Zero-point correction = 0.422894
Sum of electronic and thermal Enthalpies = -2233.311647
Sum of electronic and thermal Free Energies = -2233.397817

$[La(DO2A2P)]^{3-}$ I_{2a} $\Delta(\lambda_{1a}\delta_{1b}\lambda_{2a}\delta_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.839471	1.579642	-1.596588
2	6	1.739700	0.841642	-2.503461
3	6	2.723278	-0.116503	-1.820208
4	7	2.139828	-1.124223	-0.918956
5	6	1.618856	-2.317469	-1.596230
6	6	0.291489	-2.153237	-2.360052
7	7	-0.839526	-1.579632	-1.596564

8	6	-1.739793	-0.841716	-2.503459
9	6	-2.723360	0.116472	-1.820244
10	7	-2.139942	1.124163	-0.918934
11	6	-1.618900	2.317433	-1.596113
12	6	-0.291634	2.153095	-2.360063
13	6	1.587257	2.640957	-0.868883
14	6	0.730076	3.350689	0.207946
15	8	0.040811	2.558682	0.943486
16	8	0.780855	4.589928	0.268861
17	6	3.155147	-1.514828	0.110878
18	6	-1.587320	-2.640856	-0.868730
19	6	-0.730080	-3.350580	0.208054
20	8	-0.780747	-4.589828	0.268893
21	8	-0.040729	-2.558574	0.943512
22	6	-3.155355	1.514718	0.110826
23	1	2.448345	2.181597	-0.356572
24	1	1.958085	3.392007	-1.590548
25	1	4.080021	-1.866229	-0.388204
26	1	2.734575	-2.353665	0.671393
27	1	-1.958247	-3.391926	-1.590321
28	1	-2.448349	-2.181424	-0.356378
29	1	-2.735038	2.353772	0.671207
30	1	-4.080310	1.865773	-0.388346
31	1	2.344704	1.550683	-3.108439
32	1	1.112877	0.299369	-3.216344
33	1	3.425960	0.461740	-1.206083
34	1	3.305136	-0.611354	-2.629677
35	1	2.359294	-2.702965	-2.333528
36	1	1.491949	-3.088489	-0.838142
37	1	0.016441	-3.151863	-2.751211
38	1	0.462531	-1.523586	-3.237506
39	1	-1.113016	-0.299494	-3.216421
40	1	-2.344813	-1.550820	-3.108349
41	1	-3.305158	0.611361	-2.629733
42	1	-3.426084	-0.461767	-1.206169
43	1	-1.491789	3.088297	-0.837907
44	1	-2.359359	2.703162	-2.333271
45	1	-0.462759	1.523256	-3.237362
46	1	-0.016661	3.151649	-2.751462
47	15	-3.539367	0.169941	1.381895
48	8	-4.481681	0.825905	2.373936
49	8	-2.058216	-0.075546	1.930497
50	8	-4.047943	-1.048901	0.589123
51	15	3.539410	-0.169995	1.381821
52	8	4.481740	-0.826003	2.373815
53	8	4.048039	1.048785	0.588987
54	8	2.058309	0.075637	1.930493
55	57	0.000044	0.000044	0.771869

HF = -2233.7790201 Hartree
Zero-point correction = 0.423464
Sum of electronic and thermal Enthalpies = -2233.325272
Sum of electronic and thermal Free Energies = -2233.412468

$[La(DO2A2P)]^{3-}$ TS_{2a-3a} $\Delta(\lambda_{1a}\delta_{1b}\lambda_{2a}X_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.056601	-1.530108	1.490701
2	6	2.231000	-0.962505	2.218300
3	6	2.771196	0.465196	1.873801
4	7	2.133493	1.274996	0.813902
5	6	1.584090	2.528594	1.346204
6	6	0.325091	2.336990	2.197304
7	7	-0.830208	1.733687	1.506805
8	6	-1.718405	1.089184	2.492405
9	6	-2.670903	0.043382	1.908305
10	7	-2.048700	-1.011916	1.090303
11	6	-1.434997	-2.090615	1.876802
12	6	-0.033397	-1.809712	2.451801
13	6	1.507904	-2.775706	0.799699
14	6	0.496505	-3.405808	-0.180900
15	8	-0.156198	-2.572209	-0.900599
16	8	0.425508	-4.646608	-0.207001
17	6	3.109092	1.554399	-0.284698
18	6	-1.589611	2.735586	0.710606
19	6	-0.796413	3.338789	-0.476694
20	8	-0.896417	4.560489	-0.672093
21	8	-0.111011	2.493291	-1.155095
22	6	-3.072300	-1.543818	0.130604
23	1	2.400403	-2.489803	0.224199
24	1	1.789207	-3.534506	1.552199
25	1	4.021991	2.022201	0.134701
26	1	2.639589	2.276698	-0.958497
27	1	-1.922913	3.557084	1.371407
28	1	-2.476310	2.239484	0.284006
29	1	-2.620198	-2.399516	-0.375597
30	1	-3.961298	-1.896721	0.689804
31	1	3.072702	-1.635703	2.047799
32	1	2.011201	-0.990607	3.297500
33	1	3.806996	0.303599	1.568700
34	1	2.776395	1.054096	2.807102
35	1	2.330489	3.047295	1.988103
36	1	1.373788	3.186794	0.506504
37	1	0.047289	3.317388	2.635205
38	1	0.587594	1.683490	3.039004
39	1	-1.086503	0.641685	3.265504
40	1	-2.338507	1.849682	3.012606
41	1	-3.225201	-0.406720	2.761805
42	1	-3.401405	0.537680	1.253705
43	1	-1.389495	-2.980514	1.249501
44	1	-2.078596	-2.349817	2.746802
45	1	-0.091299	-0.957312	3.131502
46	1	0.236705	-2.687411	3.076800
47	15	-3.567604	-0.321918	-1.229395
48	8	-4.515102	-1.097220	-2.126095
49	8	-2.123905	-0.048114	-1.855096
50	8	-4.108407	0.935380	-0.519594
51	15	3.529395	0.034001	-1.312900
52	8	4.514693	0.514904	-2.363300
53	8	3.988499	-1.044299	-0.315501
54	8	2.064795	-0.278303	-1.875199
55	57	-0.017904	-0.033309	-0.771097

HF = -2233.7628818 Hartree

Zero-point correction = 0.423267
Sum of electronic and thermal Enthalpies = -2233.309811
Sum of electronic and thermal Free Energies = -2233.396245

$[La(DO2A2P)]^{3-}$ I_{3a} $\Delta(\lambda_{1a}\delta_{1b}\lambda_{2a}\lambda_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.192241	-1.576082	1.393552
2	6	2.415196	-0.941710	1.939454
3	6	2.289553	0.563484	2.158733
4	7	2.024418	1.329752	0.937195
5	6	1.499283	2.666116	1.254430
6	6	0.152206	2.678784	1.997528
7	7	-0.911120	1.838988	1.400322
8	6	-1.666416	1.137247	2.453432
9	6	-2.568344	0.004847	1.957359
10	7	-1.915675	-1.049879	1.157854
11	6	-1.249854	-2.083750	1.968291
12	6	0.182372	-1.772787	2.445201
13	6	1.572107	-2.854352	0.740850
14	6	0.522494	-3.427094	-0.238283
15	8	-0.070013	-2.553584	-0.963065
16	8	0.373859	-4.660978	-0.262232
17	6	3.226203	1.450234	0.051610
18	6	-1.801912	2.665420	0.540689
19	6	-1.033973	3.300697	-0.646247
20	8	-1.254351	4.493218	-0.910099
21	8	-0.221982	2.505599	-1.244894
22	6	-2.935356	-1.661165	0.237408
23	1	2.473209	-2.640569	0.150398
24	1	1.812300	-3.617082	1.503980
25	1	4.121004	1.647345	0.674730
26	1	3.064165	2.338012	-0.565337
27	1	-2.257598	3.470982	1.145298
28	1	-2.609590	2.035824	0.133191
29	1	-2.446240	-2.496697	-0.267057
30	1	-3.782641	-2.055322	0.831668
31	1	3.222306	-1.115706	1.213914
32	1	2.692162	-1.411047	2.907598
33	1	3.229502	0.913772	2.638639
34	1	1.488201	0.767189	2.876467
35	1	2.220416	3.244254	1.875954
36	1	1.382138	3.191297	0.307573
37	1	-0.180684	3.729590	2.050409
38	1	0.303448	2.361017	3.036086
39	1	-0.938424	0.755286	3.177486
40	1	-2.313098	1.847548	3.013069
41	1	-3.053813	-0.438836	2.853848
42	1	-3.360237	0.421412	1.319369
43	1	-1.226932	-3.004857	1.384181
44	1	-1.848662	-2.304095	2.878380
45	1	0.171879	-0.877028	3.071471
46	1	0.492323	-2.609925	3.107466
47	15	-3.553927	-0.509294	-1.131801

48	8	-4.433527	-1.380824	-2.008114
49	8	-2.149840	-0.104023	-1.776394
50	8	-4.204475	0.699709	-0.430225
51	15	3.592512	0.101537	-1.239294
52	8	4.568603	0.792641	-2.175458
53	8	4.082089	-1.157771	-0.504547
54	8	2.123326	-0.090964	-1.830341
55	57	-0.001646	-0.009394	-0.777098

HF = -2233.7773806 Hartree
Zero-point correction = 0.422957
Sum of electronic and thermal Enthalpies = -2233.324009
Sum of electronic and thermal Free Energies = -2233.411533

$[La(DO2A2P)]^{3-}$ $TS_{3a\text{-}SAP}$ $\Delta(\lambda_{1a}X_{1b}\lambda_{2a}\lambda_{2b})$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.231724	1.648280	1.306891
2	6	-2.407707	1.003996	1.934859
3	6	-2.206822	-0.473087	2.256111
4	7	-1.881206	-1.306039	1.091454
5	6	-1.253006	-2.566772	1.520236
6	6	0.135546	-2.406341	2.156486
7	7	1.165825	-1.734102	1.335341
8	6	2.209233	-1.127211	2.208401
9	6	2.589847	0.382476	2.052735
10	7	1.888265	1.249946	1.076536
11	6	1.170838	2.350046	1.742295
12	6	-0.198874	1.954233	2.308691
13	6	-1.687405	2.858043	0.576367
14	6	-0.714407	3.404997	-0.495965
15	8	-0.057382	2.516863	-1.144979
16	8	-0.682067	4.636935	-0.654720
17	6	-3.074033	-1.586307	0.226865
18	6	1.824732	-2.709607	0.412591
19	6	0.918659	-3.306335	-0.686821
20	8	1.102564	-4.496949	-0.987463
21	8	0.063828	-2.499360	-1.204539
22	6	2.868990	1.776704	0.069230
23	1	-2.603481	2.565913	0.046382
24	1	-1.930561	3.668496	1.287592
25	1	-3.928329	-1.876771	0.870177
26	1	-2.809334	-2.456168	-0.379295
27	1	2.241617	-3.544235	1.004890
28	1	2.656804	-2.171060	-0.066120
29	1	2.334208	2.497356	-0.553467
30	1	3.690383	2.305016	0.591379
31	1	-3.245362	1.084984	1.226766
32	1	-2.677116	1.530112	2.875844
33	1	-3.134835	-0.841980	2.742620
34	1	-1.409252	-0.586817	2.997822
35	1	-1.889784	-3.095181	2.265033
36	1	-1.180113	-3.205819	0.642785
37	1	0.480607	-3.418053	2.450256

38	1	0.031806	-1.841884	3.088399
39	1	1.909122	-1.287246	3.254285
40	1	3.140106	-1.681930	2.057378
41	1	2.500039	0.843754	3.051274
42	1	3.642436	0.376624	1.764520
43	1	1.049783	3.163768	1.028600
44	1	1.771381	2.758090	2.582273
45	1	-0.068341	1.070240	2.945568
46	1	-0.550431	2.774649	2.971319
47	15	3.542195	0.448180	-1.085616
48	8	4.460635	1.177371	-2.049556
49	8	2.160095	-0.041789	-1.720956
50	8	4.153044	-0.640449	-0.182864
51	15	-3.621489	-0.320916	-1.087593
52	8	-4.545002	-1.143234	-1.969568
53	8	-4.227828	0.903206	-0.379003
54	8	-2.200334	0.011667	-1.727338
55	57	-0.022703	-0.004746	-0.760426

HF = -2233.7625292 Hartree
Zero-point correction = 0.422918
Sum of electronic and thermal Enthalpies = -2233.309754
Sum of electronic and thermal Free Energies = -2233.396203

$[La(DO2A2P)]^{3-}$ SAP $\Delta(\lambda_{1a}\lambda_{1b}\lambda_{2a}\lambda_{2b})$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.293023	1.759141	1.218241
2	6	-2.432804	1.081944	1.876293
3	6	-2.133614	-0.358428	2.285550
4	7	-1.773599	-1.250356	1.173403
5	6	-1.110771	-2.460578	1.696531
6	6	0.320524	-2.238951	2.210493
7	7	1.293386	-1.759161	1.218100
8	6	2.433237	-1.082173	1.876256
9	6	2.134138	0.358161	2.285683
10	7	1.773970	1.250148	1.173630
11	6	1.111188	2.460347	1.696877
12	6	-0.320155	2.238747	2.210726
13	6	-1.797575	2.859594	0.360922
14	6	-0.783068	3.394741	-0.678715
15	8	-0.023503	2.507205	-1.208160
16	8	-0.811322	4.611150	-0.927758
17	6	-2.954063	-1.629317	0.324980
18	6	1.797753	-2.859452	0.360477
19	6	0.782888	-3.394563	-0.678840
20	8	0.810957	-4.610995	-0.927790
21	8	0.023211	-2.507015	-1.208109
22	6	2.954276	1.629131	0.324997
23	1	-2.654342	2.455769	-0.193478
24	1	-2.146716	3.702521	0.984933
25	1	-3.784666	-1.950750	0.984134
26	1	-2.634383	-2.497763	-0.255450
27	1	2.147152	-3.702424	0.984280

28	1	2.654301	-2.455513	-0.194175
29	1	2.634528	2.497699	-0.255212
30	1	3.785054	1.950387	0.984016
31	1	-3.274305	1.070264	1.166616
32	1	-2.743557	1.640279	2.784899
33	1	-3.028779	-0.752674	2.812237
34	1	-1.316285	-0.378931	3.017110
35	1	-1.700096	-2.901101	2.530394
36	1	-1.092892	-3.198891	0.896500
37	1	0.669086	-3.196443	2.650536
38	1	0.301898	-1.518199	3.035092
39	1	2.743954	-1.640657	2.784781
40	1	3.274747	-1.070443	1.166585
41	1	1.316895	0.378617	3.017337
42	1	3.029373	0.752352	2.812291
43	1	1.093388	3.198748	0.896930
44	1	1.700513	2.900727	2.530815
45	1	-0.301607	1.517869	3.035219
46	1	-0.668674	3.196192	2.650909
47	15	3.595236	0.450048	-1.030985
48	8	4.434589	1.373912	-1.895183
49	8	2.204084	0.005426	-1.668891
50	8	4.313720	-0.735985	-0.364594
51	15	-3.595439	-0.450072	-1.030646
52	8	-4.434818	-1.373894	-1.894867
53	8	-4.313943	0.735744	-0.363891
54	8	-2.204420	-0.005194	-1.668652
55	57	-0.000120	0.000110	-0.759240

HF = -2233.7806458 Hartree
Zero-point correction = 0.422549
Sum of electronic and thermal Enthalpies = -2233.327568
Sum of electronic and thermal Free Energies = -2233.415626

[Lu(DOTA)]$^-$ A (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.062833	-0.477158	1.012849
2	6	2.560000	0.783922	1.604706
3	6	1.427475	1.699660	2.075547
4	7	0.473094	2.066224	1.010059
5	6	-0.788990	2.564508	1.598822
6	6	-1.705350	1.432913	2.070831
7	7	-2.070206	0.476864	1.006987
8	6	-2.570005	-0.783960	1.596535
9	6	-1.439341	-1.700285	2.071089
10	7	-0.482022	-2.065930	1.008394
11	6	0.779056	-2.564271	1.599409
12	6	1.693353	-1.432940	2.075598
13	6	3.062389	-1.067386	0.084143
14	6	2.442666	-2.043838	-0.945542
15	8	1.284493	-1.682921	-1.394642

16	8	3.080289	-3.047227	-1.256773
17	6	1.063761	3.063032	0.078852
18	6	2.043239	2.440035	-0.945883
19	8	3.047792	3.076627	-1.256272
20	8	1.682577	1.281542	-1.393990
21	6	-3.063344	1.066767	0.071749
22	6	-2.434714	2.043117	-0.952419
23	8	-3.064209	3.052908	-1.261384
24	8	-1.277079	1.677358	-1.397430
25	6	-1.070443	-3.061322	0.074273
26	6	-2.045898	-2.434476	-0.952084
27	8	-3.055595	-3.064277	-1.260247
28	8	-1.678596	-1.278389	-1.400380
29	1	3.491945	-0.248236	-0.498237
30	1	3.866002	-1.576090	0.636924
31	1	1.570725	3.869138	0.629397
32	1	0.244990	3.489428	-0.506430
33	1	-3.870600	1.575979	0.618725
34	1	-3.489031	0.247605	-0.513442
35	1	-0.250360	-3.487658	-0.509185
36	1	-1.579889	-3.867630	0.622265
37	1	3.161729	1.301136	0.857293
38	1	3.225870	0.583844	2.462927
39	1	1.875151	2.606112	2.521247
40	1	0.868272	1.205585	2.877022
41	1	-0.590535	3.231944	2.456240
42	1	-1.305568	3.164775	0.849740
43	1	-2.612595	1.881781	2.513804
44	1	-1.212734	0.875364	2.874473
45	1	-3.238713	-0.584743	2.452853
46	1	-3.169289	-1.301209	0.847141
47	1	-0.882769	-1.206757	2.874789
48	1	-1.888242	-2.607391	2.514052
49	1	1.297858	-3.162126	0.850005
50	1	0.579599	-3.233864	2.454939
51	1	1.197078	-0.874731	2.876428
52	1	2.598813	-1.881317	2.522367
53	71	0.004872	-0.002236	-0.645326

HF = -1485.2885873 Hartree
Zero-point correction = 0.428133
Sum of electronic and thermal Enthalpies = -1484.833339
Sum of electronic and thermal Free Energies = -1484.914019

$[Lu(DOTA)]^-$ TS_{A-IA} (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.039076	-2.163438	1.211996
2	6	1.405410	-2.274871	1.756485
3	6	1.980677	-0.959114	2.280184
4	7	2.162958	0.040876	1.214985
5	6	2.270294	1.407319	1.760488
6	6	0.951225	1.978091	2.281100
7	7	-0.044663	2.162870	1.212608
8	6	-1.412691	2.273906	1.753319

9	6	-1.988449	0.957948	2.276220
10	7	-2.168348	-0.041945	1.210619
11	6	-2.277374	-1.408285	1.755616
12	6	-0.959600	-1.980056	2.278204
13	6	-0.268851	-3.378700	0.407995
14	6	-0.169022	-3.189633	-1.127205
15	8	-0.442974	-1.993797	-1.523200
16	8	0.065598	-4.185732	-1.801409
17	6	3.379622	-0.265046	0.412375
18	6	3.191529	-0.170404	-1.123324
19	8	4.188518	0.062220	-1.797131
20	8	1.996286	-0.445754	-1.519615
21	6	0.265553	3.378928	0.410809
22	6	0.175602	3.190336	-1.124991
23	8	-0.052926	4.187318	-1.800186
24	8	0.449747	1.994301	-1.519896
25	6	-3.382223	0.264172	0.403930
26	6	-3.188647	0.172020	-1.131172
27	8	-4.183142	-0.059310	-1.809065
28	8	-1.991809	0.447466	-1.522881
29	1	0.364604	-4.220052	0.716388
30	1	-1.303285	-3.682496	0.603803
31	1	3.686725	-1.297994	0.611070
32	1	4.218488	0.371813	0.719670
33	1	1.297999	3.685230	0.613302
34	1	-0.371602	4.218591	0.715616
35	1	-4.221789	-0.373987	0.706834
36	1	-3.691425	1.296426	0.603135
37	1	2.040640	-2.648924	0.948179
38	1	1.447168	-3.026919	2.566783
39	1	2.938957	-1.174265	2.786876
40	1	1.321876	-0.546781	3.049690
41	1	3.019850	1.450177	2.573082
42	1	2.645347	2.043854	0.953787
43	1	1.161870	2.934282	2.793601
44	1	0.536278	1.314192	3.044701
45	1	-1.457334	3.026459	2.563022
46	1	-2.045837	2.646756	0.942925
47	1	-1.330937	0.545515	3.046814
48	1	-2.947623	1.172798	2.781329
49	1	-2.651439	-2.044619	0.948218
50	1	-3.028317	-1.451043	2.566922
51	1	-0.546246	-1.317355	3.043803
52	1	-1.171540	-2.936944	2.788704
53	71	0.001292	-0.000093	-0.702998

HF = -1485.2522458 Hartree
Zero-point correction = 0.425687
Sum of electronic and thermal Enthalpies = -1484.799223
Sum of electronic and thermal Free Energies = -1484.882786

[Lu(DOTA)]$^-$ IA (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.624427	-1.331277	1.132895

2	6	-2.175991	-0.477232	2.196071
3	6	-2.494367	0.936260	1.711147
4	7	-1.323792	1.628323	1.132333
5	6	-0.465866	2.185938	2.189177
6	6	0.945715	2.501531	1.697290
7	7	1.635123	1.327523	1.122080
8	6	2.196192	0.474541	2.181115
9	6	2.510770	-0.938917	1.694375
10	7	1.335575	-1.630014	1.123684
11	6	0.484578	-2.188241	2.185832
12	6	-0.929847	-2.504563	1.702721
13	6	-2.663506	-1.794108	0.181249
14	6	-2.026251	-2.406388	-1.094690
15	8	-0.865763	-1.912551	-1.394500
16	8	-2.648496	-3.277979	-1.689146
17	6	-1.791270	2.661421	0.176161
18	6	-2.421008	2.011730	-1.084871
19	8	-1.913211	0.859724	-1.393405
20	8	-3.310258	2.620814	-1.666973
21	6	2.664892	1.789604	0.159692
22	6	2.009238	2.417205	-1.099171
23	8	0.857725	1.905787	-1.403379
24	8	2.609462	3.314134	-1.678875
25	6	1.795516	-2.663187	0.163945
26	6	2.417322	-2.012429	-1.100155
27	8	1.902273	-0.863655	-1.408667
28	8	3.310072	-2.616021	-1.682868
29	1	-1.442945	-0.429108	3.009173
30	1	-3.090819	-0.921019	2.629341
31	1	-3.268454	0.892118	0.943013
32	1	-2.918960	1.516259	2.549578
33	1	-0.414865	1.457170	3.005946
34	1	-0.908137	3.103064	2.619158
35	1	0.898456	3.271293	0.924985
36	1	1.529280	2.930751	2.530875
37	1	1.469878	0.426672	3.000209
38	1	3.114455	0.919024	2.606307
39	1	3.279190	-0.894995	0.920524
40	1	2.941321	-1.519031	2.529706
41	1	0.438441	-1.460207	3.003514
42	1	0.930001	-3.105531	2.612109
43	1	-0.886721	-3.273237	0.929190
44	1	-1.506988	-2.935018	2.540240
45	1	-3.336840	-2.528964	0.648766
46	1	-3.255207	-0.935479	-0.143979
47	1	-2.518061	3.342403	0.645079
48	1	-0.932789	3.245117	-0.163985
49	1	3.349660	2.516133	0.623440
50	1	3.244692	0.928611	-0.181016
51	1	2.524605	-3.345016	0.627960
52	1	0.933662	-3.244977	-0.170969
53	71	-0.002836	-0.001675	-0.597647

HF = -1485.2831556 Hartree
Zero-point correction = 0.426810
Sum of electronic and thermal Enthalpies = -1484.828890
Sum of electronic and thermal Free Energies = -1484.910675

[Lu(DOTA)]$^-$ SAP $\Delta(\lambda\lambda\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.062833	-0.477158	1.012849
2	6	2.560000	0.783922	1.604706
3	6	1.427475	1.699660	2.075547
4	7	0.473094	2.066224	1.010059
5	6	-0.788990	2.564508	1.598822
6	6	-1.705350	1.432913	2.070831
7	7	-2.070206	0.476864	1.006987
8	6	-2.570005	-0.783960	1.596535
9	6	-1.439341	-1.700285	2.071089
10	7	-0.482022	-2.065930	1.008394
11	6	0.779056	-2.564271	1.599409
12	6	1.693353	-1.432940	2.075598
13	6	3.062389	-1.067386	0.084143
14	6	2.442666	-2.043838	-0.945542
15	8	1.284493	-1.682921	-1.394642
16	8	3.080289	-3.047227	-1.256773
17	6	1.063761	3.063032	0.078852
18	6	2.043239	2.440035	-0.945883
19	8	3.047792	3.076627	-1.256272
20	8	1.682577	1.281542	-1.393990
21	6	-3.063344	1.066767	0.071749
22	6	-2.434714	2.043117	-0.952419
23	8	-3.064209	3.052908	-1.261384
24	8	-1.277079	1.677358	-1.397430
25	6	-1.070443	-3.061322	0.074273
26	6	-2.045898	-2.434476	-0.952084
27	8	-3.055595	-3.064277	-1.260247
28	8	-1.678596	-1.278389	-1.400380
29	1	3.491945	-0.248236	-0.498237
30	1	3.866002	-1.576090	0.636924
31	1	1.570725	3.869138	0.629397
32	1	0.244990	3.489428	-0.506430
33	1	-3.870600	1.575979	0.618725
34	1	-3.489031	0.247605	-0.513442
35	1	-0.250360	-3.487658	-0.509185
36	1	-1.579889	-3.867630	0.622265
37	1	3.161729	1.301136	0.857293
38	1	3.225870	0.583844	2.462927
39	1	1.875151	2.606112	2.521247
40	1	0.868272	1.205585	2.877022
41	1	-0.590535	3.231944	2.456240
42	1	-1.305568	3.164775	0.849740
43	1	-2.612595	1.881781	2.513804
44	1	-1.212734	0.875364	2.874473
45	1	-3.238713	-0.584743	2.452853
46	1	-3.169289	-1.301209	0.847141
47	1	-0.882769	-1.206757	2.874789
48	1	-1.888242	-2.607391	2.514052
49	1	1.297858	-3.162126	0.850005
50	1	0.579599	-3.233864	2.454939
51	1	1.197078	-0.874731	2.876428

52	1	2.598813	-1.881317	2.522367
53	71	0.004872	-0.002236	-0.645326

HF = -1485.2885873 Hartree
Zero-point correction = 0.428133
Sum of electronic and thermal Enthalpies = -1484.833339
Sum of electronic and thermal Free Energies = -1484.914019

[Lu(DOTA)]$^-$ TS_{SAP-1} $\Delta(X\lambda\lambda\lambda)$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.097305	2.043300	1.145907
2	6	-1.310103	2.138758	2.001505
3	6	-2.401860	1.025415	1.879995
4	7	-2.171519	-0.144891	0.992789
5	6	-2.107387	-1.423199	1.735481
6	6	-0.692207	-1.775776	2.201783
7	7	0.266085	-1.984419	1.094484
8	6	1.650378	-2.089794	1.610187
9	6	2.267848	-0.738729	1.968896
10	7	2.256801	0.227879	0.855102
11	6	2.394371	1.606769	1.359811
12	6	1.108896	2.114032	2.008511
13	6	-0.086145	3.155805	0.146614
14	6	0.969049	2.985757	-0.971584
15	8	1.092887	1.775753	-1.413091
16	8	1.587402	3.979027	-1.346477
17	6	-3.242217	-0.163129	-0.047314
18	6	-3.020155	0.981565	-1.058407
19	8	-3.982420	1.638818	-1.445005
20	8	-1.778546	1.131503	-1.406003
21	6	-0.075576	-3.198296	0.302576
22	6	-1.193262	-2.971032	-0.741626
23	8	-1.993309	-3.882489	-0.948034
24	8	-1.163800	-1.812930	-1.310419
25	6	3.308787	-0.082670	-0.143897
26	6	2.919129	-1.240944	-1.092605
27	8	3.778387	-2.062687	-1.405808
28	8	1.685032	-1.214477	-1.477408
29	1	-1.060643	3.159559	-0.347589
30	1	0.072404	4.120194	0.652020
31	1	-4.239314	-0.075280	0.406184
32	1	-3.172965	-1.101930	-0.599220
33	1	-0.347222	-4.036386	0.961070
34	1	0.813411	-3.475739	-0.269724
35	1	3.429235	0.801927	-0.775191
36	1	4.268574	-0.309123	0.344004
37	1	-1.797452	3.102384	1.814909
38	1	-0.989503	2.174235	3.048306
39	1	-3.321434	1.513265	1.543096
40	1	-2.609882	0.660120	2.894492
41	1	-2.761589	-1.401771	2.623379
42	1	-2.488727	-2.219076	1.094175
43	1	-0.746056	-2.680977	2.834377

44	1	-0.312567	-0.966099	2.836388
45	1	1.688942	-2.740802	2.501883
46	1	2.260055	-2.569621	0.844085
47	1	1.724068	-0.301705	2.811098
48	1	3.299838	-0.913384	2.322798
49	1	2.675907	2.250059	0.527316
50	1	3.204273	1.681022	2.108913
51	1	0.904463	1.521237	2.905507
52	1	1.277049	3.150021	2.351217
53	71	-0.004108	-0.009895	-0.633705

HF = -1485.2659033 Hartree
Zero-point correction = 0.427752
Sum of electronic and thermal Enthalpies = -1484.811444
Sum of electronic and thermal Free Energies = -1484.891824

[Lu(DOTA)]$^-$ I_1 $\Delta(\delta\lambda\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.500746	1.913540	1.266378
2	6	-0.565864	2.020188	2.281629
3	6	-1.952822	1.694201	1.739727
4	7	-2.071248	0.391821	1.050974
5	6	-2.183139	-0.765822	1.966671
6	6	-0.846535	-1.448577	2.306923
7	7	-0.086484	-1.932617	1.133541
8	6	1.275831	-2.367285	1.525329
9	6	2.242477	-1.214212	1.796798
10	7	2.370706	-0.270258	0.672086
11	6	2.868626	1.038411	1.132514
12	6	1.820293	1.815977	1.931828
13	6	0.487418	3.064578	0.322846
14	6	1.396228	2.823620	-0.912374
15	8	1.314392	1.629244	-1.403282
16	8	2.102416	3.746436	-1.308656
17	6	-3.225438	0.496486	0.113420
18	6	-2.867829	1.375594	-1.111237
19	8	-3.774011	1.972364	-1.681136
20	8	-1.604358	1.389474	-1.415804
21	6	-0.795366	-3.053533	0.457472
22	6	-1.911620	-2.579117	-0.500168
23	8	-2.968605	-3.211093	-0.533435
24	8	-1.601891	-1.534566	-1.186186
25	6	3.234572	-0.813196	-0.401900
26	6	2.510346	-1.842843	-1.300641
27	8	3.112933	-2.855940	-1.647704
28	8	1.301186	-1.505516	-1.615542
29	1	-0.528304	3.189025	-0.060894
30	1	0.797678	3.988264	0.834223
31	1	-4.109982	0.915465	0.615027
32	1	-3.472513	-0.497102	-0.262534
33	1	-1.202997	-3.762169	1.193078
34	1	-0.064407	-3.576394	-0.165342
35	1	3.507019	0.022783	-1.052773

36	1	4.153314	-1.259617	0.007957
37	1	-0.596784	3.030958	2.727761
38	1	-0.324399	1.331831	3.097869
39	1	-2.245538	2.464468	1.023472
40	1	-2.674037	1.757558	2.574430
41	1	-2.657918	-0.471963	2.918963
42	1	-2.845209	-1.501573	1.505290
43	1	-1.065361	-2.290033	2.990468
44	1	-0.206576	-0.754554	2.857683
45	1	1.237677	-3.009182	2.423737
46	1	1.673437	-2.980919	0.715848
47	1	1.912057	-0.659677	2.679264
48	1	3.225033	-1.648073	2.056666
49	1	3.166686	1.609842	0.254924
50	1	3.767183	0.927569	1.767997
51	1	1.671791	1.332654	2.902563
52	1	2.222354	2.819578	2.148440
53	71	-0.032617	-0.002904	-0.653155

HF = -1485.2782449 Hartree
Zero-point correction = 0.427661
Sum of electronic and thermal Enthalpies = -1484.823239
Sum of electronic and thermal Free Energies = -1484.904891

[Lu(DOTA)]$^-$ TS_{1-2a} $\Delta(\delta\lambda X\lambda)$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.170415	-1.801210	1.164984
2	6	-0.211460	-2.304827	2.163473
3	6	1.213241	-2.355692	1.634761
4	7	1.713515	-1.047942	1.143364
5	6	2.063142	-0.160416	2.277067
6	6	1.612802	1.343742	2.238979
7	7	0.755047	1.844769	1.125488
8	6	-0.440216	2.567055	1.629402
9	6	-1.618328	1.639844	1.923007
10	7	-2.117072	0.935105	0.727607
11	6	-3.059870	-0.139985	1.091109
12	6	-2.393256	-1.301127	1.828697
13	6	-1.509528	-2.828536	0.147081
14	6	-2.239694	-2.220097	-1.079009
15	8	-1.717400	-1.116246	-1.506908
16	8	-3.221244	-2.804585	-1.529304
17	6	2.880435	-1.345129	0.261353
18	6	2.422887	-2.015964	-1.061147
19	8	3.235545	-2.700186	-1.669757
20	8	1.180963	-1.794078	-1.381935
21	6	1.557556	2.747648	0.244987
22	6	2.552625	1.920445	-0.588326
23	8	3.748499	2.211056	-0.583834
24	8	1.986211	0.942796	-1.214727
25	6	-2.761667	1.868650	-0.228082
26	6	-1.764241	2.582948	-1.168987
27	8	-1.974052	3.758330	-1.464478

28	8	-0.787875	1.838341	-1.568299
29	1	-0.579491	-3.263348	-0.229429
30	1	-2.128550	-3.625096	0.587482
31	1	3.588602	-2.012366	0.776544
32	1	3.396847	-0.418480	0.011254
33	1	2.083690	3.506494	0.841087
34	1	0.873305	3.235488	-0.452705
35	1	-3.415217	1.276193	-0.875180
36	1	-3.379432	2.614290	0.294527
37	1	-0.492464	-3.308755	2.530270
38	1	-0.250515	-1.635535	3.031077
39	1	1.268999	-3.058582	0.803357
40	1	1.874284	-2.750135	2.426254
41	1	1.631890	-0.596361	3.184368
42	1	3.150945	-0.181116	2.425357
43	1	2.517145	1.962326	2.266775
44	1	1.083592	1.534088	3.179984
45	1	-0.202361	3.133272	2.545103
46	1	-0.736291	3.303232	0.880809
47	1	-1.305052	0.893969	2.661000
48	1	-2.425679	2.233967	2.391117
49	1	-3.513143	-0.503822	0.169611
50	1	-3.878000	0.245636	1.728118
51	1	-2.126577	-0.985608	2.842197
52	1	-3.135980	-2.107697	1.944399
53	71	0.033805	-0.023688	-0.642616

HF = -1485.2616085 Hartree
Zero-point correction = 0.427468
Sum of electronic and thermal Enthalpies = -1484.807356
Sum of electronic and thermal Free Energies = -1484.888048

[Lu(DOTA)]$^-$ TS_{1-2b} $\Delta(\delta X\lambda\lambda)$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.179979	1.970186	1.221999
2	6	-0.670930	1.639882	2.379491
3	6	-2.031025	1.045279	2.009880
4	7	-2.003915	-0.169920	1.161478
5	6	-1.901318	-1.430820	1.930677
6	6	-0.465019	-1.901017	2.181788
7	7	0.332491	-2.079713	0.951294
8	6	1.757989	-2.287710	1.282105
9	6	2.457682	-1.019109	1.755412
10	7	2.392887	0.111592	0.806513
11	6	2.699778	1.366192	1.529517
12	6	1.532774	2.385889	1.677710
13	6	-0.342618	3.070886	0.363496
14	6	0.508092	3.132490	-0.937597
15	8	0.874099	1.967192	-1.378496
16	8	0.779493	4.229891	-1.412493
17	6	-3.222909	-0.165722	0.300269
18	6	-3.119502	0.877380	-0.836129
19	8	-4.155000	1.384778	-1.253936

20	8	-1.910400	1.109284	-1.244719
21	6	-0.168099	-3.223213	0.143188
22	6	-1.379593	-2.857415	-0.743421
23	8	-2.311891	-3.658318	-0.830629
24	8	-1.277992	-1.709614	-1.318218
25	6	3.324496	-0.074904	-0.336580
26	6	2.855507	-1.129703	-1.364985
27	8	3.679413	-1.922901	-1.814380
28	8	1.600009	-1.053006	-1.666995
29	1	-1.370515	2.861784	0.068588
30	1	-0.301624	4.038585	0.884098
31	1	-4.127714	0.027675	0.894362
32	1	-3.317902	-1.143221	-0.176333
33	1	-0.414502	-4.082415	0.784485
34	1	0.633407	-3.515410	-0.541006
35	1	3.363798	0.877097	-0.874378
36	1	4.335594	-0.333501	0.014428
37	1	-0.857637	2.533981	3.003891
38	1	-0.108533	0.938083	3.006895
39	1	-2.604123	1.804278	1.472377
40	1	-2.583932	0.849076	2.944875
41	1	-2.404326	-1.337923	2.908774
42	1	-2.434012	-2.208121	1.379672
43	1	-0.510421	-2.848918	2.749986
44	1	0.047774	-1.176817	2.819893
45	1	1.870785	-3.056011	2.069105
46	1	2.259397	-2.671607	0.393308
47	1	2.009374	-0.684711	2.696609
48	1	3.508581	-1.273706	1.986120
49	1	3.512781	1.879095	1.008525
50	1	3.097971	1.124492	2.523920
51	1	1.473665	2.713287	2.726510
52	1	1.806676	3.274390	1.106413
53	71	-0.034202	0.045588	-0.640706

HF = -1485.2615715 Hartree
Zero-point correction = 0.427496
Sum of electronic and thermal Enthalpies = -1484.807277
Sum of electronic and thermal Free Energies = -1484.887903

$[Lu(DOTA)]^-$ I_{2a} $\Delta(\delta\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.343220	1.736751	-1.412589
2	6	0.871712	1.935205	-2.236695
3	6	2.173045	1.750472	-1.454461
4	7	2.287447	0.475190	-0.721194
5	6	2.660200	-0.680731	-1.559942
6	6	1.489560	-1.369530	-2.278564
7	7	0.343465	-1.736876	-1.412498
8	6	-0.871369	-1.935278	-2.236763
9	6	-2.172797	-1.750502	-1.454701
10	7	-2.287371	-0.475169	-0.721568
11	6	-2.659976	0.680696	-1.560447

12	6	-1.489188	1.369455	-2.278852
13	6	-0.643900	2.968298	-0.631276
14	6	-1.674881	2.725915	0.499126
15	8	-1.486217	1.628120	1.146406
16	8	-2.557376	3.563970	0.675963
17	6	3.251160	0.660220	0.395850
18	6	2.651214	1.525894	1.528622
19	8	3.406308	2.219378	2.199945
20	8	1.364602	1.405425	1.664211
21	6	0.644018	-2.968465	-0.631198
22	6	1.674784	-2.726156	0.499408
23	8	2.557099	-3.564343	0.676503
24	8	1.486153	-1.628286	1.146576
25	6	-3.251289	-0.660207	0.395276
26	6	-2.651531	-1.525345	1.528570
27	8	-3.406984	-2.217554	2.200792
28	8	-1.364770	-1.405842	1.663584
29	1	0.281141	3.298021	-0.148733
30	1	-1.000078	3.767806	-1.298237
31	1	4.194231	1.108179	0.049483
32	1	3.457909	-0.321047	0.828266
33	1	1.000333	-3.767926	-1.298142
34	1	-0.281112	-3.298220	-0.148852
35	1	-3.458566	0.321088	0.827375
36	1	-4.194128	-1.108563	0.048788
37	1	0.878472	2.942693	-2.687864
38	1	0.838232	1.231442	-3.071507
39	1	2.259819	2.552869	-0.717372
40	1	3.018455	1.879946	-2.155189
41	1	3.393076	-0.388857	-2.334453
42	1	3.159225	-1.409474	-0.920949
43	1	1.890110	-2.265636	-2.784798
44	1	1.108903	-0.716988	-3.067049
45	1	-0.837749	-1.231520	-3.071574
46	1	-0.878107	-2.942764	-2.687938
47	1	-3.018118	-1.880113	-2.155518
48	1	-2.259608	-2.552771	-0.717486
49	1	-3.159144	1.409469	-0.921598
50	1	-3.392685	0.388774	-2.335099
51	1	-1.108421	0.716907	-3.067278
52	1	-1.889598	2.265588	-2.785152
53	71	0.000000	-0.000067	0.624792

HF = -1485.2771022 Hartree
Zero-point correction = 0.427432
Sum of electronic and thermal Enthalpies = -1484.822227
Sum of electronic and thermal Free Energies = -1484.904179

[Lu(DOTA)]$^-$ I_{2b} $\Delta(\delta\delta\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.353671	-0.108404	0.974077
2	6	2.437015	0.940049	2.002354
3	6	1.635002	2.182453	1.634577

4	7	0.230390	1.903379	1.262719
5	6	-0.573566	1.554210	2.446574
6	6	-1.938902	0.953130	2.105551
7	7	-1.924597	-0.235838	1.215819
8	6	-1.775469	-1.525539	1.932849
9	6	-0.330350	-2.029700	2.043905
10	7	0.334812	-2.221044	0.741728
11	6	1.766515	-2.550961	0.896270
12	6	2.594110	-1.445082	1.551536
13	6	3.267773	0.158656	-0.161999
14	6	2.966089	-0.738211	-1.390184
15	8	1.708447	-0.821301	-1.687051
16	8	3.903069	-1.284051	-1.965307
17	6	-0.269497	3.087011	0.515942
18	6	0.427764	3.177075	-0.872362
19	8	0.572116	4.283405	-1.376947
20	8	0.804344	2.029995	-1.351164
21	6	-3.179638	-0.207658	0.405169
22	6	-3.134056	0.910240	-0.663109
23	8	-4.190991	1.431431	-1.002911
24	8	-1.944197	1.186113	-1.098003
25	6	-0.324378	-3.283265	-0.058366
26	6	-1.491700	-2.764354	-0.926524
27	8	-2.501816	-3.461281	-1.032057
28	8	-1.271306	-1.617286	-1.470709
29	1	3.119581	1.193561	-0.485055
30	1	4.317958	0.022187	0.140084
31	1	-0.095094	4.015858	1.079641
32	1	-1.338065	2.979066	0.327935
33	1	-4.060773	-0.064482	1.046988
34	1	-3.285419	-1.157914	-0.121989
35	1	0.418785	-3.682656	-0.755104
36	1	-0.668106	-4.110362	0.580143
37	1	3.481320	1.243687	2.198682
38	1	2.060397	0.524577	2.942981
39	1	2.103199	2.678046	0.783053
40	1	1.676246	2.896328	2.477007
41	1	-0.000227	0.841235	3.047597
42	1	-0.741241	2.438948	3.088578
43	1	-2.540070	1.718531	1.610269
44	1	-2.457628	0.717109	3.050541
45	1	-2.190762	-1.457568	2.952411
46	1	-2.369789	-2.274132	1.404236
47	1	0.257333	-1.314332	2.624926
48	1	-0.344644	-2.975620	2.618886
49	1	2.154482	-2.753677	-0.101940
50	1	1.895725	-3.472054	1.495292
51	1	2.368044	-1.405503	2.621671
52	1	3.657379	-1.726396	1.474097
53	71	-0.048960	0.074287	-0.652975

HF = -1485.2727906 Hartree
Zero-point correction = 0.427617
Sum of electronic and thermal Enthalpies = -1484.817820
Sum of electronic and thermal Free Energies = -1484.899455

$[Lu(DOTA)]^-$ TS_{2a-I3} $\Delta(\delta X \delta\lambda)$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.391843	1.683323	1.417885
2	6	-0.772951	1.722353	2.328892
3	6	-2.126156	1.617364	1.618801
4	7	-2.288580	0.440856	0.741517
5	6	-2.741894	-0.770428	1.450034
6	6	-1.626201	-1.542036	2.161937
7	7	-0.472912	-1.878865	1.299034
8	6	0.716489	-2.165573	2.126731
9	6	2.014086	-2.014602	1.344121
10	7	2.206104	-0.644812	0.826103
11	6	2.582025	0.293596	1.909189
12	6	1.657246	1.525714	2.196180
13	6	0.493358	2.938112	0.613469
14	6	1.612349	2.786782	-0.444036
15	8	1.594128	1.636975	-1.033621
16	8	2.400962	3.712568	-0.616652
17	6	-3.214181	0.777557	-0.370482
18	6	-2.556473	1.727034	-1.396798
19	8	-3.259664	2.550038	-1.972303
20	8	-1.282477	1.533612	-1.559303
21	6	-0.798335	-3.033271	0.419651
22	6	-1.741136	-2.652971	-0.750348
23	8	-2.648250	-3.429260	-1.045033
24	8	-1.457922	-1.522982	-1.300464
25	6	3.236897	-0.683841	-0.247402
26	6	2.724279	-1.398948	-1.518791
27	8	3.537866	-1.964770	-2.238688
28	8	1.440079	-1.309531	-1.700684
29	1	-0.442443	3.098220	0.074573
30	1	0.693475	3.801817	1.263957
31	1	-4.149972	1.223475	-0.002582
32	1	-3.444498	-0.147946	-0.903469
33	1	-1.242044	-3.852457	1.005463
34	1	0.129657	-3.394990	-0.032650
35	1	3.460711	0.345953	-0.532716
36	1	4.157492	-1.175050	0.102198
37	1	-0.773833	2.656360	2.920180
38	1	-0.660259	0.904460	3.044601
39	1	-2.272046	2.508959	1.003891
40	1	-2.917451	1.645086	2.389806
41	1	-3.511686	-0.523507	2.204236
42	1	-3.218808	-1.427930	0.722745
43	1	-2.067813	-2.458724	2.591751
44	1	-1.252787	-0.957032	3.005528
45	1	0.723305	-1.462562	2.968122
46	1	0.666176	-3.178167	2.564244
47	1	2.858686	-2.315407	1.989420
48	1	2.016471	-2.695213	0.490430
49	1	3.581730	0.683778	1.692579
50	1	2.683422	-0.272894	2.843796
51	1	1.405852	1.514231	3.263781
52	1	2.257059	2.427303	2.040165
53	71	0.043806	0.020204	-0.614292

HF = -1485.2644079 Hartree
Zero-point correction = 0.427029

Sum of electronic and thermal Enthalpies = -1484.810475
Sum of electronic and thermal Free Energies = -1484.891443

[Lu(DOTA)]$^-$ TS_{2b-I3} $\Delta(\delta\delta X\lambda)$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.218734	-0.566314	1.008209
2	6	2.597621	0.490038	1.963128
3	6	2.137647	1.870385	1.509847
4	7	0.701154	1.929318	1.172238
5	6	-0.139461	1.843274	2.377232
6	6	-1.597088	1.521708	2.061618
7	7	-1.797797	0.238937	1.332397
8	6	-1.868705	-0.916771	2.263278
9	6	-1.002917	-2.193643	1.968664
10	7	-0.207816	-2.275594	0.716768
11	6	1.136732	-2.836618	0.986168
12	6	2.063715	-1.858511	1.700488
13	6	3.198133	-0.654084	-0.102686
14	6	2.683568	-1.464519	-1.320002
15	8	1.450691	-1.231905	-1.631806
16	8	3.460103	-2.237080	-1.875109
17	6	0.477367	3.151650	0.360856
18	6	1.129062	2.994214	-1.042542
19	8	1.523655	4.001888	-1.615624
20	8	1.190956	1.766515	-1.463361
21	6	-3.067480	0.376262	0.550891
22	6	-2.916582	1.395266	-0.605492
23	8	-3.928731	1.949462	-1.017690
24	8	-1.695864	1.574164	-1.007782
25	6	-0.886885	-3.127119	-0.297750
26	6	-2.013513	-2.364908	-1.015345
27	8	-3.137557	-2.858707	-1.089360
28	8	-1.625509	-1.224135	-1.483225
29	1	3.389725	0.361005	-0.464669
30	1	4.147392	-1.088573	0.247913
31	1	0.883143	4.044507	0.860172
32	1	-0.592520	3.287748	0.196351
33	1	-3.885955	0.699524	1.211991
34	1	-3.337663	-0.590408	0.123074
35	1	-0.145903	-3.379672	-1.060849
36	1	-1.271070	-4.052291	0.156134
37	1	3.688723	0.516538	2.130435
38	1	2.149094	0.252162	2.932822
39	1	2.692678	2.165950	0.617855
40	1	2.385207	2.607251	2.295659
41	1	0.266665	1.055728	3.022022
42	1	-0.101682	2.780762	2.961947
43	1	-2.010813	2.318154	1.442927
44	1	-2.174593	1.524845	3.001014
45	1	-1.575681	-0.566112	3.259886
46	1	-2.917133	-1.225879	2.351267
47	1	-0.305531	-2.296718	2.805267
48	1	-1.666595	-3.067785	2.022546

49	1	1.574113	-3.127142	0.032066
50	1	1.067847	-3.753321	1.599453
51	1	1.664727	-1.652791	2.699789
52	1	3.040670	-2.352300	1.849687
53	71	-0.040197	0.098211	-0.627894

HF = -1485.2600173 Hartree
Zero-point correction = 0.427160
Sum of electronic and thermal Enthalpies = -1484.806019
Sum of electronic and thermal Free Energies = -1484.886839

$[Lu(DOTA)]^-$ I_3 $\Delta(\delta\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.516853	1.542979	1.503298
2	6	-0.567085	1.408136	2.493442
3	6	-1.973046	1.402542	1.875165
4	7	-2.213258	0.382380	0.827429
5	6	-2.762334	-0.884294	1.350312
6	6	-1.722085	-1.836163	1.939466
7	7	-0.622154	-2.172076	1.016291
8	6	0.513525	-2.760045	1.753481
9	6	1.855346	-2.400878	1.120715
10	7	2.037099	-0.949578	0.928364
11	6	2.161741	-0.242423	2.212918
12	6	1.840944	1.247273	2.105991
13	6	0.590264	2.900170	0.897218
14	6	1.543378	2.889180	-0.330626
15	8	1.625276	1.738212	-0.918822
16	8	2.128110	3.927469	-0.616190
17	6	-3.134054	0.936959	-0.201861
18	6	-2.447391	2.010874	-1.071990
19	8	-3.104808	2.977335	-1.444499
20	8	-1.203897	1.757725	-1.337793
21	6	-1.065153	-3.091401	-0.060087
22	6	-1.893620	-2.404094	-1.173133
23	8	-2.903085	-2.972797	-1.586013
24	8	-1.414686	-1.273044	-1.563991
25	6	3.189576	-0.731652	0.021951
26	6	2.860095	-1.195573	-1.424153
27	8	3.779738	-1.587748	-2.130746
28	8	1.601279	-1.112101	-1.735280
29	1	-0.396362	3.196123	0.537927
30	1	0.935905	3.642312	1.632290
31	1	-4.044206	1.354413	0.253270
32	1	-3.414266	0.120706	-0.872763
33	1	-1.639218	-3.933285	0.357716
34	1	-0.167490	-3.491932	-0.542998
35	1	3.400854	0.338589	-0.032851
36	1	4.087825	-1.256648	0.381478
37	1	-0.525323	2.229019	3.232982
38	1	-0.397862	0.481133	3.049765
39	1	-2.159292	2.381980	1.427397
40	1	-2.704574	1.297199	2.695160

41	1	-3.521784	-0.691004	2.129924
42	1	-3.279133	-1.388914	0.532754
43	1	-2.250296	-2.748750	2.273656
44	1	-1.280933	-1.387150	2.835065
45	1	0.478505	-2.405472	2.788320
46	1	0.430024	-3.858068	1.811882
47	1	2.669368	-2.824694	1.737365
48	1	1.927909	-2.865970	0.135079
49	1	3.175435	-0.353464	2.638401
50	1	1.477492	-0.706356	2.928662
51	1	1.916811	1.702586	3.108742
52	1	2.596104	1.731744	1.486544
53	71	0.093672	0.094055	-0.631544

HF = -1485.2756003 Hartree
Zero-point correction = 0.427091
Sum of electronic and thermal Enthalpies = -1484.821002
Sum of electronic and thermal Free Energies = -1484.903179

$[Lu(DOTA)]^-$ $TS_{3\text{-}TSAP}$ $\Delta(\delta\delta\delta X)$ (1 imaginary frequency)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.670509	1.646166	1.412096
2	6	-0.391488	1.629134	2.434200
3	6	-1.796586	1.694817	1.834305
4	7	-2.136059	0.545433	0.962111
5	6	-2.722124	-0.584628	1.725419
6	6	-1.963106	-1.952374	1.777822
7	7	-0.703818	-2.095453	1.003818
8	6	0.377055	-2.594814	1.876116
9	6	1.767867	-2.368201	1.295810
10	7	2.022751	-0.952118	0.974003
11	6	2.244103	-0.166026	2.197699
12	6	1.994992	1.325888	1.996293
13	6	0.796985	2.948055	0.704390
14	6	1.691871	2.785395	-0.556213
15	8	1.654498	1.599095	-1.075507
16	8	2.343328	3.753154	-0.931619
17	6	-3.097135	0.996187	-0.087287
18	6	-2.459480	1.974444	-1.094994
19	8	-3.167829	2.841784	-1.594495
20	8	-1.200294	1.761167	-1.322297
21	6	-0.922778	-3.019045	-0.143777
22	6	-1.910343	-2.388290	-1.149476
23	8	-2.904483	-3.020631	-1.498370
24	8	-1.570073	-1.193212	-1.507883
25	6	3.143153	-0.865490	0.008898
26	6	2.727613	-1.439571	-1.373098
27	8	3.590579	-1.955726	-2.071698
28	8	1.463420	-1.308896	-1.644694
29	1	-0.183396	3.275513	0.356792
30	1	1.217034	3.721133	1.364885
31	1	-3.984505	1.464042	0.364314
32	1	-3.405191	0.114603	-0.654082

33	1	-1.303235	-3.990620	0.206228
34	1	0.028712	-3.165405	-0.662580
35	1	3.394916	0.185794	-0.148007
36	1	4.033822	-1.397942	0.376297
37	1	-0.270035	2.467230	3.145196
38	1	-0.289442	0.703531	3.014704
39	1	-1.892433	2.606520	1.241701
40	1	-2.522677	1.790864	2.659207
41	1	-2.886401	-0.262214	2.762418
42	1	-3.716937	-0.782270	1.315823
43	1	-2.663554	-2.729433	1.450028
44	1	-1.743516	-2.169382	2.828822
45	1	0.294690	-2.078905	2.838014
46	1	0.252991	-3.671806	2.090421
47	1	2.518646	-2.754343	2.009409
48	1	1.886829	-2.945212	0.377312
49	1	3.271096	-0.302786	2.581995
50	1	1.574583	-0.544382	2.976103
51	1	2.126227	1.845685	2.961490
52	1	2.754814	1.726740	1.323888
53	71	0.056007	0.073494	-0.602095

HF = -1485.2625116 Hartree
Zero-point correction = 0.426749
Sum of electronic and thermal Enthalpies = -1484.808811
Sum of electronic and thermal Free Energies = -1484.890028

[Lu(DOTA)]$^-$ TSAP $\Lambda(\delta\delta\delta\delta)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.624427	-1.331277	1.132895
2	6	-2.175991	-0.477232	2.196071
3	6	-2.494367	0.936260	1.711147
4	7	-1.323792	1.628323	1.132333
5	6	-0.465866	2.185938	2.189177
6	6	0.945715	2.501531	1.697290
7	7	1.635123	1.327523	1.122080
8	6	2.196192	0.474541	2.181115
9	6	2.510770	-0.938917	1.694375
10	7	1.335575	-1.630014	1.123684
11	6	0.484578	-2.188241	2.185832
12	6	-0.929847	-2.504563	1.702721
13	6	-2.663506	-1.794108	0.181249
14	6	-2.026251	-2.406388	-1.094690
15	8	-0.865763	-1.912551	-1.394500
16	8	-2.648496	-3.277979	-1.689146
17	6	-1.791270	2.661421	0.176161
18	6	-2.421008	2.011730	-1.084871
19	8	-1.913211	0.859724	-1.393405
20	8	-3.310258	2.620814	-1.666973
21	6	2.664892	1.789604	0.159692
22	6	2.009238	2.417205	-1.099171
23	8	0.857725	1.905787	-1.403379
24	8	2.609462	3.314134	-1.678875

25	6	1.795516	-2.663187	0.163945
26	6	2.417322	-2.012429	-1.100155
27	8	1.902273	-0.863655	-1.408667
28	8	3.310072	-2.616021	-1.682868
29	1	-1.442945	-0.429108	3.009173
30	1	-3.090819	-0.921019	2.629341
31	1	-3.268454	0.892118	0.943013
32	1	-2.918960	1.516259	2.549578
33	1	-0.414865	1.457170	3.005946
34	1	-0.908137	3.103064	2.619158
35	1	0.898456	3.271293	0.924985
36	1	1.529280	2.930751	2.530875
37	1	1.469878	0.426672	3.000209
38	1	3.114455	0.919024	2.606307
39	1	3.279190	-0.894995	0.920524
40	1	2.941321	-1.519031	2.529706
41	1	0.438441	-1.460207	3.003514
42	1	0.930001	-3.105531	2.612109
43	1	-0.886721	-3.273237	0.929190
44	1	-1.506988	-2.935018	2.540240
45	1	-3.336840	-2.528964	0.648766
46	1	-3.255207	-0.935479	-0.143979
47	1	-2.518061	3.342403	0.645079
48	1	-0.932789	3.245117	-0.163985
49	1	3.349660	2.516133	0.623440
50	1	3.244692	0.928611	-0.181016
51	1	2.524605	-3.345016	0.627960
52	1	0.933662	-3.244977	-0.170969
53	71	-0.002836	-0.001675	-0.597647

HF = -1485.2831556 Hartree
Zero-point correction = 0.426810
Sum of electronic and thermal Enthalpies = -1484.828890
Sum of electronic and thermal Free Energies = -1484.910675