Electronic Supplementary Information for Dalton Transactions

The Effect of Ring Size Variation on the Structure and Stability of Lanthanide(III) Complexes with Crown Ethers Containing Picolinate Pendants†

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Supporting Information (72 pages)

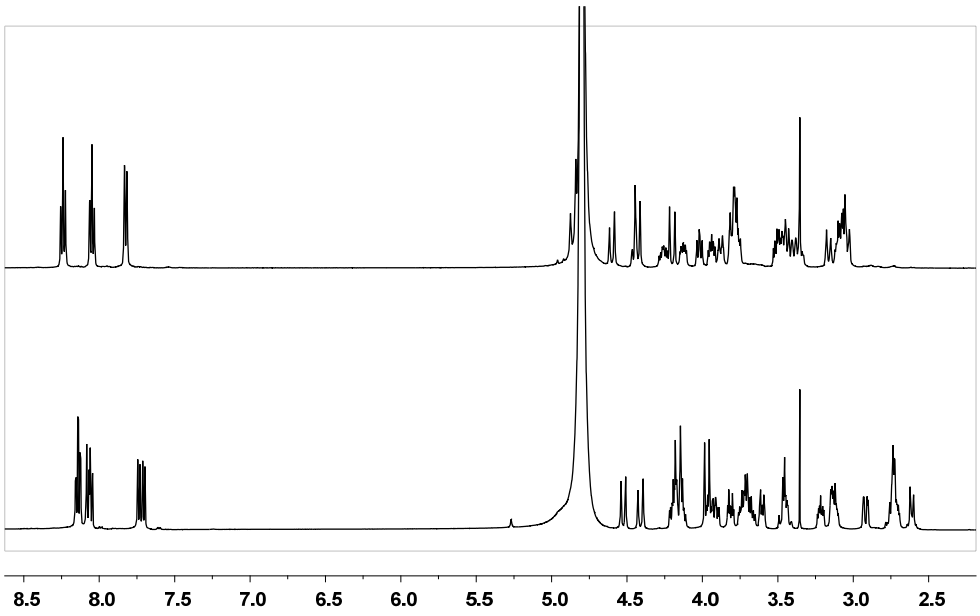

Figure S1. ^{1}H NMR spectra (500 MHz) of $[Lu(bp15c5)]^{+}$ (top) and $[La(bp15c5)]^{+}$ (bottom) complexes recorded in D_2O solution (pD = 7.0) at 298 K.

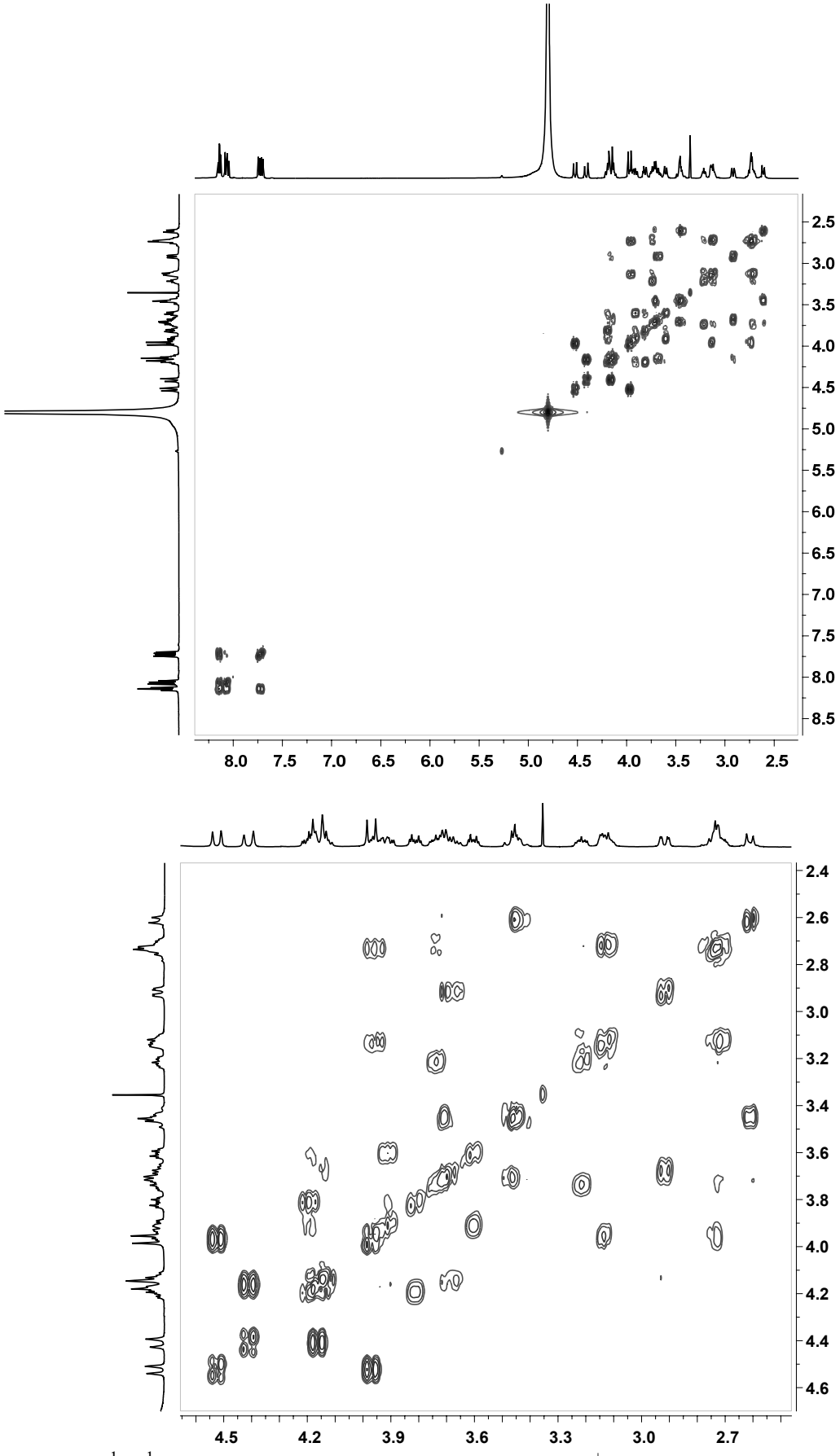

Figure S2. ^{1}H-^{1}H-COSY NMR spectrum of $[La(bp15c5)]^{+}$ recorded in D_2O solution (pD = 7.0) at 298 K.

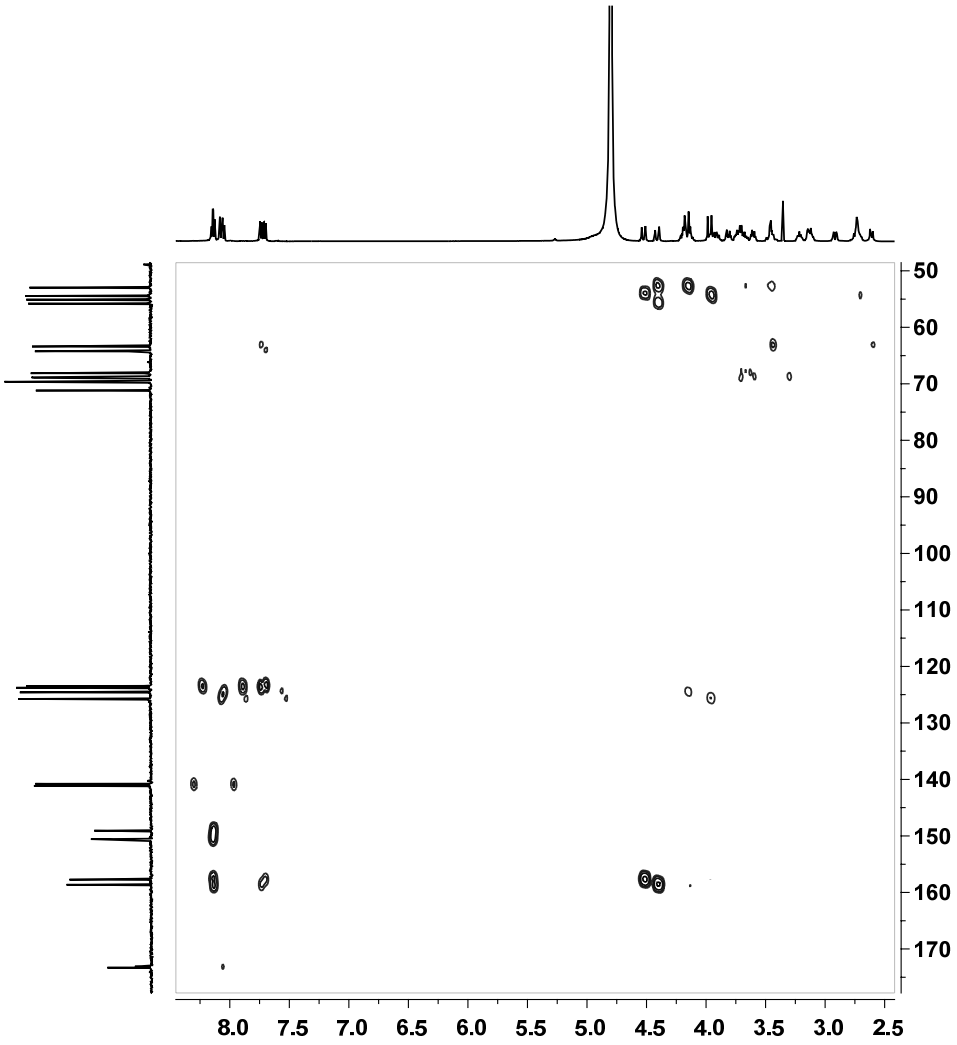

Figure S3. ^{1}H-^{13}C-HMBC NMR spectrum of $[La(bp15c5)]^{+}$ recorded in D_2O solution (pD = 7.0) at 298 K.

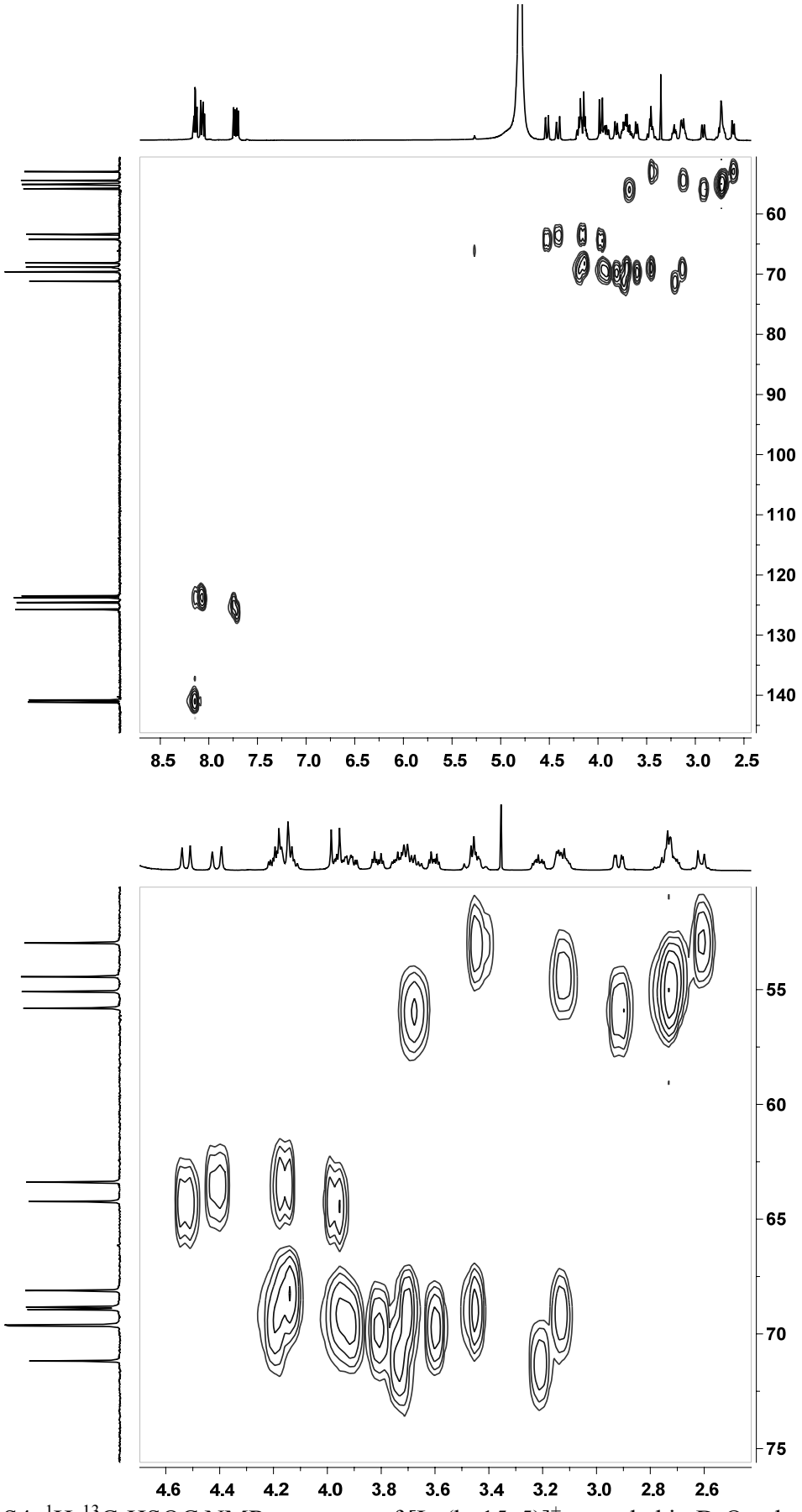

Figure S4. ^{1}H-^{13}C-HSQC NMR spectrum of $[La(bp15c5)]^{+}$ recorded in D_2O solution (pD = 7.0) at 298 K.

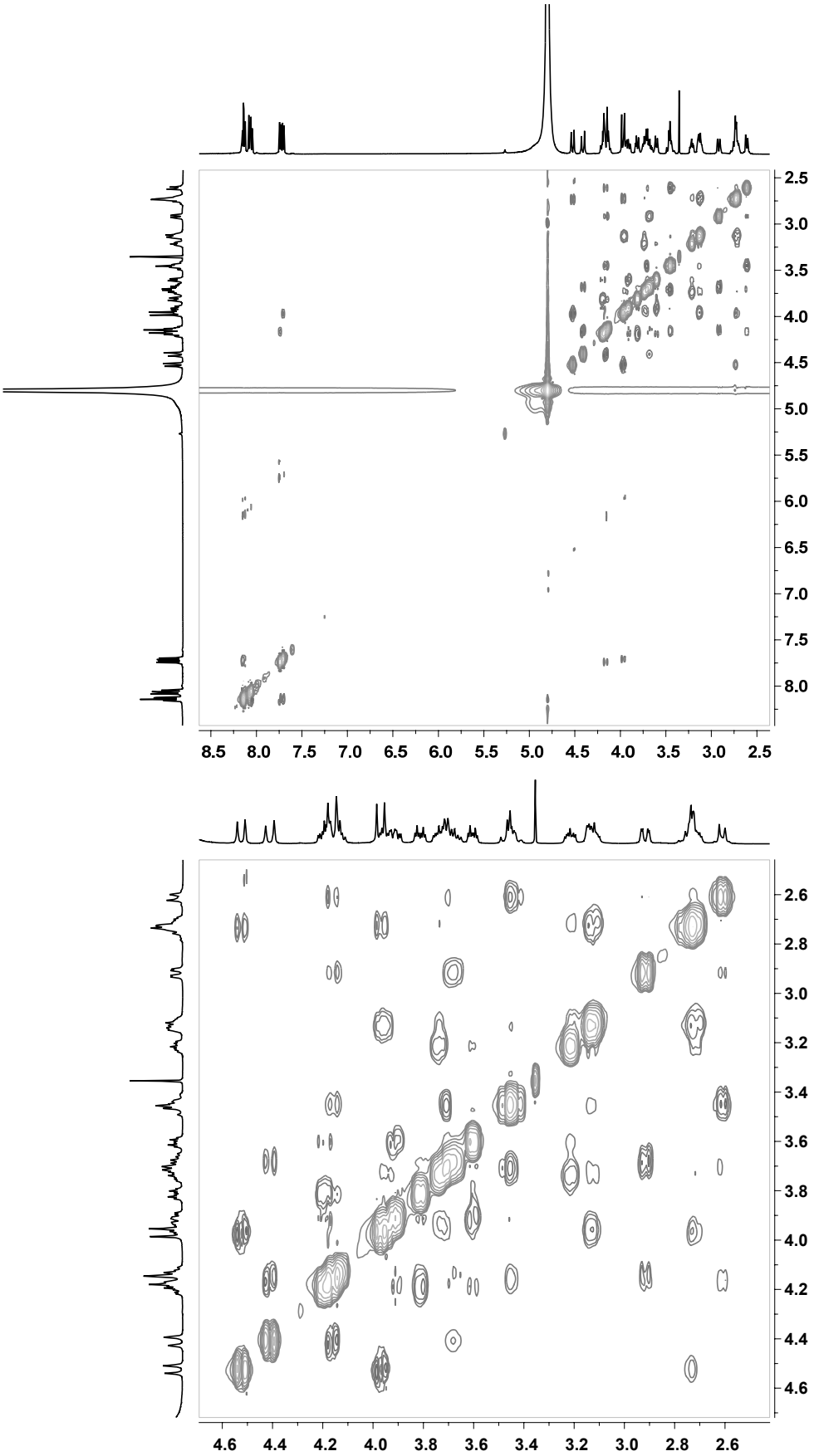

Figure S5. ^{1}H-^{1}H-NOESY NMR spectrum of $[La(bp15c5)]^{+}$ recorded in D_2O solution (pD = 7.0) at 298 K.

Table S1. ^{1}H Shifts (ppm with respect to TMS) of paramagnetic $[Ln(bp15c5)]^{+}$ complexes (Ln = Ce, Eu or Yb) recorded in D_2O solution (pD = 7.0) at 298 K.

	Ce	**Yb**	**Eu**
1	16.04	70.01	18.97
2	14.07	44.78	14.98
3	13.93	42.23	13.80
4	13.64	40.76	12.10
5	12.02	32.65	8.82
6	11.6	27.79	8.35
7	10.76	19.95	7.83
8	10.6	19.82	7.70
9	10.32	19.07	6.95
10	10.24	19.05	3.47
11	9.76	13.9	2.78
12	9.17	8.43	2.60
13	8.4	7.68	1.91
14	4..15	3.89	1.81
15	3.91	3.69	1.63
16	3.8	3.69	0.42
17	3.7	3.1	-1.05
18	2.96	-1.34	-1.32
19	1.91	-1.68	-1.70
20	0.72	-5.85	-1.79
21	0.34	-6.62	-1.79
22	0.04	-7.52	-3.48
23	-0.25	-9.38	-4.68
24	-1.51	-9.44	-7.77
25	-1.67	-9.48	-10.31
26	-2.73	-27.24	-14.80
27	-4.09	-27.24	-15.17
28	-4.74	-29.65	-15.68
29	-6.82	-39.8	-16.10
30	-8.07	-42.76	-18.37

$[Ce(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	0.060416	-0.183494	0.019497
2	7	2.624915	-1.463876	-0.319193
3	7	-1.732291	-0.395851	2.099949
4	8	1.047560	-1.243193	2.121443
5	8	-1.855990	-2.151749	-0.117049
6	8	0.277132	-2.498728	-1.464841
7	6	-2.558450	-1.626519	2.079585
8	6	-3.029057	-2.001927	0.684721
9	6	-2.107860	-2.508145	-1.482116
10	6	-0.851981	-3.181856	-2.010440
11	6	1.524716	-2.904086	-2.028431
12	1	1.752633	-2.273939	-2.897111
13	1	1.466021	-3.944944	-2.371024
14	6	2.566521	-2.813101	-0.926090
15	1	2.287361	-3.529795	-0.149452
16	1	3.552817	-3.117811	-1.312041
17	6	3.196959	-1.527321	1.048175
18	1	3.483889	-0.515291	1.340903
19	1	4.108018	-2.148127	1.069979
20	6	3.434535	-0.573050	-1.189326
21	1	3.049118	-0.666135	-2.210839
22	1	4.486183	-0.901445	-1.213991
23	6	2.227986	-2.062522	2.097835
24	1	1.937939	-3.106188	1.918772
25	1	2.721223	-2.014046	3.076755
26	6	0.250207	-1.387525	3.312178
27	1	0.882312	-1.206302	4.190736
28	1	-0.117186	-2.420151	3.371960
29	6	-0.869364	-0.350258	3.310253
30	1	-0.415199	0.642098	3.336720
31	1	-1.456914	-0.486639	4.232805
32	6	3.357724	0.877184	-0.768051
33	6	4.400563	1.776829	-0.994222
34	1	5.310643	1.446810	-1.485823
35	6	4.251438	3.099854	-0.573138
36	1	5.045019	3.820460	-0.747466
37	6	3.089346	3.473966	0.099479
38	1	2.927515	4.474159	0.484621
39	6	2.102869	2.511515	0.300204
40	6	0.845242	2.799610	1.104180
41	7	2.226023	1.250644	-0.153638
42	6	-2.588509	0.823370	2.039509
43	1	-1.983042	1.659945	2.398251
44	1	-3.458714	0.717865	2.704267
45	6	-3.032711	1.196056	0.637330
46	6	-4.216335	1.894464	0.386801
47	1	-4.902507	2.117270	1.198132
48	6	-4.491035	2.312085	-0.918054
49	1	-5.403959	2.860439	-1.131476
50	6	-3.584204	2.026640	-1.938788
51	1	-3.739771	2.333458	-2.966712
52	6	-2.427929	1.321554	-1.612374
53	6	-1.356466	0.979590	-2.646939
54	7	-2.178052	0.911059	-0.356768
55	8	-0.294243	0.414186	-2.124511
56	8	-1.555798	1.227576	-3.822983

57	8	0.666818	3.909720	1.577885
58	8	0.067159	1.757418	1.226912
59	1	-0.811351	-4.234105	-1.697367
60	1	-0.843728	-3.136331	-3.106703
61	1	-2.352266	-1.607773	-2.056040
62	1	-2.952478	-3.205111	-1.545727
63	1	-1.956391	-2.457578	2.454768
64	1	-3.428659	-1.526809	2.746889
65	1	-3.694466	-1.248221	0.250155
66	1	-3.571186	-2.956301	0.727268

HF = -1714.1526672 Hartrees
Zero-point correction = 0.541662 Hartrees
Sum of electronic and thermal Enthalpies = -1713.577896 Hartrees
Sum of electronic and thermal Free Energies = -1713.672776 Hartrees

$[Ce(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	0.057172	-0.171541	0.033796
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6	8	0.144850	-2.677759	-1.258604
7	6	-2.566071	-1.419469	2.189547
8	6	-3.112527	-1.845505	0.836120
9	6	-2.196050	-2.945141	-1.088662
10	6	-1.034382	-2.827122	-2.057082
11	6	1.358730	-2.968783	-1.948628
12	1	1.505580	-2.254672	-2.769973
13	1	1.313501	-3.979166	-2.377523
14	6	2.460168	-2.907968	-0.905945
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16	1	3.418086	-3.228437	-1.344290
17	6	3.145546	-1.625022	1.062070
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21	1	3.038232	-0.818580	-2.210780
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23	6	2.149757	-2.082098	2.124077
24	1	1.787831	-3.104815	1.956402
25	1	2.650750	-2.056033	3.099647
26	6	0.257633	-1.211683	3.363732
27	1	0.921648	-0.997142	4.210509
28	1	-0.148676	-2.221265	3.504947
29	6	-0.821773	-0.131289	3.318330
30	1	-0.332394	0.843698	3.280090
31	1	-1.397750	-0.193053	4.256031
32	6	3.398300	0.746572	-0.805966
33	6	4.478010	1.595925	-1.054152
34	1	5.375988	1.213392	-1.529714
35	6	4.381348	2.936636	-0.676938
36	1	5.204357	3.618595	-0.869316
37	6	3.231660	3.378342	-0.024668
38	1	3.107706	4.396137	0.326957
39	6	2.206469	2.463133	0.201233

40	6	0.959583	2.829914	0.988249
41	7	2.279195	1.183441	-0.209943
42	6	-2.529664	1.026667	2.007032
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44	1	-3.397839	0.980411	2.680868
45	6	-2.975195	1.331852	0.588169
46	6	-4.153192	2.025550	0.299843
47	1	-4.832358	2.308076	1.098451
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49	1	-5.341092	2.902159	-1.271195
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51	1	-3.710850	2.214403	-3.082079
52	6	-2.392158	1.290386	-1.671145
53	6	-1.355402	0.826491	-2.691801
54	7	-2.130735	0.977575	-0.391162
55	8	-0.295471	0.270824	-2.147479
56	8	-1.574616	0.968310	-3.881750
57	8	0.825825	3.961209	1.425508
58	8	0.138495	1.825909	1.140893
59	1	-1.967556	-2.249371	2.572530
60	1	-3.401847	-1.269057	2.891404
61	1	-3.843322	-1.137915	0.428869
62	1	-3.607513	-2.818354	0.951728
63	1	-0.972870	-3.739142	-2.664792
64	1	-1.134455	-1.960725	-2.718582
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Sum of electronic and thermal Free Energies = -1713.674900 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.059678	-0.179233	0.009026
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4	8	1.061776	-1.215707	2.131968
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6	8	0.273643	-2.512519	-1.447395
7	6	-2.545115	-1.590913	2.122088
8	6	-3.019765	-1.997550	0.737160
9	6	-2.110569	-2.550118	-1.422982
10	6	-0.856417	-3.226287	-1.950696
11	6	1.520484	-2.925798	-2.008418
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13	1	1.459344	-3.968912	-2.342885
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21	1	3.056588	-0.693822	-2.213883
22	1	4.493426	-0.927432	-1.217020

23	6	2.235898	-2.043944	2.111036
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35	6	4.289371	3.077105	-0.604651
36	1	5.090925	3.788451	-0.780545
37	6	3.127038	3.468139	0.057415
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50	6	-3.635119	1.991708	-1.936434
51	1	-3.806527	2.281127	-2.966878
52	6	-2.471299	1.296085	-1.615779
53	6	-1.415061	0.941454	-2.662068
54	7	-2.201403	0.907301	-0.357468
55	8	-0.344126	0.384250	-2.149105
56	8	-1.633447	1.174294	-3.837962
57	8	0.709471	3.942913	1.524568
58	8	0.072704	1.801131	1.174344
59	1	-0.798747	-4.267246	-1.604349
60	1	-0.867847	-3.216053	-3.047796
61	1	-2.364017	-1.660970	-2.010342
62	1	-2.951667	-3.252915	-1.467203
63	1	-1.942577	-2.413929	2.513709
64	1	-3.413899	-1.477360	2.788965
65	1	-3.685242	-1.253305	0.286944
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Sum of electronic and thermal Free Energies = -1713.082450Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.056997	-0.169434	0.021560
2	7	2.585441	-1.559510	-0.304840
3	7	-1.695544	-0.194216	2.136509
4	8	1.042990	-1.164923	2.150752
5	8	-1.998692	-1.978294	-0.028464

6	8	0.149660	-2.689728	-1.236782
7	6	-2.552429	-1.400077	2.217266
8	6	-3.102094	-1.846078	0.871268
9	6	-2.188632	-2.971736	-1.041653
10	6	-1.036595	-2.856181	-2.022247
11	6	1.360430	-2.984581	-1.931371
12	1	1.502018	-2.276972	-2.759276
13	1	1.314103	-3.998294	-2.352080
14	6	2.468089	-2.914419	-0.895392
15	1	2.223219	-3.625007	-0.101484
16	1	3.423528	-3.237269	-1.337414
17	6	3.157796	-1.617768	1.062778
18	1	3.503952	-0.615931	1.326371
19	1	4.032057	-2.288513	1.100826
20	6	3.430103	-0.723292	-1.195257
21	1	3.043990	-0.831712	-2.215224
22	1	4.468021	-1.093460	-1.208765
23	6	2.164223	-2.065922	2.130974
24	1	1.799549	-3.088892	1.970515
25	1	2.669191	-2.035563	3.104434
26	6	0.279169	-1.181303	3.372184
27	1	0.946108	-0.959478	4.214869
28	1	-0.127638	-2.189106	3.524480
29	6	-0.799703	-0.100346	3.321235
30	1	-0.309672	0.873811	3.268792
31	1	-1.368725	-0.150431	4.263907
32	6	3.412190	0.740809	-0.819498
33	6	4.496817	1.583618	-1.068059
34	1	5.394712	1.194434	-1.538343
35	6	4.405232	2.926773	-0.697951
36	1	5.232241	3.603756	-0.890778
37	6	3.255477	3.377280	-0.052110
38	1	3.135284	4.397351	0.294156
39	6	2.224500	2.468513	0.174600
40	6	0.977025	2.848462	0.955783
41	7	2.292712	1.186392	-0.229936
42	6	-2.518039	1.045437	2.014301
43	1	-1.880203	1.884138	2.305049
44	1	-3.375450	1.009141	2.702430
45	6	-2.985724	1.333329	0.598922
46	6	-4.171518	2.017696	0.320702
47	1	-4.840973	2.304219	1.126044
48	6	-4.471905	2.335505	-1.006497
49	1	-5.385980	2.872779	-1.241938
50	6	-3.593973	1.958260	-2.022885
51	1	-3.777332	2.176445	-3.068690
52	6	-2.434177	1.272517	-1.667927
53	6	-1.410811	0.804488	-2.700752
54	7	-2.153168	0.973692	-0.388789
55	8	-0.341439	0.254643	-2.168991
56	8	-1.648194	0.939346	-3.887978
57	8	0.853587	3.982474	1.389074
58	8	0.145291	1.853372	1.108301
59	1	-1.952340	-2.224103	2.610218
60	1	-3.386982	-1.241516	2.918803
61	1	-3.834998	-1.145486	0.456087
62	1	-3.595127	-2.817940	1.002411
63	1	-0.974208	-3.774133	-2.620776
64	1	-1.149271	-1.997179	-2.691387
65	1	-2.203107	-3.961348	-0.565718
66	1	-3.141160	-2.814956	-1.564208

HF = -1713.5650224 Hartrees
Zero-point correction = 0.541760 Hartrees
Sum of electronic and thermal Enthalpies = -1712.990283 Hartrees
Sum of electronic and thermal Free Energies = -1713.084588 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) Λ(λδ)(λδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.028627	-0.133550	-0.025957
2	7	2.626834	-1.501134	-0.335105
3	7	-1.795738	-0.210112	2.063605
4	8	0.923912	-1.290390	2.062828
5	8	-1.931018	-2.135765	-0.018512
6	8	0.254661	-2.544874	-1.381529
7	6	-2.811277	-1.296568	2.037801
8	1	-3.105478	-1.581289	3.059635
9	1	-3.702302	-0.898178	1.546799
10	6	-2.406069	-2.540779	1.265074
11	1	-1.630929	-3.135507	1.767489
12	1	-3.292610	-3.179540	1.155298
13	6	-1.950998	-3.200254	-0.979506
14	1	-2.964863	-3.324236	-1.380918
15	1	-1.642753	-4.134229	-0.491513
16	6	-0.961560	-2.852908	-2.070716
17	1	-0.824238	-3.717947	-2.731037
18	1	-1.273589	-1.991691	-2.670096
19	6	1.467286	-2.819193	-2.079893
20	1	1.629634	-2.070558	-2.866201
21	1	1.415835	-3.808967	-2.552433
22	6	2.551373	-2.815129	-1.015935
23	1	2.294462	-3.581772	-0.280508
24	1	3.522907	-3.094461	-1.451979
25	6	3.110378	-1.633251	1.059481
26	1	3.415515	-0.642695	1.405071
27	1	3.996074	-2.288145	1.116717
28	6	3.512327	-0.616735	-1.130462
29	1	3.191442	-0.686002	-2.176439
30	1	4.554548	-0.974064	-1.097044
31	6	2.064302	-2.169270	2.035557
32	1	1.729527	-3.183373	1.782236
33	1	2.515418	-2.202211	3.034902
34	6	0.107473	-1.386873	3.248587
35	1	0.749287	-1.278119	4.131860
36	1	-0.356543	-2.379982	3.290389
37	6	-0.917089	-0.254288	3.257803
38	1	-0.374938	0.693490	3.288728
39	1	-1.504555	-0.343495	4.186587
40	6	3.454795	0.829578	-0.699855
41	6	4.544633	1.687348	-0.862179
42	1	5.468020	1.318670	-1.298452
43	6	4.425635	3.015730	-0.451416
44	1	5.256040	3.704060	-0.577988
45	6	3.241360	3.434087	0.151952
46	1	3.095088	4.439226	0.530335
47	6	2.208899	2.510504	0.294693
48	6	0.930835	2.852857	1.038876
49	7	2.301591	1.243883	-0.154084

50	6	-2.515988	1.098280	1.995860
51	1	-1.804186	1.883026	2.260430
52	1	-3.350335	1.122547	2.711588
53	6	-3.006676	1.390995	0.591030
54	6	-4.187594	2.086014	0.324621
55	1	-4.840008	2.387852	1.138215
56	6	-4.505484	2.396709	-1.000775
57	1	-5.417945	2.940720	-1.226739
58	6	-3.645107	2.006187	-2.026017
59	1	-3.838857	2.222562	-3.070312
60	6	-2.487014	1.310700	-1.682812
61	6	-1.471155	0.850252	-2.725437
62	7	-2.193589	1.010075	-0.407614
63	8	-0.391614	0.309274	-2.202607
64	8	-1.716205	0.987309	-3.910451
65	8	0.772498	3.970887	1.500935
66	8	0.111942	1.840439	1.133718

HF = -1713.5603708 Hartrees
Zero-point correction = 0.541496 Hartrees
Sum of electronic and thermal Enthalpies = -1712.985779 Hartrees
Sum of electronic and thermal Free Energies = -1713.080730 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) Λ(δδ)(λδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.037362	-0.254828	0.047273
2	7	-2.819948	-1.205732	0.101560
3	7	1.984149	-0.810466	-1.819428
4	8	-0.852614	-1.406588	-2.063087
5	8	1.675317	-2.357226	0.562113
6	8	-0.759967	-2.401756	1.531190
7	6	3.002628	-1.778192	-1.333089
8	1	3.589620	-2.184814	-2.171000
9	1	3.695091	-1.238152	-0.684542
10	6	2.415706	-2.917800	-0.526242
11	1	1.755090	-3.567833	-1.118848
12	1	3.237066	-3.535722	-0.140364
13	6	1.404793	-3.312792	1.595685
14	1	2.310178	-3.488374	2.191116
15	1	1.088377	-4.260323	1.138899
16	6	0.286034	-2.757497	2.450687
17	1	-0.060008	-3.525115	3.151979
18	1	0.586960	-1.864312	3.007082
19	6	-2.093946	-2.692548	1.944456
20	1	-2.390996	-2.021659	2.760595
21	1	-2.156666	-3.724179	2.314561
22	6	-2.964831	-2.546462	0.705888
23	1	-2.637753	-3.295015	-0.020156
24	1	-4.015021	-2.768953	0.955261
25	6	-3.195418	-1.196242	-1.332565
26	1	-3.271303	-0.152780	-1.645140
27	1	-4.184142	-1.660655	-1.492361
28	6	-3.637294	-0.236321	0.872275
29	1	-3.439923	-0.401103	1.936946
30	1	-4.713339	-0.423239	0.721105
31	6	-2.194299	-1.902114	-2.251311
32	1	-2.170447	-2.983973	-2.080543

33	1	-2.508377	-1.735732	-3.286759
34	6	-0.122253	-0.931434	-3.225827
35	6	1.345800	-1.316661	-3.064851
36	6	-3.315109	1.200732	0.528885
37	6	-4.233275	2.238151	0.706701
38	1	-5.216192	2.034773	1.121031
39	6	-3.866037	3.531924	0.332449
40	1	-4.556835	4.357726	0.474763
41	6	-2.624170	3.741656	-0.267304
42	1	-2.302502	4.710727	-0.631322
43	6	-1.779436	2.647581	-0.431017
44	6	-0.480035	2.727107	-1.214240
45	7	-2.101161	1.416944	0.008036
46	6	2.657243	0.505671	-2.017364
47	1	1.952342	1.177868	-2.511274
48	1	3.547251	0.391295	-2.654816
49	6	3.037074	1.126846	-0.684336
50	6	4.161986	1.934711	-0.514075
51	1	4.833804	2.119894	-1.346510
52	6	4.401602	2.504493	0.739843
53	1	5.269297	3.140304	0.889446
54	6	3.524971	2.248737	1.793418
55	1	3.663845	2.660363	2.786465
56	6	2.423037	1.431627	1.547415
57	6	1.387193	1.109512	2.621887
58	7	2.201496	0.887878	0.339832
59	8	0.344945	0.448365	2.163510
60	8	1.580374	1.458328	3.772061
61	8	-0.079509	3.800235	-1.635119
62	8	0.069039	1.553965	-1.391858
63	1	1.401479	-2.409235	-3.049677
64	1	1.897444	-0.978494	-3.955060
65	1	-0.516269	-1.417033	-4.124830
66	1	-0.258467	0.150832	-3.298925

HF = -1713.5551936 Hartrees
Zero-point correction = 0.541385 Hartrees
Sum of electronic and thermal Enthalpies = -1712.980729 Hartrees
Sum of electronic and thermal Free Energies = -1713.075637 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δδδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.057062	-0.102077	-0.054525
2	7	2.629002	-1.504684	-0.482418
3	7	-1.627768	-0.501753	2.101478
4	8	1.118137	-1.385995	1.976752
5	8	-1.798549	-2.070119	-0.263198
6	8	0.332322	-2.181149	-1.799126
7	6	-2.404368	-1.761687	2.031468
8	6	-2.913311	-2.098175	0.637560
9	6	-1.968287	-2.896434	-1.423821
10	6	-0.907893	-2.486056	-2.442054
11	6	1.052965	-3.284108	-1.249844
12	6	2.503515	-2.833137	-1.140975
13	6	3.245467	-1.606050	0.856564
14	1	3.526409	-0.602586	1.182613
15	1	4.164209	-2.215985	0.834461

16	6	3.379272	-0.571290	-1.364512
17	1	2.885971	-0.592897	-2.343153
18	1	4.416832	-0.909371	-1.514794
19	6	2.306286	-2.191791	1.901984
20	1	2.026966	-3.231489	1.681547
21	1	2.814059	-2.180433	2.874415
22	6	0.396679	-1.530466	3.212413
23	6	-0.721083	-0.496238	3.280151
24	6	3.378600	0.850213	-0.845317
25	6	4.459120	1.713154	-1.030542
26	1	5.345323	1.373519	-1.557685
27	6	4.380106	3.012491	-0.523151
28	1	5.205187	3.704189	-0.665519
29	6	3.248531	3.397327	0.192703
30	1	3.141781	4.376785	0.644505
31	6	2.217552	2.472795	0.348364
32	6	0.987433	2.775764	1.193373
33	7	2.273883	1.240161	-0.188612
34	6	-2.522674	0.688868	2.168820
35	1	-1.915313	1.522914	2.532596
36	1	-3.338129	0.519579	2.887634
37	6	-3.073803	1.117637	0.824709
38	6	-4.315848	1.739667	0.679805
39	1	-4.972680	1.858834	1.536049
40	6	-4.687819	2.216886	-0.579965
41	1	-5.647232	2.708222	-0.713227
42	6	-3.818345	2.060965	-1.658898
43	1	-4.049526	2.415458	-2.656874
44	6	-2.599735	1.423069	-1.435328
45	6	-1.574609	1.204985	-2.544013
46	7	-2.252432	0.959611	-0.223352
47	8	-0.456520	0.668110	-2.116585
48	8	-1.854336	1.504091	-3.691692
49	8	0.890634	3.855241	1.752675
50	8	0.142948	1.779491	1.251133
51	1	3.088107	-3.594290	-0.607690
52	1	2.915181	-2.769575	-2.152137
53	1	0.981639	-4.156658	-1.912546
54	1	0.634475	-3.562572	-0.271897
55	1	-0.768320	-3.280093	-3.186881
56	1	-1.182451	-1.564308	-2.955709
57	1	-1.870635	-3.948421	-1.122488
58	1	-2.966962	-2.754195	-1.855985
59	1	-3.345310	-3.106945	0.661289
60	1	-3.683232	-1.403621	0.284938
61	1	-1.756062	-2.582949	2.344635
62	1	-3.256175	-1.738482	2.729770
63	1	-0.269081	0.497205	3.320799
64	1	-1.276350	-0.660531	4.218168
65	1	1.078499	-1.347846	4.052991
66	1	0.035487	-2.563635	3.298957

HF = -1713.5581161 Hartrees
Zero-point correction = 0.541708 Hartrees
Sum of electronic and thermal Enthalpies = -1712.983399 Hartrees
Sum of electronic and thermal Free Energies = -1713.077797 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\lambda)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.012280	0.166642	-0.000417
2	7	-2.438372	1.881194	-0.020723
3	7	1.424407	-0.617241	2.182559
4	8	-1.266954	0.355422	2.214322
5	8	2.002727	1.792613	0.837126
6	8	0.153908	2.865061	-0.557034
7	6	2.136219	0.504135	2.835908
8	6	2.910625	1.372540	1.857145
9	6	2.388288	3.003984	0.175834
10	6	1.466385	3.193114	-1.017319
11	6	-0.926882	3.329443	-1.369587
12	1	-1.012647	2.707563	-2.270217
13	1	-0.746003	4.367108	-1.679387
14	6	-2.150588	3.273883	-0.472406
15	1	-1.937978	3.891886	0.402717
16	1	-3.019390	3.716625	-0.980695
17	6	-2.963135	1.877359	1.369983
18	6	-3.375198	1.280779	-1.000587
19	1	-3.013697	1.553758	-1.999749
20	1	-4.377891	1.726089	-0.896849
21	6	-2.685129	0.623671	2.196463
22	6	-0.767878	-0.272359	3.416013
23	1	-1.557252	-0.883195	3.868147
24	1	-0.506205	0.518274	4.129144
25	6	0.403402	-1.202189	3.093511
26	1	0.013892	-2.087138	2.589209
27	1	0.852174	-1.518264	4.049612
28	6	-3.476131	-0.224585	-0.951036
29	6	-4.659700	-0.882072	-1.292678
30	1	-5.545749	-0.309317	-1.549003
31	6	-4.680078	-2.277578	-1.303426
32	1	-5.586547	-2.810094	-1.575875
33	6	-3.529083	-2.972261	-0.940005
34	1	-3.479680	-4.054291	-0.900873
35	6	-2.393974	-2.242728	-0.592000
36	6	-1.137258	-2.937939	-0.092563
37	7	-2.361473	-0.895520	-0.618250
38	6	2.369844	-1.687951	1.746359
39	1	1.791651	-2.613047	1.671502
40	1	3.152664	-1.841489	2.503724
41	6	2.990076	-1.472506	0.377378
42	6	4.226826	-2.020095	0.025444
43	1	4.828163	-2.537889	0.766561
44	6	4.663403	-1.905937	-1.296747
45	1	5.618611	-2.330538	-1.591530
46	6	3.863041	-1.251300	-2.233283
47	1	4.146317	-1.141085	-3.273742
48	6	2.647778	-0.722446	-1.804145
49	6	1.696014	0.009100	-2.748848
50	7	2.241540	-0.827929	-0.527812
51	8	0.562931	0.360561	-2.184460
52	8	2.041369	0.232593	-3.895855
53	8	-1.118765	-4.155247	-0.000321
54	8	-0.184873	-2.110747	0.235139
55	1	1.394770	1.141748	3.324987
56	1	2.821367	0.135631	3.616513

57	1	3.758547	0.845869	1.402816
58	1	3.299247	2.246975	2.395262
59	1	-3.027727	0.824373	3.218361
60	1	-3.205653	-0.263835	1.825139
61	1	-4.050514	2.059140	1.387992
62	1	-2.489383	2.709746	1.896600
63	1	1.507466	4.238593	-1.349159
64	1	1.736286	2.545490	-1.857254
65	1	2.290801	3.836571	0.884959
66	1	3.431320	2.944353	-0.160848

HF = -1713.5567968 Hartrees
Zero-point correction = 0.541870 Hartrees
Sum of electronic and thermal Enthalpies = -1712.981906 Hartrees
Sum of electronic and thermal Free Energies = -1713.076534 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) $\Lambda(\delta\lambda)(\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.010470	-0.263395	-0.045362
2	7	2.757275	-1.502981	-0.077639
3	7	-1.869053	-0.431917	2.031322
4	8	1.039400	-0.856624	2.250234
5	8	-1.771518	-2.356512	-0.055552
6	8	0.490335	-2.561149	-1.340653
7	6	-2.917947	-1.467322	1.830412
8	1	-3.409921	-1.717297	2.782808
9	1	-3.680029	-1.047824	1.170661
10	6	-2.395635	-2.730491	1.176966
11	1	-1.671792	-3.272763	1.802652
12	1	-3.240863	-3.402449	0.980166
13	6	-1.652296	-3.444227	-0.982376
14	6	-0.667878	-3.019938	-2.052629
15	6	1.767876	-2.888347	-1.887347
16	1	2.018833	-2.194127	-2.699360
17	1	1.750357	-3.904087	-2.302157
18	6	2.742501	-2.840604	-0.722182
19	1	2.405807	-3.576215	0.012455
20	1	3.747138	-3.144136	-1.057270
21	6	3.164984	-1.598137	1.350278
22	6	3.644662	-0.625604	-0.875634
23	1	3.451466	-0.831759	-1.934579
24	1	4.701771	-0.884417	-0.699718
25	6	2.464461	-0.641203	2.313067
26	6	0.307520	-0.186117	3.304471
27	6	-1.128405	-0.694132	3.294006
28	6	3.438837	0.852580	-0.647799
29	6	4.469562	1.769893	-0.869492
30	1	5.448427	1.422660	-1.186329
31	6	4.219452	3.128270	-0.675609
32	1	5.001055	3.860499	-0.855469
33	6	2.966004	3.524674	-0.212567
34	1	2.716109	4.557041	0.003573
35	6	2.003982	2.544142	0.013014
36	6	0.676308	2.872152	0.672229
37	7	2.221004	1.238134	-0.242217
38	6	-2.536182	0.901513	2.035374
39	1	-1.802366	1.650403	2.341326

40	1	-3.371135	0.911474	2.752408
41	6	-3.021992	1.274010	0.646036
42	6	-4.156379	2.054537	0.420692
43	1	-4.768204	2.385101	1.254391
44	6	-4.481335	2.411255	-0.891371
45	1	-5.358263	3.021626	-1.086136
46	6	-3.671867	1.983798	-1.942824
47	1	-3.870812	2.236610	-2.977915
48	6	-2.555352	1.206961	-1.638439
49	6	-1.574858	0.730674	-2.705990
50	7	-2.260109	0.855530	-0.377124
51	8	-0.496613	0.161627	-2.207973
52	8	-1.835218	0.889813	-3.884343
53	8	0.383377	4.030832	0.918302
54	8	-0.019207	1.805501	0.961273
55	1	-1.097438	-1.777569	3.444746
56	1	-1.659694	-0.264102	4.156856
57	1	0.763295	-0.440783	4.269463
58	1	0.367426	0.895381	3.147676
59	1	2.812049	-0.872093	3.328578
60	1	2.681839	0.409821	2.103393
61	1	4.250828	-1.452804	1.463294
62	1	2.944082	-2.612629	1.693103
63	1	-0.417320	-3.877233	-2.687502
64	1	-1.049874	-2.206837	-2.677532
65	1	-1.273444	-4.330176	-0.455479
66	1	-2.634098	-3.676710	-1.414690

HF = -1713.5548548 Hartrees
Zero-point correction = 0.541737Hartrees
Sum of electronic and thermal Enthalpies = -1712.980184 Hartrees
Sum of electronic and thermal Free Energies = -1713.074780 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\lambda\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.036526	-0.112932	-0.017139
2	7	2.645473	-1.427639	-0.362998
3	7	-1.777862	-0.449782	2.050326
4	8	0.978574	-1.381949	2.028376
5	8	-1.965359	-1.870573	-0.328623
6	8	0.305302	-2.579635	-1.423525
7	6	-2.688645	-1.622141	1.905454
8	1	-2.828849	-2.131895	2.869283
9	1	-3.668009	-1.252758	1.590936
10	6	-2.228818	-2.627041	0.852543
11	1	-1.331550	-3.182702	1.158432
12	1	-3.030245	-3.354142	0.667327
13	6	-2.059504	-2.532588	-1.592534
14	6	-0.809327	-3.350731	-1.878303
15	6	1.552482	-2.910188	-2.042288
16	1	1.708261	-2.253694	-2.907382
17	1	1.540144	-3.947037	-2.399239
18	6	2.633433	-2.771400	-0.985426
19	1	2.430614	-3.513017	-0.209130
20	1	3.616817	-3.018134	-1.416777
21	6	3.179224	-1.498088	1.018331
22	1	3.399876	-0.481271	1.348720

23	1	4.122498	-2.068710	1.054403
24	6	3.451046	-0.510258	-1.208079
25	1	3.069722	-0.587041	-2.233286
26	1	4.505711	-0.829564	-1.237122
27	6	2.211161	-2.120665	2.021075
28	1	1.997487	-3.176086	1.807542
29	1	2.669114	-2.067236	3.016783
30	6	0.145481	-1.617782	3.180351
31	1	0.761440	-1.564304	4.086664
32	1	-0.278786	-2.629139	3.121029
33	6	-0.922329	-0.533763	3.258396
34	1	-0.421365	0.431003	3.365398
35	1	-1.522676	-0.712849	4.165436
36	6	3.370057	0.931310	-0.755953
37	6	4.415163	1.833741	-0.959506
38	1	5.322948	1.514754	-1.462504
39	6	4.272857	3.144454	-0.499147
40	1	5.068230	3.866999	-0.656465
41	6	3.117691	3.501587	0.194187
42	1	2.964170	4.488731	0.614764
43	6	2.128111	2.537513	0.370964
44	6	0.884195	2.802733	1.205963
45	7	2.241124	1.292186	-0.128041
46	6	-2.572221	0.816887	2.074689
47	1	-1.905099	1.608691	2.424458
48	1	-3.415315	0.735144	2.775390
49	6	-3.058248	1.222615	0.696715
50	6	-4.286297	1.847825	0.473154
51	1	-4.977363	2.007387	1.295126
52	6	-4.602158	2.273716	-0.820813
53	1	-5.549670	2.768612	-1.012975
54	6	-3.698082	2.054371	-1.859209
55	1	-3.892748	2.357025	-2.881719
56	6	-2.496931	1.412716	-1.560351
57	6	-1.450737	1.093352	-2.627663
58	7	-2.198982	1.018097	-0.313313
59	8	-0.371865	0.514036	-2.146887
60	8	-1.680763	1.355919	-3.794316
61	8	0.721905	3.896117	1.721703
62	8	0.102570	1.760160	1.306377
63	1	-0.815680	-4.318072	-1.356197
64	1	-0.742760	-3.540362	-2.956643
65	1	-2.155832	-1.727836	-2.323531
66	1	-2.959056	-3.159483	-1.630883

HF = -1713.5558054 Hartrees
Zero-point correction = 0.541232 Hartrees
Sum of electronic and thermal Enthalpies = -1712.981341 Hartrees
Sum of electronic and thermal Free Energies = -1713.076730 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) Λ(λλ)(δδδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.009625	0.112339	-0.147785
2	7	-2.378638	1.922755	-0.267284
3	7	1.273048	-0.600612	2.208582
4	8	-1.357196	0.414216	2.059821
5	8	1.858333	1.851505	0.906712

6	8	0.228463	2.724944	-0.963903
7	6	1.908380	0.541551	2.901841
8	6	2.713687	1.437337	1.976694
9	6	2.313694	3.036657	0.238853
10	6	1.596719	3.105518	-1.103584
11	6	-0.654509	3.718116	-0.449000
12	6	-2.053298	3.264985	-0.823447
13	6	-2.843476	2.088084	1.131743
14	6	-3.393984	1.282634	-1.137396
15	1	-3.086984	1.462546	-2.174176
16	1	-4.378745	1.760834	-1.011405
17	6	-2.723323	0.866821	2.033740
18	6	-0.990728	-0.256723	3.282547
19	6	0.193853	-1.190335	3.042620
20	6	-3.526423	-0.213647	-0.967286
21	6	-4.747265	-0.854856	-1.188038
22	1	-5.632688	-0.271650	-1.421967
23	6	-4.806169	-2.247039	-1.110932
24	1	-5.742574	-2.766929	-1.290751
25	6	-3.652363	-2.953029	-0.781051
26	1	-3.628584	-4.031716	-0.678334
27	6	-2.477407	-2.239106	-0.552496
28	6	-1.215113	-2.948982	-0.085561
29	7	-2.409045	-0.897213	-0.665875
30	6	2.263643	-1.663606	1.877043
31	1	1.703057	-2.595766	1.759174
32	1	2.973000	-1.803698	2.706285
33	6	3.004429	-1.458287	0.570619
34	6	4.284445	-1.974464	0.352627
35	1	4.829994	-2.446918	1.163872
36	6	4.836442	-1.891363	-0.927981
37	1	5.828099	-2.290880	-1.119482
38	6	4.099979	-1.305285	-1.956779
39	1	4.466979	-1.228395	-2.973799
40	6	2.834823	-0.804025	-1.658114
41	6	1.940895	-0.166874	-2.719695
42	7	2.319280	-0.866747	-0.418375
43	8	0.755469	0.165102	-2.267877
44	8	2.373684	0.001432	-3.846310
45	8	-1.236055	-4.156948	0.088846
46	8	-0.214227	-2.142433	0.132505
47	1	-2.794007	4.018358	-0.513192
48	1	-2.086221	3.199381	-1.913179
49	1	-0.449600	4.687755	-0.921588
50	1	-0.521739	3.835517	0.636378
51	1	1.676684	4.112272	-1.532916
52	1	2.017319	2.393410	-1.814553
53	1	2.094995	3.905862	0.874213
54	1	3.398316	2.994680	0.075667
55	1	3.051173	2.314028	2.544969
56	1	3.597244	0.935403	1.564773
57	1	1.120600	1.154597	3.346564
58	1	2.557032	0.194919	3.722829
59	1	-0.157875	-2.074968	2.510600
60	1	0.573426	-1.510892	4.026953
61	1	-1.830991	-0.866769	3.634764
62	1	-0.789373	0.506088	4.045093
63	1	-3.023017	1.172393	3.043837
64	1	-3.367380	0.039151	1.720279
65	1	-3.892458	2.428926	1.154727
66	1	-2.241180	2.880785	1.585328

HF = -1713.5542645 Hartrees
Zero-point correction = 0.542009 Hartrees
Sum of electronic and thermal Enthalpies = -1712.979248 Hartrees
Sum of electronic and thermal Free Energies = -1713.074009 Hartrees

$[Eu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\lambda\delta)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.045155	0.135949	-0.063190
2	7	-2.648308	1.419423	-0.514839
3	7	1.676859	0.255287	2.104468
4	8	-1.098663	1.163513	2.008106
5	8	1.887419	2.036163	-0.033447
6	8	-0.299346	2.858530	-1.189439
7	6	2.531857	1.463979	2.162469
8	6	3.041636	1.892589	0.795409
9	6	2.058572	2.752688	-1.265998
10	6	0.859740	3.668508	-1.379302
11	6	-1.477273	3.622183	-0.966181
12	6	-2.668843	2.720966	-1.230826
13	6	-3.212962	1.508976	0.857263
14	1	-3.535796	0.507365	1.148839
15	1	-4.105867	2.155985	0.872411
16	6	-3.444787	0.466217	-1.341164
17	1	-3.022444	0.492449	-2.352199
18	1	-4.493610	0.793731	-1.420705
19	6	-2.262007	2.007242	1.946653
20	1	-1.947097	3.047017	1.801838
21	1	-2.795251	1.949975	2.904228
22	6	-0.350421	1.257053	3.237804
23	1	-1.026759	1.069177	4.081180
24	1	0.036415	2.279058	3.340095
25	6	0.749929	0.195693	3.264863
26	1	0.279325	-0.789059	3.243555
27	1	1.287161	0.298899	4.221913
28	6	-3.390385	-0.955771	-0.841012
29	6	-4.460286	-1.837988	-1.001199
30	1	-5.377310	-1.502338	-1.475596
31	6	-4.327760	-3.149769	-0.541927
32	1	-5.142156	-3.857445	-0.665884
33	6	-3.151146	-3.526509	0.101910
34	1	-2.995161	-4.516864	0.513931
35	6	-2.138787	-2.579373	0.239337
36	6	-0.868267	-2.875018	1.015348
37	7	-2.245591	-1.330090	-0.250239
38	6	2.510676	-0.979855	2.032647
39	1	1.874418	-1.818675	2.324595
40	1	3.351389	-0.919594	2.739488
41	6	3.016874	-1.289377	0.634704
42	6	4.211958	-1.973935	0.401861
43	1	4.857328	-2.246371	1.231369
44	6	4.553483	-2.310193	-0.910950
45	1	5.475711	-2.848114	-1.110472
46	6	3.705234	-1.951669	-1.958601
47	1	3.918410	-2.187395	-2.994914
48	6	2.533871	-1.263348	-1.649311
49	6	1.531628	-0.830530	-2.719397

50	7	2.213940	-0.944775	-0.383754
51	8	0.456183	-0.256894	-2.225370
52	8	1.785975	-1.023895	-3.893958
53	8	-0.703555	-3.972490	1.523167
54	8	-0.062202	-1.850804	1.083031
55	1	0.904990	4.440756	-0.597822
56	1	0.827717	4.158775	-2.361747
57	1	2.098858	2.041255	-2.097114
58	1	2.983955	3.338551	-1.248608
59	1	-3.599334	3.272486	-1.020479
60	1	-2.658511	2.501511	-2.301186
61	1	-1.463224	4.046660	0.047485
62	1	-1.526709	4.464215	-1.670803
63	1	3.554994	2.858453	0.890467
64	1	3.741029	1.172374	0.358310
65	1	3.382651	1.312872	2.844869
66	1	1.939679	2.291082	2.561330

HF = -1713.5554981 Hartrees
Zero-point correction = 0.541530 Hartrees
Sum of electronic and thermal Enthalpies = -1712.980797 Hartrees
Sum of electronic and thermal Free Energies = -1713.076477 Hartrees

$[Gd(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	0.060416	-0.183494	0.019497
2	7	2.624915	-1.463876	-0.319193
3	7	-1.732291	-0.395851	2.099949
4	8	1.047560	-1.243193	2.121443
5	8	-1.855990	-2.151749	-0.117049
6	8	0.277132	-2.498728	-1.464841
7	6	-2.558450	-1.626519	2.079585
8	6	-3.029057	-2.001927	0.684721
9	6	-2.107860	-2.508145	-1.482116
10	6	-0.851981	-3.181856	-2.010440
11	6	1.524716	-2.904086	-2.028431
12	1	1.752633	-2.273939	-2.897111
13	1	1.466021	-3.944944	-2.371024
14	6	2.566521	-2.813101	-0.926090
15	1	2.287361	-3.529795	-0.149452
16	1	3.552817	-3.117811	-1.312041
17	6	3.196959	-1.527321	1.048175
18	1	3.483889	-0.515291	1.340903
19	1	4.108018	-2.148127	1.069979
20	6	3.434535	-0.573050	-1.189326
21	1	3.049118	-0.666135	-2.210839
22	1	4.486183	-0.901445	-1.213991
23	6	2.227986	-2.062522	2.097835
24	1	1.937939	-3.106188	1.918772
25	1	2.721223	-2.014046	3.076755
26	6	0.250207	-1.387525	3.312178
27	1	0.882312	-1.206302	4.190736
28	1	-0.117186	-2.420151	3.371960
29	6	-0.869364	-0.350258	3.310253
30	1	-0.415199	0.642098	3.336720
31	1	-1.456914	-0.486639	4.232805
32	6	3.357724	0.877184	-0.768051

33	6	4.400563	1.776829	-0.994222
34	1	5.310643	1.446810	-1.485823
35	6	4.251438	3.099854	-0.573138
36	1	5.045019	3.820460	-0.747466
37	6	3.089346	3.473966	0.099479
38	1	2.927515	4.474159	0.484621
39	6	2.102869	2.511515	0.300204
40	6	0.845242	2.799610	1.104180
41	7	2.226023	1.250644	-0.153638
42	6	-2.588509	0.823370	2.039509
43	1	-1.983042	1.659945	2.398251
44	1	-3.458714	0.717865	2.704267
45	6	-3.032711	1.196056	0.637330
46	6	-4.216335	1.894464	0.386801
47	1	-4.902507	2.117270	1.198132
48	6	-4.491035	2.312085	-0.918054
49	1	-5.403959	2.860439	-1.131476
50	6	-3.584204	2.026640	-1.938788
51	1	-3.739771	2.333458	-2.966712
52	6	-2.427929	1.321554	-1.612374
53	6	-1.356466	0.979590	-2.646939
54	7	-2.178052	0.911059	-0.356768
55	8	-0.294243	0.414186	-2.124511
56	8	-1.555798	1.227576	-3.822983
57	8	0.666818	3.909720	1.577885
58	8	0.067159	1.757418	1.226912
59	1	-0.811351	-4.234105	-1.697367
60	1	-0.843728	-3.136331	-3.106703
61	1	-2.352266	-1.607773	-2.056040
62	1	-2.952478	-3.205111	-1.545727
63	1	-1.956391	-2.457578	2.454768
64	1	-3.428659	-1.526809	2.746889
65	1	-3.694466	-1.248221	0.250155
66	1	-3.571186	-2.956301	0.727268

HF = -1714.1526672 Hartrees
Zero-point correction = 0.541662 Hartrees
Sum of electronic and thermal Enthalpies = -1713.577896 Hartrees
Sum of electronic and thermal Free Energies = -1713.672776 Hartrees

$[Gd(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	0.057172	-0.171541	0.033796
2	7	2.574971	-1.557201	-0.305684
3	7	-1.707883	-0.213785	2.125731
4	8	1.026150	-1.183715	2.144982
5	8	-2.006510	-1.966345	-0.061477
6	8	0.144850	-2.677759	-1.258604
7	6	-2.566071	-1.419469	2.189547
8	6	-3.112527	-1.845505	0.836120
9	6	-2.196050	-2.945141	-1.088662
10	6	-1.034382	-2.827122	-2.057082
11	6	1.358730	-2.968783	-1.948628
12	1	1.505580	-2.254672	-2.769973
13	1	1.313501	-3.979166	-2.377523
14	6	2.460168	-2.907968	-0.905945
15	1	2.209706	-3.623849	-0.118574

16	1	3.418086	-3.228437	-1.344290
17	6	3.145546	-1.625022	1.062070
18	1	3.490095	-0.624817	1.333873
19	1	4.020324	-2.295259	1.096741
20	6	3.420946	-0.715124	-1.189173
21	1	3.038232	-0.818580	-2.210780
22	1	4.459571	-1.083350	-1.200909
23	6	2.149757	-2.082098	2.124077
24	1	1.787831	-3.104815	1.956402
25	1	2.650750	-2.056033	3.099647
26	6	0.257633	-1.211683	3.363732
27	1	0.921648	-0.997142	4.210509
28	1	-0.148676	-2.221265	3.504947
29	6	-0.821773	-0.131289	3.318330
30	1	-0.332394	0.843698	3.280090
31	1	-1.397750	-0.193053	4.256031
32	6	3.398300	0.746572	-0.805966
33	6	4.478010	1.595925	-1.054152
34	1	5.375988	1.213392	-1.529714
35	6	4.381348	2.936636	-0.676938
36	1	5.204357	3.618595	-0.869316
37	6	3.231660	3.378342	-0.024668
38	1	3.107706	4.396137	0.326957
39	6	2.206469	2.463133	0.201233
40	6	0.959583	2.829914	0.988249
41	7	2.279195	1.183441	-0.209943
42	6	-2.529664	1.026667	2.007032
43	1	-1.898033	1.862376	2.318745
44	1	-3.397839	0.980411	2.680868
45	6	-2.975195	1.331852	0.588169
46	6	-4.153192	2.025550	0.299843
47	1	-4.832358	2.308076	1.098451
48	6	-4.433308	2.357625	-1.028229
49	1	-5.341092	2.902159	-1.271195
50	6	-3.543244	1.985306	-2.035958
51	1	-3.710850	2.214403	-3.082079
52	6	-2.392158	1.290386	-1.671145
53	6	-1.355402	0.826491	-2.691801
54	7	-2.130735	0.977575	-0.391162
55	8	-0.295471	0.270824	-2.147479
56	8	-1.574616	0.968310	-3.881750
57	8	0.825825	3.961209	1.425508
58	8	0.138495	1.825909	1.140893
59	1	-1.967556	-2.249371	2.572530
60	1	-3.401847	-1.269057	2.891404
61	1	-3.843322	-1.137915	0.428869
62	1	-3.607513	-2.818354	0.951728
63	1	-0.972870	-3.739142	-2.664792
64	1	-1.134455	-1.960725	-2.718582
65	1	-2.222673	-3.940562	-0.625480
66	1	-3.142878	-2.773911	-1.617058

HF = -1714.1554533 Hartrees
Zero-point correction = 0.541864 Hartrees
Sum of electronic and thermal Enthalpies = -1713.580631 Hartrees
Sum of electronic and thermal Free Energies = -1713.674900 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	0.060718	-0.181386	0.049603
2	7	2.572939	-1.486520	-0.316703
3	7	-1.756034	-0.383426	2.079264
4	8	0.998468	-1.260576	2.109946
5	8	-1.902592	-2.092207	-0.153159
6	8	0.224931	-2.496085	-1.459613
7	6	-2.597033	-1.603061	2.049043
8	6	-3.073897	-1.951598	0.650357
9	6	-2.156483	-2.428707	-1.521882
10	6	-0.912190	-3.125349	-2.048933
11	6	1.464564	-2.914805	-2.026799
12	1	1.699415	-2.287330	-2.895724
13	1	1.394079	-3.955567	-2.368583
14	6	2.505686	-2.834852	-0.924559
15	1	2.219995	-3.550235	-0.149180
16	1	3.490563	-3.145516	-1.309086
17	6	3.151288	-1.558042	1.047287
18	1	3.450679	-0.550285	1.341787
19	1	4.054975	-2.189445	1.065246
20	6	3.383433	-0.601637	-1.191969
21	1	2.983166	-0.683998	-2.208423
22	1	4.431008	-0.941371	-1.229477
23	6	2.176647	-2.085247	2.095055
24	1	1.881900	-3.127825	1.918645
25	1	2.664135	-2.034584	3.076541
26	6	0.199908	-1.398008	3.302253
27	1	0.835472	-1.224569	4.179628
28	1	-0.176515	-2.427408	3.359454
29	6	-0.910573	-0.351475	3.301197
30	1	-0.450598	0.637205	3.342070
31	1	-1.509929	-0.493888	4.215135
32	6	3.323990	0.845268	-0.761490
33	6	4.366089	1.743159	-0.997886
34	1	5.266502	1.414025	-1.507505
35	6	4.228749	3.063176	-0.563706
36	1	5.022066	3.782272	-0.745210
37	6	3.078619	3.436302	0.130082
38	1	2.926320	4.434267	0.524859
39	6	2.092739	2.475377	0.337821
40	6	0.844473	2.753491	1.155548
41	7	2.204549	1.217432	-0.125821
42	6	-2.598229	0.844587	2.003120
43	1	-1.998853	1.672499	2.390269
44	1	-3.491900	0.741372	2.636235
45	6	-2.990423	1.231175	0.589226
46	6	-4.153724	1.949019	0.301164
47	1	-4.862299	2.181838	1.090159
48	6	-4.379857	2.372309	-1.011058
49	1	-5.276642	2.935485	-1.252398
50	6	-3.445755	2.073176	-2.002993
51	1	-3.563620	2.382988	-3.035042
52	6	-2.312075	1.350038	-1.640183
53	6	-1.211625	0.989003	-2.635654
54	7	-2.108928	0.934354	-0.377559
55	8	-0.179052	0.406903	-2.072196
56	8	-1.361622	1.238284	-3.818477

57	8	0.665187	3.855049	1.647897
58	8	0.069612	1.706761	1.266778
59	1	-0.909998	-4.187853	-1.769266
60	1	-0.879691	-3.046405	-3.142935
61	1	-2.380139	-1.517829	-2.087676
62	1	-3.016467	-3.105553	-1.596023
63	1	-2.003125	-2.445963	2.410734
64	1	-3.463256	-1.500881	2.721209
65	1	-3.736930	-1.186772	0.230912
66	1	-3.621519	-2.903489	0.676312

HF = -1715.9147166 Hartrees
Zero-point correction = 0.541939 Hartrees
Sum of electronic and thermal Enthalpies = -1715.339728 Hartrees
Sum of electronic and thermal Free Energies = -1715.434522 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	0.056686	-0.166384	0.064636
2	7	2.527231	-1.574500	-0.294208
3	7	-1.735100	-0.202408	2.102343
4	8	0.973146	-1.196848	2.138042
5	8	-2.042294	-1.924824	-0.096224
6	8	0.101719	-2.673477	-1.266066
7	6	-2.607707	-1.397686	2.154029
8	6	-3.152279	-1.800823	0.794107
9	6	-2.243281	-2.888061	-1.134931
10	6	-1.065127	-2.791371	-2.084319
11	6	1.316726	-2.975601	-1.946055
12	1	1.477551	-2.262243	-2.765117
13	1	1.265974	-3.985589	-2.375982
14	6	2.407995	-2.925186	-0.893719
15	1	2.143164	-3.638163	-0.108445
16	1	3.368263	-3.253041	-1.321217
17	6	3.098616	-1.647626	1.072428
18	1	3.450520	-0.650807	1.346750
19	1	3.967780	-2.325012	1.107129
20	6	3.377955	-0.739474	-1.179406
21	1	2.990377	-0.837167	-2.199386
22	1	4.413517	-1.116005	-1.193596
23	6	2.095324	-2.098800	2.128655
24	1	1.730759	-3.120407	1.961591
25	1	2.587523	-2.070260	3.108400
26	6	0.201962	-1.219377	3.356607
27	1	0.867469	-1.011156	4.203550
28	1	-0.211222	-2.226434	3.494724
29	6	-0.869459	-0.131991	3.309643
30	1	-0.374969	0.840257	3.287486
31	1	-1.459890	-0.201150	4.237724
32	6	3.365238	0.720174	-0.793346
33	6	4.442052	1.569803	-1.053651
34	1	5.332681	1.188162	-1.543502
35	6	4.351989	2.908986	-0.670060
36	1	5.172844	3.590973	-0.871233
37	6	3.211394	3.349366	-0.000610
38	1	3.093010	4.366180	0.355789
39	6	2.189606	2.433598	0.235006

40	6	0.950403	2.790560	1.033965
41	7	2.255696	1.155144	-0.180103
42	6	-2.543462	1.044954	1.967284
43	1	-1.919547	1.874072	2.309623
44	1	-3.436252	0.998380	2.608007
45	6	-2.934631	1.362904	0.535464
46	6	-4.090036	2.077213	0.207939
47	1	-4.790486	2.371443	0.983604
48	6	-4.320433	2.413614	-1.128471
49	1	-5.210216	2.973551	-1.401138
50	6	-3.404295	2.025304	-2.106627
51	1	-3.533965	2.256210	-3.157743
52	6	-2.277963	1.312271	-1.703378
53	6	-1.213397	0.827154	-2.682602
54	7	-2.064407	0.995128	-0.415569
55	8	-0.182368	0.261827	-2.093661
56	8	-1.385265	0.960868	-3.881085
57	8	0.810693	3.916132	1.482923
58	8	0.136595	1.778885	1.182673
59	1	-2.020285	-2.238545	2.530433
60	1	-3.443504	-1.243175	2.854943
61	1	-3.871834	-1.078904	0.391086
62	1	-3.661288	-2.768131	0.894942
63	1	-1.014948	-3.701947	-2.695742
64	1	-1.135723	-1.921902	-2.745547
65	1	-2.301512	-3.886851	-0.681731
66	1	-3.178665	-2.688085	-1.673768

HF = -1715.9176441 Hartrees
Zero-point correction = 0.542234 Hartrees
Sum of electronic and thermal Enthalpies = -1715.342531 Hartrees
Sum of electronic and thermal Free Energies = -1715.436618 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) Λ(λδ)(λδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.032467	-0.129311	-0.017135
2	7	-2.556319	-1.544661	0.319857
3	7	1.845855	-0.181368	-2.030966
4	8	-0.830540	-1.324458	-2.046008
5	8	2.009397	-2.060671	0.070125
6	8	-0.176388	-2.542244	1.384664
7	6	2.890807	-1.238781	-1.984644
8	1	3.202310	-1.526378	-3.000326
9	1	3.766431	-0.812379	-1.489376
10	6	2.507418	-2.479784	-1.198868
11	1	1.751530	-3.100239	-1.699853
12	1	3.406932	-3.096236	-1.068729
13	6	2.062287	-3.101241	1.054597
14	1	3.071939	-3.165324	1.480154
15	1	1.812242	-4.060167	0.582104
16	6	1.030377	-2.781285	2.112746
17	1	0.914069	-3.641349	2.784072
18	1	1.287769	-1.899724	2.708573
19	6	-1.387063	-2.822273	2.081417
20	1	-1.565055	-2.061840	2.852451
21	1	-1.323492	-3.803264	2.571247
22	6	-2.462152	-2.852118	1.010952

23	1	-2.183645	-3.619799	0.284646
24	1	-3.432354	-3.145718	1.440076
25	6	-3.027526	-1.698481	-1.076126
26	1	-3.350090	-0.718143	-1.434769
27	1	-3.898279	-2.372851	-1.135454
28	6	-3.464786	-0.675293	1.105175
29	1	-3.150516	-0.733696	2.153439
30	1	-4.499857	-1.051898	1.063512
31	6	-1.958322	-2.222354	-2.032321
32	1	-1.609528	-3.228317	-1.767314
33	1	-2.390345	-2.267478	-3.039251
34	6	-0.004798	-1.409446	-3.228708
35	1	-0.646456	-1.323147	-4.114208
36	1	0.480784	-2.392463	-3.258121
37	6	0.994577	-0.255331	-3.241930
38	1	0.434965	0.680368	-3.296567
39	1	1.600491	-0.349089	-4.158296
40	6	-3.426708	0.768355	0.669250
41	6	-4.519326	1.620915	0.842492
42	1	-5.433630	1.249367	1.295137
43	6	-4.414798	2.946884	0.421112
44	1	-5.247412	3.631015	0.555472
45	6	-3.241966	3.368502	-0.203068
46	1	-3.107912	4.371993	-0.590345
47	6	-2.207726	2.449418	-0.354040
48	6	-0.940729	2.781500	-1.115327
49	7	-2.285461	1.185384	0.103854
50	6	2.529201	1.144464	-1.941743
51	1	1.815193	1.910982	-2.248417
52	1	3.398174	1.183934	-2.613887
53	6	2.940836	1.454677	-0.515646
54	6	4.089077	2.179508	-0.191831
55	1	4.773343	2.496307	-0.972915
56	6	4.333850	2.499343	1.146735
57	1	5.220583	3.065657	1.416101
58	6	3.433537	2.089163	2.129293
59	1	3.570257	2.311218	3.181405
60	6	2.311400	1.366189	1.730023
61	6	1.253442	0.879738	2.715008
62	7	2.088795	1.055352	0.442830
63	8	0.215539	0.320667	2.129859
64	8	1.430140	1.011366	3.912587
65	8	-0.776284	3.891957	-1.592076
66	8	-0.130451	1.760375	-1.207752

HF = -1715.9122743 Hartrees
Zero-point correction = 0.541940 Hartrees
Sum of electronic and thermal Enthalpies = -1715.337311 Hartrees
Sum of electronic and thermal Free Energies = -1715.432186 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) $\Lambda(\delta\delta)(\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.036450	-0.257447	0.011927
2	7	-2.793553	-1.203367	0.081898
3	7	2.022731	-0.811143	-1.772066
4	8	-0.793683	-1.426774	-2.041246
5	8	1.686974	-2.307348	0.618574

6	8	-0.753221	-2.384756	1.530821
7	6	3.044198	-1.760589	-1.257228
8	1	3.647773	-2.173440	-2.079981
9	1	3.721102	-1.204401	-0.605742
10	6	2.451573	-2.888250	-0.440968
11	1	1.806778	-3.555146	-1.032243
12	1	3.268982	-3.492070	-0.025595
13	6	1.424260	-3.238921	1.675404
14	1	2.322826	-3.370626	2.292095
15	1	1.143488	-4.207909	1.241168
16	6	0.272793	-2.690926	2.487754
17	1	-0.074255	-3.451356	3.196678
18	1	0.535844	-1.778591	3.031300
19	6	-2.088344	-2.660045	1.946820
20	1	-2.384369	-1.970306	2.747340
21	1	-2.156926	-3.683409	2.338846
22	6	-2.952019	-2.534326	0.703157
23	1	-2.624283	-3.296320	-0.008316
24	1	-4.005247	-2.746141	0.948212
25	6	-3.150270	-1.214946	-1.355781
26	1	-3.224435	-0.177113	-1.687147
27	1	-4.134765	-1.685377	-1.523587
28	6	-3.616820	-0.223453	0.831635
29	1	-3.439943	-0.382300	1.900451
30	1	-4.691355	-0.402029	0.661103
31	6	-2.131083	-1.934163	-2.242103
32	1	-2.103363	-3.011798	-2.048110
33	1	-2.425759	-1.790690	-3.286311
34	6	-0.054277	-0.981035	-3.211999
35	6	1.416226	-1.340433	-3.022477
36	6	-3.273514	1.206437	0.485515
37	6	-4.173694	2.260669	0.659522
38	1	-5.159205	2.075913	1.076386
39	6	-3.785488	3.545812	0.278058
40	1	-4.461821	4.383992	0.417267
41	6	-2.541371	3.731024	-0.326083
42	1	-2.204789	4.692338	-0.697207
43	6	-1.717508	2.621259	-0.484440
44	6	-0.422269	2.660859	-1.271962
45	7	-2.057865	1.398841	-0.037434
46	6	2.689364	0.507923	-1.965276
47	1	2.001960	1.166014	-2.499757
48	1	3.608125	0.392568	-2.560252
49	6	3.002744	1.146978	-0.623903
50	6	4.106220	1.973960	-0.411004
51	1	4.809795	2.164387	-1.215527
52	6	4.283580	2.556134	0.847499
53	1	5.134328	3.206383	1.028898
54	6	3.366269	2.294801	1.864453
55	1	3.455213	2.716296	2.859089
56	6	2.289345	1.458780	1.576930
57	6	1.209661	1.126592	2.601450
58	7	2.128198	0.901268	0.365898
59	8	0.204797	0.442036	2.095010
60	8	1.335987	1.485342	3.757628
61	8	0.011186	3.714664	-1.707805
62	8	0.089648	1.468254	-1.438753
63	1	1.489507	-2.431668	-2.993103
64	1	1.977048	-1.004203	-3.907591
65	1	-0.431725	-1.504606	-4.096423
66	1	-0.205914	0.095173	-3.322756

HF = -1715.9071018 Hartrees
Zero-point correction = 0.541878 Hartrees
Sum of electronic and thermal Enthalpies = -1715.332255 Hartrees
Sum of electronic and thermal Free Energies = -1715.426932 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δδδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.137731	0.097186	0.009099
2	7	-2.205611	1.754745	-0.747401
3	7	1.710545	0.384980	1.943304
4	8	-0.890743	1.661734	1.790147
5	8	3.056550	1.256800	-0.595651
6	8	0.568231	2.392820	-1.079721
7	6	2.730406	1.463799	1.818322
8	6	3.715371	1.311437	0.659530
9	6	2.958606	2.469745	-1.326769
10	6	1.634328	2.429144	-2.060125
11	6	-0.395050	3.452854	-1.120152
12	6	-1.747777	2.906122	-1.561012
13	6	-2.886552	2.163899	0.509592
14	1	-3.455277	1.303363	0.865653
15	1	-3.606984	2.976098	0.320499
16	6	-3.115395	0.904994	-1.571425
17	1	-2.594535	0.697912	-2.513067
18	1	-4.047913	1.436407	-1.815569
19	6	-1.961591	2.606631	1.646380
20	1	-1.544379	3.608773	1.493239
21	1	-2.547513	2.632640	2.574180
22	6	-0.082334	1.844543	2.971036
23	6	0.851611	0.648912	3.132677
24	6	-3.422509	-0.412003	-0.894043
25	6	-4.624024	-1.100006	-1.061013
26	1	-5.406842	-0.691606	-1.692588
27	6	-4.797653	-2.319451	-0.399609
28	1	-5.721253	-2.877404	-0.522370
29	6	-3.789547	-2.796751	0.436853
30	1	-3.878807	-3.718487	1.000304
31	6	-2.624603	-2.043240	0.561386
32	6	-1.490476	-2.427969	1.500126
33	7	-2.445253	-0.893494	-0.111363
34	6	2.353034	-0.960317	2.077967
35	1	1.639158	-1.608863	2.592213
36	1	3.259903	-0.897142	2.696733
37	6	2.661421	-1.615190	0.742205
38	6	3.710727	-2.518415	0.558116
39	1	4.384624	-2.752157	1.376855
40	6	3.873295	-3.116426	-0.694505
41	1	4.680456	-3.825106	-0.855333
42	6	3.003933	-2.790731	-1.736216
43	1	3.093834	-3.213573	-2.730187
44	6	1.984351	-1.879072	-1.476732
45	6	0.992365	-1.420535	-2.542327
46	7	1.825836	-1.326248	-0.263528
47	8	0.089507	-0.575655	-2.085439
48	8	1.099581	-1.823613	-3.685351
49	8	-1.584981	-3.428297	2.190131

50	8	-0.497596	-1.576205	1.471050
51	1	-2.493271	3.717926	-1.560724
52	1	-1.642694	2.559760	-2.592886
53	1	-0.076717	4.229791	-1.823441
54	1	-0.428970	3.909903	-0.128674
55	1	1.519082	3.307533	-2.703035
56	1	1.554476	1.526124	-2.670680
57	1	2.988337	3.342062	-0.658653
58	1	3.786400	2.555282	-2.045860
59	1	4.422728	2.150461	0.700738
60	1	4.301515	0.393786	0.752607
61	1	2.202824	2.415216	1.697142
62	1	3.312778	1.529167	2.753460
63	1	0.241190	-0.241983	3.291592
64	1	1.460471	0.817118	4.035796
65	1	-0.737851	1.891506	3.849382
66	1	0.448564	2.801624	2.893047

HF = -1715.906025 Hartrees
Zero-point correction = 0.541491 Hartrees
Sum of electronic and thermal Enthalpies = -1715.331453 Hartrees
Sum of electronic and thermal Free Energies = -1715.426889 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\lambda)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.013310	0.146408	0.035150
2	7	-2.385107	1.896276	-0.006729
3	7	1.450908	-0.597080	2.171989
4	8	-1.223833	0.365120	2.209058
5	8	2.038100	1.772592	0.796678
6	8	0.203761	2.825146	-0.598240
7	6	2.169686	0.526174	2.813643
8	6	2.947623	1.371145	1.820005
9	6	2.447969	2.948836	0.090947
10	6	1.509542	3.122988	-1.090730
11	6	-0.881341	3.304143	-1.394394
12	1	-0.997863	2.674882	-2.285687
13	1	-0.685267	4.335321	-1.716773
14	6	-2.085061	3.281153	-0.471186
15	1	-1.840767	3.898919	0.395863
16	1	-2.957830	3.736360	-0.961639
17	6	-2.905627	1.911175	1.383876
18	6	-3.331600	1.300716	-0.978756
19	1	-2.975407	1.568784	-1.980780
20	1	-4.331365	1.751073	-0.868633
21	6	-2.638269	0.657799	2.212016
22	6	-0.723795	-0.250520	3.418045
23	1	-1.513893	-0.856490	3.875076
24	1	-0.463536	0.548714	4.121980
25	6	0.448755	-1.179833	3.103220
26	1	0.061547	-2.075939	2.618443
27	1	0.910509	-1.474085	4.059940
28	6	-3.436893	-0.202923	-0.925842
29	6	-4.616170	-0.859220	-1.285409
30	1	-5.495983	-0.284663	-1.558635
31	6	-4.640308	-2.254244	-1.291922
32	1	-5.543476	-2.785550	-1.577280

33	6	-3.496417	-2.950136	-0.908030
34	1	-3.449501	-4.032156	-0.865356
35	6	-2.366720	-2.221019	-0.544780
36	6	-1.116687	-2.909366	-0.028727
37	7	-2.329844	-0.873918	-0.571710
38	6	2.396707	-1.661705	1.722619
39	1	1.832792	-2.597607	1.685669
40	1	3.209522	-1.788635	2.452536
41	6	2.960093	-1.459701	0.327406
42	6	4.179675	-2.011890	-0.073852
43	1	4.813095	-2.522626	0.645112
44	6	4.556712	-1.912953	-1.415475
45	1	5.498012	-2.341075	-1.747498
46	6	3.713804	-1.271643	-2.323843
47	1	3.948949	-1.176990	-3.377772
48	6	2.519161	-0.738626	-1.846284
49	6	1.514961	-0.027890	-2.749396
50	7	2.173483	-0.824100	-0.550871
51	8	0.405737	0.310665	-2.131264
52	8	1.798743	0.192388	-3.913624
53	8	-1.089218	-4.125139	0.075003
54	8	-0.171778	-2.072649	0.300094
55	1	1.432487	1.175795	3.293270
56	1	2.851473	0.161915	3.599003
57	1	3.792168	0.830664	1.374548
58	1	3.342985	2.254256	2.339138
59	1	-2.959783	0.867414	3.238708
60	1	-3.178049	-0.222916	1.852926
61	1	-3.990337	2.107876	1.405766
62	1	-2.417970	2.740157	1.903211
63	1	1.559457	4.159429	-1.448895
64	1	1.757598	2.454885	-1.921308
65	1	2.385541	3.806711	0.773589
66	1	3.483666	2.848251	-0.258824

HF = -1715.9094183 Hartrees
Zero-point correction = 0.542287 Hartrees
Sum of electronic and thermal Enthalpies = -1715.334210 Hartrees
Sum of electronic and thermal Free Energies = -1715.428574 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) $\Lambda(\delta\lambda)(\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.009032	-0.257250	-0.011954
2	7	2.758796	-1.475410	-0.055235
3	7	-1.912464	-0.523560	1.973740
4	8	0.981475	-0.916609	2.229495
5	8	-1.755240	-2.321051	-0.197473
6	8	0.534016	-2.488106	-1.401294
7	6	-2.953895	-1.550132	1.702403
8	1	-3.461591	-1.850697	2.631508
9	1	-3.706639	-1.101643	1.050965
10	6	-2.407814	-2.770709	0.994125
11	1	-1.695468	-3.343182	1.605974
12	1	-3.241888	-3.435894	0.736711
13	6	-1.630026	-3.352339	-1.186170
14	6	-0.594400	-2.891013	-2.189141
15	6	1.822769	-2.821718	-1.913327

16	1	2.105298	-2.120629	-2.708599
17	1	1.806683	-3.832120	-2.341565
18	6	2.762159	-2.800684	-0.720597
19	1	2.400671	-3.546653	-0.008387
20	1	3.775512	-3.102260	-1.031007
21	6	3.150152	-1.588999	1.374058
22	6	3.642104	-0.574262	-0.828655
23	1	3.476900	-0.775188	-1.892860
24	1	4.701341	-0.808411	-0.631929
25	6	2.401225	-0.675704	2.341029
26	6	0.222235	-0.321818	3.310961
27	6	-1.206276	-0.841156	3.241609
28	6	3.393969	0.895591	-0.593854
29	6	4.394888	1.845404	-0.818354
30	1	5.380536	1.529480	-1.146784
31	6	4.107005	3.193883	-0.611692
32	1	4.864654	3.950332	-0.793678
33	6	2.847332	3.549265	-0.131135
34	1	2.570138	4.571798	0.098138
35	6	1.919013	2.538156	0.095671
36	6	0.592981	2.809343	0.778021
37	7	2.170133	1.241310	-0.174518
38	6	-2.585377	0.805150	2.014173
39	1	-1.870830	1.542607	2.385148
40	1	-3.450777	0.778488	2.693598
41	6	-3.010769	1.232830	0.621684
42	6	-4.135021	2.021159	0.374331
43	1	-4.783425	2.321217	1.191749
44	6	-4.402564	2.425117	-0.936946
45	1	-5.271268	3.041756	-1.148037
46	6	-3.545904	2.037112	-1.966228
47	1	-3.699002	2.327715	-2.999203
48	6	-2.442160	1.251800	-1.639575
49	6	-1.407425	0.815656	-2.669365
50	7	-2.203178	0.852213	-0.380864
51	8	-0.348335	0.247649	-2.129607
52	8	-1.608992	0.998158	-3.855673
53	8	0.250921	3.950595	1.039434
54	8	-0.048442	1.708844	1.071864
55	1	-1.169054	-1.930511	3.339251
56	1	-1.763621	-0.458786	4.110505
57	1	0.664414	-0.634358	4.264998
58	1	0.274528	0.767244	3.223403
59	1	2.721167	-0.928782	3.360029
60	1	2.601593	0.385292	2.168663
61	1	4.228147	-1.407812	1.507501
62	1	2.961157	-2.617733	1.692858
63	1	-0.326780	-3.720927	-2.852884
64	1	-0.934369	-2.044426	-2.792786
65	1	-1.292911	-4.278154	-0.701426
66	1	-2.601405	-3.531315	-1.664921

HF = -1715.9059945 Hartrees
Zero-point correction = 0.542029 Hartrees
Sum of electronic and thermal Enthalpies = -1715.331044 Hartrees
Sum of electronic and thermal Free Energies = -1715.425932 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) Λ(λδ)(λλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	0.034288	-0.119393	0.033056
2	7	2.611865	-1.414091	-0.346383
3	7	-1.826000	-0.489942	2.002549
4	8	0.917680	-1.410954	2.009649
5	8	-1.940682	-1.824896	-0.405657
6	8	0.314746	-2.580590	-1.441342
7	6	-2.733671	-1.657591	1.807962
8	1	-2.891708	-2.194586	2.753794
9	1	-3.707240	-1.280067	1.485187
10	6	-2.248406	-2.626574	0.734283
11	1	-1.365590	-3.201796	1.045064
12	1	-3.048693	-3.338330	0.493958
13	6	-2.032996	-2.429892	-1.697991
14	6	-0.803598	-3.277405	-1.990574
15	6	1.566508	-2.903083	-2.047790
16	1	1.730501	-2.247242	-2.912214
17	1	1.566503	-3.941674	-2.401938
18	6	2.628936	-2.754932	-0.975201
19	1	2.423864	-3.502883	-0.205777
20	1	3.622868	-2.984761	-1.391156
21	6	3.138297	-1.487186	1.036983
22	1	3.346370	-0.471295	1.377549
23	1	4.086280	-2.049508	1.077449
24	6	3.404858	-0.481040	-1.185355
25	1	3.020477	-0.553051	-2.209424
26	1	4.463606	-0.786159	-1.217916
27	6	2.164726	-2.128228	2.021924
28	1	1.971257	-3.185900	1.801912
29	1	2.602042	-2.069005	3.026264
30	6	0.068625	-1.677417	3.145211
31	1	0.672574	-1.641859	4.060114
32	1	-0.346990	-2.689855	3.054426
33	6	-1.006842	-0.602414	3.232547
34	1	-0.515468	0.360992	3.381810
35	1	-1.630068	-0.814813	4.116509
36	6	3.303161	0.953738	-0.721300
37	6	4.322300	1.883092	-0.936488
38	1	5.226754	1.590708	-1.461166
39	6	4.158524	3.185318	-0.460157
40	1	4.933269	3.928040	-0.626079
41	6	3.008958	3.508580	0.259399
42	1	2.840511	4.487983	0.692247
43	6	2.047489	2.519000	0.444536
44	6	0.810258	2.735387	1.298273
45	7	2.180008	1.281409	-0.067796
46	6	-2.618835	0.777381	2.022429
47	1	-1.972526	1.557318	2.431562
48	1	-3.499924	0.677511	2.671817
49	6	-3.025967	1.222939	0.631277
50	6	-4.230164	1.873505	0.356406
51	1	-4.961212	2.027762	1.144105
52	6	-4.470802	2.330827	-0.942960
53	1	-5.398990	2.845560	-1.173444
54	6	-3.517875	2.116302	-1.938101
55	1	-3.654824	2.441565	-2.963033
56	6	-2.345270	1.448194	-1.590035

57	6	-1.249097	1.121916	-2.601936
58	7	-2.118982	1.024998	-0.337257
59	8	-0.213839	0.509013	-2.068677
60	8	-1.404216	1.406370	-3.775633
61	8	0.614238	3.813460	1.833313
62	8	0.066301	1.663540	1.390858
63	1	-0.866510	-4.275961	-1.534729
64	1	-0.699212	-3.399845	-3.075796
65	1	-2.089172	-1.593768	-2.396642
66	1	-2.952804	-3.022416	-1.777174

HF = -1715.9084236 Hartrees
Zero-point correction = 0.541482 Hartrees
Sum of electronic and thermal Enthalpies = -1715.333743 Hartrees
Sum of electronic and thermal Free Energies = -1715.429140 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\lambda)(\delta\delta\delta)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.109389	0.113819	-0.022033
2	7	-2.181947	1.817984	-0.739356
3	7	1.648150	0.238409	2.003360
4	8	-0.898222	1.610679	1.790352
5	8	3.093631	1.298854	-0.399104
6	8	0.643238	2.494045	-0.840713
7	6	2.662807	1.329120	2.007866
8	6	3.697639	1.267235	0.884591
9	6	3.029257	2.560328	-1.047947
10	6	1.719316	2.599658	-1.805710
11	6	-0.373405	3.505575	-0.899169
12	6	-1.630701	2.940398	-1.538980
13	6	-2.829879	2.328744	0.508832
14	6	-3.113581	1.020611	-1.576961
15	1	-2.607618	0.822065	-2.529173
16	1	-4.031997	1.583791	-1.802340
17	6	-2.340164	1.690534	1.815284
18	6	-0.203676	1.602132	3.064111
19	6	0.734237	0.398983	3.170833
20	6	-3.448625	-0.304052	-0.933310
21	6	-4.671307	-0.953324	-1.107173
22	1	-5.453876	-0.495660	-1.704429
23	6	-4.864164	-2.198365	-0.502887
24	1	-5.804261	-2.726574	-0.631970
25	6	-3.848783	-2.742657	0.282410
26	1	-3.946683	-3.691407	0.797545
27	6	-2.664097	-2.023601	0.419814
28	6	-1.525255	-2.485102	1.314803
29	7	-2.467410	-0.842597	-0.193550
30	6	2.296980	-1.109689	2.053311
31	1	1.575913	-1.799621	2.498366
32	1	3.186374	-1.089226	2.699555
33	6	2.648524	-1.662685	0.682001
34	6	3.704199	-2.551679	0.466750
35	1	4.350512	-2.846038	1.288192
36	6	3.909432	-3.056398	-0.820079
37	1	4.722190	-3.752651	-1.005138
38	6	3.075619	-2.653786	-1.864135
39	1	3.199805	-3.002783	-2.882772

40	6	2.047483	-1.761640	-1.573209
41	6	1.092818	-1.222961	-2.635821
42	7	1.847630	-1.299523	-0.328226
43	8	0.175897	-0.408463	-2.149486
44	8	1.237096	-1.542868	-3.800403
45	8	-1.623453	-3.527123	1.939691
46	8	-0.523313	-1.644091	1.331121
47	1	-2.375815	3.740736	-1.676338
48	1	-1.372395	2.553602	-2.529054
49	1	-0.016411	4.368420	-1.470967
50	1	-0.553602	3.836517	0.127579
51	1	1.627767	3.536407	-2.364763
52	1	1.640901	1.760032	-2.501877
53	1	3.059385	3.383052	-0.320329
54	1	3.872437	2.679750	-1.743694
55	1	4.394706	2.105570	1.015482
56	1	4.289276	0.349619	0.937574
57	1	2.132552	2.284076	1.937634
58	1	3.204777	1.324117	2.969220
59	1	0.130835	-0.508104	3.226114
60	1	1.301770	0.497298	4.110935
61	1	-0.931163	1.542300	3.879582
62	1	0.321558	2.558663	3.149061
63	1	-2.657012	2.323676	2.651572
64	1	-2.748130	0.685920	1.962966
65	1	-3.917563	2.191374	0.456877
66	1	-2.657148	3.406744	0.572175

HF = -1715.9019841 Hartrees
Zero-point correction = 0.541658 Hartrees
Sum of electronic and thermal Enthalpies = -1715.327312 Hartrees
Sum of electronic and thermal Free Energies = -1715.422507 Hartrees

$[Ho(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δλδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.038708	0.115626	-0.016506
2	7	-2.577306	1.463080	-0.507762
3	7	1.704602	0.207187	2.080624
4	8	-1.040308	1.143638	2.005353
5	8	1.938072	1.944782	-0.073858
6	8	-0.233298	2.893013	-1.129357
7	6	2.568598	1.408528	2.134743
8	6	3.085397	1.817386	0.765402
9	6	2.102474	2.705685	-1.280754
10	6	0.940806	3.673711	-1.322694
11	6	-1.403926	3.668727	-0.930546
12	6	-2.589927	2.768071	-1.218736
13	6	-3.148274	1.553524	0.860756
14	1	-3.499736	0.559221	1.143793
15	1	-4.022829	2.224869	0.880076
16	6	-3.372944	0.522627	-1.348170
17	1	-2.928401	0.540430	-2.349633
18	1	-4.415038	0.865784	-1.447376
19	6	-2.184239	2.016993	1.952933
20	1	-1.841095	3.048424	1.815715
21	1	-2.714504	1.964117	2.912093
22	6	-0.295667	1.213367	3.240713

23	1	-0.978238	1.018551	4.077120
24	1	0.095795	2.231877	3.357235
25	6	0.799789	0.147270	3.257263
26	1	0.327629	-0.836185	3.245101
27	1	1.352596	0.253342	4.204967
28	6	-3.347922	-0.897525	-0.845841
29	6	-4.424600	-1.767880	-1.025993
30	1	-5.326784	-1.422427	-1.521267
31	6	-4.318536	-3.079218	-0.559459
32	1	-5.138930	-3.777199	-0.697771
33	6	-3.159806	-3.468013	0.109530
34	1	-3.024368	-4.458772	0.527852
35	6	-2.139675	-2.532653	0.262751
36	6	-0.884638	-2.835210	1.055602
37	7	-2.220759	-1.282812	-0.230094
38	6	2.529664	-1.031619	1.976672
39	1	1.905690	-1.867971	2.299347
40	1	3.401840	-0.972747	2.644277
41	6	2.971210	-1.340981	0.556746
42	6	4.146061	-2.038236	0.265076
43	1	4.822214	-2.329577	1.063061
44	6	4.428237	-2.361051	-1.065025
45	1	5.334116	-2.908102	-1.309481
46	6	3.543223	-1.976310	-2.072626
47	1	3.711949	-2.199014	-3.119970
48	6	2.394901	-1.278687	-1.705405
49	6	1.353351	-0.809542	-2.719411
50	7	2.131612	-0.975242	-0.423293
51	8	0.310618	-0.231765	-2.161881
52	8	1.548670	-0.978905	-3.908436
53	8	-0.734608	-3.924841	1.583415
54	8	-0.067365	-1.818282	1.112768
55	1	1.036828	4.415769	-0.516022
56	1	0.899898	4.201688	-2.285668
57	1	2.084511	2.026899	-2.139133
58	1	3.054552	3.246531	-1.271827
59	1	-3.526971	3.313573	-1.022742
60	1	-2.558281	2.551260	-2.289022
61	1	-1.409483	4.096716	0.082104
62	1	-1.435101	4.509331	-1.638317
63	1	3.597505	2.784673	0.849988
64	1	3.790066	1.092108	0.344109
65	1	3.414774	1.255868	2.822697
66	1	1.980615	2.243626	2.523084

HF = -1715.9077935 Hartrees
Zero-point correction = 0.541888 Hartrees
Sum of electronic and thermal Enthalpies = -1715.332804 Hartrees
Sum of electronic and thermal Free Energies = -1715.428550 Hartrees

$[Yb(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.059974	-0.165437	0.077002
2	7	2.508850	-1.539597	-0.300275
3	7	-1.772432	-0.297795	2.076253
4	8	0.950787	-1.225650	2.117184
5	8	-1.966721	-2.039787	-0.115229

6	8	0.139472	-2.529767	-1.403756
7	6	-2.637759	-1.500221	2.078033
8	6	-3.130016	-1.863512	0.689489
9	6	-2.235314	-2.383259	-1.477896
10	6	-1.012697	-3.120741	-2.000155
11	6	1.364395	-2.969909	-1.981720
12	1	1.600065	-2.351888	-2.857269
13	1	1.276685	-4.012614	-2.314532
14	6	2.415125	-2.895024	-0.889588
15	1	2.123553	-3.595906	-0.103235
16	1	3.392441	-3.225423	-1.276516
17	6	3.092881	-1.606700	1.061155
18	1	3.424088	-0.604663	1.340519
19	1	3.976604	-2.265349	1.085721
20	6	3.333340	-0.685245	-1.192189
21	1	2.922341	-0.768292	-2.204097
22	1	4.372166	-1.050305	-1.232993
23	6	2.103312	-2.087999	2.115528
24	1	1.774198	-3.122192	1.952556
25	1	2.589768	-2.038659	3.097314
26	6	0.160208	-1.314139	3.321094
27	1	0.808472	-1.128073	4.186235
28	1	-0.232667	-2.334939	3.409173
29	6	-0.932904	-0.250252	3.300581
30	1	-0.459110	0.732025	3.323173
31	1	-1.536451	-0.367470	4.215312
32	6	3.309756	0.765669	-0.776483
33	6	4.365983	1.640934	-1.034952
34	1	5.252722	1.289105	-1.553272
35	6	4.260699	2.967220	-0.611604
36	1	5.065741	3.668676	-0.809648
37	6	3.126352	3.369821	0.091925
38	1	2.998454	4.374539	0.478155
39	6	2.124816	2.430339	0.319378
40	6	0.887716	2.736737	1.139631
41	7	2.206500	1.165307	-0.130227
42	6	-2.591145	0.941750	1.954777
43	1	-1.989838	1.768876	2.339966
44	1	-3.503004	0.866781	2.565411
45	6	-2.940689	1.300540	0.522489
46	6	-4.081730	2.033716	0.187042
47	1	-4.802573	2.303808	0.952700
48	6	-4.270426	2.422586	-1.141534
49	1	-5.149648	2.996620	-1.419165
50	6	-3.321973	2.074491	-2.103607
51	1	-3.411811	2.354820	-3.146850
52	6	-2.211809	1.340569	-1.693998
53	6	-1.096458	0.923751	-2.648701
54	7	-2.044339	0.958859	-0.415400
55	8	-0.088545	0.346671	-2.037955
56	8	-1.213993	1.127955	-3.843819
57	8	0.731042	3.839315	1.636620
58	8	0.089588	1.706337	1.247603
59	1	-1.047362	-4.183307	-1.722142
60	1	-0.971665	-3.042522	-3.094034
61	1	-2.435699	-1.472131	-2.052261
62	1	-3.115251	-3.035135	-1.542490
63	1	-2.058317	-2.347913	2.451735
64	1	-3.496275	-1.366418	2.754458
65	1	-3.781577	-1.092895	0.261425
66	1	-3.697293	-2.803300	0.734694

HF = -1717.6625976 Hartrees
Zero-point correction = 0.542342 Hartrees
Sum of electronic and thermal Enthalpies = -1717.087297 Hartrees
Sum of electronic and thermal Free Energies = -1717.181900 Hartrees

$[Yb(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.056879	-0.150581	0.091644
2	7	2.472772	-1.609507	-0.272018
3	7	-1.756263	-0.148350	2.086028
4	8	0.924296	-1.173832	2.142666
5	8	-2.084795	-1.884434	-0.092996
6	8	0.041750	-2.700689	-1.236951
7	6	-2.646045	-1.330241	2.148386
8	6	-3.194451	-1.735441	0.791613
9	6	-2.306046	-2.846655	-1.127546
10	6	-1.117338	-2.790948	-2.066058
11	6	1.254211	-3.017790	-1.910833
12	1	1.424134	-2.311868	-2.734343
13	1	1.197727	-4.031078	-2.333000
14	6	2.340756	-2.966711	-0.854872
15	1	2.064014	-3.666567	-0.061930
16	1	3.300092	-3.309568	-1.272442
17	6	3.045775	-1.676312	1.093789
18	1	3.416536	-0.683579	1.357668
19	1	3.901588	-2.369880	1.136537
20	6	3.332740	-0.797155	-1.168626
21	1	2.937612	-0.895889	-2.185351
22	1	4.361967	-1.190540	-1.183815
23	6	2.031162	-2.096446	2.150486
24	1	1.647678	-3.112500	1.993602
25	1	2.517188	-2.064010	3.132952
26	6	0.154570	-1.169569	3.363690
27	1	0.825096	-0.957639	4.205478
28	1	-0.268849	-2.170260	3.515130
29	6	-0.905411	-0.072637	3.302399
30	1	-0.403015	0.895069	3.278797
31	1	-1.505944	-0.131740	4.224622
32	6	3.343805	0.664242	-0.793909
33	6	4.427332	1.499628	-1.072460
34	1	5.307370	1.104066	-1.570328
35	6	4.357766	2.842166	-0.697006
36	1	5.184379	3.512872	-0.911954
37	6	3.229413	3.300915	-0.018800
38	1	3.126599	4.321800	0.330780
39	6	2.200082	2.398643	0.233044
40	6	0.968668	2.770825	1.033469
41	7	2.246950	1.116031	-0.171153
42	6	-2.548122	1.105369	1.918848
43	1	-1.927639	1.932577	2.271379
44	1	-3.459306	1.073121	2.533874
45	6	-2.895130	1.409543	0.472922
46	6	-4.028612	2.137795	0.101970
47	1	-4.744126	2.457363	0.853473
48	6	-4.217840	2.454192	-1.245685
49	1	-5.090127	3.024317	-1.551679

50	6	-3.283313	2.032385	-2.192374
51	1	-3.381589	2.246321	-3.250489
52	6	-2.180823	1.308550	-1.746278
53	6	-1.096845	0.786576	-2.682340
54	7	-2.006598	1.010818	-0.447855
55	8	-0.092225	0.222330	-2.048023
56	8	-1.229497	0.892508	-3.888448
57	8	0.838555	3.896213	1.484861
58	8	0.144219	1.766502	1.179981
59	1	-2.071092	-2.176450	2.531996
60	1	-3.479430	-1.156870	2.847782
61	1	-3.902162	-1.005289	0.381494
62	1	-3.720244	-2.693101	0.899669
63	1	-1.087929	-3.707208	-2.670925
64	1	-1.157790	-1.926264	-2.736358
65	1	-2.397326	-3.840851	-0.669429
66	1	-3.231209	-2.622944	-1.674967

HF = -1717.665603 Hartrees
Zero-point correction = 0.542536 Hartrees
Sum of electronic and thermal Enthalpies = -1717.090254 Hartrees
Sum of electronic and thermal Free Energies = -1717.184215 Hartrees

$[La(bp15c5)]^+$ (vacuum) Λ(λδ)(δλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.056519	-0.148166	-0.081045
2	7	2.707343	-1.489847	-0.296262
3	7	-1.668982	-0.257803	2.172757
4	8	1.147918	-1.110743	2.171941
5	8	-1.788460	-2.265066	0.116956
6	8	0.319880	-2.587063	-1.400511
7	6	-2.496190	-1.488271	2.253279
8	6	-2.959882	-2.015072	0.902491
9	6	-2.052604	-2.772579	-1.199511
10	6	-0.785495	-3.444332	-1.697823
11	6	1.579358	-3.014750	-1.930464
12	1	1.805066	-2.423983	-2.826207
13	1	1.528244	-4.068509	-2.228466
14	6	2.627302	-2.867386	-0.835415
15	1	2.347239	-3.539098	-0.019548
16	1	3.607728	-3.204217	-1.210811
17	6	3.273187	-1.491924	1.076132
18	1	3.572919	-0.469696	1.316878
19	1	4.177570	-2.120810	1.129499
20	6	3.532699	-0.647724	-1.200534
21	1	3.148508	-0.777643	-2.219443
22	1	4.577948	-0.996984	-1.212990
23	6	2.304258	-1.960869	2.158335
24	1	1.985430	-3.003177	2.022105
25	1	2.817763	-1.892171	3.126057
26	6	0.362405	-1.194347	3.373121
27	1	1.002507	-0.978903	4.238653
28	1	-0.015574	-2.219031	3.485973
29	6	-0.748760	-0.147716	3.337721
30	1	-0.284201	0.840133	3.281938
31	1	-1.298113	-0.210303	4.291457
32	6	3.493535	0.824459	-0.841221

33	6	4.586347	1.664731	-1.056779
34	1	5.502237	1.272260	-1.488019
35	6	4.480142	3.012031	-0.702848
36	1	5.313959	3.687239	-0.871249
37	6	3.308654	3.468632	-0.103325
38	1	3.177285	4.491463	0.230318
39	6	2.266593	2.563731	0.095110
40	6	0.995932	2.969488	0.838805
41	7	2.351433	1.278904	-0.299092
42	6	-2.518193	0.966529	2.097727
43	1	-1.866115	1.819777	2.309017
44	1	-3.305464	0.936325	2.865952
45	6	-3.122091	1.223015	0.729674
46	6	-4.354936	1.856297	0.561298
47	1	-4.964155	2.108889	1.423705
48	6	-4.779454	2.171257	-0.732873
49	1	-5.732368	2.669691	-0.885320
50	6	-3.971715	1.845010	-1.821346
51	1	-4.245933	2.069719	-2.845664
52	6	-2.758234	1.204056	-1.574636
53	6	-1.803023	0.817439	-2.706833
54	7	-2.360278	0.899971	-0.327446
55	8	-0.678752	0.290706	-2.288427
56	8	-2.146537	1.004057	-3.861518
57	8	0.891858	4.113321	1.252040
58	8	0.138443	1.997073	0.982305
59	1	-0.633769	-4.409386	-1.195408
60	1	-0.866681	-3.613102	-2.778902
61	1	-2.346819	-1.946596	-1.857004
62	1	-2.864693	-3.509804	-1.168513
63	1	-1.900748	-2.277303	2.718439
64	1	-3.374646	-1.325670	2.896767
65	1	-3.621369	-1.314624	0.382826
66	1	-3.505765	-2.956125	1.055028

HF = -1709.8299463 Hartrees
Zero-point correction = 0.540801 Hartrees
Sum of electronic and thermal Enthalpies = -1709.255781 Hartrees
Sum of electronic and thermal Free Energies = -1709.351631 Hartrees

$[La(bp15c5)]^+$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.060965	-0.146731	-0.060266
2	7	2.656164	-1.582708	-0.298769
3	7	-1.641564	-0.104474	2.186616
4	8	1.137837	-1.073503	2.185032
5	8	-1.971502	-2.031281	0.115540
6	8	0.183080	-2.780412	-1.125146
7	6	-2.503282	-1.302843	2.333403
8	6	-3.063259	-1.839875	1.021636
9	6	-2.145805	-3.107239	-0.814114
10	6	-1.035218	-3.017941	-1.847045
11	6	1.382063	-3.078522	-1.842480
12	1	1.490452	-2.398975	-2.699452
13	1	1.342524	-4.106349	-2.227715
14	6	2.521506	-2.956982	-0.842228
15	1	2.306336	-3.640716	-0.016582

16	1	3.462996	-3.293438	-1.303753
17	6	3.226144	-1.597624	1.072285
18	1	3.581885	-0.589803	1.298897
19	1	4.095668	-2.273147	1.132370
20	6	3.508033	-0.779700	-1.214342
21	1	3.115389	-0.911371	-2.230226
22	1	4.539772	-1.167219	-1.226024
23	6	2.236625	-1.999643	2.164204
24	1	1.847235	-3.017830	2.029109
25	1	2.760273	-1.963488	3.128075
26	6	0.373967	-1.064559	3.403876
27	1	1.039464	-0.829263	4.244626
28	1	-0.039168	-2.066858	3.577014
29	6	-0.700137	0.021689	3.334768
30	1	-0.202535	0.989227	3.229897
31	1	-1.238172	0.019233	4.297027
32	6	3.524376	0.697540	-0.878540
33	6	4.646214	1.493149	-1.115338
34	1	5.545508	1.058865	-1.541639
35	6	4.589993	2.850698	-0.790708
36	1	5.446977	3.491751	-0.976091
37	6	3.436989	3.362255	-0.199844
38	1	3.342178	4.396896	0.109186
39	6	2.364593	2.499292	0.022581
40	6	1.110744	2.968232	0.756313
41	7	2.401801	1.203235	-0.341230
42	6	-2.451804	1.143968	2.061637
43	1	-1.771055	1.983132	2.234801
44	1	-3.237378	1.171408	2.831686
45	6	-3.053590	1.354458	0.683190
46	6	-4.282423	1.988030	0.485303
47	1	-4.886741	2.291956	1.334640
48	6	-4.711029	2.231757	-0.822836
49	1	-5.660440	2.729366	-0.998694
50	6	-3.916909	1.829082	-1.896192
51	1	-4.202862	1.986665	-2.929859
52	6	-2.705901	1.195251	-1.619749
53	6	-1.778622	0.699748	-2.732742
54	7	-2.298973	0.973853	-0.359084
55	8	-0.649077	0.191670	-2.297411
56	8	-2.145656	0.783699	-3.892011
57	8	1.039663	4.129084	1.127009
58	8	0.227495	2.025847	0.939910
59	1	-1.905415	-2.102033	2.777578
60	1	-3.337178	-1.100955	3.024814
61	1	-3.802341	-1.171229	0.568296
62	1	-3.550818	-2.801819	1.226102
63	1	-0.973844	-3.964670	-2.398764
64	1	-1.201156	-2.196546	-2.552940
65	1	-2.099206	-4.058104	-0.266649
66	1	-3.119706	-3.032549	-1.314896

HF = -1709.8320387 Hartrees
Zero-point correction = 0.540866 Hartrees
Sum of electronic and thermal Enthalpies = -1709.257973 Hartrees
Sum of electronic and thermal Free Energies = -1709.352934 Hartrees

$[La(bp15c5)]^+$ (vacuum) Λ(λδ)(λδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.028120	-0.110701	-0.114021
2	7	2.696452	-1.509297	-0.335945
3	7	-1.714354	-0.122936	2.124628
4	8	1.038862	-1.178708	2.107239
5	8	-1.887281	-2.202927	0.140297
6	8	0.296392	-2.641918	-1.279536
7	6	-2.716616	-1.221244	2.170749
8	1	-2.990840	-1.454185	3.211489
9	1	-3.619249	-0.856201	1.675404
10	6	-2.320723	-2.511641	1.466005
11	1	-1.527096	-3.065939	1.985554
12	1	-3.205854	-3.161220	1.430223
13	6	-1.871626	-3.346860	-0.725532
14	1	-2.887598	-3.561349	-1.081042
15	1	-1.496586	-4.216958	-0.170254
16	6	-0.940799	-3.046240	-1.883097
17	1	-0.799211	-3.952083	-2.484844
18	1	-1.313833	-2.240480	-2.524216
19	6	1.500701	-2.939219	-1.986119
20	1	1.635262	-2.239041	-2.821511
21	1	1.456973	-3.955948	-2.397633
22	6	2.614130	-2.855840	-0.952130
23	1	2.391876	-3.587777	-0.171254
24	1	3.575379	-3.145915	-1.404024
25	6	3.196839	-1.573432	1.058785
26	1	3.504369	-0.566380	1.350332
27	1	4.086061	-2.221746	1.133553
28	6	3.570502	-0.654784	-1.177639
29	1	3.226172	-0.755315	-2.214365
30	1	4.609976	-1.021108	-1.158450
31	6	2.172962	-2.062989	2.082924
32	1	1.828753	-3.085830	1.880876
33	1	2.654414	-2.058978	3.069030
34	6	0.245896	-1.231644	3.308097
35	1	0.899193	-1.074829	4.176114
36	1	-0.206976	-2.226013	3.406249
37	6	-0.790939	-0.109266	3.286603
38	1	-0.255370	0.843551	3.255619
39	1	-1.346822	-0.152223	4.238060
40	6	3.543946	0.808160	-0.790512
41	6	4.664422	1.624336	-0.953776
42	1	5.585750	1.212885	-1.354703
43	6	4.578843	2.969570	-0.589637
44	1	5.434319	3.626175	-0.718111
45	6	3.395506	3.446183	-0.031150
46	1	3.273413	4.467812	0.309590
47	6	2.326456	2.563718	0.116843
48	6	1.043369	2.996290	0.817280
49	7	2.390921	1.279927	-0.287259
50	6	-2.444189	1.181817	2.045249
51	1	-1.708590	1.977155	2.192444
52	1	-3.203453	1.252070	2.837932
53	6	-3.074716	1.396662	0.682024
54	6	-4.296608	2.046505	0.501374
55	1	-4.875585	2.374033	1.359376
56	6	-4.751732	2.276807	-0.800600

57	1	-5.697406	2.785803	-0.962709
58	6	-3.987527	1.847438	-1.884405
59	1	-4.292199	1.996493	-2.913872
60	6	-2.780377	1.198756	-1.624876
61	6	-1.875716	0.693770	-2.750326
62	7	-2.351163	0.983966	-0.371211
63	8	-0.736672	0.190254	-2.331096
64	8	-2.258802	0.772860	-3.904284
65	8	0.950908	4.137731	1.239926
66	8	0.158705	2.044051	0.919460

HF = -1709.828853 Hartrees
Zero-point correction = 0.540623 Hartrees
Sum of electronic and thermal Enthalpies = -1709.254911 Hartrees
Sum of electronic and thermal Free Energies = -1709.350586 Hartrees

$[La(bp15c5)]^+$ (vacuum) $\Lambda(\delta\delta)(\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.026440	-0.218798	-0.130044
2	7	2.848482	-1.273781	-0.160089
3	7	-1.892953	-0.620640	1.970581
4	8	0.939889	-1.310422	2.101119
5	8	-1.692457	-2.445597	-0.269234
6	8	0.691654	-2.555824	-1.428986
7	6	-2.918373	-1.640421	1.624221
8	1	-3.472719	-1.959466	2.520836
9	1	-3.638201	-1.175908	0.947736
10	6	-2.358005	-2.865372	0.926735
11	1	-1.652276	-3.427792	1.555454
12	1	-3.191378	-3.534254	0.674017
13	6	-1.443680	-3.524284	-1.179609
14	1	-2.377530	-3.819051	-1.676093
15	1	-1.048542	-4.385424	-0.623488
16	6	-0.418433	-3.055901	-2.194056
17	1	-0.106566	-3.900090	-2.819488
18	1	-0.803449	-2.254466	-2.834429
19	6	2.007996	-2.841345	-1.903986
20	1	2.251319	-2.194890	-2.757455
21	1	2.068991	-3.883926	-2.241472
22	6	2.943900	-2.641173	-0.718244
23	1	2.650389	-3.355833	0.054814
24	1	3.977374	-2.885334	-1.013028
25	6	3.261014	-1.220928	1.264879
26	1	3.383017	-0.168779	1.531073
27	1	4.238211	-1.712054	1.416186
28	6	3.674968	-0.355418	-0.983036
29	1	3.424145	-0.533780	-2.035325
30	1	4.746726	-0.591340	-0.875562
31	6	2.266465	-1.852612	2.245003
32	1	2.187501	-2.936073	2.104624
33	1	2.632951	-1.676987	3.262044
34	6	0.310038	-0.656463	3.233000
35	6	-1.177835	-1.003519	3.221020
36	6	3.444214	1.105941	-0.659045
37	6	4.438399	2.068834	-0.841945
38	1	5.410227	1.784935	-1.234489
39	6	4.161599	3.394875	-0.502440

40	1	4.914305	4.164037	-0.648718
41	6	2.927732	3.708932	0.064615
42	1	2.669279	4.707539	0.397728
43	6	1.998164	2.685239	0.237384
44	6	0.688883	2.912052	0.984904
45	7	2.238554	1.422097	-0.162861
46	6	-2.563889	0.706991	2.096531
47	1	-1.820503	1.425958	2.451616
48	1	-3.383779	0.655210	2.829352
49	6	-3.087802	1.200426	0.757997
50	6	-4.246177	1.968904	0.635863
51	1	-4.835846	2.215771	1.513394
52	6	-4.627236	2.417122	-0.632445
53	1	-5.522724	3.020896	-0.747541
54	6	-3.857115	2.079890	-1.744518
55	1	-4.109710	2.393782	-2.750759
56	6	-2.712818	1.308370	-1.544573
57	6	-1.795413	0.906353	-2.701417
58	7	-2.353047	0.886569	-0.321500
59	8	-0.690185	0.305474	-2.319146
60	8	-2.134530	1.154200	-3.844669
61	8	0.405463	4.035085	1.370795
62	8	0.005563	1.815974	1.171149
63	1	-1.265934	-2.086728	3.345523
64	1	-1.652586	-0.540095	4.098568
65	1	0.753532	-1.026356	4.163846
66	1	0.476683	0.422209	3.151404

HF = -1709.8233795 Hartrees
Zero-point correction = 0.540340 Hartrees
Sum of electronic and thermal Enthalpies = -1709.249661 Hartrees
Sum of electronic and thermal Free Energies = -1709.345637 Hartrees

$[La(bp15c5)]^+$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\delta)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.052357	-0.071826	-0.153494
2	7	2.661917	-1.579706	-0.436893
3	7	-1.557190	-0.204659	2.191699
4	8	1.198274	-1.160944	2.063159
5	8	-1.793102	-2.138656	0.087941
6	8	0.262792	-2.446730	-1.598049
7	6	-2.366119	-1.442362	2.314574
8	6	-2.895511	-1.990278	0.995317
9	6	-1.986685	-3.144220	-0.918565
10	6	-1.027353	-2.852528	-2.069155
11	6	1.066398	-3.448966	-0.976347
12	6	2.504085	-2.943570	-1.011722
13	6	3.274173	-1.606998	0.910480
14	1	3.614119	-0.597124	1.149702
15	1	4.158809	-2.265579	0.932512
16	6	3.461105	-0.732192	-1.365911
17	1	2.980681	-0.795940	-2.349571
18	1	4.484252	-1.123239	-1.482293
19	6	2.327169	-2.047738	2.019881
20	1	1.976708	-3.081036	1.891091
21	1	2.867856	-1.995426	2.973480
22	6	0.505263	-1.156355	3.321543

23	6	-0.582165	-0.086432	3.309799
24	6	3.523588	0.721369	-0.941496
25	6	4.668512	1.496566	-1.126746
26	1	5.556263	1.062007	-1.575870
27	6	4.651558	2.833752	-0.720851
28	1	5.528233	3.458421	-0.864959
29	6	3.512419	3.343466	-0.103116
30	1	3.447913	4.359508	0.268729
31	6	2.412190	2.502149	0.062383
32	6	1.169714	2.967603	0.819923
33	7	2.413307	1.230199	-0.378909
34	6	-2.415024	1.015637	2.168389
35	1	-1.754042	1.871287	2.340255
36	1	-3.152730	0.982586	2.984201
37	6	-3.102061	1.261079	0.839904
38	6	-4.365550	1.846524	0.740616
39	1	-4.936057	2.075959	1.635401
40	6	-4.872544	2.142181	-0.528184
41	1	-5.850499	2.604013	-0.628367
42	6	-4.115786	1.839523	-1.659050
43	1	-4.456808	2.044743	-2.667272
44	6	-2.866298	1.246791	-1.478910
45	6	-1.973041	0.871197	-2.661629
46	7	-2.384907	0.968666	-0.256076
47	8	-0.807013	0.387041	-2.308775
48	8	-2.395850	1.018530	-3.795437
49	8	1.147708	4.097215	1.280939
50	8	0.242241	2.054844	0.922750
51	1	3.157036	-3.665099	-0.500651
52	1	2.816622	-2.919741	-2.059178
53	1	0.997922	-4.391750	-1.535555
54	1	0.717340	-3.635164	0.049076
55	1	-0.937614	-3.732443	-2.719199
56	1	-1.373118	-2.004173	-2.661898
57	1	-1.812356	-4.130578	-0.467634
58	1	-3.016119	-3.117463	-1.297430
59	1	-3.348746	-2.970609	1.190636
60	1	-3.653863	-1.345103	0.540524
61	1	-1.739481	-2.220418	2.755120
62	1	-3.214221	-1.287514	3.000088
63	1	-0.102816	0.890507	3.206278
64	1	-1.087962	-0.112844	4.289139
65	1	1.212593	-0.909986	4.124255
66	1	0.115220	-2.162784	3.522827

HF = -1709.8261075 Hartrees
Zero-point correction = 0.541243 Hartrees
Sum of electronic and thermal Enthalpies = -1709.251707 Hartrees
Sum of electronic and thermal Free Energies = -1709.346662 Hartrees

$[La(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\lambda)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	-0.010408	0.176735	-0.099994
2	7	-2.501610	1.900500	-0.001558
3	7	1.358583	-0.763869	2.159276
4	8	-1.343488	0.265573	2.201541
5	8	1.964494	1.766462	0.980730

6	8	0.108224	2.965319	-0.373999
7	6	2.071831	0.314038	2.883765
8	6	2.854964	1.258593	1.979545
9	6	2.317191	3.058088	0.465597
10	6	1.439079	3.344502	-0.743243
11	6	-0.945859	3.445484	-1.213889
12	1	-0.972481	2.874212	-2.152835
13	1	-0.779010	4.501771	-1.462396
14	6	-2.216859	3.315347	-0.388903
15	1	-2.072623	3.907786	0.517237
16	1	-3.064522	3.757249	-0.931506
17	6	-3.021346	1.831566	1.391513
18	6	-3.438886	1.335261	-1.004245
19	1	-3.064000	1.630139	-1.992933
20	1	-4.435544	1.793625	-0.898701
21	6	-2.758310	0.541120	2.167973
22	6	-0.864591	-0.435052	3.367773
23	1	-1.665718	-1.057554	3.782603
24	1	-0.592748	0.307918	4.127078
25	6	0.291111	-1.370005	3.003045
26	1	-0.111473	-2.206678	2.428904
27	1	0.704218	-1.769324	3.944279
28	6	-3.571346	-0.171551	-0.993416
29	6	-4.785609	-0.791192	-1.293342
30	1	-5.669785	-0.192376	-1.489357
31	6	-4.839678	-2.185930	-1.340884
32	1	-5.771133	-2.689300	-1.582944
33	6	-3.690917	-2.917646	-1.052879
34	1	-3.667557	-4.001180	-1.044312
35	6	-2.519810	-2.226841	-0.741078
36	6	-1.261762	-2.981166	-0.317669
37	7	-2.458053	-0.880467	-0.736585
38	6	2.286665	-1.844669	1.709735
39	1	1.669779	-2.725445	1.507455
40	1	2.991411	-2.102687	2.514331
41	6	3.036891	-1.551628	0.423031
42	6	4.305281	-2.077094	0.163871
43	1	4.831090	-2.644056	0.926095
44	6	4.874268	-1.872650	-1.095964
45	1	5.856186	-2.278884	-1.320675
46	6	4.174133	-1.146197	-2.058591
47	1	4.565193	-0.956415	-3.051511
48	6	2.918241	-0.643196	-1.721790
49	6	2.089044	0.180552	-2.709726
50	7	2.378387	-0.846859	-0.508322
51	8	0.909459	0.529008	-2.252489
52	8	2.569041	0.467716	-3.792862
53	8	-1.298078	-4.200904	-0.261179
54	8	-0.260346	-2.207823	-0.010921
55	1	1.329941	0.914561	3.416866
56	1	2.755988	-0.106885	3.638508
57	1	3.708909	0.770681	1.496105
58	1	3.235019	2.085178	2.593716
59	1	-3.121352	0.702711	3.190210
60	1	-3.278189	-0.326756	1.751398
61	1	-4.107305	2.021418	1.419246
62	1	-2.540145	2.634718	1.955174
63	1	1.481065	4.416529	-0.975726
64	1	1.751573	2.775203	-1.625036
65	1	2.155329	3.805387	1.253430
66	1	3.373223	3.078213	0.167339

HF = -1709.8238988 Hartrees
Zero-point correction = 0.540883 Hartrees
Sum of electronic and thermal Enthalpies = -1709.249714 Hartrees
Sum of electronic and thermal Free Energies = -1709.345333 Hartrees

$[La(bp15c5)]^{+}$ (vacuum) Λ(δλ)(λδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	-0.010125	-0.258299	-0.115692
2	7	2.785717	-1.527884	-0.089976
3	7	-1.811986	-0.333964	2.095582
4	8	1.125076	-0.786571	2.278551
5	8	-1.782939	-2.412422	0.097232
6	8	0.479990	-2.686963	-1.249617
7	6	-2.864114	-1.378023	1.965864
8	1	-3.338628	-1.577275	2.939282
9	1	-3.638572	-0.990811	1.300992
10	6	-2.366531	-2.686152	1.376526
11	1	-1.624922	-3.188988	2.014474
12	1	-3.222457	-3.363347	1.258715
13	6	-1.637251	-3.576705	-0.727405
14	6	-0.701818	-3.221784	-1.867741
15	6	1.751856	-3.027686	-1.804808
16	1	1.974582	-2.381091	-2.663822
17	1	1.742702	-4.066578	-2.157783
18	6	2.756963	-2.897742	-0.668388
19	1	2.448554	-3.595684	0.113715
20	1	3.753843	-3.212606	-1.016102
21	6	3.222659	-1.557382	1.335161
22	6	3.661378	-0.689038	-0.943785
23	1	3.412235	-0.910351	-1.988624
24	1	4.717076	-0.977703	-0.811431
25	6	2.547887	-0.558983	2.276959
26	6	0.411384	-0.036748	3.288620
27	6	-1.026052	-0.543304	3.342571
28	6	3.516143	0.801589	-0.734155
29	6	4.587922	1.670304	-0.951501
30	1	5.556508	1.278520	-1.247167
31	6	4.391016	3.041689	-0.781682
32	1	5.205682	3.737514	-0.959639
33	6	3.148612	3.498504	-0.347346
34	1	2.939149	4.544341	-0.154394
35	6	2.139367	2.564560	-0.120789
36	6	0.813284	2.976713	0.507399
37	7	2.308856	1.247422	-0.353196
38	6	-2.467535	1.007212	2.074339
39	1	-1.703255	1.759773	2.286968
40	1	-3.244854	1.066231	2.851519
41	6	-3.057962	1.323975	0.710852
42	6	-4.214122	2.087192	0.544496
43	1	-4.762307	2.449078	1.408897
44	6	-4.644961	2.383457	-0.752214
45	1	-5.539699	2.980333	-0.903131
46	6	-3.922273	1.908202	-1.845337
47	1	-4.210584	2.106443	-2.871219
48	6	-2.777504	1.150684	-1.599829
49	6	-1.903731	0.612808	-2.733788

50	7	-2.374473	0.867891	-0.350790
51	8	-0.785770	0.056183	-2.322622
52	8	-2.283635	0.724304	-3.885604
53	8	0.590193	4.159121	0.713596
54	8	0.050345	1.963666	0.811037
55	1	-0.989593	-1.618815	3.541037
56	1	-1.529625	-0.074662	4.202021
57	1	0.882093	-0.213779	4.264126
58	1	0.466496	1.031265	3.050382
59	1	2.937941	-0.738368	3.287913
60	1	2.750526	0.481719	2.008514
61	1	4.310823	-1.408630	1.415777
62	1	3.009992	-2.555303	1.727851
63	1	-0.462394	-4.122365	-2.444345
64	1	-1.129298	-2.465668	-2.535026
65	1	-1.207736	-4.393495	-0.131718
66	1	-2.617754	-3.889513	-1.109358

HF = -1709.8240453 Hartrees
Zero-point correction = 0.540831 Hartrees
Sum of electronic and thermal Enthalpies = -1709.250054 Hartrees
Sum of electronic and thermal Free Energies = -1709.345213 Hartrees

$[La(bp15c5)]^+$ (vacuum) Λ(λδ)(λλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.007297	-0.064206	-0.164273
2	7	2.701314	-1.458520	-0.358218
3	7	-1.681550	-0.219028	2.131837
4	8	1.062976	-1.200646	2.071822
5	8	-1.837393	-2.133258	0.036748
6	8	0.310367	-2.553084	-1.590443
7	6	-2.561593	-1.416055	2.188395
8	1	-2.726355	-1.734861	3.228989
9	1	-3.534493	-1.132260	1.779491
10	6	-2.069032	-2.604105	1.367241
11	1	-1.155670	-3.056128	1.774215
12	1	-2.850791	-3.374532	1.360044
13	6	-1.914287	-3.093034	-1.026394
14	6	-0.545383	-3.666966	-1.336913
15	6	1.611857	-2.871547	-2.094528
16	1	1.821870	-2.147532	-2.887611
17	1	1.612987	-3.868606	-2.549849
18	6	2.634511	-2.807840	-0.966407
19	1	2.337730	-3.523565	-0.194031
20	1	3.623746	-3.127939	-1.333729
21	6	3.226442	-1.520989	1.026384
22	1	3.514779	-0.509591	1.321152
23	1	4.131811	-2.149121	1.079738
24	6	3.558979	-0.583829	-1.198008
25	1	3.212068	-0.670489	-2.234287
26	1	4.603061	-0.937274	-1.188896
27	6	2.229204	-2.038092	2.058924
28	1	1.927456	-3.078361	1.875351
29	1	2.714185	-2.003099	3.042633
30	6	0.323370	-1.221304	3.305953
31	1	1.005910	-1.010652	4.139225
32	1	-0.099223	-2.221947	3.466542

33	6	-0.742600	-0.132027	3.276017
34	1	-0.241762	0.836887	3.203113
35	1	-1.281451	-0.165598	4.237834
36	6	3.516202	0.873748	-0.785894
37	6	4.626525	1.705977	-0.934607
38	1	5.551740	1.314391	-1.346350
39	6	4.526145	3.042110	-0.540660
40	1	5.373666	3.711056	-0.657697
41	6	3.340249	3.493156	0.033489
42	1	3.209202	4.505327	0.398250
43	6	2.281033	2.596017	0.165166
44	6	0.996438	2.997736	0.884528
45	7	2.359658	1.323381	-0.270080
46	6	-2.517516	1.019440	2.085145
47	1	-1.845319	1.866396	2.251074
48	1	-3.270623	1.010923	2.886631
49	6	-3.176135	1.229378	0.735562
50	6	-4.456604	1.765224	0.590673
51	1	-5.061961	1.983700	1.465073
52	6	-4.935499	2.029010	-0.696579
53	1	-5.927106	2.451348	-0.830953
54	6	-4.132741	1.748654	-1.800590
55	1	-4.448982	1.935728	-2.820347
56	6	-2.867468	1.205246	-1.576751
57	6	-1.915483	0.872703	-2.728196
58	7	-2.418065	0.952021	-0.337538
59	8	-0.740511	0.442127	-2.331977
60	8	-2.297998	1.013946	-3.876113
61	8	0.899130	4.126327	1.338593
62	8	0.118840	2.036026	0.968812
63	1	-0.161208	-4.270977	-0.500778
64	1	-0.610060	-4.308646	-2.225619
65	1	-2.289619	-2.547720	-1.896286
66	1	-2.623968	-3.889271	-0.772591

HF = -1709.8239253 Hartrees
Zero-point correction = 0.540615 Hartrees
Sum of electronic and thermal Enthalpies = -1709.249955 Hartrees
Sum of electronic and thermal Free Energies = -1709.345892 Hartrees

$[La(bp15c5)]^+$ (vacuum) Λ(λλ)(δδδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	-0.038913	0.127121	-0.203677
2	7	-2.685401	1.503563	-0.525926
3	7	1.543533	-0.100114	2.181467
4	8	-1.248213	0.876833	2.040226
5	8	1.852154	2.083580	0.435569
6	8	-0.259556	3.001893	-0.865225
7	6	2.420758	1.055736	2.489549
8	6	2.977012	1.740347	1.249222
9	6	2.109529	2.973865	-0.660866
10	6	0.885604	3.854145	-0.789479
11	6	-1.482476	3.725870	-0.771149
12	6	-2.615148	2.818214	-1.211072
13	6	-3.250366	1.587981	0.849085
14	1	-3.711829	0.623504	1.074466
15	1	-4.049616	2.346149	0.892430

16	6	-3.547646	0.629029	-1.372177
17	1	-3.157165	0.684407	-2.395305
18	1	-4.580269	1.011110	-1.407402
19	6	-2.269829	1.885203	1.986962
20	1	-1.796589	2.870561	1.903448
21	1	-2.842700	1.868160	2.923529
22	6	-0.548099	0.797916	3.296818
23	1	-1.263481	0.540220	4.088369
24	1	-0.128122	1.784211	3.533120
25	6	0.517078	-0.298037	3.238826
26	1	0.023511	-1.250743	3.031412
27	1	0.973749	-0.367984	4.239892
28	6	-3.553125	-0.818007	-0.939827
29	6	-4.694761	-1.612467	-1.054991
30	1	-5.619762	-1.187027	-1.431952
31	6	-4.623309	-2.955745	-0.679470
32	1	-5.495463	-3.596546	-0.769860
33	6	-3.428178	-3.450556	-0.165017
34	1	-3.310671	-4.472574	0.176216
35	6	-2.337425	-2.587123	-0.065210
36	6	-1.034885	-3.043225	0.576328
37	7	-2.392069	-1.304357	-0.470346
38	6	2.347597	-1.342990	1.997156
39	1	1.653070	-2.186634	2.034636
40	1	3.078066	-1.454641	2.812460
41	6	3.046130	-1.419115	0.651098
42	6	4.280635	-2.049130	0.481023
43	1	4.813750	-2.449681	1.337801
44	6	4.809297	-2.162612	-0.807983
45	1	5.765608	-2.654306	-0.961064
46	6	4.103571	-1.639952	-1.890799
47	1	4.464394	-1.697513	-2.911270
48	6	2.880660	-1.017718	-1.642445
49	6	2.038388	-0.416418	-2.770558
50	7	2.378923	-0.915614	-0.400221
51	8	0.888065	0.073001	-2.367546
52	8	2.476493	-0.421596	-3.906982
53	8	-0.952650	-4.176233	1.024810
54	8	-0.117356	-2.118777	0.609763
55	1	0.798903	4.506036	0.091522
56	1	0.952556	4.480313	-1.689300
57	1	2.284176	2.394254	-1.574340
58	1	2.989737	3.593998	-0.455625
59	1	-3.567321	3.365779	-1.111383
60	1	-2.466391	2.617512	-2.275763
61	1	-1.610496	4.114723	0.248617
62	1	-1.462365	4.591069	-1.448469
63	1	3.506771	2.653427	1.552049
64	1	3.672463	1.106580	0.691072
65	1	3.252337	0.753250	3.144406
66	1	1.838719	1.801264	3.035980

HF = -1709.8236577 Hartrees
Zero-point correction = 0.541155 Hartrees
Sum of electronic and thermal Enthalpies = -1709.249274 Hartrees
Sum of electronic and thermal Free Energies = -1709.344626 Hartrees

$[La(bp15c5)]^+$ (vacuum) Λ(λδ)(δλδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	-0.038913	0.127121	-0.203677
2	7	-2.685401	1.503563	-0.525926
3	7	1.543533	-0.100114	2.181467
4	8	-1.248213	0.876833	2.040226
5	8	1.852154	2.083580	0.435569
6	8	-0.259556	3.001893	-0.865225
7	6	2.420758	1.055736	2.489549
8	6	2.977012	1.740347	1.249222
9	6	2.109529	2.973865	-0.660866
10	6	0.885604	3.854145	-0.789479
11	6	-1.482476	3.725870	-0.771149
12	6	-2.615148	2.818214	-1.211072
13	6	-3.250366	1.587981	0.849085
14	1	-3.711829	0.623504	1.074466
15	1	-4.049616	2.346149	0.892430
16	6	-3.547646	0.629029	-1.372177
17	1	-3.157165	0.684407	-2.395305
18	1	-4.580269	1.011110	-1.407402
19	6	-2.269829	1.885203	1.986962
20	1	-1.796589	2.870561	1.903448
21	1	-2.842700	1.868160	2.923529
22	6	-0.548099	0.797916	3.296818
23	1	-1.263481	0.540220	4.088369
24	1	-0.128122	1.784211	3.533120
25	6	0.517078	-0.298037	3.238826
26	1	0.023511	-1.250743	3.031412
27	1	0.973749	-0.367984	4.239892
28	6	-3.553125	-0.818007	-0.939827
29	6	-4.694761	-1.612467	-1.054991
30	1	-5.619762	-1.187027	-1.431952
31	6	-4.623309	-2.955745	-0.679470
32	1	-5.495463	-3.596546	-0.769860
33	6	-3.428178	-3.450556	-0.165017
34	1	-3.310671	-4.472574	0.176216
35	6	-2.337425	-2.587123	-0.065210
36	6	-1.034885	-3.043225	0.576328
37	7	-2.392069	-1.304357	-0.470346
38	6	2.347597	-1.342990	1.997156
39	1	1.653070	-2.186634	2.034636
40	1	3.078066	-1.454641	2.812460
41	6	3.046130	-1.419115	0.651098
42	6	4.280635	-2.049130	0.481023
43	1	4.813750	-2.449681	1.337801
44	6	4.809297	-2.162612	-0.807983
45	1	5.765608	-2.654306	-0.961064
46	6	4.103571	-1.639952	-1.890799
47	1	4.464394	-1.697513	-2.911270
48	6	2.880660	-1.017718	-1.642445
49	6	2.038388	-0.416418	-2.770558
50	7	2.378923	-0.915614	-0.400221
51	8	0.888065	0.073001	-2.367546
52	8	2.476493	-0.421596	-3.906982
53	8	-0.952650	-4.176233	1.024810
54	8	-0.117356	-2.118777	0.609763
55	1	0.798903	4.506036	0.091522
56	1	0.952556	4.480313	-1.689300

57	1	2.284176	2.394254	-1.574340
58	1	2.989737	3.593998	-0.455625
59	1	-3.567321	3.365779	-1.111383
60	1	-2.466391	2.617512	-2.275763
61	1	-1.610496	4.114723	0.248617
62	1	-1.462365	4.591069	-1.448469
63	1	3.506771	2.653427	1.552049
64	1	3.672463	1.106580	0.691072
65	1	3.252337	0.753250	3.144406
66	1	1.838719	1.801264	3.035980

HF = -1709.8248594 Hartrees
Zero-point correction = 0.541179 Hartrees
Sum of electronic and thermal Enthalpies = -1709.250454 Hartrees
Sum of electronic and thermal Free Energies = -1709.346033 Hartrees

$[Nd(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	60	0.060111	-0.169995	-0.027798
2	7	2.667321	-1.476376	-0.310044
3	7	-1.694768	-0.323327	2.143676
4	8	1.104735	-1.175160	2.150815
5	8	-1.822181	-2.218419	0.012168
6	8	0.296244	-2.539853	-1.428901
7	6	-2.520070	-1.555564	2.181403
8	6	-2.991993	-2.012787	0.809998
9	6	-2.086637	-2.644089	-1.331972
10	6	-0.827280	-3.313624	-1.854947
11	6	1.547602	-2.957145	-1.980842
12	1	1.771957	-2.346036	-2.863566
13	1	1.490877	-4.004500	-2.301326
14	6	2.595787	-2.839604	-0.884590
15	1	2.318126	-3.534951	-0.088081
16	1	3.577884	-3.160400	-1.268888
17	6	3.238750	-1.509955	1.059334
18	1	3.533386	-0.492550	1.325182
19	1	4.146155	-2.135594	1.094788
20	6	3.483979	-0.609691	-1.198494
21	1	3.098876	-0.722312	-2.218676
22	1	4.532615	-0.948107	-1.217562
23	6	2.272170	-2.011261	2.128855
24	1	1.966144	-3.054256	1.972176
25	1	2.778765	-1.952914	3.100647
26	6	0.316610	-1.282170	3.349911
27	1	0.955063	-1.079446	4.219447
28	1	-0.056838	-2.310293	3.443058
29	6	-0.797907	-0.238809	3.328183
30	1	-0.337186	0.751468	3.304870
31	1	-1.362967	-0.331414	4.270114
32	6	3.425470	0.852393	-0.809499
33	6	4.493879	1.722131	-1.031747
34	1	5.407732	1.359878	-1.492703
35	6	4.365741	3.058454	-0.646027
36	1	5.179939	3.756190	-0.818433
37	6	3.197999	3.475164	-0.010257
38	1	3.051190	4.487528	0.348084
39	6	2.182975	2.541690	0.190694

40	6	0.918150	2.890126	0.965608
41	7	2.287380	1.267793	-0.231726
42	6	-2.549462	0.897081	2.074310
43	1	-1.918797	1.745379	2.355484
44	1	-3.377655	0.829320	2.795396
45	6	-3.077907	1.206941	0.686099
46	6	-4.287784	1.872169	0.476325
47	1	-4.934394	2.110772	1.315178
48	6	-4.640272	2.236861	-0.826075
49	1	-5.574403	2.759891	-1.009173
50	6	-3.784149	1.930266	-1.883269
51	1	-4.000865	2.195311	-2.911724
52	6	-2.597786	1.257360	-1.596413
53	6	-1.585202	0.893231	-2.683475
54	7	-2.271329	0.901130	-0.342113
55	8	-0.489944	0.346458	-2.214235
56	8	-1.859077	1.111165	-3.850921
57	8	0.779243	4.017859	1.410984
58	8	0.097290	1.883907	1.097772
59	1	-0.730080	-4.330560	-1.451022
60	1	-0.870912	-3.367236	-2.949945
61	1	-2.359133	-1.776051	-1.942188
62	1	-2.915082	-3.363104	-1.348992
63	1	-1.919072	-2.364913	2.602606
64	1	-3.392014	-1.422404	2.840425
65	1	-3.655336	-1.285455	0.330505
66	1	-3.537297	-2.960737	0.913481

HF = -1711.7413125 Hartrees
Zero-point correction = 0.541350 Hartrees
Sum of electronic and thermal Enthalpies = -1711.166800 Hartrees
Sum of electronic and thermal Free Energies = -1711.261777 Hartrees

$[Nd(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	60	0.058365	-0.161072	-0.017340
2	7	2.619518	-1.567996	-0.302248
3	7	-1.664661	-0.143350	2.164264
4	8	1.091901	-1.114735	2.168251
5	8	-1.982320	-2.007510	0.054285
6	8	0.166303	-2.736375	-1.173260
7	6	-2.522603	-1.346054	2.285090
8	6	-3.079100	-1.842556	0.958221
9	6	-2.165939	-3.047776	-0.912652
10	6	-1.037813	-2.945963	-1.923328
11	6	1.369546	-3.032850	-1.882343
12	1	1.491315	-2.340185	-2.726237
13	1	1.326172	-4.054425	-2.283480
14	6	2.495711	-2.933834	-0.867135
15	1	2.269610	-3.630624	-0.055637
16	1	3.443813	-3.261368	-1.321328
17	6	3.193156	-1.601129	1.066314
18	1	3.542445	-0.595051	1.309124
19	1	4.066312	-2.272647	1.115093
20	6	3.463425	-0.747625	-1.208694
21	1	3.070627	-0.868937	-2.225187
22	1	4.498969	-1.124332	-1.224566

23	6	2.203776	-2.026080	2.148883
24	1	1.828686	-3.047844	2.003834
25	1	2.719317	-1.989418	3.116786
26	6	0.332603	-1.110819	3.391197
27	1	1.001848	-0.877720	4.229243
28	1	-0.077492	-2.114590	3.561328
29	6	-0.743588	-0.026924	3.328318
30	1	-0.249827	0.943741	3.243438
31	1	-1.294929	-0.048347	4.282611
32	6	3.460256	0.723280	-0.853557
33	6	4.561122	1.545196	-1.099479
34	1	5.459619	1.135421	-1.550743
35	6	4.485102	2.895483	-0.751232
36	1	5.325221	3.556543	-0.942716
37	6	3.334005	3.373718	-0.128827
38	1	3.225114	4.400685	0.200299
39	6	2.284488	2.485420	0.097740
40	6	1.034013	2.906448	0.858168
41	7	2.339053	1.196317	-0.286898
42	6	-2.483236	1.098695	2.036171
43	1	-1.824098	1.940539	2.265595
44	1	-3.306490	1.094908	2.765918
45	6	-3.017015	1.342337	0.635699
46	6	-4.224227	2.001663	0.392568
47	1	-4.862851	2.299298	1.218627
48	6	-4.586059	2.280277	-0.928354
49	1	-5.517483	2.798249	-1.137686
50	6	-3.747583	1.888069	-1.971712
51	1	-3.979602	2.075190	-3.013848
52	6	-2.563036	1.227069	-1.651028
53	6	-1.584430	0.744539	-2.722290
54	7	-2.221919	0.968559	-0.377901
55	8	-0.486318	0.211929	-2.234786
56	8	-1.881943	0.857008	-3.898461
57	8	0.939345	4.050866	1.271574
58	8	0.172889	1.938505	1.016198
59	1	-1.922352	-2.156009	2.705808
60	1	-3.355732	-1.163491	2.982553
61	1	-3.815269	-1.158958	0.522131
62	1	-3.569429	-2.809422	1.129830
63	1	-0.974887	-3.880916	-2.494671
64	1	-1.181036	-2.108509	-2.614219
65	1	-2.146272	-4.016682	-0.396152
66	1	-3.131468	-2.936485	-1.422705

HF = -1711.7437715 Hartrees
Zero-point correction = 0.541375 Hartrees
Sum of electronic and thermal Enthalpies = -1711.169326 Hartrees
Sum of electronic and thermal Free Energies = -1711.263865 Hartrees

$[Pr(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	59	0.059535	-0.163959	-0.042373
2	7	2.677863	-1.481752	-0.307205
3	7	-1.686701	-0.304058	2.153109
4	8	1.117647	-1.158204	2.157246
5	8	-1.814440	-2.233195	0.043489

6	8	0.300112	-2.552337	-1.421952
7	6	-2.512835	-1.535695	2.204156
8	6	-2.983873	-2.013383	0.838939
9	6	-2.080492	-2.681797	-1.293090
10	6	-0.819412	-3.351533	-1.810959
11	6	1.553401	-2.973315	-1.968236
12	1	1.778295	-2.367789	-2.854541
13	1	1.497461	-4.022376	-2.282700
14	6	2.602100	-2.848756	-0.872518
15	1	2.323401	-3.537589	-0.070676
16	1	3.583207	-3.174975	-1.254973
17	6	3.248237	-1.507713	1.062948
18	1	3.545546	-0.489290	1.321930
19	1	4.154142	-2.135301	1.102692
20	6	3.497614	-0.622318	-1.200052
21	1	3.112689	-0.739430	-2.219931
22	1	4.545033	-0.964634	-1.217413
23	6	2.281139	-1.999334	2.136680
24	1	1.970507	-3.041897	1.985720
25	1	2.790489	-1.938731	3.106964
26	6	0.330838	-1.256871	3.357493
27	1	0.970313	-1.049968	4.225374
28	1	-0.044502	-2.283704	3.457555
29	6	-0.782172	-0.211822	3.331478
30	1	-0.319713	0.777536	3.297638
31	1	-1.342192	-0.294701	4.277348
32	6	3.445772	0.842807	-0.819332
33	6	4.521685	1.703460	-1.040332
34	1	5.435827	1.331954	-1.493289
35	6	4.400684	3.043157	-0.663779
36	1	5.220892	3.733964	-0.835629
37	6	3.232284	3.472149	-0.037713
38	1	3.090648	4.487729	0.313510
39	6	2.208981	2.547443	0.163323
40	6	0.942978	2.913170	0.930460
41	7	2.306926	1.270278	-0.251109
42	6	-2.539513	0.917735	2.082060
43	1	-1.901689	1.767622	2.342241
44	1	-3.355695	0.861308	2.817745
45	6	-3.090555	1.211885	0.699217
46	6	-4.307594	1.867408	0.501418
47	1	-4.943564	2.109445	1.347385
48	6	-4.681153	2.218152	-0.799050
49	1	-5.621118	2.733722	-0.973272
50	6	-3.838765	1.906845	-1.865726
51	1	-4.072285	2.160724	-2.893320
52	6	-2.644035	1.243564	-1.590518
53	6	-1.647484	0.874455	-2.691345
54	7	-2.296762	0.901881	-0.337827
55	8	-0.543075	0.334172	-2.237007
56	8	-1.941940	1.083909	-3.855406
57	8	0.814753	4.046092	1.365884
58	8	0.111394	1.916770	1.067618
59	1	-0.705998	-4.355065	-1.378717
60	1	-0.875729	-3.437597	-2.903302
61	1	-2.360556	-1.825253	-1.916255
62	1	-2.904062	-3.406684	-1.295887
63	1	-1.913209	-2.339514	2.637678
64	1	-3.385965	-1.393591	2.859711
65	1	-3.646686	-1.293448	0.347879
66	1	-3.529931	-2.959142	0.957656

HF = -1711.1181101 Hartrees
Zero-point correction = 0.541194 Hartrees
Sum of electronic and thermal Enthalpies = -1710.543703 Hartrees
Sum of electronic and thermal Free Energies = -1710.638893 Hartrees

$[Pr(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	59	0.059247	-0.157482	-0.031470
2	7	2.631519	-1.571465	-0.301409
3	7	-1.655928	-0.129149	2.172254
4	8	1.106976	-1.100783	2.173491
5	8	-1.978533	-2.015247	0.076519
6	8	0.172148	-2.751454	-1.154680
7	6	-2.515164	-1.330230	2.303121
8	6	-3.073302	-1.840843	0.981645
9	6	-2.158576	-3.070080	-0.875366
10	6	-1.036879	-2.973610	-1.894191
11	6	1.373495	-3.047819	-1.867814
12	1	1.489354	-2.359448	-2.716191
13	1	1.331464	-4.071501	-2.263553
14	6	2.505111	-2.940359	-0.858889
15	1	2.284442	-3.633020	-0.042381
16	1	3.450813	-3.269716	-1.316721
17	6	3.204310	-1.597795	1.067876
18	1	3.554698	-0.590744	1.305120
19	1	4.076917	-2.269767	1.120306
20	6	3.476932	-0.756284	-1.211430
21	1	3.083625	-0.881297	-2.227454
22	1	4.511519	-1.135671	-1.226532
23	6	2.215357	-2.015994	2.153758
24	1	1.836527	-3.036945	2.012151
25	1	2.733674	-1.978869	3.120235
26	6	0.347384	-1.093543	3.395774
27	1	1.016210	-0.859077	4.233861
28	1	-0.064110	-2.096367	3.568428
29	6	-0.727664	-0.008402	3.330430
30	1	-0.232323	0.960930	3.237546
31	1	-1.274053	-0.022358	4.287733
32	6	3.478959	0.716750	-0.862640
33	6	4.585725	1.531274	-1.106325
34	1	5.484663	1.114410	-1.550158
35	6	4.515007	2.883851	-0.765477
36	1	5.359855	3.539295	-0.955505
37	6	3.363103	3.371681	-0.152294
38	1	3.257991	4.400939	0.170818
39	6	2.307050	2.490567	0.073332
40	6	1.055477	2.925776	0.826149
41	7	2.357039	1.199244	-0.304783
42	6	-2.471824	1.114788	2.043909
43	1	-1.805279	1.956124	2.253862
44	1	-3.283083	1.121962	2.787037
45	6	-3.027669	1.346222	0.649864
46	6	-4.241801	1.997471	0.420228
47	1	-4.869569	2.297980	1.253524
48	6	-4.624787	2.264051	-0.897305
49	1	-5.561885	2.775716	-1.096619

50	6	-3.800359	1.867487	-1.950068
51	1	-4.049357	2.044682	-2.990009
52	6	-2.607513	1.214793	-1.642589
53	6	-1.645195	0.727537	-2.727256
54	7	-2.245600	0.968998	-0.372721
55	8	-0.537298	0.201150	-2.256160
56	8	-1.964210	0.832273	-3.898598
57	8	0.968840	4.074801	1.228633
58	8	0.186584	1.966075	0.989960
59	1	-1.915716	-2.136405	2.732113
60	1	-3.348343	-1.140501	2.998638
61	1	-3.810365	-1.162205	0.539739
62	1	-3.562887	-2.805960	1.164731
63	1	-0.973789	-3.913931	-2.456605
64	1	-1.188862	-2.143437	-2.592219
65	1	-2.128787	-4.031836	-0.346179
66	1	-3.127247	-2.973203	-1.382340

HF = -1711.1204654 Hartrees
Zero-point correction = 0.541225 Hartrees
Sum of electronic and thermal Enthalpies = -1710.546126 Hartrees
Sum of electronic and thermal Free Energies = -1710.640807 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\lambda\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	0.060405	-0.170260	0.088028
2	7	2.510356	-1.519278	-0.300962
3	7	-1.795312	-0.344883	2.049588
4	8	0.928064	-1.267446	2.100315
5	8	-1.967006	-2.021311	-0.186161
6	8	0.159391	-2.539181	-1.416203
7	6	-2.665635	-1.543329	2.010079
8	6	-3.141269	-1.867383	0.606169
9	6	-2.210237	-2.353714	-1.556295
10	6	-0.983503	-3.100924	-2.056821
11	6	1.391298	-2.955596	-1.995176
12	1	1.620237	-2.327382	-2.865469
13	1	1.321002	-3.997382	-2.335709
14	6	2.437376	-2.872040	-0.899926
15	1	2.154044	-3.582377	-0.119214
16	1	3.420559	-3.185483	-1.285894
17	6	3.089059	-1.590410	1.062419
18	1	3.401189	-0.585923	1.354347
19	1	3.983832	-2.234048	1.085004
20	6	3.327838	-0.648771	-1.183808
21	1	2.920197	-0.728250	-2.197297
22	1	4.370853	-1.001820	-1.224156
23	6	2.101827	-2.100906	2.105301
24	1	1.799919	-3.142100	1.934975
25	1	2.577400	-2.043756	3.091952
26	6	0.120478	-1.394402	3.290031
27	1	0.756296	-1.234071	4.169345
28	1	-0.271000	-2.418285	3.340447
29	6	-0.974383	-0.332279	3.287242
30	1	-0.503004	0.649406	3.346912
31	1	-1.591064	-0.479185	4.188787
32	6	3.286986	0.798157	-0.756228

33	6	4.328756	1.691289	-1.012659
34	1	5.217017	1.357790	-1.540419
35	6	4.207262	3.011464	-0.574830
36	1	5.000764	3.726405	-0.771283
37	6	3.072593	3.390734	0.141367
38	1	2.933590	4.389477	0.539148
39	6	2.086780	2.434341	0.366050
40	6	0.850957	2.708656	1.198928
41	7	2.183101	1.175907	-0.098581
42	6	-2.608511	0.900395	1.945625
43	1	-2.013852	1.715375	2.365051
44	1	-3.532770	0.811370	2.535233
45	6	-2.928772	1.295871	0.516232
46	6	-4.059022	2.043513	0.176232
47	1	-4.791592	2.302273	0.934650
48	6	-4.222166	2.461046	-1.147040
49	1	-5.092324	3.047402	-1.427473
50	6	-3.261027	2.124028	-2.100477
51	1	-3.332066	2.424634	-3.139523
52	6	-2.163779	1.373045	-1.687260
53	6	-1.039149	0.958577	-2.631400
54	7	-2.018629	0.967773	-0.413230
55	8	-0.054842	0.345357	-2.016864
56	8	-1.129160	1.194475	-3.823053
57	8	0.672893	3.804144	1.704448
58	8	0.078009	1.659100	1.306703
59	1	-1.041543	-4.168081	-1.801129
60	1	-0.909237	-3.002722	-3.147323
61	1	-2.388039	-1.437091	-2.128999
62	1	-3.095711	-2.995217	-1.643219
63	1	-2.093515	-2.402700	2.368212
64	1	-3.531474	-1.423302	2.679667
65	1	-3.787251	-1.084645	0.191651
66	1	-3.709143	-2.807766	0.618037

HF = -1718.2176357 Hartrees
Zero-point correction = 0.542314 Hartrees
Sum of electronic and thermal Enthalpies = -1717.642345 Hartrees
Sum of electronic and thermal Free Energies = -1717.737071 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	0.057304	-0.143675	0.104795
2	7	2.455426	-1.618831	-0.263830
3	7	-1.768172	-0.140306	2.074570
4	8	0.900721	-1.180733	2.141843
5	8	-2.101821	-1.866871	-0.111843
6	8	0.025699	-2.717413	-1.234477
7	6	-2.666198	-1.316573	2.129305
8	6	-3.212956	-1.712609	0.769294
9	6	-2.323386	-2.831858	-1.143629
10	6	-1.126947	-2.791821	-2.072549
11	6	1.240662	-3.028700	-1.904895
12	1	1.411835	-2.319423	-2.725206
13	1	1.189477	-4.040920	-2.330703
14	6	2.322668	-2.977177	-0.844691
15	1	2.041053	-3.674904	-0.051631

16	1	3.283446	-3.322430	-1.256881
17	6	3.026169	-1.686165	1.102706
18	1	3.398471	-0.694236	1.367397
19	1	3.880276	-2.381685	1.147624
20	6	3.320113	-0.811447	-1.160229
21	1	2.926000	-0.909838	-2.177259
22	1	4.347740	-1.209099	-1.172870
23	6	2.007567	-2.103969	2.156021
24	1	1.623807	-3.119828	1.999487
25	1	2.488992	-2.069474	3.140595
26	6	0.127077	-1.174905	3.360819
27	1	0.796299	-0.968196	4.204840
28	1	-0.301713	-2.173787	3.508423
29	6	-0.926909	-0.072603	3.297919
30	1	-0.419906	0.892762	3.282230
31	1	-1.534714	-0.133218	4.215214
32	6	3.336458	0.650232	-0.788148
33	6	4.420378	1.483051	-1.073409
34	1	5.297343	1.084572	-1.574361
35	6	4.355154	2.826537	-0.700960
36	1	5.182168	3.495053	-0.921094
37	6	3.230309	3.289466	-0.019511
38	1	3.130646	4.311686	0.327069
39	6	2.200775	2.389525	0.238843
40	6	0.971429	2.763956	1.040175
41	7	2.243657	1.105579	-0.161380
42	6	-2.551777	1.118230	1.903113
43	1	-1.931828	1.941381	2.265723
44	1	-3.470319	1.088383	2.507071
45	6	-2.879818	1.426241	0.453766
46	6	-4.003757	2.161830	0.068533
47	1	-4.725419	2.487987	0.811259
48	6	-4.175692	2.476311	-1.281908
49	1	-5.040263	3.052146	-1.598887
50	6	-3.234434	2.044495	-2.217496
51	1	-3.320206	2.255498	-3.277290
52	6	-2.142257	1.314151	-1.757275
53	6	-1.052401	0.778419	-2.677854
54	7	-1.983800	1.019736	-0.456143
55	8	-0.059989	0.209975	-2.028387
56	8	-1.170100	0.877545	-3.886134
57	8	0.838577	3.890778	1.486693
58	8	0.149485	1.757829	1.192330
59	1	-2.098121	-2.168102	2.511354
60	1	-3.500286	-1.139849	2.827002
61	1	-3.914115	-0.975668	0.359889
62	1	-3.746769	-2.666349	0.872682
63	1	-1.105688	-3.708425	-2.677617
64	1	-1.151373	-1.926973	-2.743549
65	1	-2.426941	-3.823193	-0.681847
66	1	-3.242247	-2.602746	-1.699447

HF = -1718.2207713 Hartrees
Zero-point correction = 0.542597 Hartrees
Sum of electronic and thermal Enthalpies = -1717.645365 Hartrees
Sum of electronic and thermal Free Energies = -1717.739373 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) Λ(λδ)(λδλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	-0.038306	-0.107326	-0.060939
2	7	-2.456816	-1.626763	0.291197
3	7	1.886660	-0.082205	-2.006357
4	8	-0.737380	-1.306918	-2.052438
5	8	2.122929	-1.967156	0.076915
6	8	-0.051249	-2.588964	1.343221
7	6	2.970748	-1.100778	-1.967165
8	1	3.295643	-1.364729	-2.984865
9	1	3.828629	-0.648076	-1.464254
10	6	2.631063	-2.360900	-1.194030
11	1	1.895751	-3.001864	-1.700497
12	1	3.551346	-2.948151	-1.072476
13	6	2.219127	-3.009096	1.055406
14	1	3.223097	-3.018162	1.499034
15	1	2.033320	-3.978174	0.574176
16	6	1.150265	-2.757829	2.094355
17	1	1.073628	-3.627524	2.759798
18	1	1.345162	-1.867767	2.701688
19	6	-1.254313	-2.893991	2.037903
20	1	-1.449350	-2.138879	2.809767
21	1	-1.173535	-3.875683	2.524897
22	6	-2.324860	-2.940880	0.965176
23	1	-2.022138	-3.690475	0.229713
24	1	-3.288169	-3.267090	1.385831
25	6	-2.924701	-1.781937	-1.105291
26	1	-3.287970	-0.812442	-1.454244
27	1	-3.765907	-2.491794	-1.173781
28	6	-3.392211	-0.800213	1.090427
29	1	-3.065077	-0.852686	2.134773
30	1	-4.412083	-1.216498	1.053505
31	6	-1.830308	-2.249850	-2.060251
32	1	-1.441681	-3.243189	-1.804999
33	1	-2.250085	-2.297373	-3.071912
34	6	0.096304	-1.350951	-3.234278
35	1	-0.546451	-1.277765	-4.119799
36	1	0.613002	-2.317533	-3.269016
37	6	1.058257	-0.166228	-3.231179
38	1	0.471994	0.752428	-3.287263
39	1	1.678778	-0.236941	-4.139732
40	6	-3.410790	0.645305	0.665131
41	6	-4.525602	1.463378	0.863038
42	1	-5.420080	1.061119	1.328798
43	6	-4.468535	2.794632	0.449899
44	1	-5.319296	3.451959	0.602864
45	6	-3.318507	3.257279	-0.188290
46	1	-3.220846	4.268066	-0.567455
47	6	-2.260367	2.370732	-0.361410
48	6	-1.008373	2.739816	-1.125344
49	7	-2.293455	1.100638	0.083818
50	6	2.518258	1.264418	-1.870296
51	1	1.792173	2.012935	-2.191831
52	1	3.411269	1.346422	-2.505588
53	6	2.860886	1.556238	-0.422374
54	6	3.970212	2.308597	-0.032559
55	1	4.674926	2.666925	-0.776563
56	6	4.150108	2.600393	1.322646

57	1	5.006256	3.186995	1.642704
58	6	3.224807	2.135522	2.256724
59	1	3.312046	2.333139	3.318952
60	6	2.144176	1.389439	1.792457
61	6	1.060863	0.841418	2.713114
62	7	1.983936	1.105521	0.489807
63	8	0.066141	0.276710	2.062040
64	8	1.179998	0.933345	3.921452
65	8	-0.869134	3.853035	-1.602250
66	8	-0.172050	1.738138	-1.217395

HF = -1718.214945 Hartrees
Zero-point correction = 0.542326 Hartrees
Sum of electronic and thermal Enthalpies = -1717.639669 Hartrees
Sum of electronic and thermal Free Energies = -1717.734480 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) $\Lambda(\delta\delta)(\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	-0.032563	-0.248701	-0.020975
2	7	-2.761316	-1.224737	0.064338
3	7	2.061968	-0.773974	-1.738736
4	8	-0.731406	-1.423723	-2.026270
5	8	1.719482	-2.260416	0.642982
6	8	-0.724256	-2.414394	1.508125
7	6	3.092934	-1.706354	-1.212130
8	1	3.712773	-2.109343	-2.027526
9	1	3.753083	-1.139616	-0.552400
10	6	2.504923	-2.838501	-0.401372
11	1	1.876650	-3.516000	-0.998431
12	1	3.323984	-3.430252	0.027940
13	6	1.473041	-3.186938	1.707758
14	1	2.365245	-3.278006	2.340859
15	1	1.235201	-4.170784	1.281677
16	6	0.287538	-2.673431	2.490554
17	1	-0.047394	-3.442014	3.197213
18	1	0.505659	-1.749621	3.034469
19	6	-2.058822	-2.664070	1.936804
20	1	-2.342551	-1.953982	2.723956
21	1	-2.138308	-3.678521	2.350245
22	6	-2.923947	-2.550882	0.694900
23	1	-2.598313	-3.320486	-0.009200
24	1	-3.977968	-2.756688	0.940752
25	6	-3.101219	-1.251993	-1.376124
26	1	-3.187550	-0.218819	-1.719205
27	1	-4.075287	-1.740240	-1.553327
28	6	-3.596900	-0.245472	0.799586
29	1	-3.434192	-0.401012	1.870928
30	1	-4.668589	-0.426372	0.614012
31	6	-2.056387	-1.964064	-2.236289
32	1	-2.007039	-3.036936	-2.022733
33	1	-2.337258	-1.844401	-3.286980
34	6	0.008337	-0.988361	-3.202734
35	6	1.484357	-1.313165	-2.997433
36	6	-3.250310	1.182783	0.455801
37	6	-4.144888	2.241401	0.635315
38	1	-5.129416	2.060231	1.056067
39	6	-3.752564	3.525249	0.254986

40	1	-4.424401	4.366303	0.398444
41	6	-2.509336	3.705949	-0.353225
42	1	-2.169683	4.666575	-0.723408
43	6	-1.692689	2.592148	-0.515609
44	6	-0.399308	2.617478	-1.302082
45	7	-2.036663	1.370043	-0.070993
46	6	2.712327	0.554955	-1.912845
47	1	2.036759	1.201739	-2.474532
48	1	3.655537	0.454076	-2.470902
49	6	2.963283	1.194395	-0.558596
50	6	4.042157	2.040034	-0.298307
51	1	4.770888	2.250186	-1.075031
52	6	4.163210	2.614657	0.970289
53	1	4.994766	3.278575	1.187546
54	6	3.214603	2.328211	1.951255
55	1	3.259714	2.742702	2.951790
56	6	2.164774	1.475757	1.617095
57	6	1.052222	1.111590	2.592193
58	7	2.057757	0.925035	0.396862
59	8	0.083886	0.413748	2.034286
60	8	1.121004	1.455930	3.757388
61	8	0.050980	3.661487	-1.743702
62	8	0.096919	1.416351	-1.462115
63	1	1.583178	-2.402324	-2.968509
64	1	2.046739	-0.962765	-3.875943
65	1	-0.353376	-1.540188	-4.076179
66	1	-0.165975	0.081042	-3.336962

HF = -1718.2094663 Hartrees
Zero-point correction = 0.542236 Hartrees
Sum of electronic and thermal Enthalpies = -1717.634313 Hartrees
Sum of electronic and thermal Free Energies = -1717.729084 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\delta)(\delta\delta\delta)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	0.176246	-0.083350	0.050560
2	7	2.003072	-1.808882	-0.876853
3	7	-1.711644	-0.413335	1.887369
4	8	0.806690	-1.787247	1.674437
5	8	-3.415857	-0.956446	-0.632489
6	8	-0.858882	-2.174590	-1.071169
7	6	-2.759591	-1.461492	1.703317
8	6	-3.869690	-1.170384	0.689551
9	6	-3.248414	-2.094444	-1.463414
10	6	-1.874355	-2.026978	-2.099013
11	6	0.019683	-3.300927	-1.210836
12	6	1.380010	-2.848773	-1.729774
13	6	2.712885	-2.373033	0.302332
14	1	3.391773	-1.602380	0.670534
15	1	3.329737	-3.238741	0.013672
16	6	2.946749	-0.987208	-1.691703
17	1	2.403354	-0.667624	-2.587360
18	1	3.817387	-1.577960	-2.013503
19	6	1.810183	-2.792017	1.465616
20	1	1.323496	-3.760683	1.301407
21	1	2.425231	-2.882283	2.369894
22	6	0.001873	-1.989201	2.856003

23	6	-0.878242	-0.763794	3.072324
24	6	3.388297	0.246649	-0.935676
25	6	4.627412	0.863271	-1.105390
26	1	5.352908	0.456216	-1.802845
27	6	4.913344	2.011573	-0.360139
28	1	5.869176	2.512629	-0.481604
29	6	3.974996	2.493663	0.552210
30	1	4.152234	3.363700	1.174062
31	6	2.764155	1.815611	0.669119
32	6	1.676445	2.210151	1.656418
33	7	2.483243	0.732283	-0.073451
34	6	-2.306821	0.944356	2.080215
35	1	-1.581901	1.537067	2.644626
36	1	-3.229804	0.891116	2.674563
37	6	-2.546764	1.671848	0.769676
38	6	-3.548113	2.627973	0.592589
39	1	-4.241623	2.852629	1.397337
40	6	-3.637618	3.291724	-0.634003
41	1	-4.408041	4.041377	-0.789004
42	6	-2.741139	2.981244	-1.657075
43	1	-2.772270	3.457905	-2.630063
44	6	-1.772611	2.013978	-1.405676
45	6	-0.752876	1.565530	-2.446553
46	7	-1.686793	1.392867	-0.218309
47	8	0.082087	0.652256	-1.991958
48	8	-0.780889	2.030622	-3.570572
49	8	1.854835	3.137089	2.426082
50	8	0.614387	1.446581	1.567807
51	1	2.041923	-3.722268	-1.845313
52	1	1.230642	-2.415434	-2.722670
53	1	-0.408553	-4.031019	-1.905769
54	1	0.082621	-3.785320	-0.235314
55	1	-1.757017	-2.818456	-2.846419
56	1	-1.716193	-1.062484	-2.585084
57	1	-3.355122	-3.027728	-0.893837
58	1	-4.013143	-2.087141	-2.253288
59	1	-4.576956	-2.011248	0.733449
60	1	-4.428717	-0.273181	0.967892
61	1	-2.257247	-2.389704	1.415243
62	1	-3.256935	-1.645159	2.671338
63	1	-0.231676	0.091347	3.277368
64	1	-1.503541	-0.948288	3.960716
65	1	0.663000	-2.104301	3.723484
66	1	-0.571148	-2.917312	2.737611

HF = -1718.2123353 Hartrees
Zero-point correction = 0.542220 Hartrees
Sum of electronic and thermal Enthalpies = -1717.637337 Hartrees
Sum of electronic and thermal Free Energies = -1717.731320 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) $\Lambda(\lambda\lambda)(\delta\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	-0.019146	0.112790	0.055463
2	7	-2.298909	1.940871	0.038415
3	7	1.459681	-0.659192	2.142304
4	8	-1.187076	0.317955	2.196281
5	8	2.100489	1.713882	0.828011

6	8	0.301878	2.810300	-0.554993
7	6	2.189212	0.436397	2.819431
8	6	2.992037	1.287582	1.852770
9	6	2.548290	2.874034	0.122936
10	6	1.610119	3.075768	-1.053968
11	6	-0.772217	3.329254	-1.338406
12	1	-0.912025	2.714878	-2.236307
13	1	-0.550697	4.359687	-1.647093
14	6	-1.968110	3.325268	-0.406295
15	1	-1.700260	3.922202	0.468375
16	1	-2.834109	3.809352	-0.880707
17	6	-2.813760	1.950203	1.429940
18	6	-3.265040	1.387238	-0.938411
19	1	-2.905844	1.661129	-1.937515
20	1	-4.252251	1.861380	-0.815828
21	6	-2.588035	0.671265	2.228814
22	6	-0.705837	-0.336098	3.393890
23	1	-1.507580	-0.947003	3.823122
24	1	-0.447458	0.441758	4.121922
25	6	0.463063	-1.263610	3.064216
26	1	0.074873	-2.150716	2.564963
27	1	0.926621	-1.573322	4.015018
28	6	-3.406883	-0.112897	-0.908350
29	6	-4.598166	-0.737214	-1.285794
30	1	-5.461797	-0.138422	-1.558585
31	6	-4.655324	-2.130818	-1.310237
32	1	-5.568490	-2.637032	-1.608977
33	6	-3.530603	-2.858352	-0.927446
34	1	-3.509264	-3.941642	-0.898572
35	6	-2.387575	-2.159646	-0.548529
36	6	-1.153094	-2.875711	-0.039862
37	7	-2.318949	-0.813670	-0.555086
38	6	2.400601	-1.709585	1.652579
39	1	1.846065	-2.651138	1.618065
40	1	3.235214	-1.839742	2.356525
41	6	2.920404	-1.478946	0.245221
42	6	4.123615	-2.026126	-0.208877
43	1	4.778777	-2.554043	0.477469
44	6	4.455539	-1.901178	-1.560139
45	1	5.383772	-2.324890	-1.932177
46	6	3.583383	-1.241702	-2.427205
47	1	3.781631	-1.129188	-3.486963
48	6	2.407905	-0.715910	-1.898154
49	6	1.367310	0.006502	-2.746978
50	7	2.107790	-0.822493	-0.592881
51	8	0.283327	0.326857	-2.076041
52	8	1.600045	0.249801	-3.917738
53	8	-1.147542	-4.090970	0.068425
54	8	-0.187887	-2.056931	0.278992
55	1	1.457481	1.087318	3.305666
56	1	2.854647	0.040391	3.603324
57	1	3.836619	0.742607	1.411151
58	1	3.393146	2.156284	2.392165
59	1	-2.881664	0.872803	3.265269
60	1	-3.170055	-0.179020	1.863073
61	1	-3.890252	2.186868	1.461657
62	1	-2.292626	2.749957	1.962433
63	1	1.685169	4.111048	-1.411525
64	1	1.840100	2.405162	-1.888091
65	1	2.515852	3.734940	0.804250
66	1	3.579567	2.740195	-0.229670

HF = -1718.2125413 Hartrees
Zero-point correction = 0.542611 Hartrees
Sum of electronic and thermal Enthalpies = -1717.637071 Hartrees
Sum of electronic and thermal Free Energies = -1717.731350 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) $\Lambda(\delta\lambda)(\lambda\delta\lambda)$ (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	-0.016277	-0.236094	0.016830
2	7	2.743640	-1.496986	-0.050691
3	7	-1.933376	-0.508194	1.957421
4	8	0.942883	-0.916565	2.207689
5	8	-1.765504	-2.279787	-0.213602
6	8	0.514946	-2.480353	-1.399016
7	6	-2.975855	-1.532491	1.682348
8	1	-3.484131	-1.836275	2.609883
9	1	-3.728387	-1.082255	1.031722
10	6	-2.423909	-2.745272	0.968128
11	1	-1.713764	-3.321740	1.578765
12	1	-3.254315	-3.410045	0.698518
13	6	-1.664390	-3.294037	-1.222552
14	6	-0.608649	-2.844535	-2.207939
15	6	1.800190	-2.780798	-1.936964
16	1	2.072131	-2.040758	-2.700020
17	1	1.787453	-3.770833	-2.410913
18	6	2.744721	-2.803775	-0.749815
19	1	2.382662	-3.569496	-0.059306
20	1	3.756691	-3.098306	-1.070762
21	6	3.105817	-1.645408	1.379887
22	6	3.644736	-0.587218	-0.789296
23	1	3.516349	-0.783827	-1.859286
24	1	4.698769	-0.815218	-0.559046
25	6	2.369239	-0.721274	2.344018
26	6	0.194430	-0.325388	3.300780
27	6	-1.239954	-0.825148	3.231436
28	6	3.381835	0.880275	-0.560254
29	6	4.376404	1.835817	-0.792764
30	1	5.362896	1.523232	-1.121996
31	6	4.081811	3.183317	-0.594024
32	1	4.834409	3.943299	-0.782118
33	6	2.820228	3.533541	-0.114037
34	1	2.536512	4.555780	0.108536
35	6	1.899847	2.517592	0.119427
36	6	0.571828	2.781234	0.795044
37	7	2.157031	1.219432	-0.140575
38	6	-2.605333	0.820709	1.982309
39	1	-1.900692	1.558707	2.369929
40	1	-3.487871	0.795509	2.639206
41	6	-2.993767	1.240832	0.577055
42	6	-4.110682	2.026694	0.291730
43	1	-4.781768	2.332695	1.088371
44	6	-4.341698	2.420586	-1.029575
45	1	-5.204700	3.034627	-1.269625
46	6	-3.455401	2.026912	-2.031439
47	1	-3.579170	2.310873	-3.070218
48	6	-2.360643	1.246233	-1.666882
49	6	-1.289901	0.805324	-2.654593

50	7	-2.158233	0.853502	-0.399738
51	8	-0.244930	0.257328	-2.067649
52	8	-1.450616	0.963589	-3.850450
53	8	0.214675	3.917737	1.055284
54	8	-0.060403	1.673848	1.087598
55	1	-1.218415	-1.914183	3.336916
56	1	-1.795239	-0.428656	4.095188
57	1	0.637308	-0.656397	4.247898
58	1	0.261266	0.763307	3.225677
59	1	2.662028	-0.996110	3.365198
60	1	2.604247	0.335231	2.188793
61	1	4.186879	-1.502903	1.537347
62	1	2.875354	-2.671449	1.679974
63	1	-0.352183	-3.674739	-2.876409
64	1	-0.921739	-1.986463	-2.809948
65	1	-1.356092	-4.237989	-0.754260
66	1	-2.638102	-3.435919	-1.708881

HF = -1718.207837 Hartrees
Zero-point correction = 0.542356 Hartrees
Sum of electronic and thermal Enthalpies = -1717.632624 Hartrees
Sum of electronic and thermal Free Energies = -1717.727506 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) Λ(λδ)(λλλ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	0.026499	-0.109946	0.078391
2	7	2.591038	-1.402004	-0.313935
3	7	-1.870781	-0.485450	1.960099
4	8	0.862332	-1.387339	2.010376
5	8	-1.887179	-1.808360	-0.443970
6	8	0.348592	-2.644948	-1.408888
7	6	-2.769469	-1.654427	1.735088
8	1	-2.958359	-2.191934	2.674871
9	1	-3.732091	-1.278400	1.379436
10	6	-2.243399	-2.617765	0.676583
11	1	-1.375104	-3.197398	1.017273
12	1	-3.034859	-3.325393	0.398751
13	6	-1.973603	-2.397259	-1.745206
14	6	-0.768252	-3.286854	-2.016718
15	6	1.605485	-2.941047	-2.008545
16	1	1.759885	-2.291035	-2.879624
17	1	1.638020	-3.984298	-2.349613
18	6	2.652166	-2.749212	-0.928302
19	1	2.460632	-3.494322	-0.152831
20	1	3.657264	-2.953489	-1.330146
21	6	3.101875	-1.453357	1.075356
22	1	3.296237	-0.433012	1.410108
23	1	4.053621	-2.007332	1.136428
24	6	3.368934	-0.461369	-1.156926
25	1	2.983886	-0.543785	-2.179803
26	1	4.432718	-0.748968	-1.187831
27	6	2.116899	-2.094818	2.047490
28	1	1.933003	-3.154234	1.829335
29	1	2.533674	-2.025972	3.059607
30	6	0.000092	-1.665397	3.135139
31	1	0.592976	-1.627556	4.056831
32	1	-0.403008	-2.681617	3.033735

33	6	-1.087285	-0.602272	3.211895
34	1	-0.610237	0.363668	3.385972
35	1	-1.731582	-0.834060	4.075519
36	6	3.244506	0.972702	-0.700818
37	6	4.241332	1.921828	-0.935393
38	1	5.143613	1.644403	-1.471784
39	6	4.058748	3.223017	-0.464111
40	1	4.816064	3.980011	-0.645183
41	6	2.912537	3.527731	0.269307
42	1	2.729989	4.506350	0.698221
43	6	1.974782	2.519786	0.471831
44	6	0.739975	2.710137	1.331102
45	7	2.124867	1.281271	-0.033451
46	6	-2.667293	0.779152	1.955760
47	1	-2.045827	1.557967	2.402972
48	1	-3.578941	0.670871	2.559798
49	6	-3.006430	1.230993	0.548593
50	6	-4.188741	1.895039	0.216889
51	1	-4.952475	2.062170	0.970198
52	6	-4.365870	2.348090	-1.094064
53	1	-5.276320	2.873255	-1.367659
54	6	-3.373955	2.114273	-2.046176
55	1	-3.463152	2.433289	-3.078329
56	6	-2.227183	1.433442	-1.642804
57	6	-1.092592	1.075104	-2.598022
58	7	-2.060422	1.017391	-0.378157
59	8	-0.098995	0.445084	-2.007852
60	8	-1.182959	1.348825	-3.780860
61	8	0.515998	3.781899	1.867111
62	8	0.023529	1.618777	1.425553
63	1	-0.886872	-4.293099	-1.589163
64	1	-0.629566	-3.388285	-3.100433
65	1	-1.983818	-1.553829	-2.436331
66	1	-2.913802	-2.952881	-1.847423

HF = -1718.2117647 Hartrees
Zero-point correction = 0.541756 Hartrees
Sum of electronic and thermal Enthalpies = -1717.636873 Hartrees
Sum of electronic and thermal Free Energies = -1717.732202 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) Λ(λλ)(δδδ) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	0.166327	-0.066187	0.014007
2	7	1.958866	-1.868893	-0.896140
3	7	-1.622121	-0.295442	1.963853
4	8	0.852278	-1.684765	1.671951
5	8	-3.537616	-1.024669	-0.368096
6	8	-0.940600	-2.200930	-0.885213
7	6	-2.635497	-1.393794	1.919444
8	6	-3.845180	-1.198561	1.000516
9	6	-3.355058	-2.191874	-1.154674
10	6	-2.014940	-2.112891	-1.859099
11	6	-0.042696	-3.312091	-1.051905
12	6	1.234803	-2.852852	-1.738970
13	6	2.617581	-2.554614	0.258872
14	6	2.926199	-1.096840	-1.718811
15	1	2.394240	-0.759962	-2.615868

16	1	3.770299	-1.724252	-2.041703
17	6	2.264258	-1.983826	1.637764
18	6	0.198761	-1.726839	2.966146
19	6	-0.717816	-0.516146	3.127721
20	6	3.417414	0.125142	-0.977753
21	6	4.687578	0.677493	-1.143516
22	1	5.406173	0.209446	-1.809137
23	6	5.010908	1.842584	-0.442008
24	1	5.991545	2.293876	-0.560944
25	6	4.072420	2.409678	0.419970
26	1	4.272073	3.301903	1.002375
27	6	2.830163	1.791787	0.537956
28	6	1.741942	2.287633	1.477035
29	7	2.516210	0.683898	-0.155799
30	6	-2.253596	1.054563	2.070153
31	1	-1.525831	1.713259	2.551934
32	1	-3.148511	1.027950	2.707126
33	6	-2.569390	1.665388	0.716255
34	6	-3.609507	2.571774	0.506583
35	1	-4.282657	2.832268	1.317762
36	6	-3.764431	3.140393	-0.760575
37	1	-4.566605	3.849945	-0.941130
38	6	-2.891113	2.788218	-1.790075
39	1	-2.970559	3.193409	-2.792252
40	6	-1.880544	1.874575	-1.505576
41	6	-0.876489	1.393211	-2.548616
42	7	-1.735055	1.342030	-0.281057
43	8	0.008083	0.544036	-2.063234
44	8	-0.958827	1.779501	-3.699210
45	8	1.944896	3.249205	2.196520
46	8	0.651748	1.562651	1.412327
47	1	1.868376	-3.722009	-1.977551
48	1	0.971426	-2.364078	-2.681247
49	1	-0.526312	-4.101959	-1.635528
50	1	0.155736	-3.710064	-0.053070
51	1	-1.917494	-2.926285	-2.585552
52	1	-1.910911	-1.163943	-2.388135
53	1	-3.407678	-3.102033	-0.541961
54	1	-4.151475	-2.243635	-1.910568
55	1	-4.504427	-2.066513	1.148950
56	1	-4.418332	-0.314894	1.293765
57	1	-2.117582	-2.314026	1.632926
58	1	-3.041524	-1.547579	2.934092
59	1	-0.098231	0.376300	3.224575
60	1	-1.291058	-0.646381	4.060172
61	1	0.951926	-1.696677	3.759652
62	1	-0.334684	-2.680632	3.034704
63	1	2.498105	-2.733929	2.401122
64	1	2.821402	-1.069407	1.863476
65	1	3.708636	-2.524082	0.148292
66	1	2.335061	-3.610770	0.241831

HF = -1718.2085561 Hartrees
Zero-point correction = 0.541923 Hartrees
Sum of electronic and thermal Enthalpies = -1717.633735 Hartrees
Sum of electronic and thermal Free Energies = -1717.728238 Hartrees

$[Lu(bp15c5)]^{+}$ (vacuum) Λ(λδ)(δλδ) (0 imaginary frequencies)

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	71	0	-0.033390	0.076630	0.020379
2	7	0	-2.491937	1.538499	-0.494775
3	7	0	1.721826	0.098029	2.063656
4	8	0	-0.984859	1.085631	2.009493
5	8	0	1.995061	1.870488	-0.053740
6	8	0	-0.136361	2.965462	-1.029560
7	6	0	2.603766	1.284047	2.148136
8	6	0	3.133276	1.711648	0.790800
9	6	0	2.174961	2.694218	-1.216886
10	6	0	1.058628	3.715003	-1.186974
11	6	0	-1.303010	3.748030	-0.861783
12	6	0	-2.476983	2.848646	-1.197660
13	6	0	-3.066710	1.634800	0.870754
14	1	0	-3.476311	0.657891	1.136016
15	1	0	-3.901258	2.354688	0.900424
16	6	0	-3.305000	0.628526	-1.349703
17	1	0	-2.846022	0.636916	-2.344639
18	1	0	-4.334931	1.003744	-1.459821
19	6	0	-2.079792	2.023455	1.970254
20	1	0	-1.675107	3.034011	1.849376
21	1	0	-2.610733	1.984473	2.929449
22	6	0	-0.250994	1.100530	3.255034
23	1	0	-0.946947	0.891940	4.076607
24	1	0	0.155582	2.108282	3.406223
25	6	0	0.828496	0.018939	3.246971
26	1	0	0.345660	-0.958405	3.218368
27	1	0	1.389552	0.100547	4.192111
28	6	0	-3.329633	-0.793151	-0.856262
29	6	0	-4.429653	-1.629648	-1.056914
30	1	0	-5.314181	-1.252368	-1.560683
31	6	0	-4.370081	-2.947280	-0.601003
32	1	0	-5.209998	-3.618308	-0.754542
33	6	0	-3.230271	-3.377929	0.075000
34	1	0	-3.128382	-4.376964	0.483049
35	6	0	-2.184358	-2.475434	0.246142
36	6	0	-0.940082	-2.823826	1.032382
37	7	0	-2.222345	-1.217020	-0.230321
38	6	0	2.529848	-1.146729	1.908029
39	1	0	1.909372	-1.985045	2.231645
40	1	0	3.423562	-1.111735	2.547966
41	6	0	2.922640	-1.419994	0.466642
42	6	0	4.076646	-2.122890	0.112081
43	1	0	4.772901	-2.453567	0.876764
44	6	0	4.312954	-2.398419	-1.237585
45	1	0	5.202191	-2.948939	-1.530485
46	6	0	3.404838	-1.961038	-2.202638
47	1	0	3.539622	-2.144176	-3.262518
48	6	0	2.279203	-1.262732	-1.773239
49	6	0	1.212647	-0.733320	-2.727993
50	7	0	2.059285	-1.007087	-0.472766
51	8	0	0.198397	-0.169656	-2.106085
52	8	0	1.363010	-0.846821	-3.929971
53	8	0	-0.820781	-3.916964	1.559902
54	8	0	-0.088151	-1.834316	1.082911
55	1	0	1.192321	4.405336	-0.339967
56	1	0	1.033299	4.300034	-2.117564

57	1	0	2.109806	2.067579	-2.111751
58	1	0	3.153055	3.185698	-1.196267
59	1	0	-3.422378	3.390325	-1.032935
60	1	0	-2.403840	2.635778	-2.266620
61	1	0	-1.343748	4.169267	0.153376
62	1	0	-1.309942	4.594437	-1.563851
63	1	0	3.659434	2.668860	0.899510
64	1	0	3.831949	0.985342	0.360170
65	1	0	3.443313	1.103474	2.837593
66	1	0	2.026492	2.119927	2.550411

HF = -1718.210919 Hartrees
Zero-point correction = 0.542189 Hartrees
Sum of electronic and thermal Enthalpies = -1717.635670 Hartrees
Sum of electronic and thermal Free Energies = -1717.731497 Hartrees