Eight-Coordinate Zn(II), Cd(II) and Pb(II) Complexes Based on a 1,7-diaza-12-crown-4 Platform Endowed with a Remarkable Selectivity over Ca(II)

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Supporting Information

[Pb(bp12c4)]; Δ(δδδδ) ; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.79843	1.96298	1.04343
2	6	1.06437	2.74545	2.05219
3	6	-0.12807	1.98869	2.65279
4	6	-1.97185	2.73583	1.30182
5	6	-2.96907	2.21825	0.26618
6	7	-2.33278	1.71755	-0.957
7	6	-1.83918	2.78559	-1.83266
8	6	-0.51285	2.47031	-2.54488
9	6	1.18451	3.28713	-1.025
10	6	2.2801	2.76997	-0.08837
11	6	2.88007	1.19348	1.67692
12	6	-3.14439	0.7208	-1.66848
13	1	0.70246	3.66838	1.59082
14	1	1.72899	3.06483	2.87495
15	1	0.18973	1.02285	3.05878
16	1	-0.55165	2.58068	3.48037
17	1	-1.38685	3.57432	0.89479
18	1	-2.53333	3.12715	2.16698
19	1	-3.51778	1.39428	0.7276
20	1	-3.70305	3.02082	0.05988
21	1	-1.7062	3.68929	-1.22992
22	1	-2.57995	3.05348	-2.60991
23	1	-0.61804	1.57295	-3.1635
24	1	-0.26944	3.30804	-3.21891
25	1	0.44159	3.8804	-0.47265
26	1	1.65339	3.96386	-1.75939
27	1	2.94925	2.14172	-0.68392
28	1	2.87154	3.64068	0.25478
29	1	3.69439	1.85459	2.0287
30	1	2.45867	0.71852	2.57174
31	1	-4.09854	1.14424	-2.03669
32	1	-2.58181	0.40955	-2.55877
33	8	-1.13322	1.66945	1.70213
34	8	0.58077	2.19051	-1.68291
35	6	3.47771	0.09768	0.80995
36	6	4.85589	-0.11778	0.75677
37	6	5.34408	-1.18426	-0.00426
38	1	5.53169	0.53433	1.30245
39	6	3.08439	-1.69522	-0.62511
40	6	4.45045	-1.98397	-0.70795
41	1	6.41302	-1.37467	-0.05277
42	1	4.76081	-2.81513	-1.33001
43	6	-3.44655	-0.50847	-0.81959
44	6	-4.7174	-1.08209	-0.75219
45	6	-2.62183	-2.01317	0.75985
46	6	-4.91574	-2.1819	0.09065
47	1	-5.53674	-0.67136	-1.33512
48	6	-3.86411	-2.64514	0.87575
49	1	-5.89504	-2.64942	0.15081
50	1	-3.96838	-3.45981	1.58271
51	7	-2.43223	-1.00516	-0.09744
52	7	2.62686	-0.68993	0.13387
53	6	2.07326	-2.50677	-1.4545
54	8	0.84371	-2.11168	-1.39225
55	8	2.52258	-3.43361	-2.12326
56	6	-1.45168	-2.38853	1.68295
57	8	-1.66216	-3.2497	2.53055
58	8	-0.35124	-1.72036	1.51469
59	82	0.08357	-0.35713	-0.19466

HF= -1527.8574513 Hartrees
Zero-point correction = 0.474425
Sum of electronic and thermal Enthalpies = -1527.352208
Sum of electronic and thermal Free Energies = -1527.445210

[Pb(bp12c4)]; Δ(λλλλ) ; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.8742	1.75956	1.36249
2	6	-2.42453	2.7267	0.39925
3	6	-2.40485	2.27104	-1.07025
4	6	-0.27193	2.96347	-1.94209
5	6	1.06736	2.39676	-2.41388
6	7	1.87585	1.75903	-1.3624
7	6	2.42675	2.72549	-0.39884
8	6	2.4066	2.26927	1.07048

9	6	0.27425	2.96254	1.9427
10	6	-1.06536	2.39648	2.41423
11	6	-2.89309	0.86754	1.93624
12	6	2.89407	0.8663	-1.93615
13	1	-1.85571	3.65791	0.47985
14	1	-3.46795	2.99069	0.65224
15	1	-3.02993	1.38731	-1.20782
16	1	-2.82914	3.07874	-1.68916
17	1	-0.13068	3.68514	-1.12395
18	1	-0.72225	3.51731	-2.78296
19	1	0.84476	1.63884	-3.17164
20	1	1.61686	3.21179	-2.92305
21	1	1.8585	3.65708	-0.47916
22	1	3.47036	2.98893	-0.65167
23	1	3.03123	1.38521	1.20787
24	1	2.8311	3.07653	1.68982
25	1	0.13349	3.68494	1.12511
26	1	0.7251	3.5154	2.78393
27	1	-0.84319	1.63812	3.17168
28	1	-1.61443	3.21161	2.92369
29	1	-2.41811	0.31357	2.75512
30	1	-3.73061	1.43656	2.38144
31	1	2.41872	0.31276	-2.75512
32	1	3.73211	1.43465	-2.38125
33	8	-1.11974	1.90132	-1.55004
34	8	1.12115	1.90003	1.54973
35	6	-3.45991	-0.15487	0.96189
36	6	-4.83059	-0.39448	0.85519
37	6	-5.27618	-1.37993	-0.0328
38	1	-5.53398	0.17799	1.45297
39	6	-2.99286	-1.76526	-0.65703
40	6	-4.35031	-2.07149	-0.80633
41	1	-6.3388	-1.58845	-0.12575
42	1	-4.62965	-2.82781	-1.53029
43	6	3.46003	-0.1566	-0.96176
44	6	4.8305	-0.39765	-0.85523
45	6	2.99156	-1.76584	0.65792
46	6	5.27515	-1.38326	0.03304
47	1	5.53438	0.17385	-1.45334
48	6	4.3487	-2.07347	0.8071
49	1	6.33756	-1.5929	0.12585
50	1	4.62741	-2.82974	1.53136
51	7	2.57688	-0.85004	-0.226
52	7	-2.57733	-0.84951	0.22655
53	6	-1.94313	-2.43304	-1.56298
54	8	-0.72573	-2.01377	-1.43076
55	8	-2.35149	-3.27749	-2.35501
56	6	1.9412	-2.43187	1.5644
57	8	2.3487	-3.2761	2.35705
58	8	0.72418	-2.01146	1.43195
59	82	-2.77E-04	-0.43996	-7.85E-04

HF= -1527.8543017 Hartrees
Zero-point correction = 0.474684
Sum of electronic and thermal Enthalpies = -1527.348787
Sum of electronic and thermal Free Energies = -1527.441309

[Pb(bp12c4)] ; $\Delta(\delta\lambda\delta\lambda)$; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	7	1.34743	1.76261	1.34605
2	6	0.44057	2.04993	2.47874
3	6	-0.90612	2.69534	2.16951
4	6	-2.70046	2.63492	0.63616
5	6	-3.37187	1.77996	-0.44897
6	7	-2.4777	1.08607	-1.37753
7	6	-1.91123	1.88017	-2.46848
8	6	-0.95653	3.01501	-2.07044
9	6	0.72944	3.51431	-0.46197
10	6	1.75791	2.89621	0.49746
11	6	2.54772	1.10134	1.90635
12	6	-3.07314	-0.17357	-1.85565
13	1	0.93648	2.69394	3.23046
14	1	0.24238	1.08265	2.95088
15	1	-2.38366	3.61433	0.24728
16	1	-3.45681	2.84143	1.4134
17	1	-3.95089	1.00921	0.06601
18	1	-4.10449	2.42243	-0.9766
19	1	-2.6956	2.34367	-3.10143
20	1	-1.35519	1.19021	-3.11314

21	1	-0.0447	4.0702	0.08075
22	1	1.27848	4.2548	-1.06934
23	1	2.59036	2.53233	-0.11384
24	1	2.15884	3.72893	1.10823
25	1	3.20086	1.827	2.42303
26	1	2.19502	0.38804	2.6594
27	1	-4.05271	-0.0259	-2.34689
28	1	-2.40157	-0.58959	-2.61693
29	8	-1.58994	1.95418	1.18004
30	8	0.12584	2.53683	-1.2876
31	6	3.36077	0.30165	0.90619
32	6	4.75587	0.30329	0.88729
33	6	5.41693	-0.5703	0.01622
34	1	5.31244	0.96388	1.54565
35	6	3.2797	-1.34723	-0.74278
36	6	4.67504	-1.41282	-0.80614
37	1	6.50327	-0.58797	-0.01354
38	1	5.12641	-2.11518	-1.49707
39	6	-3.21903	-1.19209	-0.73188
40	6	-4.38861	-1.91196	-0.48402
41	6	-2.16717	-2.1524	1.1152
42	6	-4.41531	-2.79718	0.60105
43	1	-5.26131	-1.77818	-1.11687
44	6	-3.3004	-2.91056	1.4272
45	1	-5.31367	-3.37256	0.80863
46	1	-3.2786	-3.54645	2.3045
47	7	-2.14161	-1.35293	0.04673
48	7	2.66381	-0.50497	0.09448
49	6	2.39412	-2.2375	-1.63125
50	8	1.12168	-2.06935	-1.48764
51	8	2.97024	-3.01241	-2.39206
52	6	-0.935	-2.12749	2.02819
53	8	-0.98538	-2.77922	3.06627
54	8	0.04636	-1.37014	1.63732
55	1	-0.58328	3.47148	-3.00207
56	1	-1.49532	3.80476	-1.53087
57	1	-0.78997	3.7435	1.85633
58	1	-1.48264	2.71563	3.11008
59	82	1.92E-01	-0.3138	-3.37E-01

HF= -1527.855001 Hartrees
Zero-point correction = 0.475299
Sum of electronic and thermal Enthalpies =-1527.349014
Sum of electronic and thermal Free Energies = -1527.440543

[Pb(bp12c4)] ; $\Delta(\lambda\delta\lambda\delta)$; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	7	1.87028	2.05994	0.87617
2	6	1.14197	2.91772	1.83639
3	6	-0.12254	2.2884	2.42192
4	6	-2.35035	1.76609	1.70769
5	6	-3.26136	1.9774	0.49337
6	7	-2.62482	1.61481	-0.78449
7	6	-2.22282	2.75285	-1.62278
8	6	-0.80792	2.67828	-2.20804
9	6	1.4786	2.68987	-1.53662
10	6	2.3708	2.81126	-0.29332
11	6	2.90715	1.28062	1.56155
12	6	-3.30552	0.5508	-1.52359
13	1	3.75164	1.9134	1.89283
14	1	2.45362	0.87015	2.47329
15	1	-4.32187	0.84054	-1.85439
16	1	-2.72962	0.35616	-2.43912
17	8	-1.15578	2.48161	1.47543
18	8	0.13777	2.96771	-1.19378
19	6	3.45512	0.10955	0.76317
20	6	4.81043	-0.22551	0.7994
21	6	5.2466	-1.36393	0.11642
22	1	5.50791	0.3921	1.35751
23	6	2.98974	-1.72066	-0.60536
24	6	4.32695	-2.12548	-0.5975
25	1	6.29635	-1.64416	0.13911
26	1	4.59897	-3.01363	-1.15533
27	6	-3.40244	-0.74215	-0.72277
28	6	-4.56204	-1.51753	-0.66028
29	6	-2.32316	-2.14831	0.79581
30	6	-4.56665	-2.66248	0.14464
31	1	-5.45E+00	-1.2254	-1.22E+00
32	6	-3.44224	-2.97736	0.904

33	1	-5.45707	-3.28312	0.19878
34	1	-3.40596	-3.82037	1.58404
35	7	-2.31223	-1.09499	-0.02767
36	7	2.58094	-0.63597	0.06831
37	6	1.94903	-2.50098	-1.4218
38	8	0.74304	-2.01982	-1.41058
39	8	2.33863	-3.48971	-2.03257
40	6	-1.09519	-2.32672	1.69515
41	8	-1.11821	-3.22369	2.52722
42	8	-0.14352	-1.44715	1.53408
43	1	-0.723	3.40969	-3.03014
44	1	-0.6167	1.68158	-2.641
45	1	-2.26171	3.66151	-1.01638
46	1	-2.92871	2.89479	-2.46051
47	1	1.56315	1.67251	-1.95291
48	1	1.84755	3.38412	-2.31171
49	1	3.36032	2.43203	-0.57415
50	1	2.5036	3.8733	-0.03911
51	1	0.81996	3.82327	1.32E+00
52	1	1.81186	3.22908	2.65602
53	1	0.02205	1.21674	2.63607
54	1	-0.37407	2.78475	3.37516
55	1	-3.5771	3.02918	0.47242
56	1	-4.17133	1.38377	0.64707
57	1	-2.13461	0.6986	1.84837
58	1	-2.86464	2.12872	2.61575
59	82	0.09971	-0.21363	-0.27964

HF= -1527.8538287 Hartrees
Zero-point correction = 0.474262
Sum of electronic and thermal Enthalpies = -1527.349524
Sum of electronic and thermal Free Energies = -1527.441924

[Cd(bp12c4)]; Δ(δδδδ) ; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.84732	1.54765	-1.29326
2	6	-1.14603	2.4201	-2.24962
3	6	0.24827	1.89488	-2.6086
4	6	1.69532	2.80367	-0.86577
5	6	2.59151	2.29699	0.26673
6	7	1.84745	1.54784	1.29297
7	6	1.14614	2.42046	2.24914
8	6	-0.24821	1.89542	2.60825
9	6	-1.695	2.80407	0.86512
10	6	-2.59134	2.29708	-0.26715
11	6	-2.65458	0.49842	-1.94899
12	6	2.65452	0.49858	1.9489
13	1	-1.05032	3.41424	-1.79945
14	1	-1.72614	2.55957	-3.17787
15	1	0.19115	0.91022	-3.07925
16	1	0.74671	2.59223	-3.29732
17	1	0.96046	3.53452	-0.496
18	1	2.31933	3.31546	-1.61414
19	1	3.33153	1.62712	-0.17606
20	1	3.14078	3.15302	0.6959
21	1	1.0505	3.41453	1.79876
22	1	1.72627	2.56022	3.17734
23	1	-0.19118	0.91084	3.07909
24	1	-0.74651	2.59305	3.2968
25	1	-0.95997	3.53463	0.49517
26	1	-2.31885	3.31619	1.61339
27	1	-3.33119	1.62728	0.17603
28	1	-3.14072	3.15288	-0.69655
29	1	-3.52648	0.92019	-2.47902
30	1	-2.01336	0.01323	-2.69446
31	1	3.52649	0.92031	2.47885
32	1	2.01327	0.01364	2.69448
33	8	1.05745	1.67997	-1.45096
34	8	-1.05736	1.68034	1.45064
35	6	-3.1148	-0.55736	-0.9537
36	6	-4.3719	-1.1599	-0.98
37	6	-4.67732	-2.10422	0.00812
38	1	-5.09528	-0.89649	-1.74637
39	6	-2.51011	-1.74027	0.96882
40	6	-3.74797	-2.39047	1.00521
41	1	-5.64764	-2.59417	0.00526
42	1	-3.94518	-3.08455	1.81362
43	6	3.11466	-0.5574	0.9538
44	6	4.3718	-1.15984	0.98012

45	6	2.51008	-1.74055	-0.96859
46	6	4.67732	-2.10418	-0.00795
47	1	5.09515	-0.89634	1.74649
48	6	3.74801	-2.3906	-1.00502
49	1	5.64768	-2.59403	-0.00505
50	1	3.94522	-3.08469	-1.81341
51	7	2.22396	-0.87445	0.00878
52	7	-2.2241	-0.87421	-0.00866
53	6	-1.45213	-1.93087	2.07659
54	8	-0.35292	-1.28051	1.91602
55	8	-1.7728	-2.66113	3.01572
56	6	1.45189	-1.93151	-2.07621
57	8	1.77264	-2.6620	-3.01517
58	8	0.35251	-1.28146	-1.91566
59	48	3.30E-05	-0.09453	1.04E-04

HF= -1572.4615629 Hartrees
Zero-point correction = 0.476673
Sum of electronic and thermal Enthalpies = -1571.955934
Sum of electronic and thermal Free Energies = -1572.042709

[Cd(bp12c4)]; Δ(λλλλ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	7	-1.43572	-1.59033	1.49494
2	6	-2.05038	-0.81718	2.58556
3	6	-2.29947	0.66341	2.25631
4	6	-0.79756	2.55309	1.99271
5	6	0.40649	2.98431	1.14164
6	7	1.43444	1.93619	0.99897
7	6	2.02455	1.48995	2.26995
8	6	2.31501	-0.01874	2.34559
9	6	0.79073	-1.89299	2.63836
10	6	-0.40481	-2.55025	1.93584
11	6	-2.40974	-2.21541	0.58447
12	6	2.42423	2.28333	-0.03476
13	1	-1.37758	-0.84677	3.44566
14	1	-3.00315	-1.26776	2.91342
15	1	-3.1383	0.79836	1.56331
16	1	-2.54714	1.18511	3.19198
17	1	-0.59703	2.6403	3.0728
18	1	-1.63623	3.22559	1.76084
19	1	0.04776	3.19163	0.13088
20	1	0.80716	3.92003	1.57259
21	1	1.3188	1.72098	3.07102
22	1	2.95585	2.03789	2.49788
23	1	3.17486	-0.30403	1.72866
24	1	2.55074	-0.26978	3.38923
25	1	0.56057	-1.61462	3.67917
26	1	1.61034	-2.62576	2.6707
27	1	-0.03572	-3.03509	1.02893
28	1	-0.8071	-3.32733	2.61139
29	1	-1.85485	-2.9242	-0.04052
30	1	-3.17913	-2.7841	1.13533
31	1	1.88375	2.80845	-0.83034
32	1	3.19761	2.96892	0.35358
33	8	-1.11735	1.20658	1.68494
34	8	1.16532	-0.73523	1.9117
35	6	-3.07674	-1.21364	-0.34795
36	6	-4.41723	-1.28242	-0.72776
37	6	-4.90513	-0.32872	-1.62868
38	1	-5.06312	-2.05991	-0.32969
39	6	-2.73144	0.68488	-1.66472
40	6	-4.06018	0.67299	-2.1008
41	1	-5.9445	-0.36477	-1.94502
42	1	-4.3879	1.4501	-2.7811
43	6	3.08398	1.06469	-0.66447
44	6	4.4259	1.01868	-1.04295
45	6	2.72377	-1.11317	-1.42552
46	6	4.90666	-0.14505	-1.65445
47	1	5.07808	1.86876	-0.8638
48	6	4.0531	-1.22968	-1.8442
49	1	5.94683	-0.20364	-1.9648
50	1	4.37488	-2.16362	-2.28955
51	7	2.27586	0.02083	-0.87462
52	7	-2.27612	-0.25494	-0.82819
53	6	-1.75235	1.80443	-2.07256
54	8	-0.57031	1.71575	-1.57219
55	8	-2.20354	2.68582	-2.80621
56	6	1.73651	-2.29458	-1.51833

57	8	2.18137	-3.3435	-1.98801
58	8	0.55533	-2.06776	-1.06079
59	48	1.52E-03	-0.02517	-2.04E-01

HF= -1572.461962 Hartrees
Zero-point correction = 0.476900
Sum of electronic and thermal Enthalpies = -1571.955857
Sum of electronic and thermal Free Energies = -1572.043521

[Cd(bp12c4)] ; Δ(δλδλ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.6409	1.1967	-1.59916
2	6	-0.76236	1.73019	-2.65409
3	6	0.34249	2.65884	-2.14934
4	6	1.79581	2.92797	-0.27588
5	6	2.47303	2.1758	0.87885
6	7	1.64055	1.19716	1.59907
7	6	0.76222	1.73135	2.65382
8	6	-0.34252	2.65993	2.14866
9	6	-1.79567	2.92849	0.27496
10	6	-2.47311	2.17593	-0.87939
11	6	-2.47139	0.08453	-2.12248
12	6	2.47066	0.08482	2.12266
13	1	-1.3311	2.27966	-3.42713
14	1	-0.28865	0.86312	-3.12145
15	1	1.13675	3.72818	0.08697
16	1	2.58712	3.41352	-0.86878
17	1	3.31318	1.62273	0.45225
18	1	2.90264	2.92874	1.56425
19	1	1.33113	2.28114	3.42651
20	1	0.2884	0.86462	3.1217
21	1	-1.1364	3.72836	-0.08828
22	1	-2.58686	3.41453	0.86762
23	1	-3.31339	1.62331	-0.4525
24	1	-2.90253	2.92864	-1.56516
25	1	-3.28821	0.45051	-2.76691
26	1	-1.81018	-0.54719	-2.7248
27	1	3.28718	0.45062	2.76757
28	1	1.80906	-0.5469	2.72456
29	8	1.05163	2.03252	-1.08496
30	8	-1.05172	2.03327	1.08451
31	6	-3.03269	-0.76529	-0.99337
32	6	-4.30689	-1.33234	-0.98672
33	6	-4.68183	-2.11268	0.11417
34	1	-4.98848	-1.16867	-1.81659
35	6	-2.54079	-1.67781	1.10119
36	6	-3.79827	-2.28433	1.17783
37	1	-5.66770	-2.56982	0.14112
38	1	-4.0455	-2.85816	2.06323
39	6	3.03243	-0.76494	0.99374
40	6	4.30674	-1.33172	0.98737
41	6	2.54104	-1.67783	-1.10078
42	6	4.68203	-2.11212	-0.11336
43	1	4.98815	-1.16784	1.81735
44	6	3.7987	-2.28413	-1.17714
45	1	5.66798	-2.56909	-0.14009
46	1	4.04611	-2.85809	-2.06237
47	7	2.19397	-0.95986	-0.02878
48	7	-2.19398	-0.96	0.02899
49	6	-1.51154	-1.75759	2.24399
50	8	-0.39694	-1.15545	2.01777
51	8	-1.85781	-2.36518	3.25862
52	6	1.51188	-1.75821	-2.24361
53	8	1.8583	-2.36612	-3.25801
54	8	0.39709	-1.15633	-2.01759
55	1	-1.02578	2.87559	2.9836
56	1	0.06402	3.6225	1.8079
57	1	-0.06393	3.6216	-1.80897
58	1	1.02575	2.87408	-2.98439
59	48	-4.00E-06	-0.09539	-1.47E-04

HF= -1572.4650608 Hartrees
Zero-point correction = 0.477671
Sum of electronic and thermal Enthalpies = -1571.958493
Sum of electronic and thermal Free Energies = -1572.044762

[Cd(bp12c4)]; Δ(λδλδ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.94183	1.54185	-1.30691
2	6	-1.25812	2.35897	-2.33686
3	6	0.2254	2.02536	-2.51313
4	6	2.2472	2.08625	-1.16919
5	6	2.67428	2.33186	0.28943
6	7	1.94184	1.542	1.30672
7	6	1.25818	2.35921	2.33663
8	6	-0.2254	2.02578	2.51283
9	6	-2.24716	2.0865	1.1689
10	6	-2.67435	2.3318	-0.28974
11	6	-2.72689	0.43785	-1.88817
12	6	2.72698	0.43808	1.88807
13	1	-3.64282	0.80536	-2.38369
14	1	-2.09967	-0.04262	-2.64845
15	1	3.64293	0.80568	2.38348
16	1	2.09981	-0.0423	2.64845
17	8	0.82797	2.14877	-1.22058
18	8	-0.82793	2.14918	1.22025
19	6	-3.09023	-0.6225	-0.86104
20	6	-4.27939	-1.35203	-0.88332
21	6	-4.4799	-2.33069	0.09666
22	1	-5.02875	-1.16153	-1.64629
23	6	-2.35364	-1.75931	1.04292
24	6	-3.51344	-2.53751	1.07933
25	1	-5.39542	-2.91663	0.09586
26	1	-3.62614	-3.26558	1.87396
27	6	3.09028	-0.6224	0.86106
28	6	4.27948	-1.35187	0.88335
29	6	2.3536	-1.7595	-1.04269
30	6	4.47998	-2.33065	-0.09651
31	1	5.0289	-1.16122	1.64623
32	6	3.51344	-2.53765	-1.07908
33	1	5.39551	-2.91655	-0.0957
34	1	3.62611	-3.26582	-1.87363
35	7	2.17017	-0.84644	-0.08172
36	7	-2.17018	-0.84637	0.08185
37	6	-1.25773	-1.86028	2.12061
38	8	-0.25737	-1.06317	1.96158
39	8	-1.4525	-2.66244	3.03431
40	6	1.25762	-1.86066	-2.1203
41	8	1.45237	-2.66294	-3.0339
42	8	0.25726	-1.06356	-1.96132
43	1	-0.67243	2.75108	3.20976
44	1	-0.3752	1.01014	2.89704
45	1	1.32604	3.4111	2.04513
46	1	1.75581	2.26429	3.31351
47	1	-2.60004	1.12083	1.54548
48	1	-2.68462	2.87898	1.79643
49	1	-3.75684	2.14859	-0.36058
50	1	-2.52025	3.39467	-0.49865
51	1	-1.3258	3.41086	-2.04532
52	1	-1.75584	2.26413	-3.31371
53	1	0.37509	1.00968	-2.8973
54	1	0.67248	2.75058	-3.21011
55	1	2.51996	3.39474	0.49812
56	1	3.75681	2.14887	0.36036
57	1	2.6002	1.1206	-1.5456
58	1	2.6846	2.87868	-1.79682
59	48	0.000005	0.11166	0.000027

HF=-1572.4544016 Hartrees
Zero-point correction = 0.476744
Sum of electronic and thermal Enthalpies = -1571.948457
Sum of electronic and thermal Free Energies = -1572.036210

[Zn(bp12c4)] ; Δ(δδδδ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.85952	-1.53987	-1.26003
2	6	1.18459	-2.40727	-2.23332
3	6	-0.20212	-1.87342	-2.60134
4	6	-1.66857	-2.77553	-0.89181
5	6	-2.58892	-2.2811	0.22363
6	7	-1.85952	-1.53962	1.26036
7	6	-1.18431	-2.40641	2.23401
8	6	0.20222	-1.87192	2.60177

9	6	1.66888	-2.77465	0.89278
10	6	2.58909	-2.28065	-0.22295
11	6	2.6481	-0.46166	-1.87627
12	6	-2.64839	-0.4614	1.8762
13	1	1.08292	-3.4047	-1.79142
14	1	1.77904	-2.53859	-3.15418
15	1	-0.12924	-0.89326	-3.07558
16	1	-0.70902	-2.56898	-3.28575
17	1	-0.9494	-3.51776	-0.51333
18	1	-2.27417	-3.27101	-1.66605
19	1	-3.32249	-1.60939	-0.22798
20	1	-3.14559	-3.14058	0.63684
21	1	-1.0823	-3.404	1.79256
22	1	-1.7787	-2.53749	3.15494
23	1	0.12901	-0.89151	3.07545
24	1	0.70932	-2.56693	3.28658
25	1	0.94988	-3.51726	0.51474
26	1	2.2746	-3.26954	1.6673
27	1	3.32252	-1.60852	0.22828
28	1	3.14595	-3.14022	-0.63569
29	1	3.56319	-0.83883	-2.36667
30	1	2.02135	0.00968	-2.64112
31	1	-3.56355	-0.83856	2.36649
32	1	-2.02187	0.01013	2.64111
33	8	-1.00481	-1.64853	-1.44124
34	8	1.00488	-1.64747	1.44155
35	6	3.00689	0.59905	-0.85026
36	6	4.22339	1.28106	-0.82605
37	6	4.44139	2.22736	0.18167
38	1	4.98369	1.07367	-1.57357
39	6	2.27186	1.71909	1.05758
40	6	3.46258	2.44324	1.14891
41	1	5.37953	2.77517	0.21646
42	1	3.58666	3.13939	1.97011
43	6	-3.00706	0.59915	0.84997
44	6	-4.2235	1.28133	0.82567
45	6	-2.27193	1.71876	-1.05806
46	6	-4.44135	2.22751	-0.18217
47	1	-4.98378	1.07417	1.57324
48	6	-3.4625	2.44314	-1.14944
49	1	-5.37941	2.77545	-0.21704
50	1	-3.58645	3.13925	-1.9707
51	7	-2.06718	0.84187	-0.06981
52	7	2.06699	0.84211	0.06943
53	6	1.14812	1.83628	2.09546
54	8	0.09648	1.13788	1.82682
55	8	1.3538	2.54991	3.07647
56	6	-1.14819	1.83564	-2.09597
57	8	-1.35349	2.5497	-3.07672
58	8	-0.09691	1.13659	-1.82754
59	30	-4.90E-05	0.09995	1.40E-05

HF= -1590.0100682 Hartrees
Zero-point correction = 0.477522
Sum of electronic and thermal Enthalpies = -1589.503911
Sum of electronic and thermal Free Energies = -1589.589467

[Zn(bp12c4)]; Δ(λλλλ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	7	1.53096	1.07272	-1.84891
2	6	2.27408	2.23504	-1.34252
3	6	2.3245	2.31545	0.18875
4	6	0.7074	2.63198	1.9359
5	6	-0.53019	1.94529	2.52984
6	7	-1.4778	1.48934	1.50152
7	6	-2.02886	2.57287	0.67935
8	6	-2.39399	2.13437	-0.74505
9	6	-0.61402	2.23351	-2.36776
10	6	0.55561	1.40675	-2.89473
11	6	2.3931	-0.06169	-2.20204
12	6	-2.4915	0.58662	2.06731
13	1	1.79008	3.14557	-1.70794
14	1	3.30519	2.25323	-1.73214
15	1	3.05265	1.6161	0.61661
16	1	2.62354	3.33411	0.47685
17	1	0.54796	3.70982	1.77224
18	1	1.53641	2.52928	2.65032
19	1	-0.20358	1.04657	3.0543
20	1	-0.99052	2.63489	3.26102

21	1	-1.2734	3.35864	0.6039
22	1	-2.92136	3.02957	1.14659
23	1	-3.23533	1.43718	-0.74367
24	1	-2.69956	3.01761	-1.32202
25	1	-0.27753	3.19111	-1.94286
26	1	-1.28649	2.4625	-3.20833
27	1	0.15285	0.46445	-3.27322
28	1	1.01092	1.95493	-3.74047
29	1	1.7677	-0.79739	-2.71732
30	1	3.21755	0.23453	-2.87446
31	1	-2.00719	0.02374	2.87155
32	1	-3.3381	1.1424	2.50694
33	8	1.02761	2.02038	0.69331
34	8	-1.30343	1.47501	-1.38515
35	6	2.95019	-0.74106	-0.96495
36	6	4.23474	-1.27966	-0.88291
37	6	4.62077	-1.92073	0.29901
38	1	4.91647	-1.19858	-1.72462
39	6	2.46155	-1.4275	1.20789
40	6	3.72829	-1.99345	1.36619
41	1	5.616	-2.34957	0.38361
42	1	3.97385	-2.46243	2.31179
43	6	-3.00415	-0.42935	1.06072
44	6	-4.3033	-0.93972	1.07085
45	6	-2.44219	-1.7319	-0.7882
46	6	-4.65511	-1.89497	0.1117
47	1	-5.02249	-0.59491	1.80836
48	6	-3.71891	-2.29416	-0.84021
49	1	-5.65992	-2.30953	0.10275
50	1	-3.93993	-3.01007	-1.62314
51	7	-2.11237	-0.84188	0.1551
52	7	2.10226	-0.82831	0.06686
53	6	1.41401	-1.42031	2.32602
54	8	0.27905	-0.91122	1.98589
55	8	1.74665	-1.86891	3.42289
56	6	-1.3574	-2.04538	-1.82502
57	8	-1.65543	-2.8047	-2.74678
58	8	-0.23586	-1.44524	-1.61841
59	30	-1.91E-02	-0.17071	3.89E-02

HF= -1590.0091733 Hartrees
Zero-point correction = 0.477709
Sum of electronic and thermal Enthalpies = -1589.502520
Sum of electronic and thermal Free Energies = -1589.589262

[Zn(bp12c4)] ; $\Delta(\delta\lambda\delta\lambda)$; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	7	-1.67158	-1.1977	1.55029
2	6	-0.83771	-1.73127	2.6355
3	6	0.29155	-2.64077	2.15907
4	6	1.7689	-2.91328	0.32639
5	6	2.48221	-2.17483	-0.80973
6	7	1.67122	-1.197	-1.551
7	6	0.8372	-1.72954	-2.63659
8	6	-0.29268	-2.63871	-2.16094
9	6	-1.77026	-2.9123	-0.32864
10	6	-2.48299	-2.17479	0.80849
11	6	-2.52265	-0.0929	2.03778
12	6	2.52275	-0.09226	-2.03782
13	1	-1.43142	-2.29502	3.37982
14	1	-0.39343	-0.8657	3.13108
15	1	1.11581	-3.71145	-0.05233
16	1	2.53731	-3.40162	0.94734
17	1	3.31447	-1.62511	-0.363
18	1	2.92671	-2.93225	-1.48122
19	1	1.43072	-2.29318	-3.38116
20	1	0.39347	-0.86345	-3.13175
21	1	-1.1181	-3.71172	0.04897
22	1	-2.5391	-3.39894	-0.9504
23	1	-3.31543	-1.62461	0.36268
24	1	-2.9272	-2.93279	1.47951
25	1	-3.39166	-0.45866	2.61095
26	1	-1.90428	0.5259	2.69347
27	1	3.39172	-0.45805	-2.61101
28	1	1.90472	0.52707	-2.69333
29	8	1.00633	-2.00722	1.10429
30	8	-1.00668	-2.00592	-1.10518
31	6	-2.9787	0.77397	0.88144
32	6	-4.22532	1.39631	0.80636

33	6	-4.51363	2.1883	-0.31028
34	1	-4.95319	1.26237	1.60143
35	6	-2.34443	1.6645	-1.17487
36	6	-3.5671	2.32156	-1.32396
37	1	-5.47732	2.68497	-0.3885
38	1	-3.73924	2.90515	-2.22077
39	6	2.97894	0.7739	-0.881
40	6	4.22556	1.39624	-0.80575
41	6	2.34502	1.66309	1.17599
42	6	4.51406	2.18748	0.31137
43	1	4.95329	1.26283	-1.60103
44	6	3.5677	2.32001	1.32533
45	1	5.47775	2.68412	0.38975
46	1	3.74006	2.90294	2.22255
47	7	2.07641	0.92505	0.09413
48	7	-2.076	0.92574	-0.09346
49	6	-1.23836	1.71074	-2.22984
50	8	-0.16127	1.09013	-1.88633
51	8	-1.46959	2.30376	-3.28299
52	6	1.23912	1.70857	2.23116
53	8	1.47077	2.30021	3.28498
54	8	0.16169	1.08889	1.88702
55	1	-0.96551	-2.84147	-3.0081
56	1	0.0928	-3.60977	-1.81816
57	1	-0.09467	-3.6111	1.81495
58	1	0.96398	-2.84516	3.00616
59	30	7.30E-05	0.14496	3.90E-05

HF= -1590.0098215 Hartrees
Zero-point correction = 0.478406
Sum of electronic and thermal Enthalpies = -1589.502745
Sum of electronic and thermal Free Energies = -1589.588205

[Zn(bp12c4)]; Δ(λδλδ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.6726	-1.1982	1.54895
2	6	2.48309	-2.17533	0.80619
3	6	1.76847	-2.91409	-0.32882
4	6	0.28969	-2.64103	-2.16044
5	6	-0.83994	-1.7312	-2.63533
6	7	-1.67276	-1.19781	-1.54918
7	6	-2.48357	-2.17484	-0.80664
8	6	-1.76952	-2.9134	0.32893
9	6	-0.29052	-2.64059	2.16035
10	6	0.8398	-1.73151	2.63515
11	6	2.52464	-0.09384	2.03575
12	1	2.92959	-2.93237	1.47679
13	1	3.31392	-1.6247	0.3579
14	1	-0.09617	-3.61143	-1.81629
15	1	0.96119	-2.84513	-3.00834
16	1	-0.39592	-0.86547	-3.13086
17	1	-1.43445	-2.29444	-3.3794
18	1	-2.92962	-2.93206	-1.47733
19	1	-3.31472	-1.62421	-0.35897
20	1	0.09455	-3.61158	1.81692
21	1	-0.9625	-2.84356	3.00812
22	1	0.39641	-0.86571	3.13111
23	1	1.43423	-2.29532	3.37886
24	8	1.00564	-2.00785	-1.10624
25	8	-1.00553	-2.00741	1.10552
26	6	2.97915	0.77382	0.87936
27	6	4.22502	1.39766	0.8041
28	6	4.51203	2.19042	-0.31233
29	1	4.95336	1.26421	1.59882
30	6	2.34307	1.66458	-1.17629
31	6	3.56497	2.32303	-1.3256
32	1	5.47511	2.68822	-0.39069
33	1	3.73608	2.90723	-2.22222
34	7	2.07593	0.925	-0.09512
35	6	1.23636	1.71035	-2.23061
36	8	0.16019	1.08824	-1.88697
37	8	1.46629	2.30455	-3.28338
38	1	-2.53762	-3.40091	0.95092
39	1	-1.11738	-3.71219	-0.05008
40	1	1.11538	-3.71182	0.05077
41	1	2.53616	-3.40298	-0.95024
42	1	3.39452	-0.46029	2.60715
43	1	1.90766	0.52465	2.69302
44	6	-2.5245	-0.09315	-2.0359

45	7	-2.07566	0.92528	0.09515
46	6	-2.34278	1.66464	1.17648
47	6	-3.56462	2.32314	1.32592
48	6	-1.23612	1.71002	2.23088
49	8	-0.15989	1.0881	1.88704
50	8	-1.46613	2.30375	3.2839
51	6	-4.51166	2.19086	0.31258
52	6	-2.97888	0.77438	-0.87938
53	6	-4.22469	1.39833	-0.80402
54	1	-1.90719	0.52531	-2.69295
55	1	-3.39434	-0.45926	-2.60749
56	1	-3.73573	2.90712	2.22268
57	1	-5.4747	2.6887	0.39102
58	1	-4.95302	1.26512	-1.59879
59	30	8.70E-05	0.14381	4.00E-06

HF= -1590.0019305 Hartrees
Zero-point correction = 0.477747
Sum of electronic and thermal Enthalpies = -1589.495364
Sum of electronic and thermal Free Energies = -1589.581869

[Ca(bp12c4)]; Δ(δδδδ) ; B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Número	Número	Coordenadas (Angstroms)		
Centro	Atómico	X	Y	Z
1	7	-1.87529	1.52911	-1.29767
2	6	-1.16654	2.39984	-2.25822
3	6	0.23196	1.87098	-2.59591
4	6	1.68408	2.79828	-0.85784
5	6	2.59769	2.29283	0.26092
6	7	1.87549	1.52931	1.29736
7	6	1.16684	2.40018	2.25784
8	6	-0.23163	1.87133	2.59572
9	6	-1.68342	2.79838	0.85732
10	6	-2.59726	2.29288	-0.26124
11	6	-2.74327	0.53303	-1.97019
12	6	2.74317	0.53309	1.97003
13	1	-1.07381	3.39868	-1.81773
14	1	-1.73981	2.52864	-3.19104
15	1	0.18628	0.87876	-3.05561
16	1	0.74338	2.55513	-3.28744
17	1	0.96239	3.54024	-0.48398
18	1	2.29845	3.29407	-1.62396
19	1	3.33517	1.62953	-0.19507
20	1	3.1457	3.1511	0.68696
21	1	1.0741	3.39898	1.81725
22	1	1.74023	2.52915	3.19057
23	1	-0.18585	0.87919	3.05559
24	1	-0.74304	2.55561	3.28713
25	1	-0.96147	3.53995	0.48323
26	1	-2.29758	3.29465	1.6233
27	1	-3.33479	1.6298	0.195
28	1	-3.1452	3.15113	-0.68737
29	1	-3.59182	1.0149	-2.48624
30	1	-2.13547	0.03893	-2.73909
31	1	3.59175	1.01484	2.48615
32	1	2.13519	0.03913	2.73888
33	8	1.02029	1.67431	-1.41767
34	8	-1.02001	1.67436	1.41756
35	6	-3.25751	-0.51867	-0.99529
36	6	-4.54524	-1.05038	-1.04623
37	6	-4.91050	-1.99565	-0.07965
38	1	-5.2465	-0.73391	-1.81318
39	6	-2.736	-1.76018	0.90996
40	6	-4.00685	-2.34598	0.9198
41	1	-5.90525	-2.43372	-0.10049
42	1	-4.24719	-3.04156	1.71537
43	6	3.25733	-0.51876	0.99529
44	6	4.5451	-1.05045	1.04629
45	6	2.73586	-1.7606	-0.90974
46	6	4.91036	-1.99587	0.07987
47	1	5.24632	-0.73388	1.81321
48	6	4.00667	-2.34641	-0.91949
49	1	5.90512	-2.43389	0.10074
50	1	4.24697	-3.04219	-1.7149
51	7	2.38415	-0.89404	0.05124
52	7	-2.38432	-0.8938	-0.0512
53	6	-1.70676	-2.02073	2.03788
54	8	-0.58663	-1.41375	1.89563
55	8	-2.08482	-2.75199	2.9562
56	6	1.70647	-2.02143	-2.0375

57	8	2.08375	-2.7543	-2.95483
58	8	0.58694	-1.41318	-1.89591
59	20	-1.36E-04	-0.15475	-4.80E-05

HF= -1561.0621832 Hartrees
Zero-point correction = 0.476690
Sum of electronic and thermal Enthalpies = -1560.556750
Sum of electronic and thermal Free Energies = -1560.642932

[Ca(bp12c4)]; Δ(λλλλ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Número	Número	Coordenadas (Angstroms)		
Centro	Atómico	X	Y	Z
1	7	-1.42948	-1.79749	1.18704
2	6	-1.99158	-1.18151	2.40416
3	6	-2.27698	0.32511	2.28598
4	6	-0.82467	2.27306	2.21718
5	6	0.38011	2.81562	1.43331
6	7	1.42964	1.80297	1.17884
7	6	1.99031	1.19254	2.39938
8	6	2.27755	-0.31422	2.28761
9	6	0.82428	-2.26192	2.22911
10	6	-0.37994	-2.80863	1.44744
11	6	-2.4605	-2.32424	0.26907
12	6	2.46168	2.32496	0.25937
13	1	-1.27128	-1.30807	3.21518
14	1	-2.91913	-1.68855	2.72002
15	1	-3.1441	0.5368	1.6503
16	1	-2.49007	0.71266	3.29267
17	1	-0.63226	2.23097	3.30063
18	1	-1.67107	2.95667	2.05958
19	1	0.02321	3.1372	0.44996
20	1	0.76337	3.70099	1.97189
21	1	1.2684	1.32144	3.20859
22	1	2.91679	1.70185	2.71485
23	1	3.14568	-0.52746	1.65386
24	1	2.48989	-0.69745	3.29608
25	1	0.63031	-2.21162	3.31193
26	1	1.66993	-2.94792	2.07789
27	1	-0.02241	-3.1354	0.46603
28	1	-0.76338	-3.69121	1.99044
29	1	-1.94477	-2.94953	-0.46987
30	1	-3.18085	-2.9721	0.79778
31	1	1.94706	2.94793	-0.4823
32	1	3.18239	2.9742	0.78589
33	8	-1.12551	0.96689	1.74592
34	8	1.12766	-0.95978	1.74859
35	6	-3.19829	-1.22445	-0.48212
36	6	-4.56388	-1.26527	-0.7627
37	6	-5.12463	-0.20872	-1.4903
38	1	-5.17411	-2.097	-0.42212
39	6	-2.96375	0.83526	-1.55143
40	6	-4.32257	0.85934	-1.88407
41	1	-6.18508	-0.21837	-1.72968
42	1	-4.70544	1.71729	-2.42439
43	6	3.19884	1.22158	-0.48724
44	6	4.5644	1.26065	-0.76803
45	6	2.96334	-0.84235	-1.54819
46	6	5.1247	0.2009	-1.49135
47	1	5.17506	2.09348	-0.43087
48	6	4.32214	-0.86838	-1.88075
49	1	6.18514	0.20912	-1.73082
50	1	4.70459	-1.72866	-2.41765
51	7	2.43203	0.19831	-0.88904
52	7	-2.43196	-0.20247	-0.8881
53	6	-2.02777	2.02741	-1.86302
54	8	-0.82128	1.88236	-1.45405
55	8	-2.54568	2.99207	-2.4307
56	6	2.02687	-2.03532	-1.85525
57	8	2.54447	-3.0024	-2.41914
58	8	0.82037	-1.88819	-1.44708
59	20	9.80E-05	-6.43E-04	-2.97E-01

HF= -1561.064106 Hartrees
Zero-point correction = 0.476847
Sum of electronic and thermal Enthalpies = -1560.558207
Sum of electronic and thermal Free Energies = -1560.645965

[Ca(bp12c4)] ; Δ(δλδλ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Número	Número	Coordenadas (Angstroms)		
Centro	Atómico	X	Y	Z
1	7	-1.65434	-1.16618	1.62043
2	6	-0.75077	-1.68746	2.66489
3	6	0.34917	-2.61682	2.14707
4	6	1.78794	-2.90261	0.25682
5	6	2.4732	-2.16146	-0.90334
6	7	1.65438	-1.16602	-1.62049
7	6	0.75073	-1.68707	-2.66498
8	6	-0.3492	-2.61651	-2.14726
9	6	-1.78813	-2.90245	-0.25716
10	6	-2.47327	-2.16144	0.90316
11	6	-2.50822	-0.07748	2.16895
12	6	2.5084	-0.07738	-2.16893
13	1	-1.3	-2.23108	3.45556
14	1	-0.26981	-0.81432	3.11723
15	1	1.13707	-3.71181	-0.10032
16	1	2.57475	-3.37199	0.86713
17	1	3.32385	-1.6214	-0.48152
18	1	2.88662	-2.92288	-1.58913
19	1	1.29989	-2.23056	-3.45578
20	1	0.26977	-0.81384	-3.11713
21	1	-1.1374	-3.71182	0.09981
22	1	-2.575	-3.3716	-0.86756
23	1	-3.32389	-1.62123	0.48147
24	1	-2.88673	-2.92293	1.58885
25	1	-3.28681	-0.46901	2.84476
26	1	-1.84878	0.574	2.75457
27	1	3.28703	-0.46896	-2.84466
28	1	1.84905	0.57415	-2.75461
29	8	1.02299	-2.00259	1.04827
30	8	-1.02305	-2.00239	-1.04841
31	6	-3.13551	0.75188	1.05603
32	6	-4.43374	1.26019	1.08353
33	6	-4.86848	2.02317	-0.00838
34	1	-5.08855	1.06766	1.92868
35	6	-2.73441	1.68037	-1.04986
36	6	-4.01962	2.23146	-1.09336
37	1	-5.87387	2.43686	-0.01108
38	1	-4.31464	2.7923	-1.97269
39	6	3.13561	0.75194	-1.05594
40	6	4.43386	1.26021	-1.08332
41	6	2.7344	1.68032	1.04998
42	6	4.86853	2.02315	0.00865
43	1	5.08873	1.06769	-1.92842
44	6	4.0196	2.2314	1.09358
45	1	5.87393	2.43682	0.01144
46	1	4.31459	2.79218	1.97296
47	7	2.32487	0.98049	-0.01537
48	7	-2.32484	0.98044	0.01542
49	6	-1.73544	1.79602	-2.22536
50	8	-0.60006	1.23519	-2.01493
51	8	-2.13808	2.38434	-3.23142
52	6	1.73542	1.79577	2.22549
53	8	2.13801	2.38405	3.23161
54	8	0.60006	1.23493	2.01498
55	1	-1.05889	-2.80862	-2.96493
56	1	0.0567	-3.58816	-1.83339
57	1	-0.05672	-3.5885	1.83312
58	1	1.05888	-2.80899	2.96471
59	20	1.10E-05	1.25E-01	-6.60E-05

HF= -1561.0664535 Hartrees
Zero-point correction = 0.477803
Sum of electronic and thermal Enthalpies = -1560.560044
Sum of electronic and thermal Free Energies = -1560.645502

[Ca(bp12c4)] ; Δ(λδλδ); B3LYP/LanL2dz/6-31G(d) (vacuo); 0 imaginary frequencies

Número	Número	Coordenadas (Angstroms)		
Centro	Atómico	X	Y	Z
1	7	-1.90546	1.52658	-1.37673
2	6	-1.18122	2.31877	-2.40645
3	6	0.30602	1.97012	-2.52067
4	6	2.27911	2.09534	-1.09361
5	6	2.63455	2.35927	0.38092
6	7	1.90594	1.52781	1.37535
7	6	1.18183	2.32054	2.40481
8	6	-0.30571	1.97294	2.51852

9	6	-2.27858	2.09699	1.09153
10	6	-2.63491	2.35843	-0.38325
11	6	-2.74206	0.46787	-1.98638
12	6	2.74336	0.46999	1.98539
13	1	-3.60702	0.89491	-2.52307
14	1	-2.11813	-0.05118	-2.72527
15	1	3.60875	0.89786	2.52072
16	1	2.12029	-0.04829	2.72553
17	8	0.85911	2.11692	-1.20615
18	8	-0.85851	2.1192	1.2038
19	6	-3.21861	-0.55888	-0.97066
20	6	-4.46737	-1.17843	-1.02334
21	6	-4.7775	-2.13161	-0.04618
22	1	-5.17877	-0.9255	-1.80431
23	6	-2.63492	-1.73762	0.95705
24	6	-3.8588	-2.41307	0.96276
25	1	-5.74047	-2.63548	-0.06876
26	1	-4.0562	-3.12119	1.75919
27	6	3.21921	-0.55798	0.97056
28	6	4.46796	-1.17758	1.02337
29	6	2.63437	-1.7392	-0.95528
30	6	4.77741	-2.1321	0.04733
31	1	5.17981	-0.92365	1.80359
32	6	3.85813	-2.41484	-0.96071
33	1	5.74037	-2.63604	0.07005
34	1	4.05499	-3.12411	-1.75625
35	7	2.33689	-0.85473	0.00848
36	7	-2.33684	-0.85447	-0.00771
37	6	-1.58971	-1.90694	2.08284
38	8	-0.54417	-1.17212	1.94859
39	8	-1.87835	-2.6895	2.98948
40	6	1.58858	-1.90993	-2.08033
41	8	1.8763	-2.69442	-2.98559
42	8	0.54362	-1.17413	-1.94703
43	1	-0.78628	2.67622	3.21479
44	1	-0.4661	0.94676	2.8762
45	1	1.25459	3.38109	2.14766
46	1	1.6452	2.19831	3.39439
47	1	-2.67284	1.13973	1.44897
48	1	-2.71965	2.89979	1.70266
49	1	-3.72182	2.23208	-0.49427
50	1	-2.41515	3.41059	-0.58567
51	1	-1.25283	3.37928	-2.14891
52	1	-1.64521	2.19722	-3.39586
53	1	0.46582	0.94368	-2.87783
54	1	0.78678	2.67278	-3.21743
55	1	2.41277	3.41133	0.58161
56	1	3.72165	2.23496	0.49262
57	1	2.67381	1.1377	-1.44949
58	1	2.72011	2.89741	-1.70575
59	20	4.80E-05	5.09E-02	2.59E-04

HF= -1561.0557611 Hartrees
Zero-point correction = 0.476820
Sum of electronic and thermal Enthalpies =-1560.549976
Sum of electronic and thermal Free Energies = -1560.637406