Supplementary material

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Figure S1 - Lowest energy conformer of $[L2H_2]^{2+}$
Figure S2 - Lowest energy conformer of $[L2H_3]^{3+}$

S1 - Cartesian Coordinates (lowest energy conformer), atomic charges and atom types for the $[L1H_4]^{4+}$

	x	y	z	atom type	atomic charge
N1	2.4720	1.7350	4.3530	N3	-0.1232858
C2	3.1620	0.4470	4.1790	C4	-0.1168203
C3	3.3910	-0.1330	2.7450	C4	-0.2887998
N4	4.3990	0.5060	1.9020	N3	0.7529426
C5	4.0100	1.8710	1.5900	C4	-0.2847452
C6	5.0060	2.8300	0.8760	C4	-0.1128383
N7	4.7000	4.2340	1.1840	N3	-0.1304092
C8	5.6730	5.1830	0.6400	C4	-0.09859705
C9	7.1640	5.1070	1.0910	C4	-0.2995677
N10	7.4930	5.5200	2.4540	N3	0.7620044
C11	7.0840	4.5130	3.4270	C4	-0.2966194
C12	7.1150	4.9060	4.9300	C4	-0.1052728
N13	6.4990	3.8810	5.7790	N3	-0.134572
C14	6.1240	4.3970	7.0950	C4	-0.09803104
C15	5.3050	3.4490	8.0240	C4	-0.2981758
N16	3.9320	3.1270	7.6490	N3	0.7308006
C17	3.8490	2.3590	6.4050	C4	-0.287056
C18	2.4430	2.1470	5.7660	C4	-0.1077161
C19	1.1390	1.7280	3.7340	C4	-0.09953547
C20	0.2220	2.9720	3.8930	C4	-0.1379271
C21	0.7670	4.3160	3.3260	C4	-0.2595148
N22	0.4280	4.7040	1.9540	N3	0.7595921
C23	1.1920	5.8670	1.4960	C4	-0.2751694
C24	2.7500	5.8220	1.5280	C4	-0.1230512
C25	3.3320	4.6000	0.7870	C4	-0.1042886
C26	4.6850	-0.2560	0.7110	C4	-0.3168936
C27	8.8940	5.8440	2.5880	C4	-0.3035707
C28	7.3490	2.7030	5.8890	C4	-0.1239672
C29	3.2300	2.4650	8.7260	C4	-0.2639089
C30	-0.9890	4.9280	1.7700	C4	-0.3261709
H31	4.1760	0.5070	4.6380	H	0.08973336
H32	2.6130	-0.3250	4.7850	H	0.1315051
H33	2.4330	-0.2510	2.1880	H	0.1252506
H34	3.7390	-1.1880	2.8880	H	0.1635857
H35	3.0710	1.7820	0.9950	H	0.1638026
H36	5.0160	2.6780	-0.2360	H	0.1345687
H37	6.0330	2.5970	1.2390	H	0.07480919
H38	5.6390	5.1160	-0.4810	H	0.1283238
H39	5.3280	6.2210	0.8660	H	0.09504187
H40	7.7000	5.8200	0.4150	H	0.1642817
H41	7.6410	4.1280	0.8540	H	0.1378438
H42	6.0290	4.2480	3.2040	H	0.1414788
H43	7.7110	3.6110	3.2440	H	0.1606733
H44	6.5450	5.8620	5.0290	H	0.0702315
H45	8.1460	5.1230	5.3160	H	0.1331677
H46	7.0600	4.7080	7.6310	H	0.09761429
H47	5.5450	5.3480	6.9730	H	0.1295662
H48	5.2510	3.9860	9.0030	H	0.1291959
H49	5.8650	2.5170	8.2740	H	0.163027
H50	4.4360	2.9090	5.6420	H	0.1175251
H51	4.3520	1.3830	6.6020	H	0.1629232
H52	1.8230	1.4150	6.3480	H	0.1272562
H53	1.9230	3.1310	5.8350	H	0.1044365
H54	1.2550	1.5810	2.6370	H	0.05151916
H55	0.5720	0.8360	4.1110	H	0.1243639
H56	-0.0560	3.0880	4.9720	H	0.1204497

H57	1.8710	4.2590	3.4290	H	0.06074953
H58	0.4310	5.1560	3.9830	H	0.1547314
H59	0.8940	6.0610	0.4360	H	0.154878
H60	0.8600	6.7660	2.0710	H	0.07020187
H61	3.1380	5.8680	2.5750	H	0.1228747
H62	3.1340	6.7640	1.0550	H	0.1264696
H63	3.2600	4.7320	-0.3240	H	0.1207596
H64	2.6300	3.7790	1.0240	H	0.04614156
H65	5.0740	-1.2660	0.9780	H	0.1033732
H66	5.4890	0.2280	0.1140	H	0.1029828
H67	3.7890	-0.3940	0.0620	H	0.1618072
H68	9.1180	6.2550	3.5970	H	0.163775
H69	9.1800	6.6610	1.8860	H	0.08838391
H70	9.5550	4.9680	2.3960	H	0.1012784
H71	7.5820	2.2640	4.8950	H	0.05357218
H72	6.8520	1.8800	6.4460	H	0.06990606
H73	8.3130	2.9270	6.4070	H	0.1040697
H74	2.1540	2.3320	8.4810	H	0.1104235
H75	3.2450	3.0880	9.6510	H	0.1556007
H76	-1.5860	4.0170	1.9820	H	0.1354437
H77	-1.2170	5.1790	0.7090	H	0.1376659
H78	-1.3700	5.7610	2.4060	H	0.156918
H79	3.4560	4.0150	7.4820	HB	0.003589272
H80	6.9620	6.3700	2.6480	HB	0.005359113
H81	0.6890	3.9210	1.3510	HB	0.0073663
H82	5.2620	0.5540	2.4470	HB	0.01293588
H83	-0.7760	2.7140	3.4570	H	0.1145327
H84	3.6740	1.4730	8.9710	H	0.09118342
H85	3.7890	2.3550	2.5630	H	0.1320156

S2 - Cartesian Coordinates for the $[L1H_4F]^{3+}$ lowest energy conformer

	x	y	z
N1	4.8880	0.9910	3.8690
C2	4.8580	0.9150	5.3300
C3	5.5230	2.1160	6.0450
N4	5.0140	3.4260	5.6470
C5	5.9350	4.4780	6.0690
C6	5.6640	5.8520	5.4100
N7	5.4170	5.7220	3.9780
C8	4.7730	6.9130	3.4280
C9	3.2640	7.0220	3.7840
N10	2.3950	5.9160	3.3760
C11	1.0180	6.1700	3.8050
C12	-0.0190	5.0570	3.4980
N13	0.4090	3.7610	4.0110
C14	-0.2440	2.6420	3.3410
C15	0.5340	1.3140	3.5370
N16	1.9620	1.3410	3.2160
C17	2.5730	0.0460	3.5260
C18	4.1000	-0.0800	3.2650
C19	6.2500	1.0950	3.3430
C20	6.3870	1.2150	1.8100
C21	7.7990	1.6640	1.3520
N22	8.2860	3.0060	1.6700
C23	7.4760	4.0880	1.1150
C24	6.2430	4.5920	1.9120
C25	6.6070	5.3220	3.2220
C26	3.6970	3.6550	6.1960
C27	2.4630	5.7110	1.9500
C28	0.2390	3.6890	5.4560
C29	2.1850	1.7010	1.8370
C30	9.6650	3.1330	1.2400
H31	3.8080	0.8450	5.6910
H32	5.3350	-0.0430	5.6660
H33	6.6190	2.0530	5.8690
H34	5.4250	2.0090	7.1530
H35	5.9100	4.5680	7.1820
H36	6.5090	6.5670	5.5930
H37	4.7940	6.3190	5.9250
H38	5.3250	7.8260	3.7750
H49	4.8900	6.9630	2.3210
H50	2.8720	7.9630	3.3290
H51	3.1500	7.1590	4.8820
H52	1.0200	6.3610	4.9010
H53	0.6580	7.1180	3.3370
H54	-0.1900	5.0180	2.3970
H55	-1.0320	5.3140	3.9070
H56	-1.2980	2.5460	3.7080
H57	-0.3710	2.8450	2.2490
H58	0.0340	0.5240	2.9260
H59	0.4150	0.9840	4.5930
H60	2.3520	-0.2110	4.5860
H61	2.0510	-0.7430	2.9320
H62	4.4830	-1.0750	3.6140
H63	4.2470	-0.1100	2.1620
H64	6.6990	2.0300	3.7410

H65	6.8620	0.2320	3.7090
H66	5.5890	1.8600	1.3730
H67	7.8560	1.5260	0.2450
H68	8.5210	0.9290	1.7810
H69	8.1220	4.9870	0.9760
H70	7.1700	3.8050	0.0790
H71	5.4920	3.8010	2.1580
H72	5.6880	5.2900	1.2380
H73	7.2610	6.2110	3.0410
H74	7.2180	4.6000	3.8040
H75	3.3150	4.6380	5.8590
H76	3.6670	3.5960	7.3070
H77	3.0090	2.9150	5.7450
H78	1.8380	4.8420	1.6790
H79	3.4840	5.3960	1.6620
H80	2.1450	6.6070	1.3710
H81	-0.8330	3.7850	5.7490
H82	0.8070	4.4880	5.9780
H83	0.6140	2.7320	5.8760
H84	3.2700	1.8380	1.6600
H85	1.7640	2.7050	1.6570
H86	10.1030	4.0980	1.5830
H87	9.7570	3.0710	0.1300
H88	10.3050	2.3420	1.6900
H89	2.3950	2.0340	3.8200
H90	2.7120	5.0820	3.8570
H91	8.2780	3.1070	2.6860
H92	4.9670	3.4470	4.6300
H93	6.2080	0.2060	1.3540
H94	1.7500	0.9630	1.1250
H95	6.9810	4.1820	5.8370
F96	3.4200	3.5020	3.5450

S3 - Cartesian Coordinates for the $[L1H_4Cl]^{3+}$ lowest energy conformer

	x	y	z
N1	0.9610	3.8120	2.2890
C2	0.6750	4.0760	3.7010
C3	0.5370	2.8040	4.5870
N4	1.6310	1.8380	4.5100
C5	1.3220	0.6130	5.2430
C6	2.3140	-0.5760	5.0690
N7	2.4580	-1.0300	3.6850
C8	3.6460	-1.8740	3.4900
C9	5.0450	-1.2030	3.6360
N10	5.4110	-0.1210	2.7230
C11	6.7510	0.3870	3.0170
C12	7.1040	1.7630	2.3880
N13	6.1910	2.8400	2.7710
C14	6.4070	4.0490	1.9780
C15	5.2100	5.0400	2.0320
N16	3.9160	4.5190	1.5910
C17	2.8390	5.4720	1.8690
C18	1.3790	5.0170	1.5720
C19	-0.1430	3.1110	1.6260
C20	0.1990	2.5610	0.2220
C21	-0.6140	1.3080	-0.2040
N22	0.0000	0.0000	0.0000
C23	0.2440	-0.3160	1.3980
C24	0.9600	-1.6530	1.7260
C25	1.2590	-1.7560	3.2420
C26	2.8630	2.4270	4.9840
C27	5.3140	-0.5420	1.3430
C28	6.2720	3.1260	4.1970
C29	3.9690	4.1520	0.1940
C30	1.4590	4.7360	4.1380
H31	-0.2590	4.6930	3.7760
H32	-0.4170	2.2930	4.3300
H33	0.4030	3.1150	5.6510
H34	1.2310	0.8550	6.3290
H35	2.0000	-1.4420	5.7100
H36	3.2980	-0.2820	5.4950
H37	3.5920	-2.7320	4.2110
H38	3.5930	-2.3740	2.4940
H49	5.8190	-2.0030	3.5330
H50	5.1570	-0.8250	4.6740
H51	6.8980	0.4570	4.1160
H52	7.5030	-0.3710	2.6860
H53	7.1140	1.6580	1.2780
H54	8.1560	2.0560	2.6480
H55	7.3440	4.5580	2.3230
H56	6.6380	3.7910	0.9150
H57	5.4650	5.9420	1.4250
H58	5.1090	5.4200	3.0720
H59	2.9030	5.7710	2.9380
H60	3.0460	6.4050	1.2900
H61	0.6570	5.8460	1.7940
H62	1.2660	4.8870	0.4720
H63	-0.4370	2.2380	2.2420
H64	-1.0480	3.7680	1.5770
H65	1.2920	2.3430	0.1500

H66	-0.7950	1.3960	-1.3020
H67	-1.6320	1.3130	0.2510
H68	0.8980	0.4870	1.8010
H69	-0.7270	-0.2730	1.9440
H70	1.9030	-1.7670	1.1370
H71	0.3100	-2.5240	1.4520
H72	1.3260	-2.8290	3.5550
H73	0.3430	-1.4070	3.7660
H74	3.1240	3.3080	4.3640
H75	3.6990	1.7160	4.8340
H76	2.8040	2.7220	6.0550
H77	4.2550	-0.7680	1.1060
H78	5.9560	-1.4230	1.1190
H79	5.5740	0.2930	0.6590
H80	5.9910	2.2440	4.8090
H81	5.5620	3.9220	4.5040
H82	7.2980	3.4480	4.4990
H83	2.9980	3.7410	-0.1420
H84	4.6770	3.3090	0.0590
H85	3.7270	3.6900	2.1460
H86	4.7660	0.6430	2.8940
H87	-0.8870	-1.0190	-0.5940
H88	1.7360	1.5830	3.5330
H89	0.0120	3.3740	-0.5250
H90	4.2530	5.0070	-0.4600
H91	0.3050	0.2790	4.9430
H92	-1.1280	-0.7610	-1.6280
H93	-1.8180	-1.1060	-0.0320
H94	-0.3940	-1.9910	-0.6140
H95	0.8940	-0.0230	-0.5020
Cl96	3.1700	1.6250	1.9400

S4 - Cartesian Coordinates for the $[L1H_4Br]^{3+}$ lowest energy conformer

	x	y	z
N1	5.7890	0.8480	3.3420
C2	7.1500	1.3290	3.5750
C3	7.5280	2.5930	2.7450
N4	6.6840	3.7740	2.9080
C5	7.0560	4.8380	1.9790
C6	6.1410	6.0960	1.9580
N7	4.7130	5.8210	1.7850
C8	3.8860	6.9990	2.0620
C9	3.7220	7.3400	3.5750
N10	3.1030	6.3260	4.4310
C11	3.1730	6.6920	5.8460
C12	2.8410	5.5690	6.8720
N13	3.7570	4.4260	6.8440
C14	3.2200	3.2790	7.5820
C15	3.9970	1.9470	7.3660
N16	4.0330	1.4390	5.9950
C17	5.0880	0.4440	5.8070
C18	5.3400	-0.1060	4.3680
C19	5.6600	0.2420	2.0080
C20	4.2600	0.4040	1.3650
C21	4.1680	1.7210	0.5460
N22	2.8610	2.1110	0.0390
C23	2.8430	3.4260	-0.5960
C24	2.9900	4.6780	0.3150
C25	4.4290	5.2230	0.4760
C26	6.7170	4.2460	4.2720
C27	1.7350	6.0680	4.0400
C28	5.0750	4.8010	7.3380
C29	2.7370	0.9230	5.6080
C30	7.3170	1.5420	4.6540
H31	7.8740	0.4970	3.3610
H32	7.5430	2.3280	1.6660
H33	8.5830	2.8730	2.9810
H34	8.1020	5.1600	2.2070
H35	6.4810	6.7950	1.1480
H36	6.3150	6.6770	2.8910
H37	4.3030	7.8780	1.5050
H38	2.8740	6.8880	1.6110
H49	3.1280	8.2810	3.6700
H50	4.7240	7.5840	3.9880
H51	4.1840	7.0900	6.0750
H52	2.4910	7.5590	6.0210
H53	1.7960	5.2230	6.6980
H54	2.8100	5.9900	7.9120
H55	3.1960	3.5270	8.6750
H56	2.1430	3.1320	7.3230
H57	3.5700	1.1590	8.0330
H58	5.0330	2.0800	7.7450
H59	6.0410	0.8660	6.1930
H60	4.8590	-0.4180	6.4800
H61	6.0940	-0.9340	4.4340
H62	4.4210	-0.6310	4.0150
H63	6.3950	0.6560	1.2850
H64	5.9510	-0.8390	2.0530
H65	3.4730	0.3680	2.1580

H66	4.8860	1.6830	-0.3060
H67	4.4980	2.5300	1.2280
H68	3.5730	3.4460	-1.4390
H69	1.8450	3.5120	-1.0870
H70	2.5380	4.4660	1.3120
H71	2.3600	5.5030	-0.1080
H72	4.6580	5.9510	-0.3430
H73	5.1140	4.3690	0.3080
H74	6.0290	5.1070	4.3950
H75	7.7420	4.5310	4.5990
H76	6.3050	3.4590	4.9320
H77	1.3410	5.1960	4.6030
H78	1.6720	5.7550	2.9800
H79	1.0730	6.9490	4.1970
H80	5.5220	5.6250	6.7430
H81	5.8060	3.9700	7.2540
H82	5.0440	5.1250	8.4070
H83	2.7370	0.6230	4.5410
H84	1.9720	1.7240	5.6680
H85	4.2720	2.2270	5.4040
H86	3.6490	5.4780	4.3200
H87	2.4080	1.1210	-0.9590
H88	5.7310	3.4980	2.6810
H89	4.0840	-0.4790	0.7000
H90	2.4220	0.0570	6.2330
H91	7.1150	4.4160	0.9520
H92	2.3000	0.1390	-0.5000
H93	3.1140	1.0480	-1.7870
H94	1.4300	1.3980	-1.3580
H95	2.1900	2.1110	0.8130
Br96	3.5900	3.3370	3.6150

S5 - Cartesian Coordinates (lowest energy conformer), atomic charges and atom types for the $[L1H_5]^{5+}$

	x	y	z	Atom type	Atomic charge
N1	5.4210	5.6650	2.8550	N3	-0.1216898
C2	6.8560	5.3360	2.7840	C4	-0.09342241
C3	7.6720	5.0890	4.0950	C4	-0.2384157
N4	7.4340	3.8290	4.8030	N3	0.6604352
C5	6.0560	3.7710	5.2700	C4	-0.2772446
C6	5.4380	2.4520	5.8210	C4	-0.08209562
N7	3.9640	2.4490	5.7340	N3	-0.122262
C8	3.3420	1.2290	6.2690	C4	-0.1083059
C9	3.7140	-0.1830	5.7050	C4	-0.2322025
N10	3.0000	-0.7140	4.5340	N3	0.6610193
C11	3.3340	0.0200	3.2890	C4	-0.2758989
C12	2.6200	-0.3680	1.9160	C4	-0.2227201
N13	3.0630	0.2740	0.6510	N3	0.5989084
C14	2.9190	1.7450	0.6550	C4	-0.2314615
C15	3.6200	2.6010	-0.4990	C4	-0.263258
N16	3.8350	4.0500	-0.2550	N3	0.638669
C17	4.8290	4.2840	0.8030	C4	-0.2340288
C18	4.7950	5.6680	1.5210	C4	-0.09098673
C19	5.1820	6.8940	3.6260	C4	-0.08346033
C20	3.7410	7.4670	3.7380	C4	-0.1279807
C21	2.6610	6.5630	4.4020	C4	-0.2226081
N22	2.4950	6.5890	5.8600	N3	0.6310811
C23	1.6130	5.5190	6.3450	C4	-0.2321215
C24	1.9550	4.0350	5.9940	C4	-0.1128306
C25	3.3940	3.6440	6.3860	C4	-0.09205294
C26	8.3830	3.6030	5.8690	C4	-0.2643509
C27	3.2200	-2.1400	4.3940	C4	-0.2682991
C28	2.4250	-0.3120	-0.5110	C4	-0.2543359
C29	4.1690	4.7760	-1.4640	C4	-0.2541728
C30	2.0530	7.8790	6.3520	C4	-0.259542
H31	6.9920	4.4020	2.1940	H	0.04073244
H32	7.3710	6.1400	2.1910	H	0.1274478
H33	7.6060	5.9540	4.7970	H	0.1486242
H34	8.7510	5.0810	3.7950	H	0.1573641
H35	5.9750	4.5790	6.0340	H	0.1317404
H36	5.7580	2.2690	6.8810	H	0.1203215
H37	5.8320	1.6140	5.2020	H	0.04982603
H38	3.5410	1.2180	7.3760	H	0.1336564
H39	2.2310	1.3310	6.2000	H	0.09879076
H40	3.4760	-0.8840	6.5460	H	0.1672165
H41	4.8150	-0.3100	5.5800	H	0.1323267
H42	3.1060	1.0820	3.5350	H	0.1159651
H43	4.4420	-0.0640	3.1530	H	0.1343547
H44	1.5110	-0.2390	2.0090	H	0.1343604
H45	2.7670	-1.4630	1.7320	H	0.1739063
H46	1.8200	1.9700	0.6810	H	0.1856284
H47	3.3080	2.0790	1.6370	H	0.1397849
H48	2.9940	2.5270	-1.4280	H	0.1915308
H49	4.6100	2.1640	-0.7930	H	0.1644456
H50	4.6930	3.5430	1.6180	H	0.03886974
H51	5.8420	4.1000	0.3680	H	0.1365385
H52	5.2530	6.4820	0.8990	H	0.1192607
H53	3.7190	5.9280	1.6410	H	0.08281481
H54	5.5210	6.7270	4.6730	H	0.05262637
H55	5.8340	7.7080	3.2110	H	0.1108472

H56	3.4010	7.7810	2.7190	H	0.1083821
H57	2.9040	5.5300	4.0770	H	0.07147163
H58	1.6640	6.8110	3.9590	H	0.1295434
H59	1.5880	5.5900	7.4610	H	0.1480781
H60	0.5650	5.7380	6.0180	H	0.1449576
H61	1.7860	3.8380	4.9090	H	0.04879284
H62	1.2240	3.3720	6.5290	H	0.1226686
H63	3.4970	3.5780	7.5000	H	0.1110622
H64	3.9650	4.5420	6.0930	H	0.03514504
H65	8.3480	4.3950	6.6540	H	0.1496519
H66	9.4240	3.5680	5.4710	H	0.1211986
H67	8.2130	2.6160	6.3550	H	0.1404946
H68	2.5580	-2.5840	3.6190	H	0.1192795
H69	2.9320	-2.6920	5.3220	H	0.1631981
H70	4.2820	-2.3970	4.1700	H	0.1366228
H71	2.8400	0.1050	-1.4560	H	0.1127326
H72	1.3190	-0.1680	-0.5170	H	0.1171713
H73	2.6220	-1.4090	-0.5840	H	0.1662672
H74	4.2810	5.8660	-1.2590	H	0.1328732
H75	3.3560	4.7090	-2.2250	H	0.1570941
H76	1.9670	7.8790	7.4640	H	0.1264144
H77	1.0620	8.1810	5.9370	H	0.1455399
H78	2.7840	8.6850	6.1280	H	0.1382546
H79	2.9440	4.4280	0.0820	HB	0.06665945
H80	1.9990	-0.5820	4.7090	HB	0.07001472
H81	3.4180	6.4180	6.2660	HB	0.04800367
H82	7.5570	3.0750	4.1220	HB	0.03589618
H83	4.0650	0.0790	0.5660	HB	0.04005408
H84	3.8040	8.4680	4.2380	H	0.128407
H85	5.1140	4.4200	-1.9390	H	0.1417254
H86	5.4200	4.0160	4.3960	H	0.1089978

S6 - Cartesian Coordinates for the $[L1H_5F]^{4+}$ lowest energy conformer

	x	y	z
N1	3.1270	0.9150	3.0010
C2	3.5240	0.2640	4.2570
C3	5.0120	-0.1110	4.5250
N4	5.9290	0.9800	4.8470
C5	6.0460	1.9110	3.7390
C6	6.8600	3.2140	3.9460
N7	6.4590	4.2470	2.9890
C8	6.9960	5.5720	3.2970
C9	6.4380	6.2050	4.6050
N10	4.9820	6.1970	4.7470
C11	4.5610	6.6800	6.0800
C12	3.0270	6.6440	6.4520
N13	2.4520	5.3010	6.6260
C14	1.0710	5.1430	6.1450
C15	0.6720	3.7040	5.6180
N16	1.3120	3.2040	4.3800
C17	0.9600	1.8040	4.1270
C18	1.6670	1.0780	2.9420
C19	3.6390	0.2030	1.8200
C20	3.2880	0.7490	0.4080
C21	3.8080	2.1800	0.0800
N22	5.0830	2.3310	-0.6300
C23	5.5310	3.7240	-0.7110
C24	5.7120	4.5200	0.6120
C25	6.7010	3.8630	1.5960
C26	7.2210	0.4860	5.2720
C27	4.3550	6.9540	3.6840
C28	2.5940	4.8430	7.9950
C29	0.9820	4.0210	3.2290
C30	5.0550	1.7390	-1.9540
H31	3.2490	0.9410	5.0980
H32	2.9070	-0.6670	4.3780
H33	5.4340	-0.7560	3.7190
H34	5.0020	-0.7840	5.4180
H35	6.4560	1.3330	2.8810
H36	7.9660	3.0480	3.8760
H37	6.6370	3.5710	4.9780
H38	8.1160	5.5180	3.3440
H39	6.8120	6.2690	2.4450
H40	6.8070	7.2580	4.6870
H41	6.8890	5.6810	5.4770
H42	5.1150	6.0900	6.8480
H43	4.9270	7.7320	6.1940
H44	2.4650	7.2110	5.6780
H45	2.8240	7.2480	7.3730
H46	0.3710	5.4990	6.9450
H47	0.8860	5.8650	5.3190
H48	-0.4370	3.6620	5.4620
H49	0.8680	2.9590	6.4240
H50	1.1220	1.2060	5.0510
H51	-0.1450	1.7410	3.9580
H52	1.1990	0.0640	2.8330
H53	1.3880	1.6060	2.0040
H54	4.7490	0.1860	1.8540
H55	3.3060	-0.8660	1.8740
H56	2.1810	0.6990	0.2570

H57	3.8720	2.7000	1.0600
H58	3.0320	2.7220	-0.5140
H59	6.5220	3.7380	-1.2280
H60	4.8360	4.2910	-1.3800
H61	4.7260	4.6720	1.1110
H62	6.0680	5.5550	0.3670
H63	7.7660	4.0590	1.3070
H64	6.5660	2.7730	1.4630
H65	7.8780	1.3200	5.6040
H66	7.7440	-0.0800	4.4670
H67	7.1220	-0.1830	6.1590
H68	4.6030	8.0390	3.7300
H69	3.2570	6.8110	3.7200
H70	4.6360	6.5430	2.6950
H71	3.6600	4.8820	8.3110
H72	2.2730	3.7830	8.0940
H73	1.9990	5.4540	8.7160
H74	-0.0980	3.9700	2.9610
H75	1.6130	3.7240	2.3690
H76	4.8810	0.6430	-1.9180
H77	6.0390	1.8490	-2.4680
H78	4.2760	2.1990	-2.6070
H79	2.3210	3.2130	4.5180
H80	4.7090	5.2210	4.6600
H81	5.7870	1.8220	-0.0890
H82	5.5240	1.4920	5.6330
H83	3.0330	4.6600	6.0950
H84	3.6250	-0.0080	-0.3420
H85	1.2690	5.0780	3.3980
H86	5.0160	2.2600	3.4980
F86	3.2600	4.5460	4.5160

S7 - Cartesian Coordinates (lowest energy conformer), atomic charges and atom types for the $[L2H_4]^{4+}$

	x	y	z	Atomic charge	Atom type
N1	3.5240	-1.4650	1.0300	0.7259588	N3
C2	4.6770	-0.7110	1.5710	-0.2980494	C4
C3	4.8940	0.8530	1.3740	-0.2766681	C4
N4	4.0710	1.8350	2.1010	0.7075005	N3
C5	4.1540	3.1480	1.5030	-0.3181839	C4
C6	4.4000	1.8900	3.5400	-0.2643037	C4
C7	3.3660	2.4960	4.5880	-0.2895546	C4
N8	2.3370	1.6070	5.1520	0.727057	N3
C9	1.6200	0.9160	4.0870	-0.2894888	C4
C10	0.7870	1.7600	3.0920	-0.1259804	C4
C11	0.3990	0.9740	1.8230	0.07917881	C4
O12	1.5920	0.6560	1.1130	-0.3882146	O2
C13	1.3050	0.2410	-0.2150	0.05549169	C4
C14	2.6310	-0.0490	-0.9350	-0.1264687	C4
C15	3.3620	-1.3140	-0.4130	-0.2939849	C4
C16	3.6080	-2.8820	1.3970	-0.2780766	C4
C17	3.5510	-3.3040	2.8970	-0.1111536	C4
N18	2.3670	-2.8940	3.6610	-0.08677816	N3
C19	1.1320	-3.3170	3.0210	-0.1245866	C4
C20	2.4530	-3.3710	5.0490	-0.07618618	C4
C21	1.2800	-2.9530	5.9750	-0.2933164	C4
N22	1.5680	-2.9520	7.4060	0.7603545	N3
C23	1.8640	-4.2730	7.9070	-0.3177056	C4
C24	0.5340	-2.3030	8.2000	-0.2909327	C4
C25	0.0330	-0.8990	7.7530	-0.0898633	C4
N26	1.0680	0.0460	7.3300	-0.1561999	N3
C27	2.0460	0.2850	8.3790	-0.1242929	C4
C28	0.4710	1.2950	6.8470	-0.09147644	C4
C29	1.4730	2.2440	6.1300	-0.2831178	C4
H30	2.6780	-1.0980	1.4700	0.03790569	HB
H31	2.4160	-2.3940	7.5280	0.01884282	HB
H32	2.8460	0.8790	5.6650	0.04854214	HB
H33	4.7500	-0.9700	2.6490	0.1839141	H
H34	5.5820	-1.2100	1.1320	0.1608645	H
H35	5.9630	1.0890	1.6170	0.1234637	H
H36	4.8750	1.0980	0.2860	0.1861262	H
H37	3.5290	3.8910	2.0450	0.1340538	H
H38	3.7570	3.1360	0.4610	0.1410244	H
H39	5.1980	3.5410	1.4640	0.1640172	H
H40	5.3750	2.4450	3.6190	0.1864678	H
H41	4.6660	0.8680	3.8950	0.1083565	H
H42	3.9560	2.8510	5.4740	0.1744226	H
H43	2.8820	3.4350	4.2220	0.1662953	H
H44	0.9490	0.1590	4.5520	0.1385145	H
H45	2.3510	0.2910	3.5310	0.05984437	H
H46	1.3150	2.6810	2.7510	0.07391131	H
H47	-0.1640	2.1220	3.5660	0.1258847	H
H48	-0.1290	0.0240	2.0790	0.06230313	H
H49	-0.2810	1.6010	1.1880	0.1140401	H
H50	0.7590	1.0590	-0.7560	0.107258	H
H51	0.6530	-0.6670	-0.1940	0.06883222	H
H52	3.2580	0.8690	-0.9360	0.07861942	H
H53	2.3980	-0.1810	-2.0300	0.1549342	H

H54	2.7290	-2.1510	-0.7950	0.1476875	H
H55	4.3400	-1.4660	-0.9340	0.1559653	H
H56	2.7960	-3.4480	0.8820	0.1579423	H
H57	4.5380	-3.3120	0.9480	0.08765632	H
H58	3.6140	-4.4260	2.9260	0.1205376	H
H59	4.4790	-2.9970	3.4390	0.1163832	H
H60	1.0810	-4.4270	2.9080	0.08962464	H
H61	1.0050	-2.8440	2.0230	0.0657931	H
H62	0.2340	-2.9900	3.5900	0.08481431	H
H63	3.3830	-2.9440	5.4930	0.01151711	H
H64	2.5610	-4.4870	5.0500	0.09286726	H
H65	1.0140	-1.9170	5.6820	0.1006021	H
H66	0.3830	-3.5970	5.8080	0.159485	H
H67	2.1250	-4.2410	8.9910	0.1528939	H
H68	2.7530	-4.7060	7.4000	0.1447133	H
H69	1.0050	-4.9730	7.7800	0.113968	H
H70	-0.3490	-2.9860	8.2670	0.1601272	H
H71	0.9080	-2.2310	9.2500	0.1536906	H
H72	-0.7080	-1.0360	6.9270	0.08446968	H
H73	-0.5720	-0.4470	8.5860	0.1307657	H
H74	2.8690	0.9460	8.0300	0.04530966	H
H75	2.5490	-0.6560	8.6930	0.054793	H
H76	1.5850	0.7460	9.2890	0.110348	H
H77	-0.0230	1.8310	7.7040	0.1379838	H
H78	-0.3800	1.0720	6.1580	0.0925715	H
H79	0.9060	3.0810	5.6540	0.1555846	H
H80	2.1020	2.7380	6.9100	0.1510302	H
H81	3.1010	1.5280	2.0240	0.0414778	HB

S8 - Cartesian Coordinates for the $[L2H_4F]^{3+}$ lowest energy conformer

	x	y	z
N1	3.9170	-2.2430	4.9260
C2	5.0810	-2.7320	4.1490
C3	5.3170	-2.0170	2.7650
N4	4.2130	-2.2140	1.8210
C5	4.3150	-3.5140	1.1860
C6	4.0440	-1.1640	0.8120
C7	2.5660	-1.0590	0.2830
N8	1.5350	-0.7250	1.2950
C9	0.2450	-1.2670	0.8900
C10	0.1030	-2.8080	1.0380
C11	0.0390	-3.3320	2.4880
O12	1.3320	-3.4740	3.0750
C13	1.2230	-3.9910	4.3980
C14	2.5890	-4.4200	4.9770
C15	3.3730	-3.3160	5.7480
C16	4.2800	-1.0610	5.7130
C17	3.1240	-0.2660	6.3850
N18	3.5160	1.0310	6.9470
C19	4.6920	0.9350	7.8000
C20	2.4260	1.6770	7.6760
C21	1.3150	2.2890	6.7940
N22	1.6810	3.4020	5.9250
C23	2.3560	4.4630	6.6360
C24	0.5230	3.9260	5.2080
C25	-0.1200	2.9520	4.1900
N26	0.8570	2.5000	3.2040
C27	1.1290	3.5260	2.2070
C28	0.4790	1.2220	2.6070
C29	1.4830	0.7170	1.5370
H30	3.1690	-2.0070	4.2870
H31	2.3340	3.0420	5.2250
H32	1.7590	-1.2020	2.1640
H33	5.9940	-2.6480	4.7900
H34	4.9960	-3.8290	3.9940
H35	5.4010	-0.9250	2.9710
H36	6.2860	-2.2880	2.2750
H37	5.2250	-3.6030	0.5490
H38	3.4210	-3.7230	0.5630
H39	4.3320	-4.3250	1.9430
H40	4.8030	-1.2950	0.0020
H41	4.2960	-0.1830	1.2760
H42	2.5030	-0.3120	-0.5460
H43	2.2870	-2.0030	-0.2300
H44	0.0060	-0.9300	-0.1480
H45	-0.5550	-0.8410	1.5340
H46	0.8650	-3.3980	0.4790
H47	-0.8670	-3.0970	0.5520
H48	-0.5790	-2.6500	3.1200
H49	-0.4490	-4.3400	2.4710
H50	0.5610	-4.8950	4.3730
H51	0.7350	-3.2230	5.0450
H52	3.1720	-4.9200	4.1690
H53	2.3820	-5.2540	5.7020
H54	2.6480	-2.8790	6.4680

H55	4.1890	-3.7550	6.3720
H56	5.0340	-1.3680	6.4740
H57	4.7670	-0.3380	5.0180
H58	2.3510	-0.0880	5.5970
H59	2.6510	-0.8670	7.1980
H60	4.9640	1.9280	8.2270
H61	5.5930	0.6450	7.2170
H62	4.5390	0.2250	8.6460
H63	2.8210	2.4870	8.3300
H64	1.9900	0.9560	8.4140
H65	0.8860	1.4760	6.1730
H66	0.4990	2.6320	7.4750
H67	1.7470	4.8510	7.4840
H68	2.6070	5.3080	5.9560
H69	3.3400	4.1120	7.0150
H70	-0.2440	4.2720	5.9430
H71	0.8230	4.8520	4.6690
H72	-0.5790	2.0870	4.7250
H73	-0.9910	3.4320	3.6700
H74	2.0010	3.2530	1.5730
H75	1.4240	4.4920	2.6690
H76	0.2490	3.7150	1.5460
H77	-0.5560	1.3100	2.1850
H78	0.4550	0.4650	3.4300
H79	1.3060	1.2520	0.5770
H80	2.4970	0.9820	1.9140
H81	3.3520	-2.2570	2.3650
F82	2.9880	-0.8690	3.1860

S9 - Cartesian Coordinates for the $[L2H_4F(H2O)]^{3+}$ lowest energy conformer

	x	y	z
N1	4.9070	-0.1340	4.7980
C2	5.6720	-1.3850	5.0110
C3	4.9520	-2.7040	4.5370
N4	3.7060	-2.9690	5.2620
C5	3.9910	-3.5530	6.5590
C6	2.7110	-3.7740	4.5460
C7	1.2390	-3.5080	5.0340
N8	0.7390	-2.1210	4.8730
C9	-0.2720	-1.8330	5.8820
C10	0.2650	-1.6380	7.3270
C11	1.0760	-0.3470	7.5610
O12	2.4330	-0.4740	7.1410
C13	3.1490	0.7280	7.4100
C14	4.6740	0.5510	7.2470
C15	5.2390	0.8440	5.8260
C16	5.1280	0.3840	3.4450
C17	4.1940	1.5310	2.9620
N18	4.2910	1.8380	1.5320
C19	5.6660	2.0200	1.0920
C20	3.4890	3.0000	1.1500
C21	1.9620	2.7680	1.1170
N22	1.4470	1.7980	0.1560
C23	1.9390	2.0270	-1.1830
C24	-0.0110	1.7570	0.1650
C25	-0.6440	1.2090	1.4670
N26	-0.1640	-0.1390	1.7560
C27	-0.8090	-1.1350	0.9120
C28	-0.2520	-0.4630	3.1770
C29	0.2420	-1.8940	3.5170
H30	3.9200	-0.3250	4.9280
H31	1.7730	0.8780	0.4480
H32	1.5000	-1.4730	5.0600
H33	6.6660	-1.2820	4.5080
H34	5.9560	-1.4770	6.0810
H35	4.7010	-2.5710	3.4590
H36	5.6070	-3.6110	4.5680
H37	4.6660	-2.9010	7.1510
H38	4.4570	-4.5620	6.4750
H39	3.0680	-3.6360	7.1680
H40	3.0050	-4.8530	4.5770
H41	2.7500	-3.5060	3.4650
H42	0.5280	-4.2010	4.5210
H43	1.1370	-3.8160	6.0960
H44	-1.0690	-2.6150	5.8450
H45	-0.7810	-0.8760	5.6320
H46	0.8440	-2.5020	7.7260
H47	-0.6280	-1.5800	8.0050
H48	0.6030	0.5120	7.0270
H49	1.0680	-0.1280	8.6600
H50	2.9490	1.0320	8.4700
H51	2.7620	1.5340	6.7410
H52	4.9600	-0.4440	7.6620
H53	5.1570	1.2760	7.9570
H54	4.8180	1.8280	5.5300
H55	6.3470	0.9890	5.8530
H56	6.1950	0.6920	3.3600

H57	4.9580	-0.4570	2.7360
H58	3.1450	1.2130	3.1790
H59	4.3900	2.4720	3.5310
H60	5.7130	2.2650	0.0050
H61	6.2450	1.0740	1.1730
H62	6.1820	2.8350	1.6520
H63	3.7940	3.3680	0.1440
H64	3.7410	3.8630	1.8180
H65	1.6360	2.4680	2.1340
H66	1.4820	3.7540	0.9080
H67	3.0370	1.8600	-1.2170
H68	1.7010	3.0520	-1.5460
H69	1.5240	1.2790	-1.8950
H70	-0.4150	2.7720	-0.0660
H71	-0.3540	1.1260	-0.6850
H72	-0.4320	1.9010	2.3170
H73	-1.7640	1.2070	1.4000
H74	-0.3110	-2.1250	1.0010
H75	-0.7220	-0.8880	-0.1680
H76	-1.8930	-1.2530	1.1530
H77	-1.3060	-0.2990	3.5210
H78	0.4070	0.2590	3.7210
H79	-0.5590	-2.6310	3.2810
H80	1.1130	-2.0910	2.8540
H81	3.2770	-2.0670	5.4690
F82	2.8370	-1.2030	4.1210
O83	2.7870	-0.7790	0.6110
H84	2.8880	-1.0880	1.5380
H85	3.1620	-1.5100	0.0710

S10 - Cartesian Coordinates for the $[L2H_4Cl]^{3+}$ lowest energy conformer

	x	y	z
N1	1.0870	1.8940	2.7830
C2	-0.3220	1.4450	2.7040
C3	-0.6830	-0.0610	3.0830
N4	0.0300	-1.1540	2.4120
C5	-0.4250	-1.2710	1.0400
C6	-0.0080	-2.4620	3.0810
C7	1.1570	-3.4680	2.6950
N8	2.5300	-3.1770	3.1720
C9	3.5370	-3.8420	2.3520
C10	3.7240	-3.3430	0.8920
C11	4.3870	-1.9620	0.7260
O12	3.5220	-0.9320	1.1790
C13	4.0290	0.3610	0.8510
C14	3.3710	1.4250	1.7560
C15	1.8300	1.4920	1.5920
C16	1.1920	3.3280	3.0190
C17	1.1580	3.6850	4.5280
N18	2.4150	3.2220	5.1030
C19	3.3670	4.3000	5.2990
C20	2.2930	2.3260	6.2420
C21	3.6080	1.5360	6.4650
N22	3.4640	0.1670	6.9510
C23	2.8560	0.1390	8.2600
C24	4.7470	-0.5280	6.9310
C25	4.7410	-2.0120	7.3740
N26	3.7060	-2.7940	6.7100
C27	3.4420	-4.0240	7.4420
C28	3.9640	-3.0520	5.2950
C29	2.6760	-3.5460	4.5810
H30	1.5120	1.4420	3.5890
H31	2.8380	-0.3280	6.3180
H32	2.6940	-2.1760	3.0780
H33	-0.8840	2.0760	3.4360
H34	-0.7480	1.7620	1.7200
H35	-0.4820	-0.1520	4.1780
H36	-1.7840	-0.2510	3.0030
H37	-0.4200	-0.2920	0.5150
H38	-1.4660	-1.6660	0.9780
H39	0.2420	-1.9380	0.4530
H40	-1.0200	-2.9170	2.9270
H41	0.0330	-2.2970	4.1820
H42	0.8980	-4.5000	3.0450
H43	1.1870	-3.5960	1.5930
H44	3.3440	-4.9430	2.3580
H45	4.5310	-3.7090	2.8360
H46	2.7920	-3.3660	0.2810
H47	4.4010	-4.0710	0.3690
H48	5.3330	-1.9190	1.3180
H49	4.6320	-1.7870	-0.3540
H50	3.8220	0.5640	-0.2290
H51	5.1360	0.3880	1.0110
H52	3.8390	2.4180	1.5390
H53	3.6750	1.1660	2.8020
H54	1.5420	2.1190	0.7140
H55	1.5560	0.4550	1.3430

H56	2.1690	3.6960	2.6290
H57	0.4190	3.8870	2.4400
H58	1.0410	4.7900	4.6780
H59	0.2770	3.2550	5.0620
H60	3.0460	4.9850	6.1200
H61	3.4880	4.9000	4.3680
H62	4.3820	3.9150	5.5460
H63	1.4870	1.5900	6.0210
H64	1.9760	2.9040	7.1470
H65	4.0990	1.4610	5.4680
H66	4.2930	2.1050	7.1370
H67	1.8750	0.6580	8.2410
H68	3.5050	0.6160	9.0290
H69	2.6320	-0.9080	8.5570
H70	5.1480	-0.4660	5.8950
H71	5.4760	0.0300	7.5680
H72	5.7410	-2.4830	7.1930
H73	4.6180	-2.0730	8.4860
H74	2.5920	-4.5900	7.0020
H75	3.1280	-3.7990	8.4870
H76	4.3350	-4.6930	7.4820
H77	4.8200	-3.7690	5.1920
H78	4.2920	-2.1090	4.8040
H79	2.5730	-4.6500	4.7000
H80	1.8310	-3.0790	5.1320
H81	1.0140	-0.8860	2.3770
Cl82	2.1280	-0.4670	4.2100

S11 - Cartesian Coordinates for the $[L2H_4Br]^{3+}$ lowest energy conformer

	x	y	z
N1	2.6030	-0.6960	6.8430
C2	2.1070	0.6160	7.3340
C3	1.2950	1.5340	6.3330
N4	2.0360	2.1790	5.2420
C5	2.8700	3.2470	5.7590
C6	1.1870	2.7080	4.1620
C7	1.9190	3.0430	2.8050
N8	2.4120	1.8960	2.0190
C9	3.5860	2.2520	1.2370
C10	4.8900	2.4850	2.0500
C11	5.3870	1.2590	2.8420
O12	4.7870	1.2010	4.1310
C13	5.1330	-0.0050	4.8080
C14	4.9900	0.1680	6.3360
C15	4.0400	-0.8400	7.0490
C16	1.8340	-1.7900	7.4420
C17	2.2760	-3.2580	7.1860
N18	2.5580	-3.5930	5.7970
C19	3.2230	-4.8860	5.7070
C20	1.3900	-3.5270	4.9260
C21	1.7810	-3.6280	3.4310
N22	0.9320	-2.9170	2.4830
C23	-0.4360	-3.3720	2.5460
C24	1.4760	-3.0280	1.1330
C25	0.7390	-2.2400	0.0220
N26	0.4720	-0.8550	0.3900
C27	-0.5070	-0.2680	-0.5130
C28	1.6680	-0.0270	0.5070
C29	1.3510	1.3300	1.1910
H30	2.4450	-0.7370	5.8410
H31	0.9340	-1.9300	2.7320
H32	2.7200	1.1800	2.6750
H33	1.4330	0.4310	8.2070
H34	2.9290	1.1620	7.8500
H35	0.5100	0.8810	5.8800
H36	0.7170	2.3260	6.8730
H37	2.2770	4.1290	6.0940
H38	3.6110	3.5710	4.9980
H39	3.4760	2.9230	6.6280
H40	0.6180	3.5910	4.5490
H41	0.3870	1.9620	3.9450
H42	1.2540	3.6510	2.1410
H43	2.7590	3.7470	2.9880
H44	3.3550	3.1310	0.5860
H45	3.8170	1.4160	0.5390
H46	4.8560	3.3720	2.7250
H47	5.6970	2.7490	1.3150
H48	5.1660	0.3180	2.2810
H49	6.4940	1.3430	2.9890
H50	6.1880	-0.2930	4.5670
H51	4.4800	-0.8200	4.4170
H52	4.7620	1.2290	6.5690
H53	6.0200	0.0520	6.7700
H54	4.3330	-1.8450	6.6670
H55	4.2430	-0.8600	8.1480
H56	1.8260	-1.6760	8.5530
H57	0.7770	-1.6690	7.1080

H58	3.1740	-3.4910	7.8130
H59	1.4960	-3.9630	7.5750
H60	4.1520	-4.9080	6.3230
H61	3.5640	-5.1010	4.6700
H62	2.5620	-5.7190	6.0430
H63	0.8850	-2.5500	5.0840
H64	0.6530	-4.3180	5.2170
H65	2.7940	-3.1730	3.3440
H66	1.8540	-4.7000	3.1320
H67	-1.0770	-2.7410	1.8940
H68	-0.8400	-3.2360	3.5710
H69	-0.5340	-4.4410	2.2510
H70	2.5390	-2.7030	1.1600
H71	1.5070	-4.1050	0.8390
H72	1.3260	-2.2670	-0.9310
H73	-0.2180	-2.7580	-0.2410
H74	-0.8020	0.7550	-0.1930
H75	-1.4540	-0.8560	-0.5040
H76	-0.1380	-0.2210	-1.5660
H77	2.1380	0.0990	-0.5030
H78	2.4150	-0.5590	1.1380
H79	1.0230	2.0740	0.4270
H80	0.4870	1.1380	1.8670
H81	2.6570	1.4780	4.8360
Br82	1.8820	-0.3190	3.8820

S12 - Cartesian Coordinates, atomic charges and atom types for the cluster $[F(H_2O)_{12}]^{12+}$

	x	y	z	Atomic charge	Atom type
F1	0.8580	0.2250	0.1630	-1	F
O2	0.8500	-2.2410	1.4560	-0.325	O2
H3	0.5470	-1.6850	0.7460	0.162	HO
H4	1.4030	-1.6290	1.9170	0.162	HO
O5	-0.9830	2.2470	0.9730	-0.325	O2
H6	-1.1850	1.5760	1.6050	0.162	HO
H7	-0.3120	1.8100	0.4570	0.162	HO
O8	2.4420	-1.8260	-1.0370	-0.325	O2
H9	1.9170	-1.0460	-0.8900	0.162	HO
H10	2.5240	-2.1550	-0.1570	0.162	HO
O11	3.2290	-0.1970	1.6170	-0.325	O2
H12	2.5830	-0.2970	0.9240	0.162	HO
H13	2.8330	0.4960	2.1220	0.162	HO
O14	0.2900	1.9880	-1.8960	-0.325	O2
H15	0.1820	1.2070	-1.3650	0.162	HO
H16	0.9960	2.4110	-1.4340	0.162	HO
O17	0.4470	0.3830	2.9480	-0.325	O2
H18	0.7720	0.5770	2.0740	0.162	HO
H19	-0.1170	-0.3510	2.7650	0.162	HO
O20	-0.5070	-1.3020	-1.7890	-0.325	O2
H21	-0.2510	-0.7150	-1.0850	0.162	HO
H22	0.3210	-1.6930	-2.0150	0.162	HO
O23	-1.7550	-0.6510	0.9760	-0.325	O2
H24	-1.9160	-0.9640	0.1000	0.162	HO
H25	-0.8690	-0.3110	0.8940	0.162	HO
O26	3.1770	1.1510	-1.2160	-0.325	O2
H27	3.5460	1.0900	-0.3500	0.162	HO
H28	2.2860	0.8570	-1.0520	0.162	HO
O29	2.0020	2.6060	1.2220	-0.325	O2
H30	1.1710	2.6750	1.6640	0.162	HO
H31	1.8640	1.8230	0.6980	0.162	HO
O32	1.7730	-0.2220	-3.6400	-0.325	O2
H33	1.0660	0.2120	-3.1870	0.162	HO
H34	2.3950	-0.3750	-2.9440	0.162	HO
O35	-2.6290	0.9920	-1.5250	-0.325	O2
H36	-2.2430	1.2950	-0.7170	0.162	HO
H37	-1.8910	0.6020	-1.9680	0.162	HO

S13 - Cartesian Coordinates, atomic charges and atom types for the cluster $[Cl(H_2O)_{12}]^{12+}$

	x	y	z	Atomic charge	Atom type
Cl1	0.7000	0.3540	-0.0440	-1	Cl
O2	0.7140	-2.5340	1.4880	-0.325	O2
H3	-0.1170	-2.5280	1.0410	0.162	HO
H4	1.0650	-1.6840	1.2580	0.162	HO
O5	-1.3990	2.4790	1.0040	-0.325	O2
H6	-1.4280	1.5420	1.1290	0.162	HO
H7	-0.6250	2.5670	0.4670	0.162	HO
O8	2.6690	-2.0190	-1.0680	-0.325	O2
H9	2.4160	-1.1080	-1.0080	0.162	HO
H10	1.9770	-2.4420	-0.5840	0.162	HO
O11	3.2520	-0.1940	1.7520	-0.325	O2
H12	2.8800	-0.7180	1.0580	0.162	HO
H13	2.6560	0.5410	1.7650	0.162	HO
O14	0.5660	3.0110	-1.7870	-0.325	O2
H15	0.2140	2.1850	-2.0820	0.162	HO
H16	0.9020	2.7730	-0.9340	0.162	HO
O17	0.3880	0.3900	3.1580	-0.325	O2
H18	0.1470	0.8280	2.3530	0.162	HO
H19	0.9500	-0.2980	2.8350	0.162	HO
O20	-0.4040	-2.2980	-1.5540	-0.325	O2
H21	-0.4280	-1.6780	-0.8380	0.162	HO
H22	0.3010	-1.9540	-2.0790	0.162	HO
O23	-1.9850	-0.8620	1.1160	-0.325	O2
H24	-1.8420	-0.5150	0.2480	0.162	HO
H25	-1.1460	-0.6910	1.5210	0.162	HO
O26	3.4360	1.3040	-1.3130	-0.325	O2
H27	3.2990	0.7650	-0.5480	0.162	HO
H28	2.5430	1.5110	-1.5520	0.162	HO
O29	1.9910	2.8940	1.3350	-0.325	O2
H30	1.2060	2.4190	1.5650	0.162	HO
H31	2.3060	2.3820	0.6050	0.162	HO
O32	1.2630	-0.0500	-3.2370	-0.325	O2
H33	0.7260	0.1720	-2.4890	0.162	HO
H34	2.1080	-0.1830	-2.8380	0.162	HO
O35	-1.8670	0.7540	-1.8590	-0.325	O2
H36	-1.5230	1.3010	-1.1680	0.162	HO
H37	-1.2400	0.0450	-1.8590	0.162	HO

S14 - Cartesian Coordinates, atomic charges and atom types for the cluster $[Br(H_2O)_{12}]^{12+}$

	x	y	z	Atomic charge	Atom type
Br1	0.7060	0.2300	-0.0820	-1	Br
O2	0.8540	-2.6180	1.6380	-0.325	O2
H3	0.1500	-2.2090	1.1580	0.162	HO
H4	1.5640	-2.0140	1.4810	0.162	HO
O5	-1.4540	2.5420	0.9280	-0.325	O2
H6	-1.4600	1.6070	1.0720	0.162	HO
H7	-0.6990	2.6420	0.3680	0.162	HO
O8	2.7990	-2.1470	-1.0890	-0.325	O2
H9	2.8270	-1.2020	-1.0530	0.162	HO
H10	1.9370	-2.3230	-0.7400	0.162	HO
O11	3.3540	-0.1770	1.8840	-0.325	O2
H12	3.0540	-0.5620	1.0740	0.162	HO
H13	2.6570	0.4350	2.0710	0.162	HO
O14	0.6720	3.1390	-1.7140	-0.325	O2
H15	0.2210	2.3130	-1.8090	0.162	HO
H16	1.2310	2.9630	-0.9720	0.162	HO
O17	0.2800	0.3380	3.2240	-0.325	O2
H18	0.1170	0.9330	2.5070	0.162	HO
H19	0.6580	-0.4020	2.7730	0.162	HO
O20	-0.5340	-2.4190	-1.6850	-0.325	O2
H21	-0.6740	-2.0230	-0.8370	0.162	HO
H22	0.1310	-1.8540	-2.0490	0.162	HO
O23	-2.1850	-0.8590	1.1360	-0.325	O2
H24	-1.9720	-0.5710	0.2610	0.162	HO
H25	-1.3720	-0.7000	1.5910	0.162	HO
O26	3.5510	1.3680	-1.3700	-0.325	O2
H27	3.3070	0.9260	-0.5700	0.162	HO
H28	2.7140	1.4490	-1.8030	0.162	HO
O29	2.0390	2.9010	1.3960	-0.325	O2
H30	1.1820	2.5070	1.4660	0.162	HO
H31	2.4690	2.3080	0.7990	0.162	HO
O32	1.2040	-0.0220	-3.3660	-0.325	O2
H33	0.5590	0.4510	-2.8610	0.162	HO
H34	1.7330	-0.4060	-2.6830	0.162	HO
O35	-1.9830	0.6920	-1.9760	-0.325	O2
H36	-1.6490	1.2180	-1.2640	0.162	HO
H37	-1.3800	-0.0370	-1.9710	0.162	HO

S15 - Cartesian Coordinates, atomic charges and atom types for the cluster of twelve H_2O

	x	y	z	Atomic charge	Atom type
O1	0.6910	-2.3950	2.2800	-0.325	O2
H2	-0.1280	-2.1610	2.6860	0.162	HO
H3	0.4490	-2.5690	1.3840	0.162	HO
O4	-1.4620	2.2370	0.8440	-0.325	O2
H5	-0.9650	3.0240	0.6880	0.162	HO
H6	-1.8400	2.0340	0.0030	0.162	HO
O7	2.8990	-0.5170	-2.2590	-0.325	O2
H8	3.3860	-1.0080	-1.6180	0.162	HO
H9	2.9020	0.3630	-1.9190	0.162	HO
O10	3.1390	-1.3460	0.7490	-0.325	O2
H11	3.2120	-1.9690	1.4540	0.162	HO
H12	2.2080	-1.2880	0.6040	0.162	HO
O13	0.7380	1.4780	-1.2180	-0.325	O2
H14	0.5200	1.2240	-0.3350	0.162	HO
H15	1.2620	2.2540	-1.1010	0.162	HO
O16	1.0420	0.7000	1.9210	-0.325	O2
H17	0.1020	0.7820	1.9580	0.162	HO
H18	1.2100	-0.1190	2.3580	0.162	HO
O19	0.2850	-1.5870	-0.7150	-0.325	O2
H20	0.8640	-1.0470	-1.2280	0.162	HO
H21	-0.4340	-1.7570	-1.3020	0.162	HO
O22	-1.7470	-0.7050	1.6160	-0.325	O2
H23	-2.2280	0.1030	1.6940	0.162	HO
H24	-1.6000	-0.7860	0.6870	0.162	HO
O25	3.5470	1.5700	0.0960	-0.325	O2
H26	2.8900	1.1390	0.6190	0.162	HO
H27	4.3080	1.0230	0.2040	0.162	HO
O28	1.3810	3.6240	0.8560	-0.325	O2
H29	1.3020	3.0230	1.5800	0.162	HO
H30	2.3030	3.6110	0.6540	0.162	HO
O31	0.1480	-0.5020	-3.5430	-0.325	O2
H32	0.5440	0.3110	-3.2700	0.162	HO
H33	0.8890	-1.0470	-3.7530	0.162	HO
O34	-2.1290	0.1890	-1.5000	-0.325	O2
H35	-2.5870	-0.1200	-2.2640	0.162	HO
H36	-1.2740	0.4160	-1.8280	0.162	HO

S16 - Cartesian Coordinates (lowest energy conformer), atomic charges and atom types for the $[L2H_2]^{2+}$

	x	y	z	Atom type	Atomic charge
N1	-0.3920	-0.9160	1.9950	N3	0.7230563
C2	0.0270	-1.4450	0.6990	C4	-0.2812724
C3	1.4330	-2.0940	0.6820	C4	-0.09176302
N4	2.5030	-1.1500	0.9960	N3	-0.06393003
C5	2.6930	-0.1950	-0.0860	C4	-0.1265931
C6	3.7450	-1.8330	1.3500	C4	-0.08111572
C7	4.8590	-0.9680	1.9890	C4	-0.07867479
N8	4.6510	-0.5800	3.3830	N3	-0.07015753
C9	3.4250	0.1670	3.6160	C4	-0.1225615
C10	3.3670	1.5980	3.0610	C4	-0.1435995
C11	1.9760	2.2370	3.1910	C4	0.07635355
O12	1.0540	1.5240	2.3840	O2	-0.3044543
C13	-0.1660	2.2240	2.2340	C4	0.04134893
C14	-1.0770	1.4350	1.2820	C4	-0.1182919
C15	-1.4760	0.0510	1.8440	C4	-0.2721381
C16	-0.7930	-2.0020	2.8900	C4	-0.2818265
C17	-0.8460	-1.6620	4.4010	C4	-0.0931716
N18	0.4270	-1.2420	4.9860	N3	-0.05817223
C19	1.4230	-2.2970	4.8920	C4	-0.135571
C20	0.2390	-0.7950	6.3680	C4	-0.08494043
C21	1.4030	0.0000	7.0060	C4	-0.08155966
N22	2.6530	-0.7020	7.2780	N3	-0.07780695
C23	2.4610	-1.8400	8.1620	C4	-0.1285276
C24	3.6810	0.2070	7.7820	C4	-0.09937334
C25	5.1050	-0.3910	7.6650	C4	-0.2861695
N26	5.4560	-0.7980	6.3110	N3	0.7530165
C27	6.5360	-1.7590	6.3200	C4	-0.3094578
C28	5.7610	0.3430	5.4590	C4	-0.2851648
C29	5.8450	0.0480	3.9420	C4	-0.09459972
H30	0.4070	-0.4340	2.4140	HB	0.1040388
H31	-0.7330	-2.1760	0.3330	H	0.1181231
H32	0.0080	-0.6410	-0.0650	H	0.129692
H33	1.4630	-2.9550	1.3870	H	0.07114351
H34	1.6330	-2.5580	-0.3170	H	0.08740127
H35	3.5420	0.4940	0.0990	H	0.06938487
H36	1.8130	0.4720	-0.2000	H	0.05438304
H37	2.8960	-0.7050	-1.0570	H	0.05457526
H38	4.1440	-2.3380	0.4350	H	0.06720191
H39	3.5340	-2.6430	2.0860	H	0.06254864
H40	5.7790	-1.5990	1.9500	H	0.0698868
H41	5.1070	-0.0780	1.3680	H	0.0605371
H42	3.2150	0.1960	4.7060	H	0.04986489
H43	2.5710	-0.4090	3.2060	H	0.09700817
H44	3.6600	1.6300	1.9870	H	0.08233613
H45	4.0940	2.2500	3.5990	H	0.06107128
H46	1.6160	2.2090	4.2470	H	0.03527898
H47	2.0340	3.2990	2.8460	H	0.06041533
H48	0.0400	3.2330	1.7960	H	0.07361948
H49	-0.6390	2.3450	3.2380	H	0.0484457
H50	-0.5980	1.3850	0.2750	H	0.08647299
H51	-2.0020	2.0480	1.1190	H	0.1092466
H52	-1.9380	0.2530	2.8360	H	0.1172011
H53	-2.2870	-0.3960	1.2190	H	0.1182885
H54	-1.7920	-2.3830	2.5680	H	0.1189933

H55	-0.1330	-2.8840	2.7570	H	0.1215782
H56	-1.6170	-0.8780	4.5870	H	0.08022833
H57	-1.2230	-2.5550	4.9630	H	0.08195072
H58	1.6610	-2.5440	3.8360	H	0.04524225
H59	1.0880	-3.2250	5.4110	H	0.05156237
H60	2.3920	-1.9820	5.3280	H	0.06859231
H61	-0.0870	-1.6430	7.0150	H	0.06298554
H62	-0.6230	-0.0850	6.3850	H	0.07025713
H63	1.6080	0.8540	6.3180	H	0.06342703
H64	1.0390	0.4500	7.9630	H	0.06532955
H65	1.7300	-2.5670	7.7470	H	0.07062066
H66	2.0960	-1.5220	9.1670	H	0.06177574
H67	3.3950	-2.4290	8.2890	H	0.04919648
H68	3.6310	1.1830	7.2440	H	0.07777983
H69	3.4540	0.4730	8.8470	H	0.09404761
H70	5.8670	0.3290	8.0510	H	0.1264161
H71	5.1760	-1.2610	8.3550	H	0.1282173
H72	7.4720	-1.3220	6.7390	H	0.1242542
H73	6.7380	-2.1390	5.2950	H	0.1231799
H74	6.2580	-2.6540	6.9200	H	0.1171947
H75	6.7210	0.8040	5.7960	H	0.1238692
H76	5.0050	1.1420	5.6110	H	0.1199434
H77	6.0560	0.9960	3.3870	H	0.08358592
H78	6.7370	-0.5880	3.7280	H	0.0853352
H79	4.6340	-1.2630	5.9160	HB	0.07338792

S17 - Cartesian Coordinates (lowest energy conformer), atomic charges and atom types for the $[L2H_3]^{3+}$

	x	y	z	Atom type	Atomic charge
N1	-0.1010	1.5030	4.4340	N3	0.7349024
C2	-0.8320	1.7510	3.1900	C4	-0.2898269
C3	-0.5540	0.7950	2.0020	C4	-0.08582211
N4	0.8100	0.8840	1.4850	N3	-0.08999109
C5	1.0500	2.1630	0.8300	C4	-0.1272497
C6	1.1510	-0.2350	0.6130	C4	-0.07672167
C7	2.6740	-0.4770	0.4250	C4	-0.2867141
N8	3.3720	-1.0070	1.5890	N3	0.755178
C9	3.3480	-0.1110	2.7390	C4	-0.286798
C10	4.0690	1.2540	2.6390	C4	-0.1121817
C11	3.8380	2.1540	3.8690	C4	0.07767057
O12	2.4610	2.4860	3.9480	O2	-0.3228946
C13	2.2200	3.5510	4.8520	C4	0.04778719
C14	0.7150	3.8720	4.8690	C4	-0.120368
C15	-0.1540	2.6660	5.3100	C4	-0.2837663
C16	-0.5810	0.2820	5.0870	C4	-0.2749348
C17	0.0880	-0.1970	6.4050	C4	-0.1081815
N18	1.4760	-0.6390	6.2390	N3	-0.06692076
C19	2.3400	-0.0290	7.2340	C4	-0.1231012
C20	1.5880	-2.1020	6.2220	C4	-0.07942963
C21	3.0290	-2.6600	6.0780	C4	-0.2947807
N22	3.1430	-4.0490	5.6520	N3	0.755918
C23	2.5130	-4.9600	6.5800	C4	-0.3150978
C24	4.5140	-4.4520	5.3730	C4	-0.2866421
C25	5.3450	-3.5600	4.4120	C4	-0.09095573
N26	4.6500	-3.1320	3.2000	N3	-0.1378055
C27	4.2470	-4.2560	2.3710	C4	-0.1231318
C28	5.4600	-2.1700	2.4480	C4	-0.09044027
C29	4.7080	-1.4860	1.2760	C4	-0.2871203
H30	0.8790	1.3510	4.1910	HB	0.06891751
H31	2.6330	-4.1260	4.7680	HB	0.035519
H32	2.8430	-1.8370	1.8720	HB	0.0335111
H33	-1.9280	1.7540	3.4070	H	0.1360039
H34	-0.6440	2.7880	2.8430	H	0.1459347
H35	-0.7870	-0.2500	2.3080	H	0.05956596
H36	-1.2760	0.9960	1.1670	H	0.1064005
H37	2.0340	2.2050	0.3180	H	0.06626201
H38	1.0700	3.0000	1.5620	H	0.07362676
H39	0.2810	2.3840	0.0510	H	0.07598579
H40	0.6390	-0.0950	-0.3760	H	0.1108378
H41	0.7340	-1.1840	1.0300	H	0.05134219
H42	2.7600	-1.2340	-0.3910	H	0.1305069
H43	3.2060	0.4170	0.0290	H	0.1468954
H44	3.7580	-0.6520	3.6170	H	0.09490329
H45	2.2880	0.0480	3.0220	H	0.1204548
H46	3.7480	1.8440	1.7490	H	0.09457821
H47	5.1730	1.1130	2.5290	H	0.08924031
H48	4.1280	1.6310	4.8110	H	0.03908479
H49	4.4480	3.0880	3.7640	H	0.0888952
H50	2.7900	4.4560	4.5220	H	0.08842146
H51	2.5700	3.2490	5.8690	H	0.04929054
H52	0.4200	4.2980	3.8800	H	0.09150743
H53	0.5600	4.7260	5.5800	H	0.1259424
H54	0.2310	2.3980	6.3150	H	0.1226434

H55	-1.2170	2.9760	5.4620	H	0.1351034
H56	-1.6730	0.4090	5.2900	H	0.1375297
H57	-0.4910	-0.5640	4.3720	H	0.1003268
H58	-0.0130	0.5510	7.2290	H	0.1086905
H59	-0.5270	-1.0300	6.8310	H	0.09576547
H60	3.4150	-0.2240	7.0220	H	0.08421075
H61	2.1020	-0.3900	8.2630	H	0.06116819
H62	2.2450	1.0810	7.2160	H	0.06955469
H63	0.9740	-2.4730	5.3660	H	0.04068393
H64	1.1390	-2.5060	7.1650	H	0.07689112
H65	3.5330	-2.0290	5.3190	H	0.1148841
H66	3.5910	-2.5440	7.0370	H	0.1447254
H67	2.9720	-4.9070	7.5940	H	0.1418518
H68	2.5860	-6.0110	6.2180	H	0.1353608
H69	1.4250	-4.7500	6.6680	H	0.1187558
H70	5.0690	-4.5380	6.3400	H	0.1480806
H71	4.4970	-5.4920	4.9680	H	0.143571
H72	5.7040	-2.6650	4.9780	H	0.08502382
H73	6.2900	-4.0980	4.1290	H	0.1158701
H74	5.1310	-4.8120	1.9780	H	0.05606478
H75	3.6290	-3.9240	1.5080	H	0.04768884
H76	3.6070	-4.9820	2.9190	H	0.0940491
H77	6.3840	-2.6770	2.0610	H	0.1156518
H78	5.8570	-1.3810	3.1340	H	0.08917344
H79	5.3220	-0.6440	0.8750	H	0.1469971
H80	4.6420	-2.2130	0.4320	H	0.1354756

S18 – Energy values (kcal/mol) for the lowest energy conformers used in ΔE reaction energy calculations.

	E (kcal/mol)
$[L1H_4]^{4+}$	383.07
$[L1H_4F]^{3+}$	53.98
$[L1H_4Cl]^{3+}$	70.91
$[L1H_4Br]^{3+}$	78.86
$[L1H_5]^{5+}$	677.93
$[L1H_5F]^{4+}$	278.63
$[L2H_4]^{4+}$	499.68
$[L2H_4F]^{3+}$	159.30
$[L2H_4F(H2O)]^{3+}$	152.02
$[L2H_4Cl]^{3+}$	186.50
$[L2H_4Br]^{3+}$	182.82
$[F(H_2O)_{12}]^{12+}$	-76.79
$[Cl(H_2O)_{12}]^{12+}$	-63.76
$[Br(H_2O)_{12}]^{12+}$	-59.14
12 H_2O	-16.97

Figure S1 - Lowest energy conformer of $[L2H_2]^{2+}$

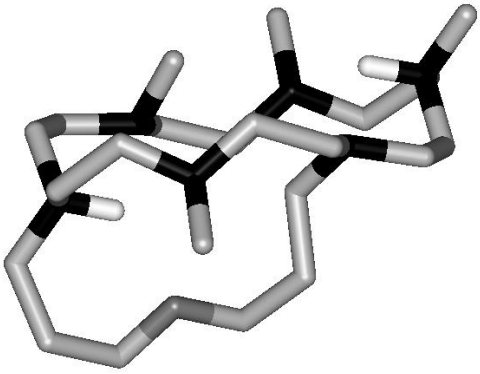

Figure S2 - Lowest energy conformer of $[L2H_3]^{3+}$