Supporting Information

Experimental and theoretical studies of halide binding with a p-xylyl based azamacrocycle

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Douglas R. Powell, and Jerzy Leszczynski and Md. Alamgir Hossain

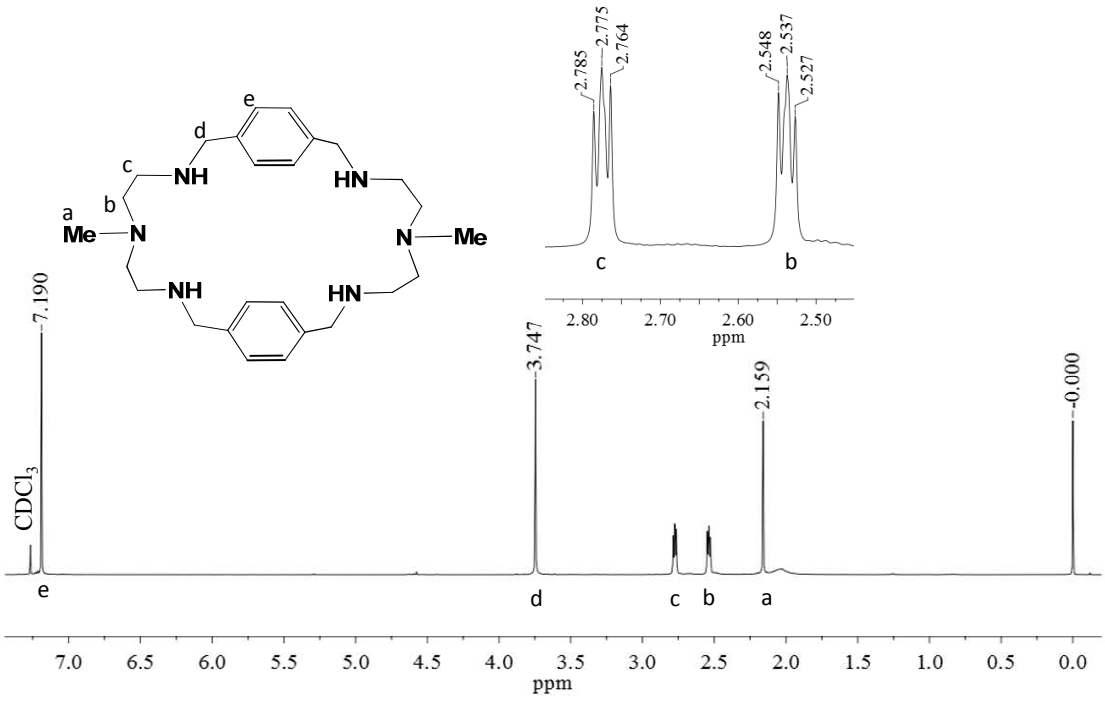

Figure S1. ^{1}H NMR spectrum of **L** in D_2O.

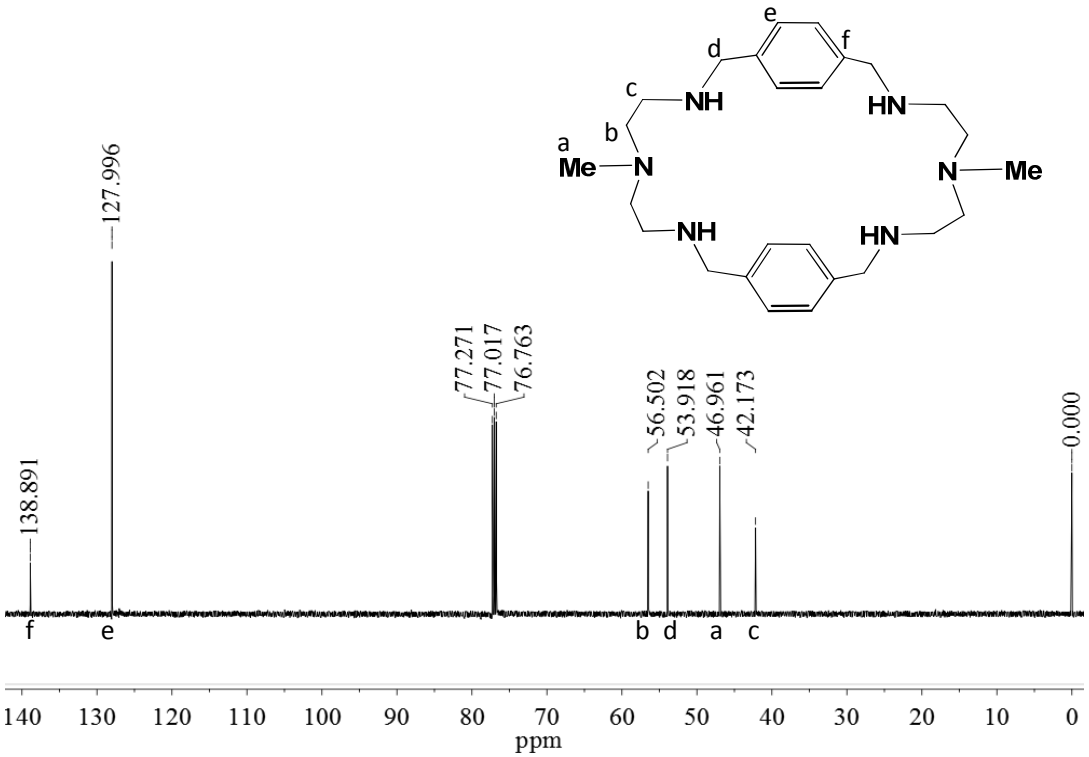

Figure S2. ^{13}C NMR spectrum of **L** in D_2O.

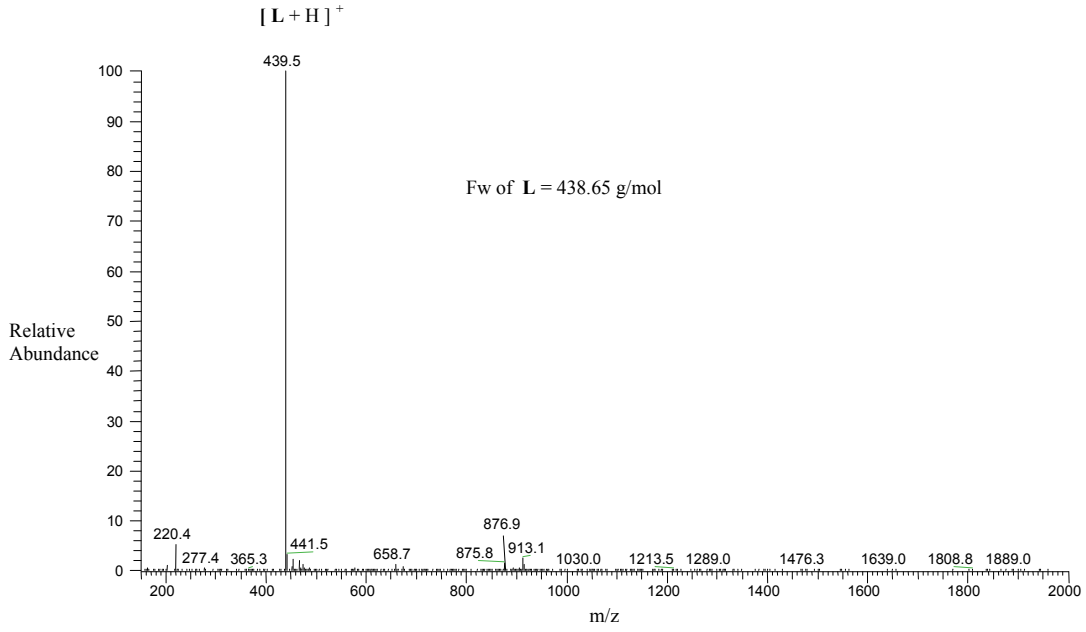

Figure S3. Mass spectrum of **L** in methanol at room temperature.

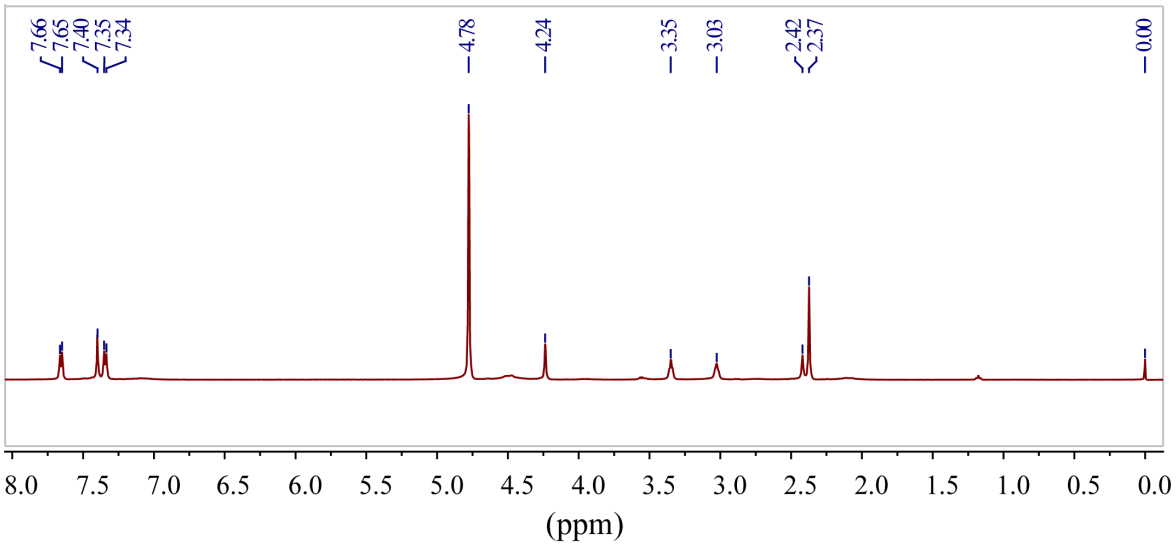

Figure S4. ^{1}H NMR spectrum of **L**-TsO complex in D_2O.

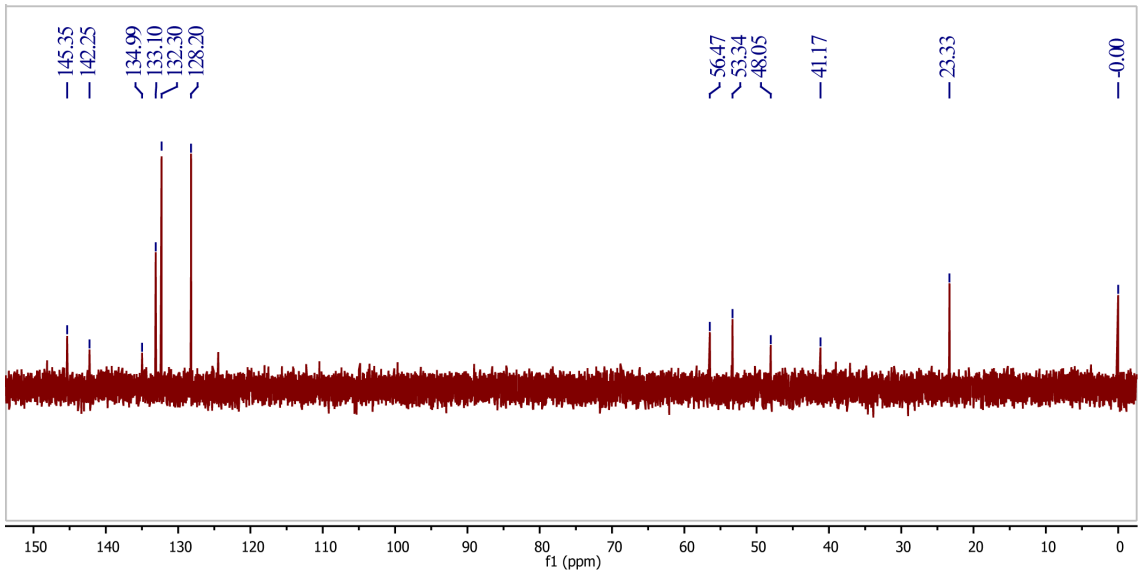

Figure S5. 13C NMR spectrum of L-TsO complex in D_2O.

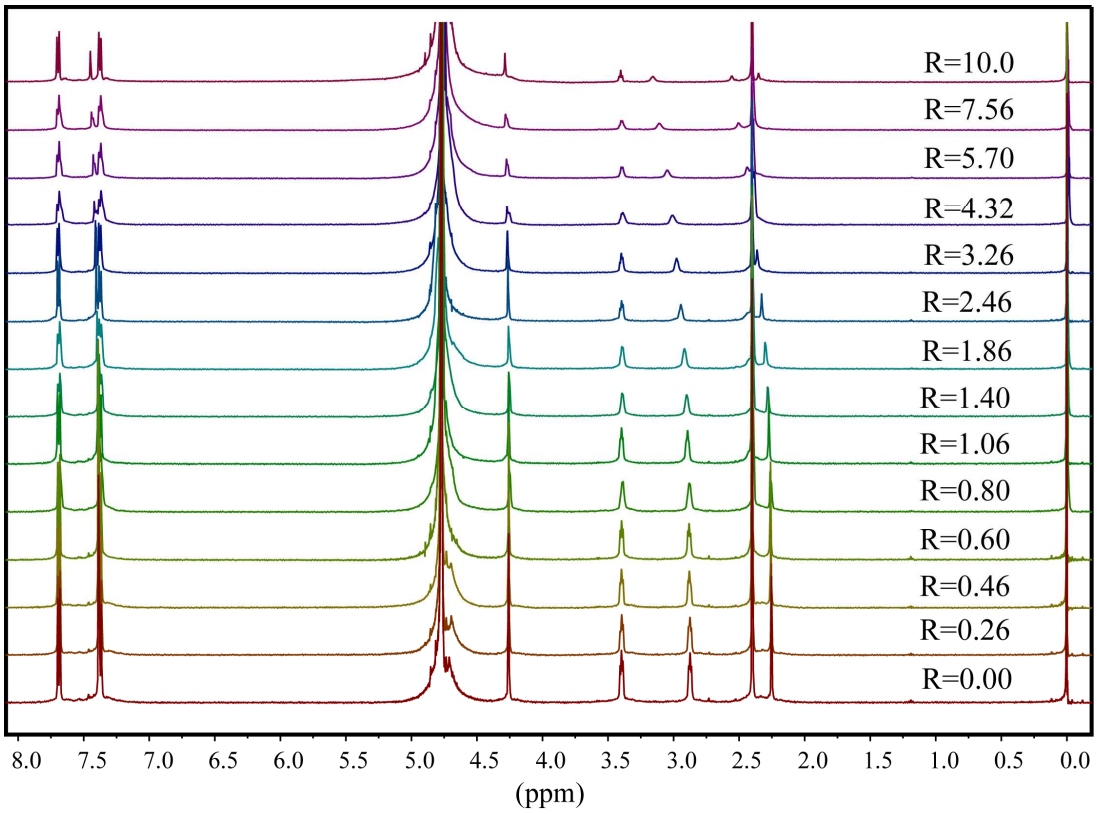

Figure S6. ^{1}H NMR spectra of L (2 mM) with an increasing amount of NaF (R = $[NaF]_0/[L]_0$) in D_2O at pH = 2.1.

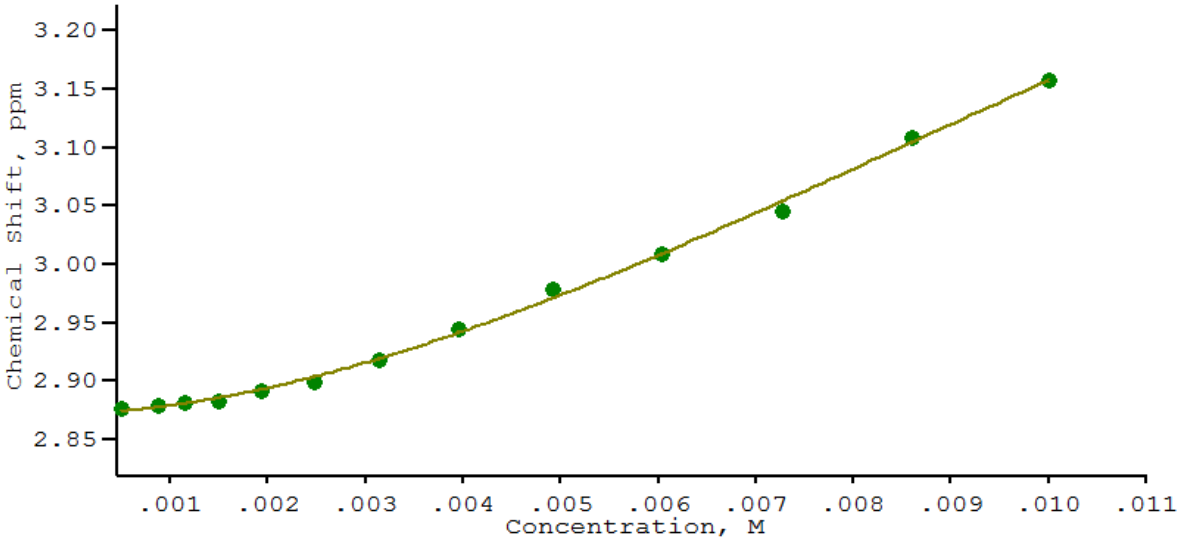

Figure S7. ^{1}H NMR titration curve of L with NaF showing the change in the chemical shifts of aliphatic CH_3NCH_2 against an increasing amount of anions in D_2O at pH = 2.1.

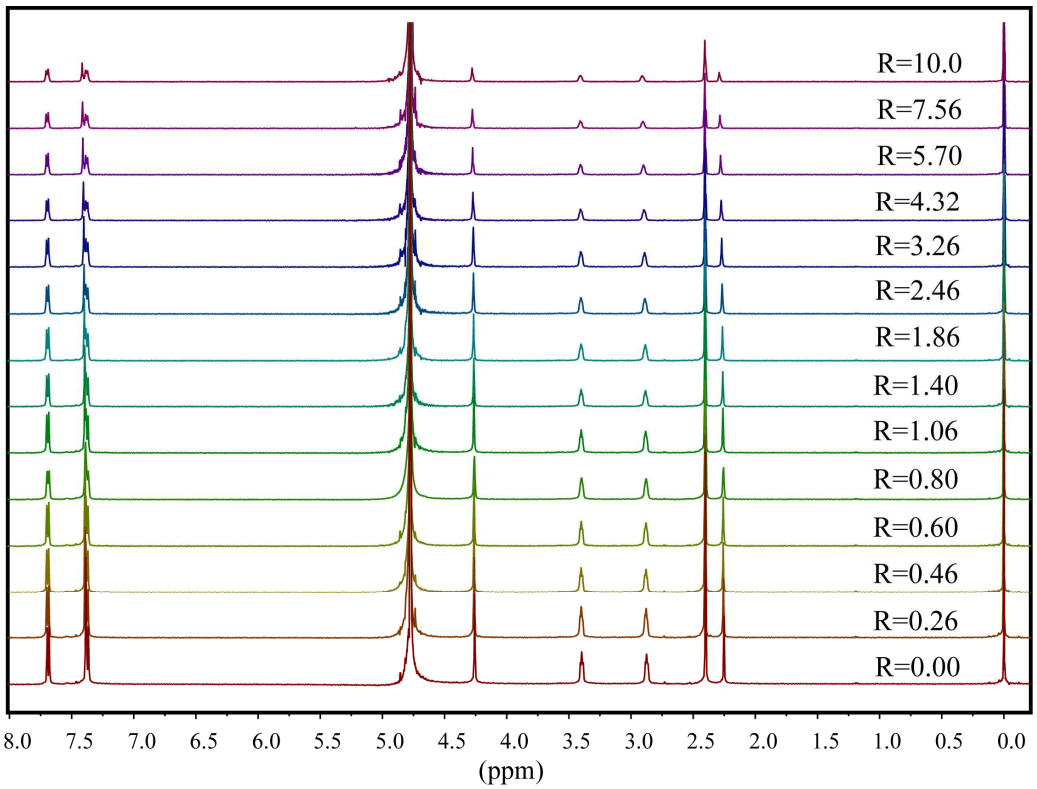

Figure S8. ^{1}H NMR spectra of L (2 mM) with an increasing amount of NaCl (R = $[NaCl]_0/[L]_0$) in D_2O at pH = 2.1.

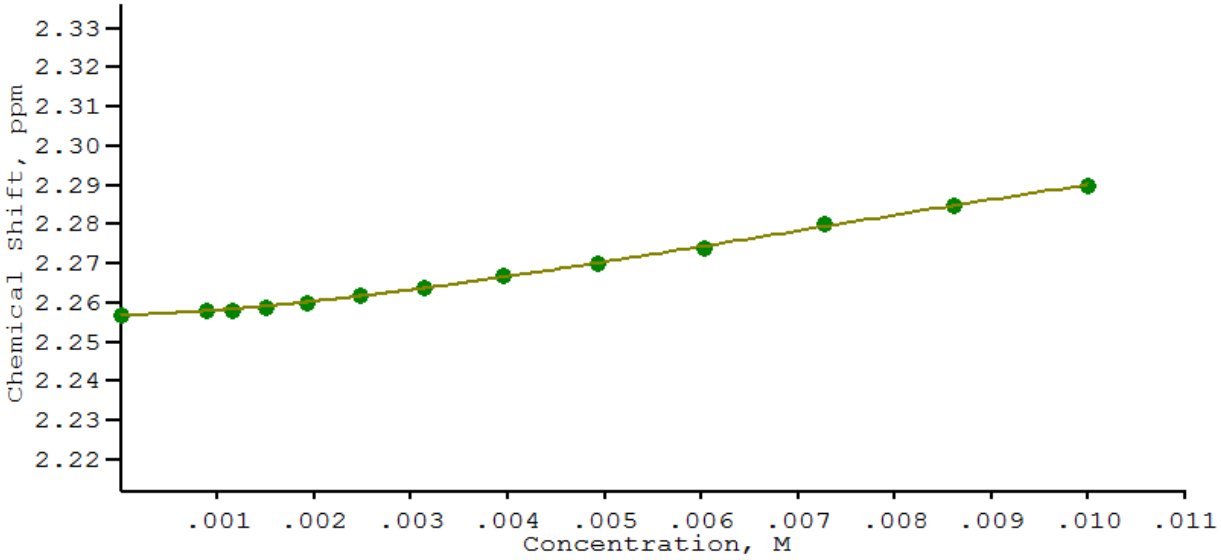

Figure S9. ^{1}H NMR titration curve of L with NaCl showing the change in the chemical shifts of aliphatic NCH_3 against an increasing amount of anions in D_2O at pH = 2.1.

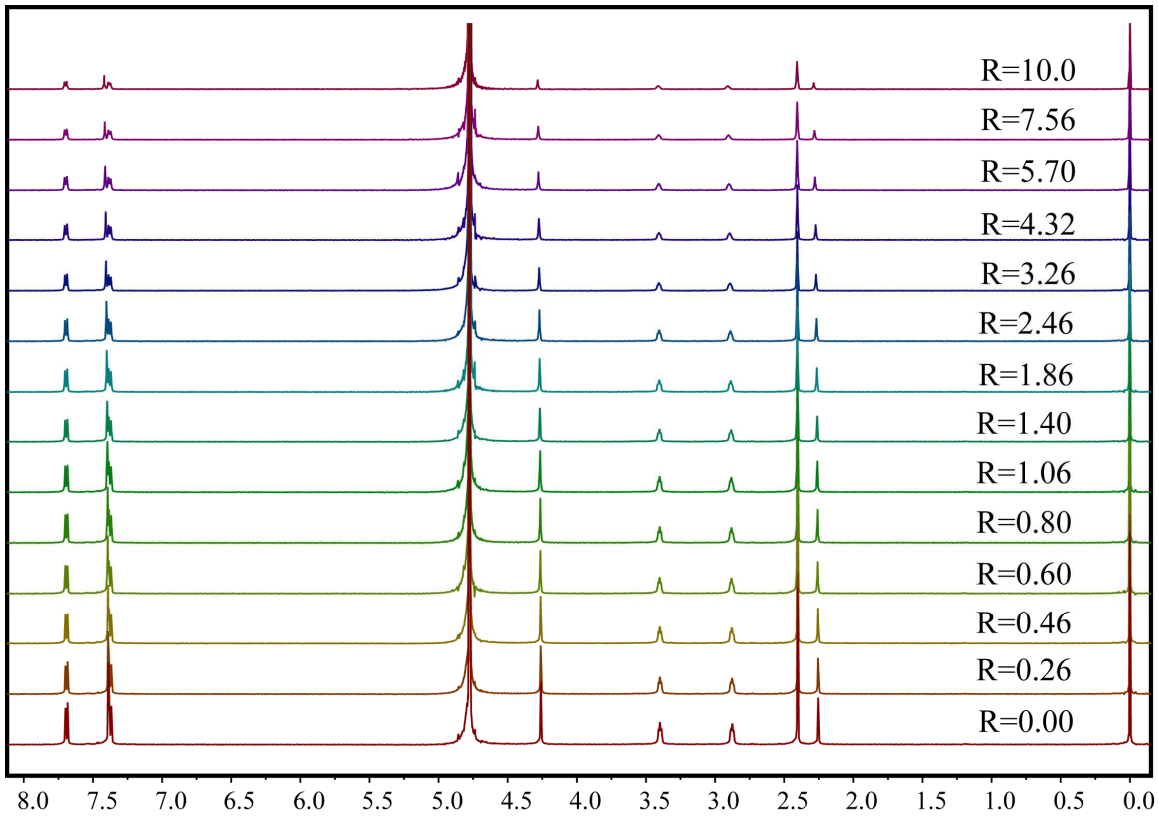

Figure S10. ^{1}H NMR spectra of L (2 mM) with an increasing amount of NaBr (R = $[NaBr]_0/[L]_0$) in D_2O at pH = 2.1.

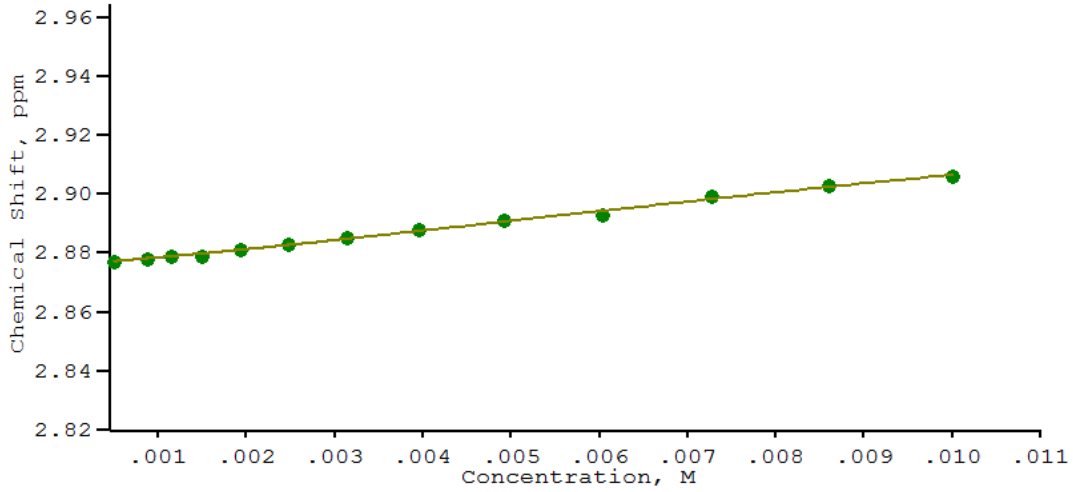

Figure S11. ^{1}H NMR titration curve of L with NaBr showing the change in the chemical shifts of aliphatic NCH_3 against an increasing amount of anions in D_2O at pH = 2.1.

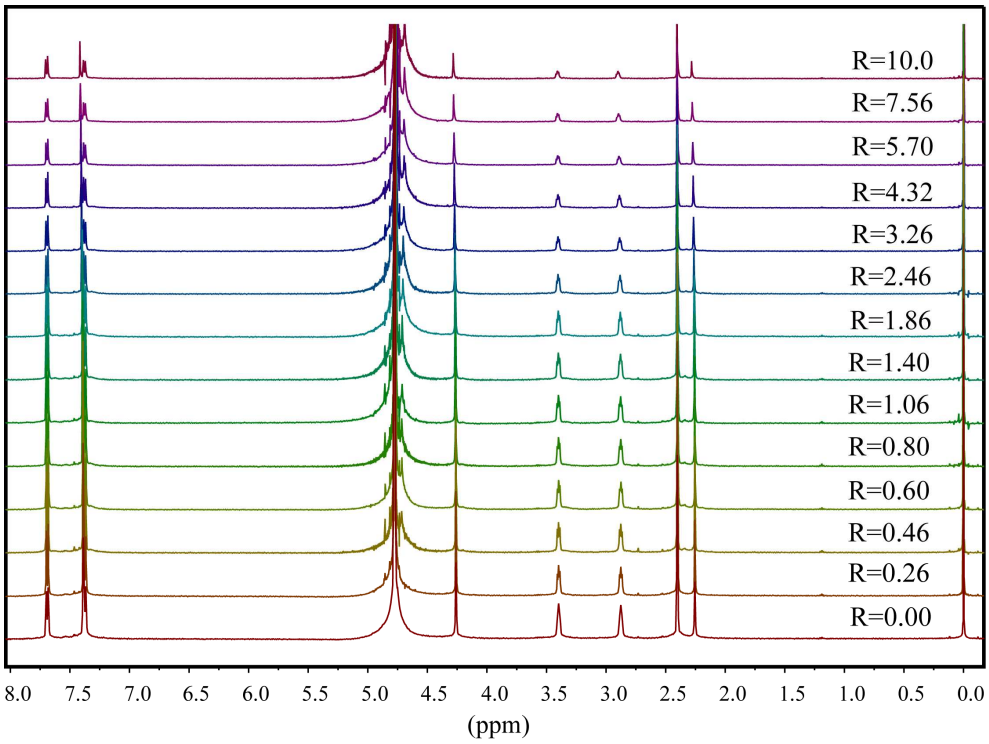

Figure S12. ^{1}H NMR spectra of L (2 mM) with an increasing amount of NaI (R = $[NaI]_0/[L]_0$) in D_2O at pH = 2.1.

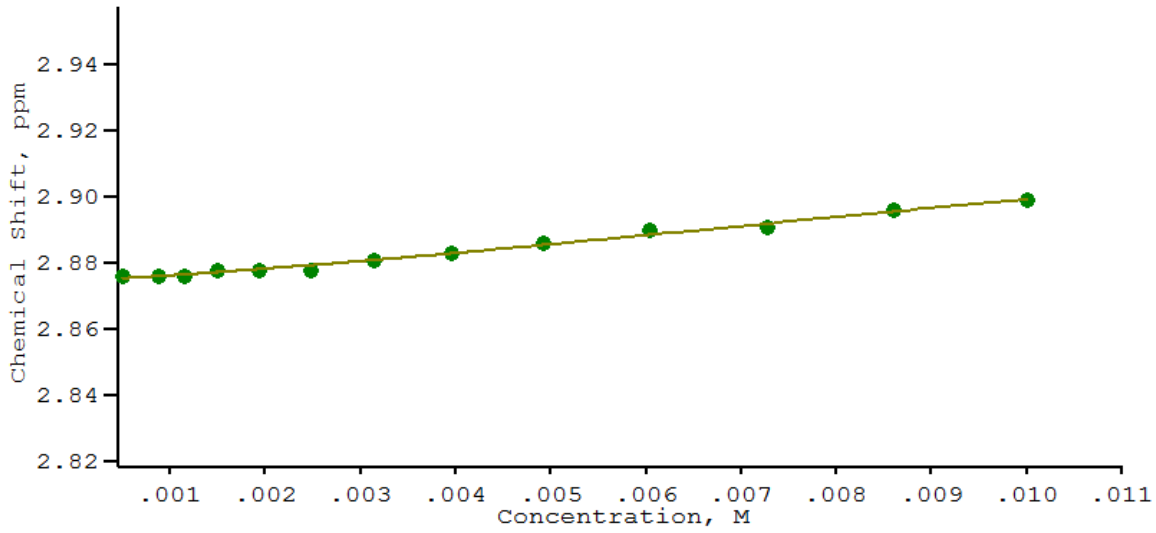

Figure S13. ^{1}H NMR titration curve of L with NaI showing the change in the chemical shifts of aliphatic NCH_3 against an increasing amount of anions in D_2O at pH = 2.1.

Table S1. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L]^{6+}$ in gas phase. Total energy: -1345.295874 au.

1	N1	-4.3950160	1.8780200	-0.2751620
2	H2	-3.6961570	1.5130680	-0.9309390
3	C3	-4.9019270	0.6927400	0.5492370
4	H4	-5.9268750	0.9294320	0.8452930
5	H5	-4.2864410	0.6296500	1.4480040
6	C6	-4.8097390	-0.6238650	-0.2529760
7	H7	-5.4474610	-0.6170520	-1.1396400
8	H8	-3.7789520	-0.8244350	-0.5583820
9	N9	-5.2301840	-1.8130020	0.5670660
10	H10	-4.8365170	-1.7688500	1.5147440
11	H11	-6.2532850	-1.8155500	0.6908360
12	C12	-4.8414950	-3.1799220	-0.0438470
13	H13	-5.3984290	-3.9148050	0.5438420
14	H14	-5.2377770	-3.1799870	-1.0604450
15	C15	-3.3541370	-3.4672310	-0.0039100
16	C16	-2.6947640	-3.6644630	1.2143320
17	H17	-3.2213960	-3.5681580	2.1605210
18	C18	-1.3726640	-4.0992970	1.2415200
19	H19	-0.9071530	-4.2996950	2.2012430
20	C20	-0.6952140	-4.3786700	0.0490450
21	C21	-1.3599780	-4.2020420	-1.1685540
22	H22	-0.8968290	-4.4952710	-2.1070070
23	C23	-2.6715880	-3.7330630	-1.1957380
24	H24	-3.1822850	-3.6608850	-2.1508250
25	C25	0.7011290	-4.9656060	0.0959120
26	H26	0.9949240	-5.2412550	1.1096510
27	H27	0.8185040	-5.8317180	-0.5595150
28	N28	1.7345750	-3.9176210	-0.3919860
29	H29	1.4467380	-3.0255930	0.0183710
30	H30	1.6061510	-3.8230420	-1.4063040
31	C31	3.1912640	-4.2228280	-0.0955840
32	H32	3.3930970	-5.2020510	-0.5378820
33	H33	3.2887380	-4.3316890	0.9876840
34	C34	4.1785740	-3.2082470	-0.7046500
35	H35	3.7958930	-2.7997510	-1.6423300
36	H36	5.1133100	-3.7248210	-0.9352610
37	N37	4.5644790	-2.0307840	0.2025240
38	H38	3.7531960	-1.7905260	0.7793560
39	C39	4.9405890	-0.7866630	-0.5942220
40	H40	4.2893720	-0.7536140	-1.4700450
41	H41	5.9694870	-0.9325230	-0.9342050
42	C42	4.7748990	0.5062550	0.2348160
43	H43	3.7480020	0.6193400	0.5938470

44	H44	5.4542580	0.5450210	1.0885140
45	N45	5.0612430	1.7333110	-0.5891380
46	H46	6.0716640	1.7963040	-0.7816740
47	H47	4.6073320	1.6806370	-1.5089020
48	C48	4.6441540	3.0683040	0.0733110
49	H49	5.2005500	3.8324260	-0.4760100
50	H50	5.0311480	3.0313020	1.0927360
51	C51	3.1576090	3.3688830	0.0323240
52	C52	2.4757820	3.6135190	1.2301000
53	H53	2.9696770	3.4661790	2.1852970
54	C54	1.2044930	4.1830420	1.2168870
55	H55	0.7689150	4.4768120	2.1687400
56	C56	0.5699640	4.4841720	0.0069000
57	C57	1.2278360	4.1848760	-1.1915230
58	H58	0.7902280	4.4646660	-2.1445250
59	C59	2.5147840	3.6514000	-1.1779490
60	H60	3.0363140	3.5579920	-2.1272530
61	C61	-0.6701630	5.3580830	-0.0253330
62	H62	-0.4982130	6.2787160	0.5388510
63	H63	-0.9591050	5.6300650	-1.0416690
64	N64	-1.9283220	4.7334520	0.6243750
65	H65	-1.6502080	4.3288310	1.5265380
66	H66	-2.5658220	5.5101120	0.8523790
67	C67	-2.6441940	3.7223600	-0.2319210
68	H68	-1.8703410	3.0551250	-0.6213020
69	H69	-3.0830210	4.2794330	-1.0621480
70	C70	-3.7015750	2.9384580	0.5771500
71	H71	-3.2225750	2.4235650	1.4114700
72	H72	-4.4873120	3.5876750	0.9721730
73	C73	-5.5155020	2.4781910	-1.1156360
74	H74	-5.9574070	1.6943670	-1.7297760
75	H75	-5.1067710	3.2535040	-1.7618550
76	H76	-6.2607830	2.8959620	-0.4382820
77	C77	5.6752980	-2.4415330	1.1614160
78	H78	5.8608340	-1.6357340	1.8698850
79	H79	6.5689190	-2.6529360	0.5728210
80	H80	5.3658460	-3.3349840	1.7029760

Table S2. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(F)]^{5+}$ in gas phase. Total energy: -1445.828645 au.

1	C1	-0.4677310	-3.8171480	-1.3229080
2	H2	-0.9310390	-3.8754860	-2.3016870
3	C3	-1.2540650	-3.6642930	-0.1786450
4	C4	-0.6359520	-3.6617610	1.0735040
5	H5	-1.2197930	-3.6293900	1.9884130

6	C6	-2.7627120	-3.6467700	-0.3232010
7	H7	-3.0453840	-3.5874340	-1.3743380
8	H8	-3.1997160	-4.5570770	0.0963690
9	N9	-3.4247680	-2.4793060	0.3689820
10	H10	-3.0315360	-1.5414050	0.0585340
11	H11	-3.2454190	-2.5454950	1.3743200
12	C12	-4.9181870	-2.4551340	0.1538290
13	H13	-5.3275970	-3.3732380	0.5790580
14	H14	-5.0832540	-2.4875010	-0.9246320
15	C15	-5.6067000	-1.2546060	0.8082430
16	H16	-5.1629990	-1.0453410	1.7830190
17	H17	-6.6605880	-1.4906890	0.9693600
18	N18	-5.5304630	0.0002470	-0.0250760
19	H19	-4.5413620	0.0001550	-0.4018870
20	C20	-5.6064090	1.2550540	0.8083210
21	H21	-5.1625870	1.0456660	1.7830170
22	H22	-6.6602400	1.4912720	0.9696090
23	C23	-4.9178180	2.4555300	0.1538960
24	H24	-5.0829500	2.4879720	-0.9245530
25	H25	-5.3270810	3.3736650	0.5791990
26	N26	-3.4243780	2.4795050	0.3689680
27	H27	-3.2449840	2.5455770	1.3743050
28	H28	-3.0312770	1.5416150	0.0584370
29	C29	-2.7621970	3.6469290	-0.3231490
30	H30	-3.1991390	4.5572640	0.0964330
31	H31	-3.0448340	3.5876540	-1.3743000
32	C32	-1.2535490	3.6643350	-0.1785420
33	C33	-0.4672280	3.8179600	-1.3227120
34	H34	-0.9305440	3.8769470	-2.3014490
35	C35	-0.6354150	3.6609420	1.0735920
36	H36	-1.2192110	3.6279570	1.9885070
37	C37	-6.5541390	0.0003970	-1.1203840
38	H38	-6.4264640	0.8853600	-1.7410620
39	H39	-7.5492980	0.0006890	-0.6745890
40	H40	-6.4269220	-0.8847670	-1.7408700
41	C41	0.7469660	3.7737980	1.1816690
42	H42	1.1992000	3.8112410	2.1674800
43	C43	1.5300690	3.9258080	0.0341630
44	C44	0.9109690	3.9661020	-1.2180120
45	H45	1.4846610	4.1665930	-2.1191800
46	C46	3.0264810	4.0677930	0.1482240
47	H47	3.3572280	4.2388880	1.1735110
48	H48	3.4426760	4.8373340	-0.5050100
49	N49	3.6711010	2.7295690	-0.3050230
50	H50	3.0916510	2.0009560	0.1208870
51	H51	3.5132670	2.6623520	-1.3173160

52	C52	5.1382820	2.5419380	0.0022440
53	H53	5.6562360	3.3994600	-0.4349860
54	H54	5.2585930	2.6102710	1.0857500
55	C55	5.7402630	1.2661710	-0.6093360
56	H56	5.2899610	1.0527610	-1.5813330
57	H57	6.8084630	1.4242490	-0.7757390
58	N58	5.6340960	-0.0002320	0.2442140
59	H59	4.7230110	-0.0001390	0.7096010
60	C60	5.7399700	-1.2665780	-0.6094530
61	H61	5.2896140	-1.0530070	-1.5813890
62	H62	6.8081300	-1.4248120	-0.7759680
63	C63	5.1378950	-2.5423430	0.0020180
64	H64	5.2586820	-2.6110630	1.0854470
65	H65	5.6554570	-3.3998390	-0.4357320
66	N66	3.6705370	-2.7295310	-0.3046590
67	H67	3.5121850	-2.6615410	-1.3168170
68	H68	3.0913870	-2.0011870	0.1221230
69	C69	3.0259530	-4.0680280	0.1478550
70	H70	3.4420980	-4.8371700	-0.5058800
71	H71	3.3567710	-4.2397320	1.1730180
72	C72	1.5295390	-3.9259440	0.0339300
73	C73	0.7464270	-3.7747040	1.1815340
74	H74	1.1986510	-3.8128280	2.1673250
75	C75	0.9104610	-3.9653780	-1.2182790
76	H76	1.4841650	-4.1652970	-2.1195690
77	C77	6.6858840	-0.0004030	1.3414180
78	H78	6.5656900	-0.8903140	1.9574910
79	H79	7.6668960	-0.0005670	0.8652120
80	H80	6.5659930	0.8895520	1.9574850
81	F81	-3.0335200	0.0000090	-0.2007090

Table S3. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(Cl)]^{5+}$ in gas phase. Total energy: -1806.198089 au.

1	C1	-0.4941290	3.9737680	1.2557190
2	H2	-0.9831190	3.8989430	2.2206280
3	C3	-1.2501280	4.0544780	0.0843800
4	C4	-0.6010380	4.2198090	-1.1405330
5	H5	-1.1661870	4.3648910	-2.0564480
6	C6	-2.7610340	4.0339660	0.1685980
7	H7	-3.0938150	4.0571020	1.2064800
8	H8	-3.2132330	4.8749350	-0.3617360
9	N9	-3.3275800	2.7633230	-0.4435830
10	H10	-2.7679240	1.9389940	-0.1249750
11	H11	-3.1979430	2.8065260	-1.4592440
12	C12	-4.7845010	2.5337870	-0.1361830

13	H13	-5.3373170	3.3830260	-0.5432030
14	H14	-4.8870240	2.5655510	0.9492340
15	C15	-5.3470470	1.2465990	-0.7523050
16	H16	-4.8974400	1.0631840	-1.7305970
17	H17	-6.4231450	1.3650420	-0.8986480
18	N18	-5.1502270	0.0001790	0.0841740
19	H19	-4.1468950	0.0000580	0.3805970
20	C20	-5.3474420	-1.2463160	-0.7521060
21	H21	-4.8981220	-1.0630880	-1.7305640
22	H22	-6.4235990	-1.3646630	-0.8981070
23	C23	-4.7848550	-2.5334740	-0.1359640
24	H24	-4.8871830	-2.5651100	0.9494770
25	H25	-5.3377910	-3.3827270	-0.5427930
26	N26	-3.3279960	-2.7631300	-0.4435760
27	H27	-3.1985000	-2.8063720	-1.4592530
28	H28	-2.7682260	-1.9388540	-0.1250490
29	C29	-2.7614760	-4.0338060	0.1685730
30	H30	-3.2137120	-4.8747490	-0.3617690
31	H31	-3.0942480	-4.0569470	1.2064580
32	C32	-1.2505710	-4.0543720	0.0843480
33	C33	-0.4945710	-3.9737040	1.2556880
34	H34	-0.9835580	-3.8988550	2.2205970
35	C35	-0.6014870	-4.2197290	-1.1405650
36	H36	-1.1666400	-4.3647750	-2.0564820
37	C37	-6.0385950	0.0003990	1.2956510
38	H38	-5.8349530	-0.8817630	1.8980710
39	H39	-7.0788990	0.0008180	0.9690570
40	H40	-5.8342640	0.8822660	1.8982670
41	C41	0.7878500	-4.2590710	-1.2031020
42	H42	1.2716340	-4.4182250	-2.1612480
43	C43	1.5414860	-4.1692650	-0.0305290
44	C44	0.8915330	-4.0496360	1.2008900
45	H45	1.4514120	-4.0685060	2.1325320
46	C46	3.0470300	-4.2157170	-0.0844180
47	H47	3.4292960	-4.4775610	-1.0719000
48	H48	3.4890090	-4.8724410	0.6678690
49	N49	3.5764300	-2.7914710	0.2320560
50	H50	3.0091880	-2.1624640	-0.3438660
51	H51	3.3115590	-2.6023480	1.2055120
52	C52	5.0569050	-2.5669570	0.0379610
53	H53	5.5611960	-3.3890990	0.5525010
54	H54	5.2702500	-2.6763570	-1.0273290
55	C55	5.5822750	-1.2593660	0.6501140
56	H56	5.0890600	-1.0543100	1.6030100
57	H57	6.6490290	-1.3773990	0.8563810
58	N58	5.4663190	-0.0002220	-0.2119770

59	H59	4.5486390	-0.0001670	-0.6643940
60	C60	5.5824670	1.2589560	0.6500430
61	H61	5.0892960	1.0540040	1.6029830
62	H62	6.6492490	1.3768890	0.8562290
63	C63	5.0571940	2.5665680	0.0378570
64	H64	5.2704750	2.6758910	-1.0274540
65	H65	5.5616080	3.3886830	0.5523190
66	N66	3.5767580	2.7912480	0.2320530
67	H67	3.3119390	2.6021710	1.2055330
68	H68	3.0094070	2.1622900	-0.3438140
69	C69	3.0474820	4.2155430	-0.0844060
70	H70	3.4895250	4.8722230	0.6678810
71	H71	3.4297610	4.4773600	-1.0718900
72	C72	1.5419350	4.1692120	-0.0305050
73	C73	0.7883010	4.2590700	-1.2030750
74	H74	1.2720890	4.4182010	-2.1612220
75	C75	0.8919790	4.0496250	1.2009170
76	H76	1.4518640	4.0684560	2.1325560
77	C77	6.5090870	-0.0003340	-1.3154090
78	H78	6.3850430	0.8884270	-1.9318100
79	H79	7.4938610	-0.0004500	-0.8468720
80	H80	6.3848360	-0.8890570	-1.9318240
81	Cl81	-2.0937250	0.0000400	0.2567330

Table S4. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(Br)]^{5+}$ in gas phase. Total energy: -3920.175348 au.

1	C1	-0.4070760	-4.1172020	-1.2153220
2	H2	-0.9042850	-4.0969070	-2.1787080
3	C3	-1.1530020	-4.1367900	-0.0351850
4	C4	-0.4943330	-4.2349410	1.1917980
5	H5	-1.0518420	-4.3339540	2.1184690
6	C6	-2.6643350	-4.1097630	-0.1071260
7	H7	-3.0067010	-4.1531760	-1.1412290
8	H8	-3.1201820	-4.9332860	0.4469370
9	N9	-3.2093970	-2.8174650	0.4815200
10	H10	-2.6162870	-2.0170810	0.1649340
11	H11	-3.0996320	-2.8526750	1.4998280
12	C12	-4.6507760	-2.5445800	0.1430690
13	H13	-5.2366650	-3.3786810	0.5349040
14	H14	-4.7301010	-2.5706610	-0.9443110
15	C15	-5.1878940	-1.2432130	0.7530620
16	H16	-4.7362010	-1.0646850	1.7313240
17	H17	-6.2664090	-1.3391970	0.8981720
18	N18	-4.9706520	0.0006850	-0.0835410
19	H19	-3.9655950	0.0003900	-0.3694350

20	C20	-5.1866650	1.2438430	0.7544660
21	H21	-4.7336340	1.0642450	1.7319180
22	H22	-6.2649700	1.3398040	0.9011370
23	C23	-4.6503100	2.5458930	0.1452910
24	H24	-4.7323550	2.5740870	-0.9418250
25	H25	-5.2348320	3.3795350	0.5401540
26	N26	-3.2080160	2.8174180	0.4809490
27	H27	-3.0961250	2.8509120	1.4990910
28	H28	-2.6159250	2.0171470	0.1621900
29	C29	-2.6633360	4.1103260	-0.1065980
30	H30	-3.1190800	4.9332450	0.4484620
31	H31	-3.0060240	4.1547340	-1.1405520
32	C32	-1.1519920	4.1373230	-0.0349180
33	C33	-0.4061900	4.1200660	-1.2151490
34	H34	-0.9034750	4.1019260	-2.1785390
35	C35	-0.4931850	4.2329980	1.1921860
36	H36	-1.0506240	4.3302540	2.1190910
37	C37	-5.8408850	0.0016830	-1.3089840
38	H38	-5.6261010	0.8827590	-1.9089560
39	H39	-6.8859260	0.0034870	-0.9977770
40	H40	-5.6291370	-0.8806900	-1.9081480
41	C41	0.8963890	4.2598720	1.2452690
42	H42	1.3888620	4.3653760	2.2064350
43	C43	1.6405230	4.2262750	0.0633150
44	C44	0.9810170	4.1820650	-1.1676410
45	H45	1.5348290	4.2445670	-2.1008350
46	C46	3.1463650	4.2462870	0.1100970
47	H47	3.5378340	4.4802870	1.1009690
48	H48	3.5959920	4.9110650	-0.6303390
49	N49	3.6504480	2.8197710	-0.2377640
50	H50	3.0723030	2.1872490	0.3236320
51	H51	3.3833980	2.6556250	-1.2153010
52	C52	5.1269380	2.5697860	-0.0470870
53	H53	5.6431010	3.3874510	-0.5568070
54	H54	5.3426910	2.6698280	1.0185940
55	C55	5.6321060	1.2574470	-0.6663910
56	H56	5.1244690	1.0557560	-1.6124190
57	H57	6.6971150	1.3654220	-0.8867200
58	N58	5.5174300	-0.0004490	0.1973500
59	H59	4.6005240	-0.0003150	0.6515660
60	C60	5.6317650	-1.2584560	-0.6662920
61	H61	5.1241330	-1.0566950	-1.6123070
62	H62	6.6967370	-1.3666870	-0.8866570
63	C63	5.1262800	-2.5706240	-0.0468770
64	H64	5.3418460	-2.6705710	1.0188500
65	H65	5.6423680	-3.3884540	-0.5564110

66	N66	3.6497810	-2.8203410	-0.2377890
67	H67	3.3829630	-2.6561170	-1.2153720
68	H68	3.0716000	-2.1877290	0.3234800
69	C69	3.1453260	-4.2467510	0.1099060
70	H70	3.5947660	-4.9115560	-0.6306240
71	H71	3.5367160	-4.4810110	1.1007460
72	C72	1.6394810	-4.2262880	0.0631130
73	C73	0.8952460	-4.2620170	1.2449350
74	H74	1.3876290	-4.3693070	2.2059470
75	C75	0.9801000	-4.1795840	-1.1678270
76	H76	1.5339510	-4.2404700	-2.1011110
77	C77	6.5636450	-0.0005480	1.2970830
78	H78	6.4414760	-0.8887580	1.9145250
79	H79	7.5469390	-0.0009700	0.8254140
80	H80	6.4420810	0.8880320	1.9141110
81	Br81	-1.7363020	-0.0005580	-0.2588780

Table S5. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(I)]^{5+}$ in gas phase. Total energy: -1357.336447 au.

1	C1	-0.4162350	-4.2882410	-1.1828150
2	H2	-0.9241700	-4.3044760	-2.1406910
3	C3	-1.1475860	-4.2837990	0.0059800
4	C4	-0.4773950	-4.3392740	1.2290360
5	H5	-1.0261240	-4.4194740	2.1627430
6	C6	-2.6580040	-4.2433310	-0.0447970
7	H7	-3.0231660	-4.3455390	-1.0668760
8	H8	-3.1209990	-5.0152310	0.5735150
9	N9	-3.1563720	-2.8973290	0.4705780
10	H10	-2.5133580	-2.1524150	0.1309390
11	H11	-3.0554550	-2.8864000	1.4909620
12	C12	-4.5779610	-2.5729110	0.1007290
13	H13	-5.2034110	-3.3693110	0.5103970
14	H14	-4.6465580	-2.6325210	-0.9856110
15	C15	-5.0783210	-1.2396930	0.6696480
16	H16	-4.6742650	-1.0757910	1.6714020
17	H17	-6.1668660	-1.2849540	0.7534760
18	N18	-4.7651290	-0.0019840	-0.1493750
19	H19	-3.7401220	-0.0014300	-0.3334780
20	C20	-5.0798110	1.2358010	0.6689740
21	H21	-4.6760910	1.0727100	1.6709950
22	H22	-6.1684310	1.2801050	0.7522880
23	C23	-4.5803650	2.5691960	0.0996470
24	H24	-4.6481070	2.6280320	-0.9867910
25	H25	-5.2069540	3.3652280	0.5082820
26	N26	-3.1593960	2.8952610	0.4704040

27	H27	-3.0592060	2.8849830	1.4908650
28	H28	-2.5154120	2.1508440	0.1315430
29	C29	-2.6620060	4.2415070	-0.0453220
30	H30	-3.1257410	5.0132430	0.5726350
31	H31	-3.0270420	4.3430860	-1.0675110
32	C32	-1.1516300	4.2831630	0.0057060
33	C33	-0.4201070	4.2875220	-1.1829840
34	H34	-0.9279130	4.3029190	-2.1409410
35	C35	-0.4816610	4.3397160	1.2288360
36	H36	-1.0305880	4.4200000	2.1624190
37	C37	-5.4941750	-0.0027250	-1.4638670
38	H38	-5.2153900	0.8775630	-2.0375020
39	H39	-6.5674530	-0.0034260	-1.2705120
40	H40	-5.2141720	-0.8828000	-2.0372340
41	C41	0.9079490	4.3417550	1.2679800
42	H42	1.4127750	4.4134270	2.2258160
43	C43	1.6384710	4.3207580	0.0775400
44	C44	0.9680780	4.3229080	-1.1479400
45	H45	1.5153770	4.3964490	-2.0840020
46	C46	3.1437670	4.2955370	0.1106870
47	H47	3.5506560	4.5119410	1.0993260
48	H48	3.6065230	4.9509730	-0.6299650
49	N49	3.6014380	2.8574850	-0.2489450
50	H50	3.0126890	2.2354500	0.3141450
51	H51	3.3197270	2.7044960	-1.2243000
52	C52	5.0735250	2.5764320	-0.0736860
53	H53	5.6003390	3.3850460	-0.5868150
54	H54	5.3012970	2.6712550	0.9898170
55	C55	5.5490960	1.2565470	-0.6987770
56	H56	5.0233340	1.0598060	-1.6359280
57	H57	6.6119570	1.3486210	-0.9361690
58	N58	5.4315830	0.0017870	0.1676680
59	H59	4.5117590	0.0008670	0.6164820
60	C60	5.5518120	-1.2531140	-0.6982830
61	H61	5.0273980	-1.0572690	-1.6363730
62	H62	6.6151560	-1.3442430	-0.9338850
63	C63	5.0765810	-2.5731900	-0.0733750
64	H64	5.3033940	-2.6675480	0.9903820
65	H65	5.6044770	-3.3815540	-0.5857930
66	N66	3.6048600	-2.8553900	-0.2498920
67	H67	3.3240170	-2.7032960	-1.2256350
68	H68	3.0151400	-2.2333710	0.3121920
69	C69	3.1478540	-4.2934910	0.1104400
70	H70	3.6109350	-4.9490800	-0.6298720
71	H71	3.5548600	-4.5091980	1.0991820
72	C72	1.6425610	-4.3195230	0.0774100

73	C73	0.9122160	-4.3403910	1.2679670
74	H74	1.4172360	-4.4112790	2.2257600
75	C75	0.9719850	-4.3226950	-1.1479690
76	H76	1.5191830	-4.3963170	-2.0840810
77	C77	6.4738980	0.0030220	1.2701510
78	H78	6.3524380	-0.8857450	1.8866730
79	H79	7.4588230	0.0059040	0.8018430
80	H80	6.3480880	0.8896820	1.8888300
81	I81	-1.2270690	-0.0001450	-0.1241800

Table S6. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(F)_2]^{4+}$ in gas phase. Total energy: -1546.315507 au.

1	C1	0.5728670	3.6526120	-1.2339990
2	H2	1.0095810	3.7673450	-2.2197800
3	C3	1.3912940	3.5460540	-0.1097410
4	C4	0.8053600	3.4454640	1.1523360
5	H5	1.4114260	3.4282680	2.0536720
6	C6	2.8905490	3.6371030	-0.2716040
7	H7	3.1676660	3.6615510	-1.3256590
8	H8	3.2942020	4.5289860	0.2141550
9	N9	3.5975350	2.4473550	0.3352800
10	H10	3.2023980	1.5363650	-0.0285450
11	H11	3.4245700	2.4487680	1.3436410
12	C12	5.0814440	2.4518630	0.0927480
13	H13	5.4842210	3.3688030	0.5262520
14	H14	5.2241220	2.5048900	-0.9879000
15	C15	5.8029460	1.2524200	0.7129130
16	H16	5.4017030	1.0447320	1.7067160
17	H17	6.8615260	1.4939940	0.8298320
18	N18	5.6899460	-0.0001070	-0.1127100
19	H19	4.6573560	-0.0001110	-0.4544940
20	C20	5.8029490	-1.2526150	0.7129530
21	H21	5.4017440	-1.0448840	1.7067620
22	H22	6.8615280	-1.4942020	0.8298410
23	C23	5.0813880	-2.4520520	0.0928420
24	H24	5.2239860	-2.5050630	-0.9878180
25	H25	5.4841840	-3.3690040	0.5263030
26	N26	3.5975000	-2.4474720	0.3354820
27	H27	3.4246300	-2.4491170	1.3438570
28	H28	3.2024740	-1.5363040	-0.0281580
29	C29	2.8903760	-3.6369860	-0.2716460
30	H30	3.2939760	-4.5290420	0.2138460
31	H31	3.1674220	-3.6611930	-1.3257250
32	C32	1.3911250	-3.5458980	-0.1097100
33	C33	0.5726650	-3.6530770	-1.2338840

34	H34	1.0093590	-3.7682300	-2.2196250
35	C35	0.8052220	-3.4447270	1.1523350
36	H36	1.4112900	-3.4270490	2.0536590
37	C37	6.6563220	-0.0001310	-1.2525000
38	H38	6.4963040	-0.8839060	-1.8672670
39	H39	7.6741190	-0.0001030	-0.8607740
40	H40	6.4962780	0.8835920	-1.8673340
41	C41	-0.5774280	-3.4231300	1.2876570
42	H42	-1.0138240	-3.3581110	2.2779830
43	C43	-1.3953790	-3.5459080	0.1651060
44	C44	-0.8094370	-3.6746620	-1.0946180
45	H45	-1.4182640	-3.8367110	-1.9797600
46	C46	-2.8941470	-3.6209570	0.3298800
47	H47	-3.1765650	-3.6011390	1.3826480
48	H48	-3.3038000	-4.5262750	-0.1241060
49	N49	-3.5848620	-2.4467720	-0.3270480
50	H50	-3.2055540	-1.5281810	0.0365240
51	H51	-3.3710210	-2.4678230	-1.3277300
52	C52	-5.0759260	-2.4511400	-0.1384540
53	H53	-5.4637130	-3.3693270	-0.5827400
54	H54	-5.2580710	-2.5002090	0.9365250
55	C55	-5.7729140	-1.2526860	-0.7878680
56	H56	-5.3313720	-1.0447320	-1.7642640
57	H57	-6.8258390	-1.4938250	-0.9477200
58	N58	-5.6938620	0.0000330	0.0417770
59	H59	-4.6793260	-0.0000110	0.4255980
60	C60	-5.7727180	1.2526740	-0.7879980
61	H61	-5.3310380	1.0445840	-1.7643030
62	H62	-6.8256050	1.4938500	-0.9480330
63	C63	-5.0757570	2.4511800	-0.1386430
64	H64	-5.2580100	2.5003930	0.9363110
65	H65	-5.4634790	3.3693200	-0.5830840
66	N66	-3.5846760	2.4467400	-0.3270930
67	H67	-3.3707510	2.4676030	-1.3277600
68	H68	-3.2054610	1.5281520	0.0366490
69	C69	-2.8939970	3.6210170	0.3296810
70	H70	-3.3036330	4.5262690	-0.1244560
71	H71	-3.1764530	3.6013650	1.3824410
72	C72	-1.3952150	3.5459710	0.1649830
73	C73	-0.5772910	3.4238240	1.2876260
74	H74	-1.0137120	3.3592740	2.2779700
75	C75	-0.8092420	3.6741410	-1.0947840
76	H76	-1.4180440	3.8356920	-1.9800350
77	C77	-6.7068420	0.0001590	1.1408420
78	H78	-6.5730550	0.8839560	1.7618660
79	H79	-7.7072280	0.0003950	0.7064820

80	H80	-6.5734320	-0.8838010	1.7617180
81	F81	3.2569500	-0.0001730	-0.3916370
82	F82	-3.2679700	0.0000290	0.4091150

Table S7. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(Cl)_2]^{4+}$ in gas phase. Total energy: -2267.041014 au.

1	C1	0.6305920	4.0625610	-1.1746830
2	H2	1.1088540	4.2218170	-2.1344840
3	C3	1.3978560	3.8849140	-0.0245930
4	C4	0.7628470	3.7188180	1.2063060
5	H5	1.3331910	3.6416130	2.1275230
6	C6	2.9038550	3.9316410	-0.1192030
7	H7	3.2290680	4.0265260	-1.1554390
8	H8	3.3316900	4.7519920	0.4618640
9	N9	3.5148490	2.6485710	0.4116050
10	H10	2.9979810	1.8316990	0.0011550
11	H11	3.3510180	2.6065590	1.4213200
12	C12	4.9823290	2.5094740	0.1274840
13	H13	5.4823220	3.3757800	0.5650760
14	H14	5.1006220	2.5712240	-0.9551490
15	C15	5.6069180	1.2428880	0.7209880
16	H16	5.2070760	1.0565250	1.7202540
17	H17	6.6843890	1.3926960	0.8200900
18	N18	5.3991020	-0.0047600	-0.1011650
19	H19	4.3830820	-0.0031420	-0.4109630
20	C20	5.6027750	-1.2528190	0.7213720
21	H21	5.2027450	-1.0650690	1.7203070
22	H22	6.6797510	-1.4056270	0.8213140
23	C23	4.9751390	-2.5178870	0.1278420
24	H24	5.0940630	-2.5804090	-0.9546760
25	H25	5.4725150	-3.3853500	0.5661240
26	N26	3.5070830	-2.6530650	0.4109620
27	H27	3.3425940	-2.6097130	1.4205160
28	H28	2.9925630	-1.8352300	-0.0004610
29	C29	2.8935320	-3.9351880	-0.1190720
30	H30	3.3197990	-4.7560070	0.4625040
31	H31	3.2185850	-4.0313550	-1.1552390
32	C32	1.3875970	-3.8858110	-0.0245130
33	C33	0.6200670	-4.0656670	-1.1740770
34	H34	1.0981200	-4.2279440	-2.1334790
35	C35	0.7528170	-3.7156830	1.2059600
36	H36	1.3232010	-3.6366160	2.1269930
37	C37	6.2483290	-0.0062810	-1.3353940
38	H38	6.0180730	-0.8863790	-1.9314440
39	H39	7.2995330	-0.0082090	-1.0460010

40	H40	6.0213090	0.8747740	-1.9312840
41	C41	-0.6332840	-3.6922640	1.2839870
42	H42	-1.1116150	-3.5612780	2.2480710
43	C43	-1.4006880	-3.8840760	0.1357300
44	C44	-0.7663490	-4.0868340	-1.0896380
45	H45	-1.3414100	-4.2973890	-1.9868800
46	C46	-2.9056300	-3.9046750	0.2296330
47	H47	-3.2398120	-3.9064690	1.2675160
48	H48	-3.3434090	-4.7611130	-0.2873720
49	N49	-3.4865200	-2.6556610	-0.4094630
50	H50	-2.9988710	-1.8190990	-0.0028780
51	H51	-3.2507150	-2.6666050	-1.4062200
52	C52	-4.9686340	-2.5087820	-0.2285700
53	H53	-5.4422970	-3.3780720	-0.6884770
54	H54	-5.1610290	-2.5574990	0.8441380
55	C55	-5.5440080	-1.2446740	-0.8746410
56	H56	-5.0651540	-1.0596560	-1.8387210
57	H57	-6.6102320	-1.3936160	-1.0589750
58	N58	-5.4015740	0.0041970	-0.0397620
59	H59	-4.4143340	0.0017180	0.3475310
60	C60	-5.5354160	1.2515480	-0.8781680
61	H61	-5.0512870	1.0624160	-1.8388240
62	H62	-6.6000660	1.4030350	-1.0692860
63	C63	-4.9600590	2.5159940	-0.2326520
64	H64	-5.1564570	2.5679000	0.8391570
65	H65	-5.4302910	3.3850840	-0.6964270
66	N66	-3.4770530	2.6593710	-0.4088560
67	H67	-3.2381500	2.6675710	-1.4049170
68	H68	-2.9925600	1.8223370	0.0005380
69	C69	-2.8953800	3.9085750	0.2289430
70	H70	-3.3320600	4.7647520	-0.2894530
71	H71	-3.2300450	3.9121220	1.2666600
72	C72	-1.3904170	3.8864120	0.1354920
73	C73	-0.6232940	3.6969720	1.2843160
74	H74	-1.1018040	3.5690960	2.2487290
75	C75	-0.7557910	4.0853590	-1.0903620
76	H76	-1.3305690	4.2941910	-1.9881990
77	C77	-6.3495090	0.0087930	1.1205690
78	H78	-6.1621610	0.8843230	1.7380380
79	H79	-7.3727420	0.0214710	0.7444780
80	H80	-6.1817440	-0.8769470	1.7290750
81	Cl81	2.4783660	-0.0004470	-0.7497490
82	Cl82	-2.5219960	-0.0000730	0.7988490

Table S8. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(Br)_2]^{4+}$ in gas phase.

Total energy: -6494.993578 au.

1	C1	0.6903180	4.1148160	-1.1585490
2	H2	1.1941860	4.2688020	-2.1059880
3	C3	1.4259680	3.9458870	0.0132710
4	C4	0.7579760	3.7881630	1.2276770
5	H5	1.3041410	3.7181200	2.1640160
6	C6	2.9344910	3.9800280	-0.0392260
7	H7	3.2906370	4.0875080	-1.0640060
8	H8	3.3554560	4.7845440	0.5681540
9	N9	3.5116900	2.6785720	0.4873340
10	H10	2.9815060	1.8818880	0.0544900
11	H11	3.3280860	2.6272020	1.4931910
12	C12	4.9785150	2.5053060	0.2241300
13	H13	5.4915400	3.3626740	0.6642410
14	H14	5.1122330	2.5577920	-0.8572000
15	C15	5.5651940	1.2281640	0.8344250
16	H16	5.1295820	1.0451310	1.8192110
17	H17	6.6407050	1.3624400	0.9703340
18	N18	5.3726760	-0.0180540	0.0050610
19	H19	4.3721320	-0.0111000	-0.3439840
20	C20	5.5460760	-1.2649300	0.8373650
21	H21	5.1058420	-1.0752100	1.8188400
22	H22	6.6191340	-1.4104910	0.9808420
23	C23	4.9499720	-2.5374140	0.2263790
24	H24	5.0889630	-2.5939390	-0.8540530
25	H25	5.4524400	-3.3986350	0.6711080
26	N26	3.4802170	-2.6964150	0.4825740
27	H27	3.2918810	-2.6389000	1.4872570
28	H28	2.9592330	-1.8967570	0.0445930
29	C29	2.8947160	-3.9954760	-0.0405250
30	H30	3.3100880	-4.8007530	0.5697090
31	H31	3.2508460	-4.1084750	-1.0647050
32	C32	1.3864370	-3.9518900	0.0114230
33	C33	0.6497750	-4.1205230	-1.1598160
34	H34	1.1527700	-4.2800420	-2.1068070
35	C35	0.7193790	-3.7870200	1.2253940
36	H36	1.2659390	-3.7170560	2.1615240
37	C37	6.2613560	-0.0256790	-1.2017680
38	H38	6.0400800	-0.9017060	-1.8072310
39	H39	7.3023320	-0.0390600	-0.8780780
40	H40	6.0618210	0.8592280	-1.8019280
41	C41	-0.6681630	-3.7548660	1.2656740
42	H42	-1.1718010	-3.6263400	2.2170960
43	C43	-1.4051150	-3.9315130	0.0950470
44	C44	-0.7388010	-4.1320160	-1.1135490

45	H45	-1.2905420	-4.3320810	-2.0276300
46	C46	-2.9126380	-3.9345520	0.1475930
47	H47	-3.2743920	-3.9303010	1.1762090
48	H48	-3.3476690	-4.7854070	-0.3808120
49	N49	-3.4597420	-2.6771920	-0.5062590
50	H5	-2.9648370	-1.8540310	-0.0819680
51	H51	-3.2044380	-2.6919040	-1.4980380
52	C52	-4.9408540	-2.4997770	-0.3500420
53	H53	-5.4233310	-3.3676860	-0.8031460
54	H54	-5.1473630	-2.5266850	0.7208970
55	C55	-5.4824550	-1.2339490	-1.0225980
56	H56	-4.9644080	-1.0524730	-1.9667940
57	H57	-6.5410410	-1.3769290	-1.2501870
58	N58	-5.3708710	0.0166530	-0.1849370
59	H59	-4.4106970	0.0079470	0.2617610
60	C60	-5.4520280	1.2628080	-1.0320510
61	H61	-4.9174230	1.0675830	-1.9642530
62	H62	-6.5042570	1.4155240	-1.2814890
63	C63	-4.9084800	2.5284710	-0.3603470
64	H64	-5.1257320	2.5636080	0.7081160
65	H65	-5.3800340	3.3972540	-0.8231080
66	N66	-3.4247400	2.6940770	-0.5041280
67	H67	-3.1613860	2.7027380	-1.4939180
68	H68	-2.9396470	1.8683220	-0.0738490
69	C69	-2.8730940	3.9499980	0.1480920
70	H70	-3.3034160	4.8017920	-0.3827050
71	H71	-3.2361370	3.9496040	1.1762540
72	C72	-1.3655920	3.9397300	0.0966080
73	C73	-0.6297290	3.7628440	1.2678540
74	H74	-1.1341620	3.6397120	2.2195760
75	C75	-0.6981410	4.1335030	-1.1124630
76	H76	-1.2487720	4.3337440	-2.0271980
77	C77	-6.3790630	0.0321080	0.9246240
78	H78	-6.2004460	0.8936230	1.5642500
79	H79	-7.3798050	0.0776620	0.4943220
80	H80	-6.2685720	-0.8664510	1.5276440
81	Br81	2.3359140	0.0001410	-0.8637290
82	Br82	-2.4262570	0.0001780	0.9557340

Table S9. Cartesian coordinates (in Å) and total energy (in au) for $[H_6L(I)_2]^{4+}$ in gas phase. Total energy: -1369.310255 au.

1	C1	-0.7391300	-4.1973010	-1.1308140
2	H2	-1.2808380	-4.3383860	-2.0591270
3	C3	-1.4263470	-4.0353570	0.0707590

4	C4	-0.7116680	-3.8931170	1.2601840
5	H5	-1.2219670	-3.8278210	2.2169440
6	C6	-2.9355980	-4.0453430	0.0775750
7	H7	-3.3355670	-4.1683840	-0.9292040
8	H8	-3.3480850	-4.8245480	0.7223200
9	N9	-3.4633660	-2.7171180	0.5947840
10	H10	-2.9235620	-1.9536250	0.1205190
11	H11	-3.2399220	-2.6461670	1.5915320
12	C12	-4.9318950	-2.5100340	0.3728470
13	H13	-5.4506820	-3.3541020	0.8316190
14	H14	-5.0961590	-2.5650850	-0.7041640
15	C15	-5.4768280	-1.2201420	0.9947820
16	H16	-5.0148510	-1.0438360	1.9687970
17	H17	-6.5511220	-1.3344320	1.1567270
18	N18	-5.2872600	0.0254970	0.1627560
19	H19	-4.2996950	0.0147070	-0.2103220
20	C20	-5.4444860	1.2700740	1.0027520
21	H21	-4.9683740	1.0815840	1.9676710
22	H22	-6.5140520	1.3988620	1.1837360
23	C23	-4.8912800	2.5559530	0.3795550
24	H24	-5.0668050	2.6179320	-0.6952340
25	H25	-5.3952240	3.4040600	0.8472700
26	N26	-3.4182800	2.7447490	0.5873980
27	H27	-3.1863580	2.6693380	1.5819340
28	H28	-2.8923070	1.9747960	0.1079980
29	C29	-2.8792090	4.0672830	0.0681780
30	H30	-3.2850240	4.8509590	0.7117710
31	H31	-3.2779600	4.1922420	-0.9388360
32	C32	-1.3701020	4.0448120	0.0623280
33	C33	-0.6803010	4.1994280	-1.1387280
34	H34	-1.2198760	4.3426400	-2.0679500
35	C35	-0.6578380	3.8999450	1.2528870
36	H36	-1.1696990	3.8403300	2.2092030
37	C37	-6.1885700	0.0399640	-1.0350920
38	H38	-5.9555000	0.9064510	-1.6496460
39	H39	-7.2254600	0.0730360	-0.7001210
40	H40	-6.0081560	-0.8517780	-1.6310530
41	C41	0.7298160	3.8707320	1.2403580
42	H42	1.2701000	3.7542300	2.1730620
43	C43	1.4201960	4.0274370	0.0389050
44	C44	0.7090470	4.2113750	-1.1462400
45	H45	1.2260990	4.3951810	-2.0835810
46	C46	2.9282830	4.0153610	0.0346580
47	H47	3.3278880	4.0305870	1.0491590
48	H48	3.3556420	4.8456630	-0.5312270
49	N49	3.4341750	2.7320980	-0.6065220

50	H50	2.9115530	1.9379170	-0.1659100
51	H51	3.1712960	2.7383980	-1.5965480
52	C52	4.9085870	2.5087470	-0.4515100
53	H53	5.4160320	3.3600890	-0.9089750
54	H54	5.1158710	2.5350560	0.6192720
55	C55	5.4140830	1.2265240	-1.1210960
56	H56	4.8900590	1.0555870	-2.0640590
57	H57	6.4757640	1.3414990	-1.3508060
58	N58	5.2784590	-0.0241260	-0.2849470
59	H59	4.3201480	-0.0108630	0.1550810
60	C60	5.3659620	-1.2645070	-1.1417180
61	H61	4.8112760	-1.0695950	-2.0623450
62	H62	6.4170190	-1.3905250	-1.4107480
63	C63	4.8632470	-2.5510220	-0.4776870
64	H64	5.0922720	-2.5944900	0.5879230
65	H65	5.3532970	-3.4008170	-0.9563200
66	N66	3.3840620	-2.7572950	-0.6082280
67	H67	3.1057460	-2.7576900	-1.5941210
68	H68	2.8779360	-1.9571730	-0.1588830
69	C69	2.8720700	-4.0356580	0.0365840
70	H70	3.2919310	-4.8699200	-0.5291510
71	H71	3.2742670	-4.0519400	1.0500480
72	C72	1.3639250	-4.0372320	0.0439050
73	C73	0.6761610	-3.8733430	1.2458710
74	H74	1.2184620	-3.7589270	2.1776730
75	C75	0.6500300	-4.2187980	-1.1399700
76	H76	1.1647100	-4.4081250	-2.0775530
77	C77	6.2681400	-0.0510050	0.8414090
78	H78	6.0561810	-0.8998550	1.4874430
79	H79	7.2741950	-0.1237370	0.4277260
80	H80	6.1673650	0.8556900	1.4334980
81	I81	-2.1121120	0.0007590	-1.0658340
82	I82	2.1466370	-0.0020850	1.0721770