Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Imaging of Al^{3+} in plants roots by the interaction with a bisphenol A based chemosensor

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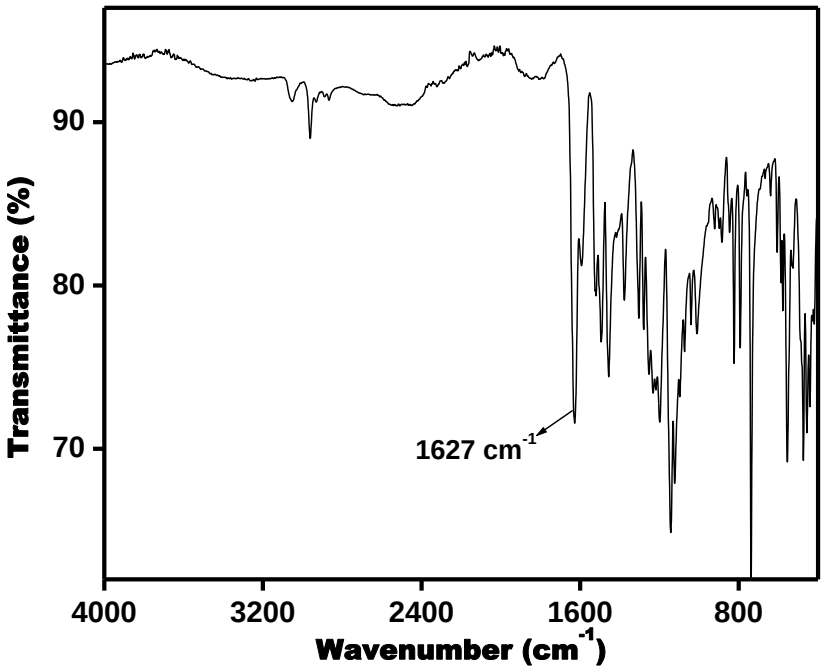


Fig. S1 FTIR spectrum of **H_4L**

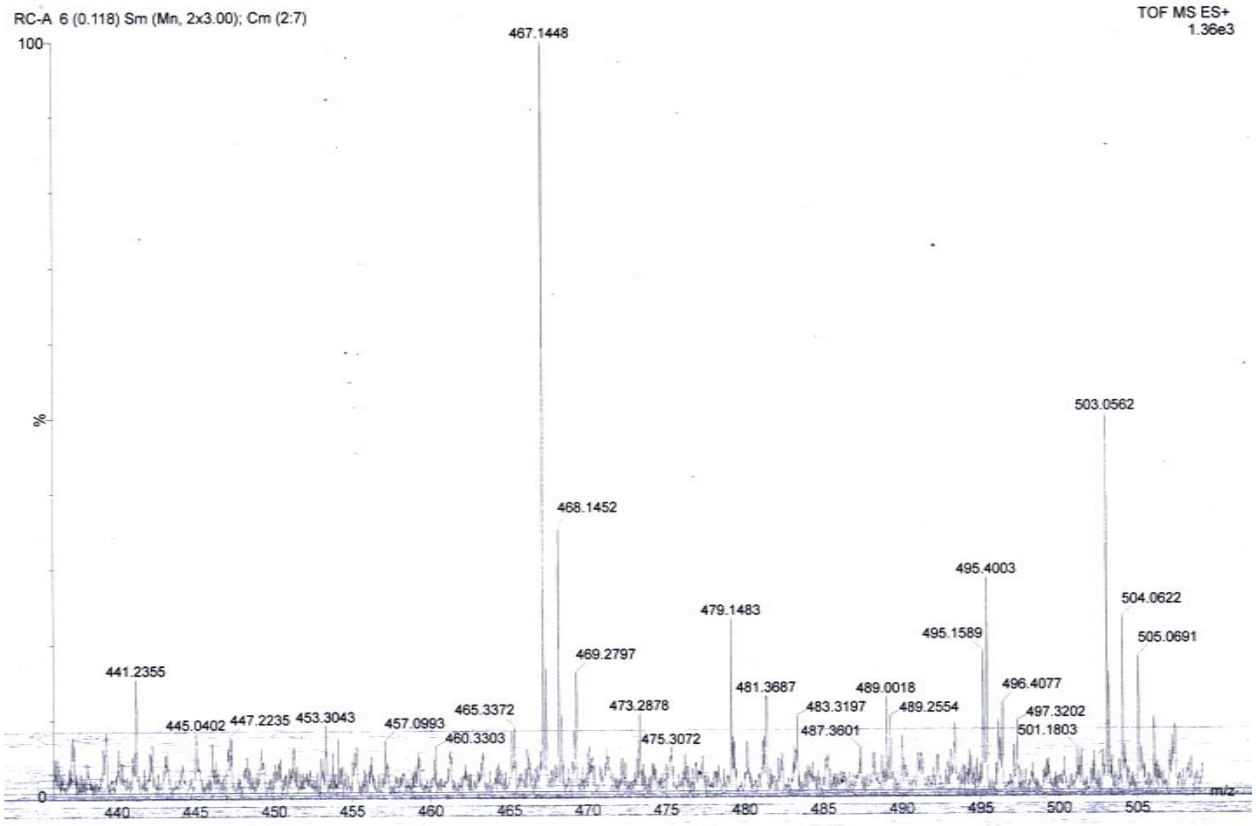


Fig. S2 ESI mass spectrum of **H_4L** in methanol

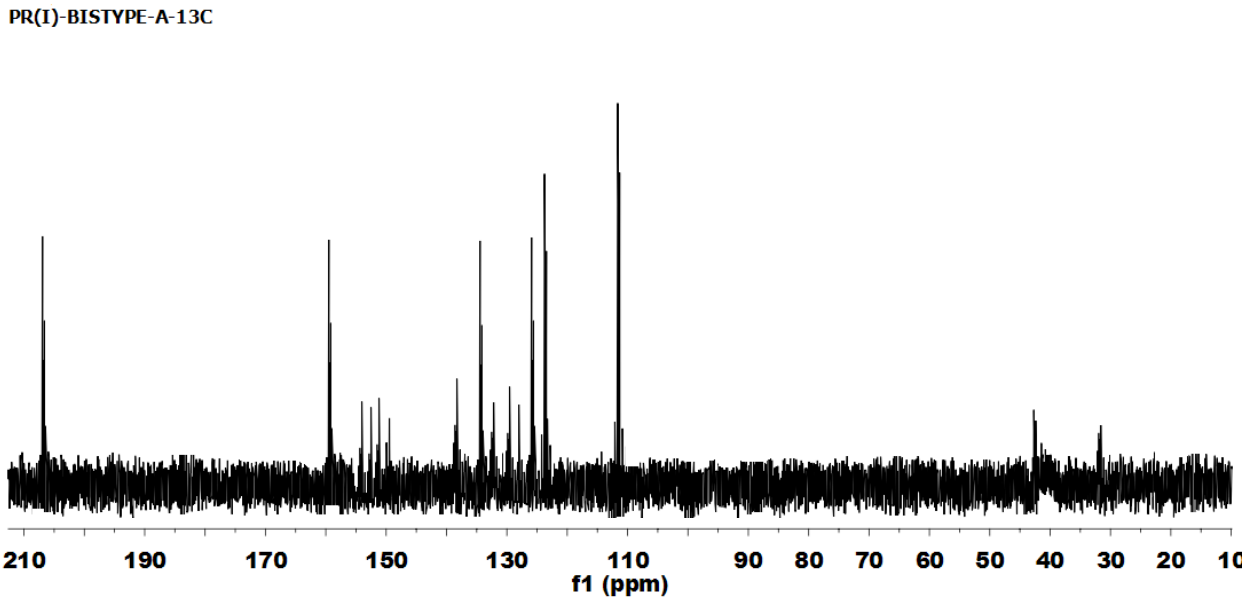


Fig. S3 ^{13}C NMR spectrum of **H_4L** in DMSO-d_6.

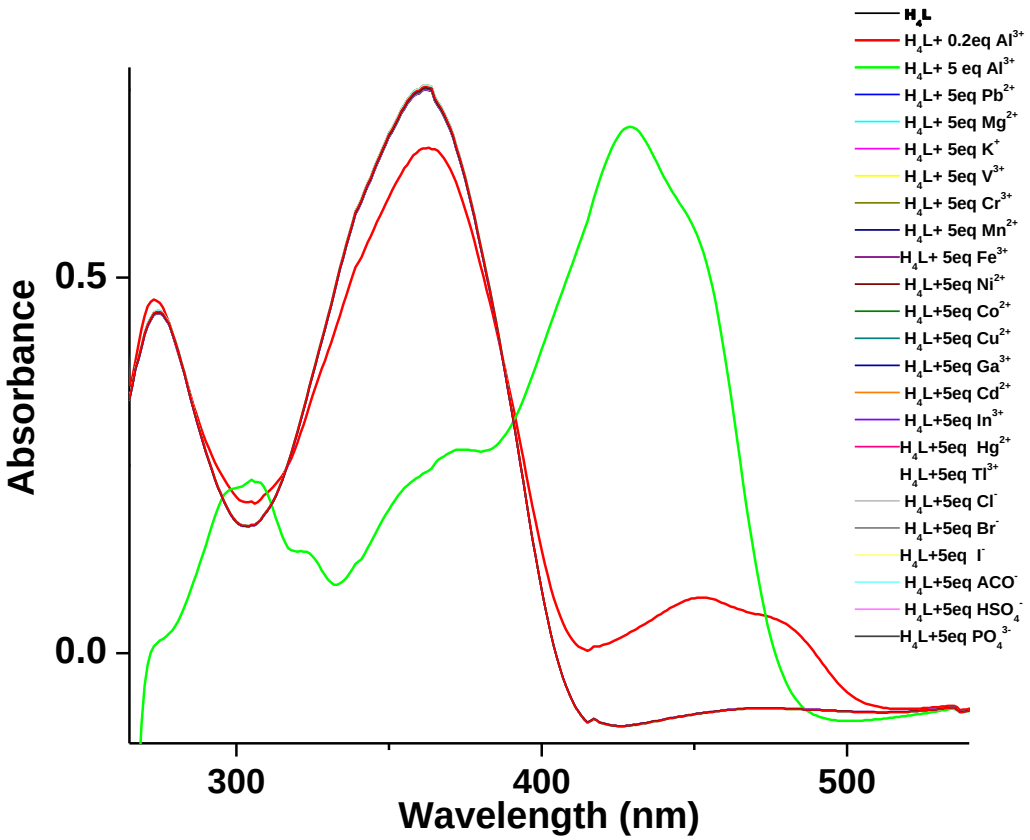


Fig. S4 Absorption spectra of **H_4L** (40 μM) in the presence of different metal ions in 10 mM HEPES buffer in H_2O/DMF = 4:1 (v/v) (pH 7.4)

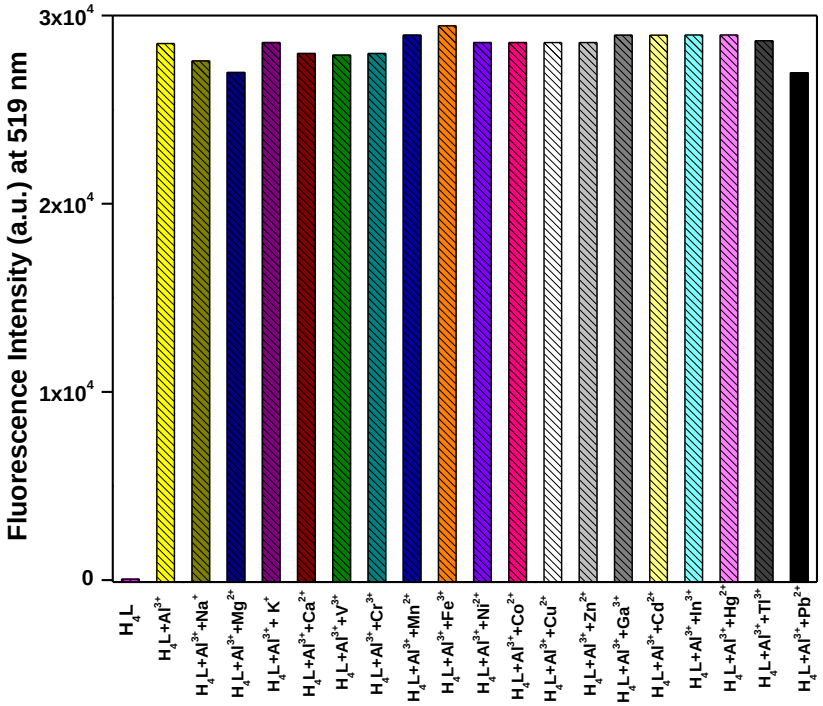


Fig. S5 Fluorescence intensity of $\mathbf{H_4L}$+Al^{3+} in the presence of different metal ions in 10 mM HEPES buffer in H_2O/DMF = 4:1 (v/v) (pH 7.4)

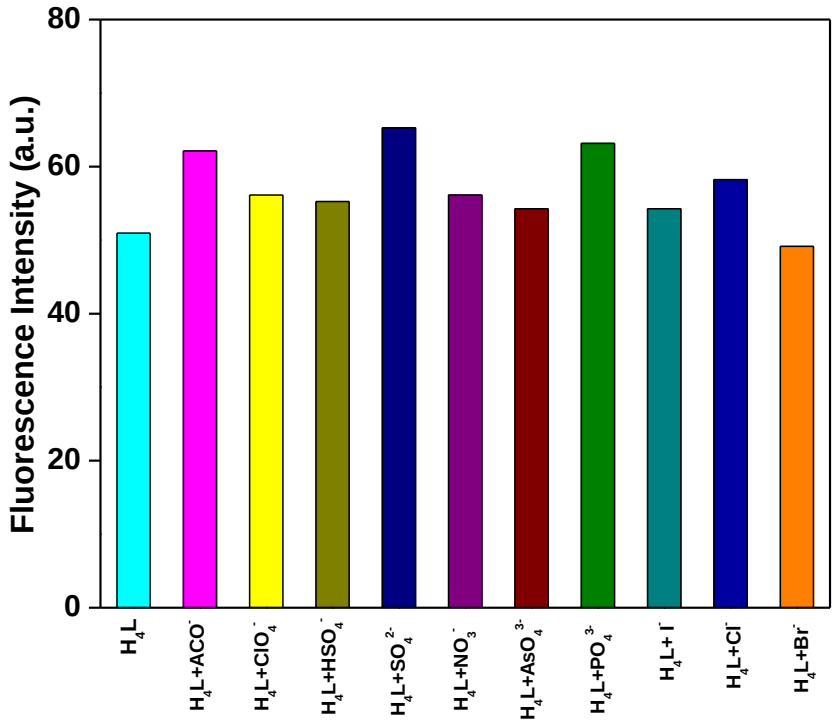


Fig. S6 Fluorescence intensity of $\mathbf{H_4L}$ (40 μM) in the presence of different anions in 10 mM HEPES buffer in H_2O/DMF = 4:1 (v/v) (pH 7.4)

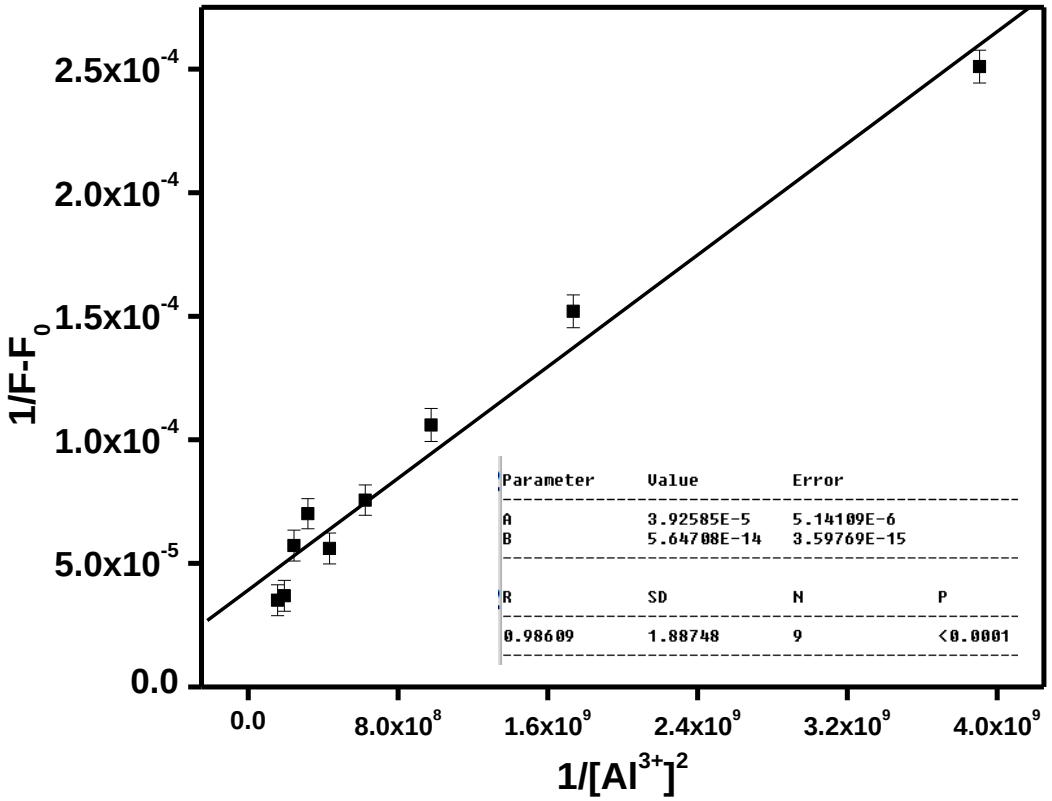


Fig. S7 A plot of $1/(F-F_0)$ vs. $1/[Al^{3+}]^2$ for the determination of association constant.

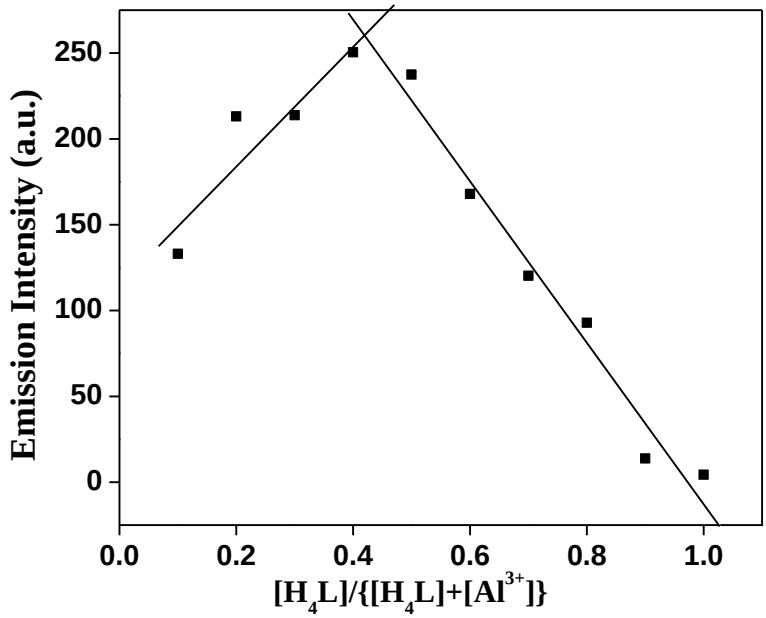


Fig. S8 Job's plot analysis indicating 1:2 (L/M) stoichiometry.

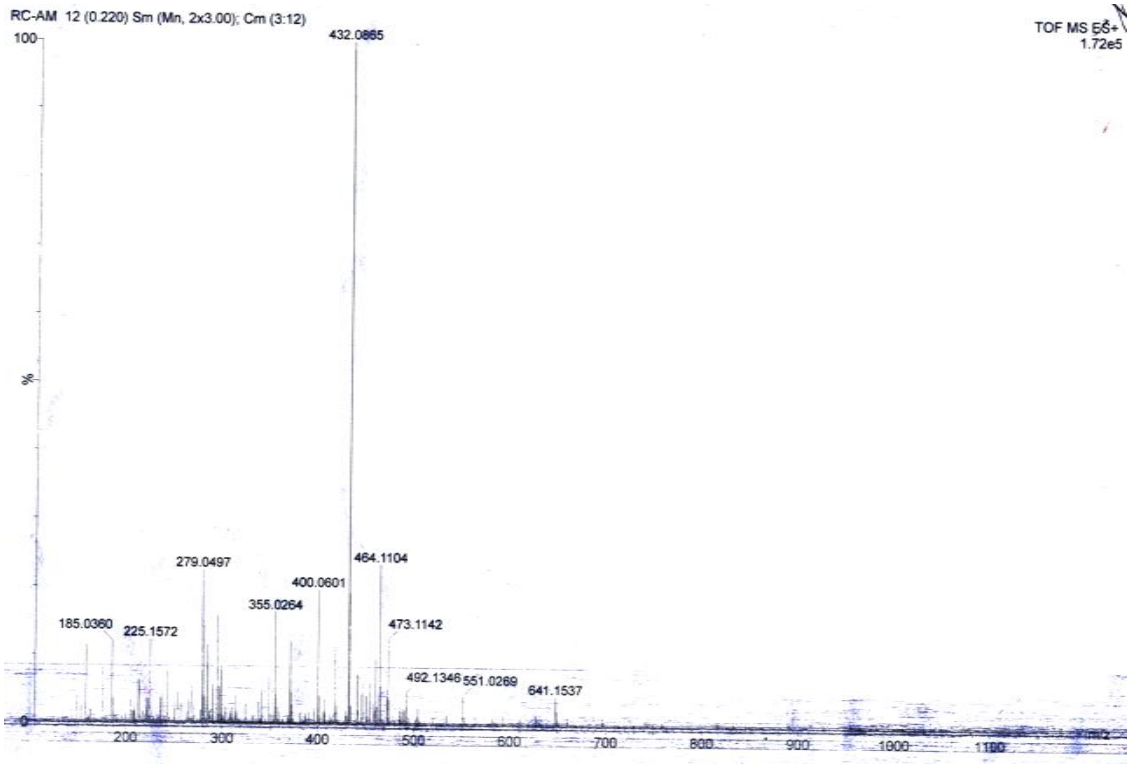


Fig. S9 ESI mass spectrum of **H_4L** with $Al(NO_3)_3$ in methanol

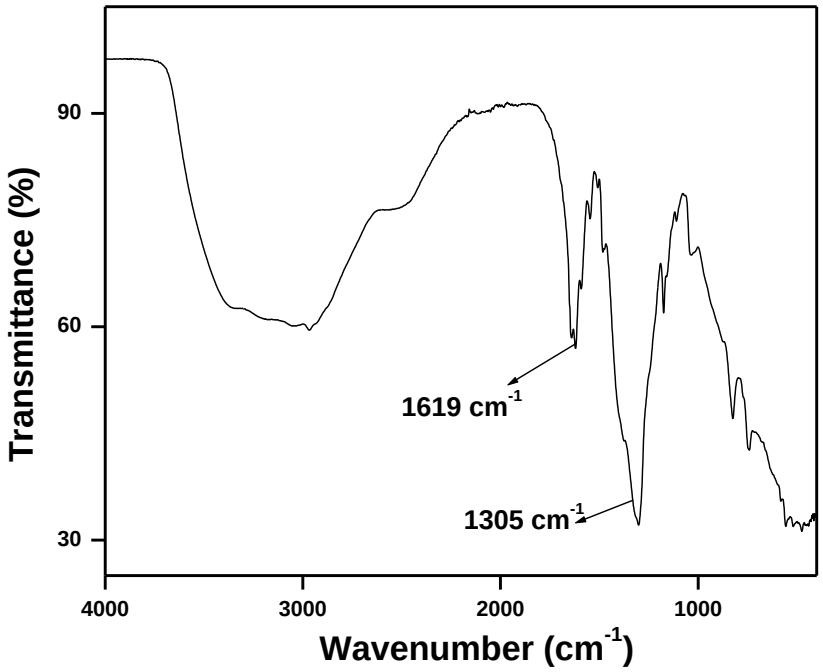


Fig. S10 FTIR spectrum of complex of **H_4L**with Al^{3+}.

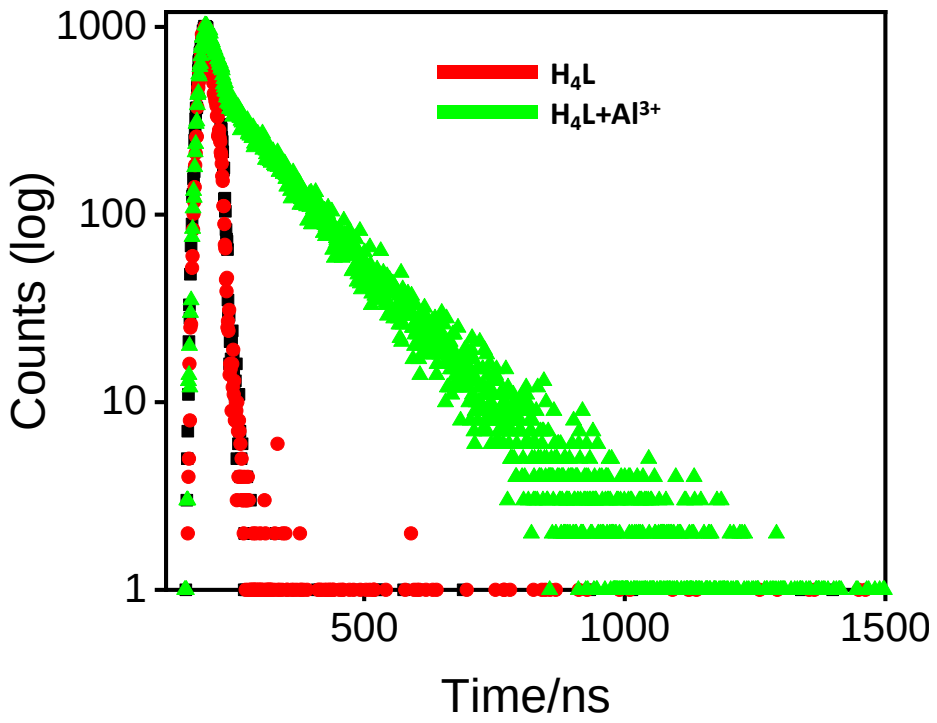


Fig. S11 Fluorescence excited state decay behavior of **H_4L** and its complex with Al^{3+}

Limit of detection (LOD) for H_4L has been determined by 3σ method by the following equation:

DL = K* Sb1/S

where K = 2 or 3 (3 in this case); here Sb1 is the standard deviation of the blank H_4L solution; and S is the slope of the calibration curve obtained from Linear dynamic plot of F.I. vs $[M^{n+}]$ in M. The LOD of H_4L has been calculated to be 4.6×10^{-7} M for Al^{3+} .

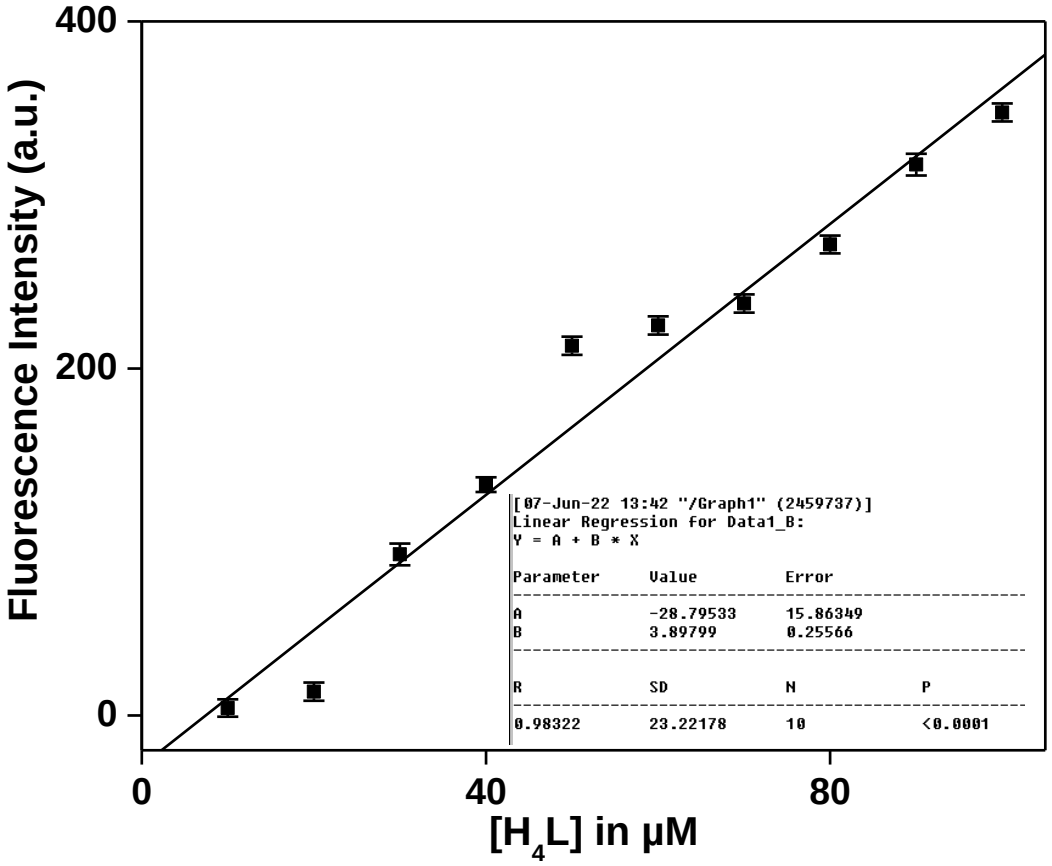


Fig. S12 Determination of Sb1 of the blank, H_4L solution.

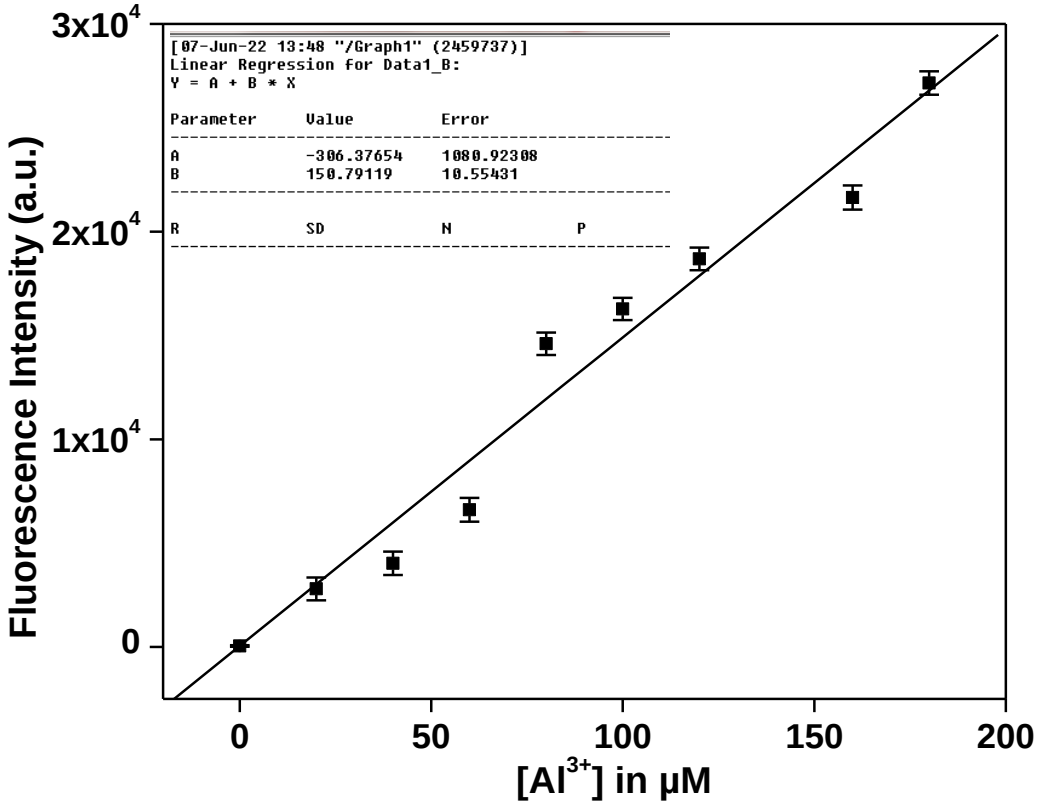
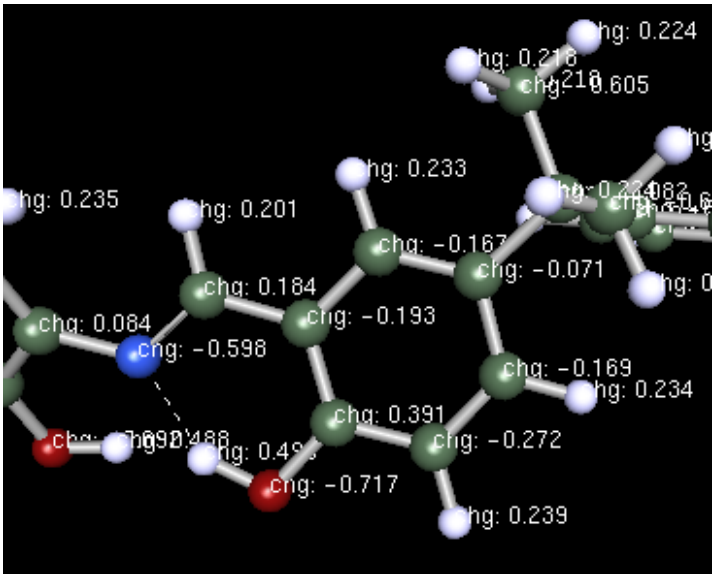


Fig. S13 Linear dynamic plot of F.I. vs. [Al^{3+}] for the determination of S (slope); [$\mathbf{H_4L}$] = 40 μM

(a)



(b)

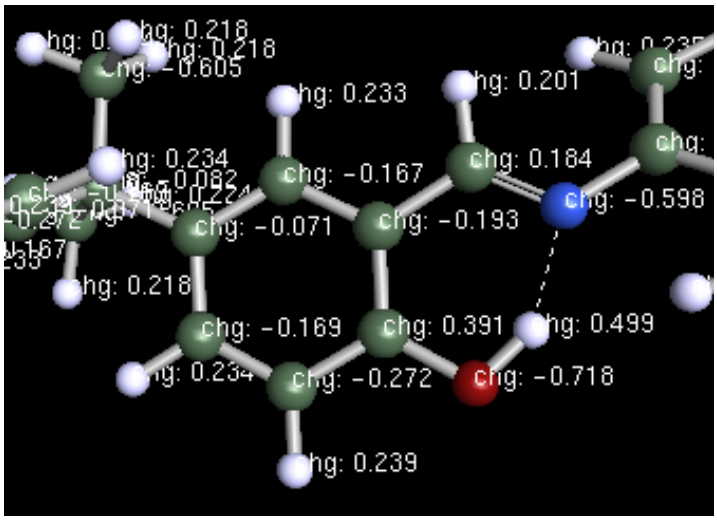
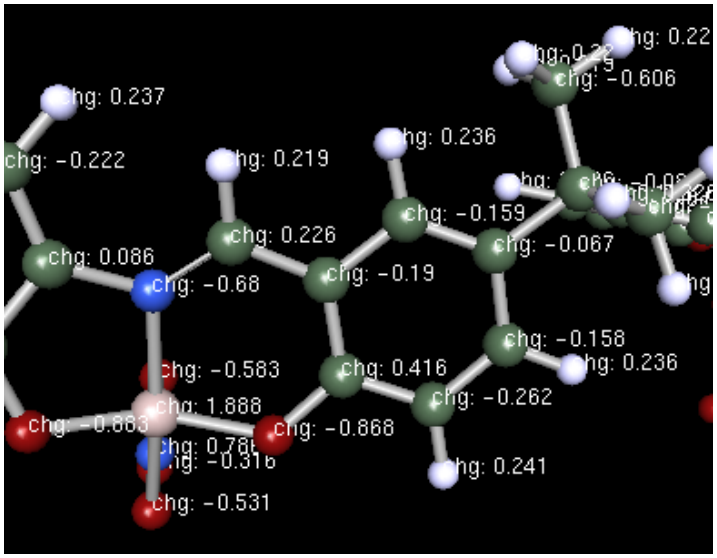


Fig. S14 NBO population of **H_4L**, pictorial diagram, blue: Nitroegn, Green: Carbon, White: Hydrogen, red: oxygen.

(a)



(b)

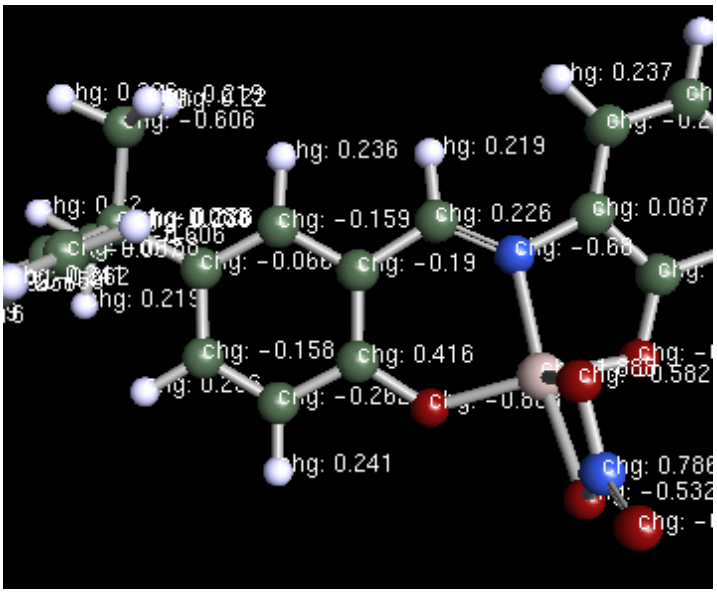


Fig. S15 NBO population of Al^{3+}-**H_4L**, pictorial diagram, blue: Nitroegn, Green: Carbon, White: Hydrogen, red: oxygen.

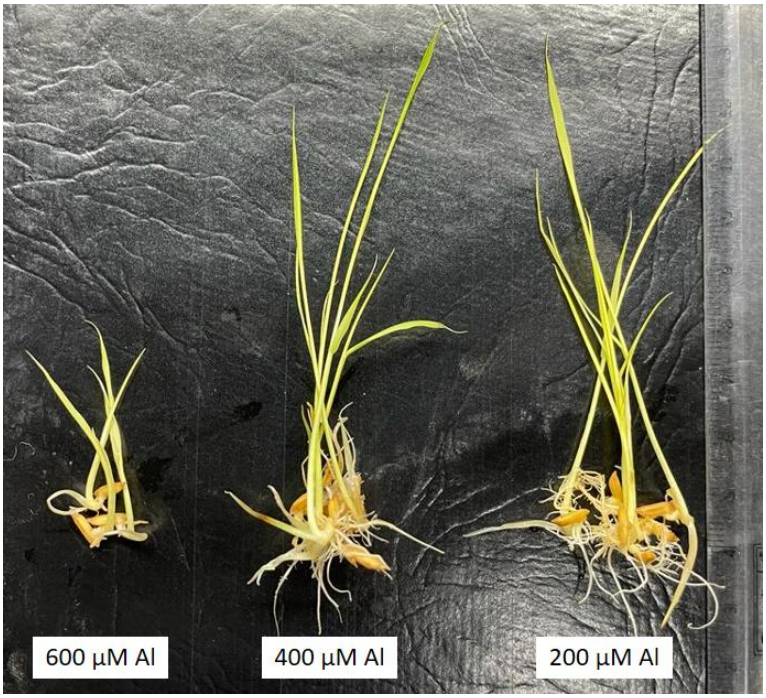


Fig. S16 Rice seedlings growth after 14 DAS under different Al treatment.

Table S1. Geometry optimized coordinates of **H_4L**.

total energy = -1529.24727693084 Hartree

61

O	8.3546748	3.2912002	0.4760588
C	4.0707569	7.0909769	0.3792825
C	4.4597374	8.5058561	0.8596100
C	3.6324215	7.1961151	-1.0974300
C	5.2504053	6.1087959	0.4526969
C	5.0199954	4.7334573	0.2206075
C	6.0477754	3.7973880	0.2276792
C	7.3699503	4.2016400	0.4778518
C	7.6312401	5.5778416	0.7226634
C	6.5610337	6.5020052	0.7024056
C	8.9775319	6.0423560	0.9857700
C	2.9397829	6.5785077	1.2846622
C	3.2235426	6.2621851	2.6329982
C	2.2404001	5.8329879	3.5172025
C	0.9116191	5.6927096	3.0825590
C	0.5974586	5.9963423	1.7293272
C	1.6229575	6.4355344	0.8602587
C	-0.7572291	5.8650711	1.2343308
H	9.2124939	3.7946161	0.6432035
H	3.5727765	9.1595404	0.8299550
H	5.2303191	8.9524867	0.2095849
H	4.8412643	8.4977373	1.8934251

H	3.2846709	6.2277148	-1.4919969
H	4.4870202	7.5254606	-1.7106477
H	2.8219347	7.9329886	-1.2237951
H	3.9998325	4.3885488	0.0344623
H	5.8488499	2.7396118	0.0438464
H	6.8031765	7.5485824	0.8914005
H	9.1106394	7.1265452	1.1328388
H	4.2505854	6.3507865	2.9958558
H	2.4801100	5.5952717	4.5556032
H	1.3408038	6.6610967	-0.1688988
H	-0.9337774	6.1500307	0.1843659
O	11.7175989	3.5702902	2.3315511
N	9.9842008	5.2307783	1.0524829
C	12.1772365	4.7604893	1.8765618
C	11.3026240	5.6698436	1.2316219
C	11.8079483	6.9013873	0.7796411
C	13.1513312	7.2315314	0.9709188
C	14.0061879	6.3258719	1.6150903
C	13.5228704	5.0944126	2.0659150
H	11.1469394	7.5885363	0.2472030
H	13.5342164	8.1869709	0.6048367
H	15.0594956	6.5770499	1.7634967
H	14.1750261	4.3786231	2.5709452
H	10.7531325	3.5381549	2.1768619
O	-0.0299345	5.2834174	3.9453487
H	-0.9025322	5.2813635	3.4396160

O	-3.3242328	3.5052633	3.0426321
N	-1.7222963	5.4290560	1.9793201
C	-3.8560852	4.3660384	2.1420236
C	-3.0510013	5.3643318	1.5394928
C	-3.6300182	6.2354627	0.6002280
C	-4.9780503	6.1149954	0.2559116
C	-5.7637762	5.1203671	0.8553288
C	-5.2067417	4.2490169	1.7954314
H	-3.0234297	7.0312684	0.1627955
H	-5.4185643	6.8050252	-0.4674797
H	-6.8206225	5.0247921	0.5935727
H	-5.8043969	3.4677776	2.2699736
H	-2.3663924	3.6880142	3.1082389

Table S2. Geometry optimized coordinates of Al^{3+}-**H_4L**.

total energy = -2572.13387985363 Hartree

67

O	8.4583454	3.3134293	-0.0264057
C	4.1207071	7.0145326	0.5041020
C	4.4477861	8.2853659	1.3174807
C	3.7451361	7.4495498	-0.9288113
C	5.3194265	6.0591138	0.4113073
C	5.1382588	4.7763409	-0.1584868
C	6.1849725	3.8780429	-0.3075778
C	7.4841270	4.2051262	0.1263414

C	7.6922857	5.4954220	0.7023090
C	6.6001217	6.3931649	0.8240235
C	8.9984330	5.9632798	1.0700863
C	2.9702094	6.2814119	1.2090042
C	3.2013151	5.6854096	2.4717367
C	2.1991140	5.0367009	3.1785788
C	0.8985331	4.9262804	2.6498447
C	0.6401351	5.5231238	1.3782013
C	1.6865700	6.1930057	0.6928471
C	-0.6765312	5.5600415	0.8078721
O	11.7697841	3.4511459	0.3420083
N	10.0546083	5.2000570	1.0670638
C	12.2927458	4.6206435	0.7522963
C	11.3900854	5.6270775	1.1906430
C	11.8545734	6.8666822	1.6415128
C	13.2298558	7.1132231	1.6552385
C	14.1262504	6.1261318	1.2148833
C	13.6679182	4.8841869	0.7632107
O	-0.0312477	4.2871771	3.3534418
O	-3.3276550	3.9304565	3.0094495
N	-1.6884695	4.9129372	1.3130882
C	-3.9002412	4.5221350	1.9456500
C	-3.0405488	5.0691423	0.9547423
C	-3.5578280	5.6923442	-0.1852893
C	-4.9434164	5.7769642	-0.3443406
C	-5.7979427	5.2460135	0.6352951

C	-5.2867769	4.6215433	1.7777513
H	3.5461908	8.9149372	1.3936402
H	5.2349439	8.8825038	0.8279254
H	4.7816649	8.0466764	2.3402461
H	3.4482770	6.5933183	-1.5558907
H	4.6134644	7.9332653	-1.4052717
H	2.9161992	8.1767425	-0.9220362
H	4.1413706	4.4750578	-0.4898012
H	6.0219515	2.8945567	-0.7526930
H	6.8085242	7.3715974	1.2577436
H	9.1033542	7.0294656	1.3073326
H	4.2023185	5.7294055	2.9081100
H	2.3996744	4.5866134	4.1528246
H	1.4398141	6.6447129	-0.2683797
H	-0.8316324	6.2121646	-0.0608810
H	11.1551811	7.6311875	1.9863632
H	13.6050941	8.0751504	2.0117648
H	15.2007004	6.3274118	1.2272194
H	14.3608072	4.1124694	0.4214332
H	-2.8904413	6.1014610	-0.9467125
H	-5.3591956	6.2552155	-1.2340645
H	-6.8809131	5.3173970	0.5042376
H	-5.9468019	4.2056820	2.5418836
N	-1.3469471	1.3551145	3.0263731
O	-1.5338607	2.1255010	4.0286462
O	-1.3069932	2.0242112	1.9132327

O	-1.2218460	0.1732990	3.0890990
N	9.9692237	1.3615653	2.0558982
O	10.1152113	1.3164055	0.7871154
O	9.8709529	2.5855543	2.4799830
O	9.9262749	0.4113608	2.7712942
Al	-1.5850645	3.6936436	2.8082503
Al	10.0450916	3.3007715	0.7115550

Table S3. Vibrational dataset for **H_4L**.

Vibrational Spectrum:

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	Raman
1	a	-2.27	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	5.89	0.00496	YES	YES
9	a	13.78	0.30397	YES	YES
10	a	26.14	0.67529	YES	YES
11	a	38.39	0.33086	YES	YES
12	a	50.02	0.91183	YES	YES
13	a	56.21	0.25724	YES	YES

14	a	57.42	0.39258	YES	YES
15	a	60.12	0.58277	YES	YES
16	a	104.50	1.01283	YES	YES
17	a	126.15	0.93610	YES	YES
18	a	134.96	0.16251	YES	YES
19	a	141.60	0.32016	YES	YES
20	a	155.66	1.08546	YES	YES
21	a	160.37	2.15763	YES	YES
22	a	201.14	3.37566	YES	YES
23	a	201.26	6.47451	YES	YES
24	a	217.53	1.28188	YES	YES
25	a	225.07	0.44243	YES	YES
26	a	242.94	6.46297	YES	YES
27	a	244.08	1.85806	YES	YES
28	a	276.78	24.60093	YES	YES
29	a	299.95	2.77172	YES	YES
30	a	307.79	4.63155	YES	YES
31	a	310.35	0.96716	YES	YES
32	a	319.06	14.12246	YES	YES
33	a	327.78	0.71022	YES	YES
34	a	340.18	0.05899	YES	YES
35	a	342.93	0.02627	YES	YES
36	a	350.20	2.71382	YES	YES
37	a	355.78	4.75174	YES	YES
38	a	394.51	0.00408	YES	YES
39	a	419.68	4.67116	YES	YES

40	a	429.71	24.80334	YES	YES
41	a	445.36	1.40650	YES	YES
42	a	447.19	354.91879	YES	YES
43	a	452.70	9.14072	YES	YES
44	a	456.56	11.68007	YES	YES
45	a	460.74	19.02963	YES	YES
46	a	467.85	0.69045	YES	YES
47	a	494.11	12.73168	YES	YES
48	a	500.72	0.65254	YES	YES
49	a	500.80	1.31686	YES	YES
50	a	512.57	11.96128	YES	YES
51	a	529.67	12.45523	YES	YES
52	a	536.42	0.70298	YES	YES
53	a	548.89	23.32055	YES	YES
54	a	566.16	7.89388	YES	YES
55	a	573.89	3.81932	YES	YES
56	a	580.40	6.42569	YES	YES
57	a	582.71	1.77724	YES	YES
58	a	598.41	2.62657	YES	YES
59	a	598.93	31.92649	YES	YES
60	a	638.00	16.78876	YES	YES
61	a	652.60	22.23623	YES	YES
62	a	667.93	0.33185	YES	YES
63	a	677.58	17.92628	YES	YES
64	a	704.30	8.78744	YES	YES
65	a	757.74	5.04914	YES	YES

66	a	758.71	1.55198	YES	YES
67	a	765.01	155.19670	YES	YES
68	a	766.73	3.76089	YES	YES
69	a	776.02	22.42534	YES	YES
70	a	778.70	0.02111	YES	YES
71	a	780.68	0.38128	YES	YES
72	a	806.26	1.77201	YES	YES
73	a	813.61	24.30207	YES	YES
74	a	839.69	49.16121	YES	YES
75	a	843.00	53.14046	YES	YES
76	a	854.97	188.75910	YES	YES
77	a	855.26	155.81005	YES	YES
78	a	868.51	8.76539	YES	YES
79	a	869.11	0.12708	YES	YES
80	a	883.03	0.12541	YES	YES
81	a	883.18	7.17008	YES	YES
82	a	892.86	3.46781	YES	YES
83	a	898.25	49.27866	YES	YES
84	a	914.94	1.45212	YES	YES
85	a	927.87	5.84150	YES	YES
86	a	940.49	0.14769	YES	YES
87	a	953.28	1.81747	YES	YES
88	a	955.76	3.30128	YES	YES
89	a	964.18	1.67846	YES	YES
90	a	965.13	15.24275	YES	YES
91	a	967.44	3.17653	YES	YES

92	a	1001.95	8.21450	YES	YES
93	a	1002.23	3.84823	YES	YES
94	a	1005.29	12.79085	YES	YES
95	a	1005.53	9.39227	YES	YES
96	a	1006.85	0.89553	YES	YES
97	a	1006.87	0.47888	YES	YES
98	a	1031.32	3.61122	YES	YES
99	a	1054.58	22.04236	YES	YES
100	a	1054.65	22.83955	YES	YES
101	a	1111.65	6.33333	YES	YES
102	a	1111.93	2.65043	YES	YES
103	a	1116.57	10.08914	YES	YES
104	a	1130.44	4.33184	YES	YES
105	a	1146.03	31.43167	YES	YES
106	a	1151.60	18.09304	YES	YES
107	a	1151.64	10.17463	YES	YES
108	a	1153.21	14.03924	YES	YES
109	a	1175.58	29.53039	YES	YES
110	a	1180.73	316.09918	YES	YES
111	a	1181.21	33.49737	YES	YES
112	a	1208.05	9.28166	YES	YES
113	a	1210.40	517.68544	YES	YES
114	a	1252.89	31.55410	YES	YES
115	a	1256.10	35.48656	YES	YES
116	a	1267.05	46.50254	YES	YES
117	a	1267.86	146.08112	YES	YES

118	a	1283.44	106.18037	YES	YES
119	a	1286.72	225.68105	YES	YES
120	a	1294.79	0.83734	YES	YES
121	a	1296.00	56.12037	YES	YES
122	a	1324.69	146.26589	YES	YES
123	a	1324.98	98.56661	YES	YES
124	a	1329.40	46.81980	YES	YES
125	a	1329.46	55.45496	YES	YES
126	a	1377.33	62.10687	YES	YES
127	a	1377.58	70.18384	YES	YES
128	a	1383.49	74.66078	YES	YES
129	a	1383.59	35.48380	YES	YES
130	a	1389.73	35.38174	YES	YES
131	a	1398.83	49.91690	YES	YES
132	a	1399.15	50.73805	YES	YES
133	a	1409.98	4.14233	YES	YES
134	a	1452.02	1.87511	YES	YES
135	a	1453.20	61.11521	YES	YES
136	a	1461.89	4.41089	YES	YES
137	a	1468.75	4.48568	YES	YES
138	a	1480.44	11.37779	YES	YES
139	a	1484.61	44.66709	YES	YES
140	a	1501.92	13.74685	YES	YES
141	a	1502.05	3.02294	YES	YES
142	a	1505.65	50.70640	YES	YES
143	a	1505.85	57.64019	YES	YES

144	a	1525.65	207.52712	YES	YES
145	a	1527.54	523.12153	YES	YES
146	a	1530.32	137.72861	YES	YES
147	a	1531.38	1.20834	YES	YES
148	a	1630.17	498.05560	YES	YES
149	a	1631.17	76.92303	YES	YES
150	a	1637.53	62.09059	YES	YES
151	a	1637.84	51.63922	YES	YES
152	a	1659.47	76.45271	YES	YES
153	a	1659.76	87.46622	YES	YES
154	a	1679.34	493.92437	YES	YES
155	a	1680.06	75.10622	YES	YES
156	a	1682.52	556.26487	YES	YES
157	a	1685.34	0.94790	YES	YES
158	a	2941.05	1636.73480	YES	YES
159	a	2941.54	592.37917	YES	YES
160	a	3010.76	28.92811	YES	YES
161	a	3015.82	27.23872	YES	YES
162	a	3078.32	22.05447	YES	YES
163	a	3078.40	22.68668	YES	YES
164	a	3093.50	1.36975	YES	YES
165	a	3097.48	102.64188	YES	YES
166	a	3101.72	17.37191	YES	YES
167	a	3101.90	49.25917	YES	YES
168	a	3170.93	0.01035	YES	YES
169	a	3170.95	0.01045	YES	YES

170	a	3172.79	1.13963	YES	YES
171	a	3172.93	13.69214	YES	YES
172	a	3180.32	15.78651	YES	YES
173	a	3180.32	3.30982	YES	YES
174	a	3188.88	3.50436	YES	YES
175	a	3188.88	35.76797	YES	YES
176	a	3191.85	16.22968	YES	YES
177	a	3191.94	22.84055	YES	YES
178	a	3194.69	1.36186	YES	YES
179	a	3194.90	1.73307	YES	YES
180	a	3195.85	33.31144	YES	YES
181	a	3195.86	6.24932	YES	YES
182	a	3589.01	453.73760	YES	YES
183	a	3589.03	9.00493	YES	YES

Table S4. Vibrational dataset for Al^{3+}-**H_4L**.

Vibrational Spectrum:

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	Raman
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.03	0.05802	-	-

8	a	5.80	0.06112	YES	YES
9	a	7.00	0.17906	YES	YES
10	a	19.25	2.12908	YES	YES
11	a	34.70	0.00009	YES	YES
12	a	43.20	0.09528	YES	YES
13	a	45.42	0.53554	YES	YES
14	a	58.71	0.25022	YES	YES
15	a	63.21	4.52846	YES	YES
16	a	68.92	2.60506	YES	YES
17	a	78.84	0.00237	YES	YES
18	a	83.96	0.00123	YES	YES
19	a	100.24	0.61990	YES	YES
20	a	106.86	0.04662	YES	YES
21	a	122.50	0.01281	YES	YES
22	a	125.80	0.33435	YES	YES
23	a	135.36	0.08975	YES	YES
24	a	154.27	0.56011	YES	YES
25	a	154.84	0.30392	YES	YES
26	a	175.97	0.18706	YES	YES
27	a	187.40	4.37310	YES	YES
28	a	198.14	16.02725	YES	YES
29	a	198.28	6.89253	YES	YES
30	a	221.53	3.45560	YES	YES
31	a	223.76	2.40122	YES	YES
32	a	238.37	8.21797	YES	YES
33	a	238.64	2.12369	YES	YES

34	a	246.93	0.20038	YES	YES
35	a	261.80	16.58777	YES	YES
36	a	264.01	10.01685	YES	YES
37	a	274.13	4.66977	YES	YES
38	a	289.94	0.68112	YES	YES
39	a	293.11	0.31310	YES	YES
40	a	312.79	0.31808	YES	YES
41	a	320.77	18.09122	YES	YES
42	a	326.69	0.23205	YES	YES
43	a	336.78	7.93604	YES	YES
44	a	345.94	0.33833	YES	YES
45	a	349.22	2.99260	YES	YES
46	a	358.02	8.71079	YES	YES
47	a	368.47	0.00187	YES	YES
48	a	381.39	25.08761	YES	YES
49	a	385.46	6.49710	YES	YES
50	a	390.98	2.80687	YES	YES
51	a	398.06	53.12676	YES	YES
52	a	398.34	11.79348	YES	YES
53	a	442.64	0.44194	YES	YES
54	a	444.50	28.66836	YES	YES
55	a	458.70	4.11608	YES	YES
56	a	464.00	10.99610	YES	YES
57	a	485.66	13.86484	YES	YES
58	a	488.40	624.49546	YES	YES
59	a	494.05	8.70009	YES	YES

60	a	505.72	73.55931	YES	YES
61	a	506.05	2.14816	YES	YES
62	a	518.23	9.62103	YES	YES
63	a	528.78	28.26472	YES	YES
64	a	562.65	13.03545	YES	YES
65	a	571.56	19.54597	YES	YES
66	a	573.85	0.64394	YES	YES
67	a	577.77	52.57769	YES	YES
68	a	579.03	2.99612	YES	YES
69	a	583.25	118.59346	YES	YES
70	a	595.65	44.04377	YES	YES
71	a	617.54	76.88206	YES	YES
72	a	641.75	47.63403	YES	YES
73	a	653.61	0.37294	YES	YES
74	a	660.42	96.21353	YES	YES
75	a	667.33	14.51684	YES	YES
76	a	689.16	16.96804	YES	YES
77	a	690.48	13.30839	YES	YES
78	a	711.10	0.68399	YES	YES
79	a	711.66	0.60854	YES	YES
80	a	720.28	49.82801	YES	YES
81	a	755.76	122.62530	YES	YES
82	a	756.16	5.62645	YES	YES
83	a	766.16	114.75111	YES	YES
84	a	766.24	97.51798	YES	YES
85	a	772.98	4.16187	YES	YES

86	a	774.91	1.43985	YES	YES
87	a	781.93	1.39856	YES	YES
88	a	787.27	24.84187	YES	YES
89	a	787.63	2.54077	YES	YES
90	a	809.82	2.21049	YES	YES
91	a	809.95	76.28102	YES	YES
92	a	824.41	63.79743	YES	YES
93	a	824.44	93.99176	YES	YES
94	a	860.84	35.83157	YES	YES
95	a	864.91	82.13873	YES	YES
96	a	869.44	186.21915	YES	YES
97	a	871.10	57.83276	YES	YES
98	a	872.74	5.60357	YES	YES
99	a	881.20	303.18459	YES	YES
100	a	888.52	3.03203	YES	YES
101	a	888.58	19.18503	YES	YES
102	a	908.70	16.43371	YES	YES
103	a	913.84	1.00906	YES	YES
104	a	919.58	1.03234	YES	YES
105	a	927.20	4.38326	YES	YES
106	a	945.39	5.03652	YES	YES
107	a	956.20	3.52242	YES	YES
108	a	961.85	15.23310	YES	YES
109	a	964.88	3.52405	YES	YES
110	a	965.11	4.49015	YES	YES
111	a	971.34	5.98698	YES	YES

112	a	999.58	84.71771	YES	YES
113	a	1000.14	4.38505	YES	YES
114	a	1010.48	0.22621	YES	YES
115	a	1010.51	0.22394	YES	YES
116	a	1011.88	0.96611	YES	YES
117	a	1012.15	2.17160	YES	YES
118	a	1031.51	2.77527	YES	YES
119	a	1047.01	26.01494	YES	YES
120	a	1047.05	15.54091	YES	YES
121	a	1057.48	118.62560	YES	YES
122	a	1057.92	127.95934	YES	YES
123	a	1117.94	24.97361	YES	YES
124	a	1119.85	25.10261	YES	YES
125	a	1120.25	7.74388	YES	YES
126	a	1133.20	3.78785	YES	YES
127	a	1150.14	44.75774	YES	YES
128	a	1150.64	14.20800	YES	YES
129	a	1153.28	21.11991	YES	YES
130	a	1159.40	43.73551	YES	YES
131	a	1177.44	21.72009	YES	YES
132	a	1205.62	156.80413	YES	YES
133	a	1206.52	2.74046	YES	YES
134	a	1236.39	3.20149	YES	YES
135	a	1243.98	336.24534	YES	YES
136	a	1272.27	78.76045	YES	YES
137	a	1278.33	87.54134	YES	YES

138	a	1281.28	21.71182	YES	YES
139	a	1281.79	78.92220	YES	YES
140	a	1287.80	701.48266	YES	YES
141	a	1288.04	420.87308	YES	YES
142	a	1292.61	7.28343	YES	YES
143	a	1293.00	50.35293	YES	YES
144	a	1315.38	161.25485	YES	YES
145	a	1315.85	122.62747	YES	YES
146	a	1334.84	229.38895	YES	YES
147	a	1335.60	326.48414	YES	YES
148	a	1357.76	295.40977	YES	YES
149	a	1357.86	1.70949	YES	YES
150	a	1389.70	69.03168	YES	YES
151	a	1391.91	72.91544	YES	YES
152	a	1394.45	20.34725	YES	YES
153	a	1411.28	18.69076	YES	YES
154	a	1414.60	134.04386	YES	YES
155	a	1416.08	184.41861	YES	YES
156	a	1459.10	7.07845	YES	YES
157	a	1462.21	2.25820	YES	YES
158	a	1464.27	0.22460	YES	YES
159	a	1468.39	0.71417	YES	YES
160	a	1480.24	17.53717	YES	YES
161	a	1486.52	12.67062	YES	YES
162	a	1501.91	5.58146	YES	YES
163	a	1501.95	22.22900	YES	YES

164	a	1513.38	361.05944	YES	YES
165	a	1513.43	396.02199	YES	YES
166	a	1514.02	32.87090	YES	YES
167	a	1515.67	262.79127	YES	YES
168	a	1587.19	925.55582	YES	YES
169	a	1590.46	5.58141	YES	YES
170	a	1626.18	3.98498	YES	YES
171	a	1626.28	6.81839	YES	YES
172	a	1649.38	96.39403	YES	YES
173	a	1649.62	234.90007	YES	YES
174	a	1667.91	691.69579	YES	YES
175	a	1669.41	29.86391	YES	YES
176	a	1673.58	955.80744	YES	YES
177	a	1676.91	68.04688	YES	YES
178	a	1719.67	744.61313	YES	YES
179	a	1720.19	798.76677	YES	YES
180	a	3010.96	28.43563	YES	YES
181	a	3016.01	24.11913	YES	YES
182	a	3093.82	1.21333	YES	YES
183	a	3097.77	99.65875	YES	YES
184	a	3101.77	16.37169	YES	YES
185	a	3101.91	46.67576	YES	YES
186	a	3139.62	14.13935	YES	YES
187	a	3139.65	11.97693	YES	YES
188	a	3172.05	0.92392	YES	YES
189	a	3172.10	0.92619	YES	YES

190	a	3176.00	3.35641	YES	YES
191	a	3176.18	12.73563	YES	YES
192	a	3181.54	8.62948	YES	YES
193	a	3181.55	7.26598	YES	YES
194	a	3190.84	19.96411	YES	YES
195	a	3190.86	19.91450	YES	YES
196	a	3194.94	11.74756	YES	YES
197	a	3195.00	20.07716	YES	YES
198	a	3197.13	39.37347	YES	YES
199	a	3197.14	7.46511	YES	YES
200	a	3201.16	1.53516	YES	YES
201	a	3201.31	3.45581	YES	YES

Table S5. NBO population of **H_4L**.

atomic populations from total density:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 o	-0.71702	3.63847	5.07297	0.00558	0.00000	0.00000
2 c	-0.08191	2.85972	3.21762	0.00457	0.00000	0.00000
3 c	-0.60431	3.07131	3.52933	0.00367	0.00000	0.00000
4 c	-0.60426	3.07136	3.52924	0.00367	0.00000	0.00000
5 c	-0.07005	2.84395	3.22247	0.00363	0.00000	0.00000
6 c	-0.16872	2.93066	3.23431	0.00376	0.00000	0.00000
7 c	-0.27159	2.94196	3.32609	0.00353	0.00000	0.00000
8 c	0.39039	2.79930	2.80271	0.00759	0.00000	0.00000
9 c	-0.19216	2.86211	3.32669	0.00336	0.00000	0.00000

10 c	-0.16684	2.91332	3.24987	0.00365	0.00000	0.00000
11 c	0.18396	2.89942	2.91076	0.00587	0.00000	0.00000
12 c	-0.07019	2.84391	3.22265	0.00363	0.00000	0.00000
13 c	-0.16864	2.93065	3.23423	0.00376	0.00000	0.00000
14 c	-0.27155	2.94200	3.32602	0.00353	0.00000	0.00000
15 c	0.39046	2.79931	2.80265	0.00759	0.00000	0.00000
16 c	-0.19217	2.86209	3.32672	0.00336	0.00000	0.00000
17 c	-0.16688	2.91328	3.24996	0.00365	0.00000	0.00000
18 c	0.18390	2.89941	2.91082	0.00587	0.00000	0.00000
19 h	0.49812	0.50175	0.00013	0.00000	0.00000	0.00000
20 h	0.22354	0.77642	0.00004	0.00000	0.00000	0.00000
21 h	0.21728	0.78268	0.00004	0.00000	0.00000	0.00000
22 h	0.21777	0.78220	0.00004	0.00000	0.00000	0.00000
23 h	0.21773	0.78223	0.00004	0.00000	0.00000	0.00000
24 h	0.22354	0.77642	0.00004	0.00000	0.00000	0.00000
25 h	0.21730	0.78266	0.00004	0.00000	0.00000	0.00000
26 h	0.23338	0.76658	0.00004	0.00000	0.00000	0.00000
27 h	0.23837	0.76159	0.00004	0.00000	0.00000	0.00000
28 h	0.23245	0.76751	0.00004	0.00000	0.00000	0.00000
29 h	0.20099	0.79897	0.00004	0.00000	0.00000	0.00000
30 h	0.23334	0.76662	0.00004	0.00000	0.00000	0.00000
31 h	0.23842	0.76154	0.00004	0.00000	0.00000	0.00000
32 h	0.23241	0.76755	0.00004	0.00000	0.00000	0.00000
33 h	0.20097	0.79899	0.00004	0.00000	0.00000	0.00000
34 o	-0.69125	3.64262	5.04308	0.00555	0.00000	0.00000
35 n	-0.59778	3.32056	4.27226	0.00497	0.00000	0.00000

36 c	0.34749	2.80394	2.84120	0.00737	0.00000	0.00000
37 c	0.08384	2.81685	3.09429	0.00503	0.00000	0.00000
38 c	-0.22863	2.94022	3.28476	0.00365	0.00000	0.00000
39 c	-0.24808	2.94162	3.30281	0.00365	0.00000	0.00000
40 c	-0.21011	2.94624	3.26010	0.00377	0.00000	0.00000
41 c	-0.27986	2.94625	3.33002	0.00358	0.00000	0.00000
42 h	0.23420	0.76576	0.00004	0.00000	0.00000	0.00000
43 h	0.23053	0.76943	0.00004	0.00000	0.00000	0.00000
44 h	0.23103	0.76893	0.00004	0.00000	0.00000	0.00000
45 h	0.23689	0.76307	0.00004	0.00000	0.00000	0.00000
46 h	0.48709	0.51279	0.00012	0.00000	0.00000	0.00000
47 o	-0.71687	3.63845	5.07284	0.00558	0.00000	0.00000
48 h	0.49810	0.50177	0.00013	0.00000	0.00000	0.00000
49 o	-0.69127	3.64262	5.04310	0.00555	0.00000	0.00000
50 n	-0.59771	3.32055	4.27219	0.00497	0.00000	0.00000
51 c	0.34746	2.80395	2.84121	0.00737	0.00000	0.00000
52 c	0.08387	2.81684	3.09426	0.00503	0.00000	0.00000
53 c	-0.22865	2.94022	3.28478	0.00365	0.00000	0.00000
54 c	-0.24809	2.94162	3.30281	0.00365	0.00000	0.00000
55 c	-0.21012	2.94624	3.26011	0.00377	0.00000	0.00000
56 c	-0.27987	2.94626	3.33003	0.00358	0.00000	0.00000
57 h	0.23420	0.76576	0.00004	0.00000	0.00000	0.00000
58 h	0.23053	0.76943	0.00004	0.00000	0.00000	0.00000
59 h	0.23103	0.76893	0.00004	0.00000	0.00000	0.00000
60 h	0.23689	0.76307	0.00004	0.00000	0.00000	0.00000
61 h	0.48708	0.51280	0.00012	0.00000	0.00000	0.00000

Table S6. NBO population of Al^{3+}-**H_4L**.

atomic populations from total density:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 o	-0.86753	3.63699	5.22695	0.00358	0.00000	0.00000
2 c	-0.08271	2.85968	3.21846	0.00457	0.00000	0.00000
3 c	-0.60550	3.07141	3.53043	0.00366	0.00000	0.00000
4 c	-0.60541	3.07147	3.53028	0.00366	0.00000	0.00000
5 c	-0.06593	2.84453	3.21774	0.00366	0.00000	0.00000
6 c	-0.15792	2.93279	3.22136	0.00378	0.00000	0.00000
7 c	-0.26162	2.94566	3.31238	0.00358	0.00000	0.00000
8 c	0.41568	2.79124	2.78574	0.00735	0.00000	0.00000
9 c	-0.18980	2.86415	3.32229	0.00336	0.00000	0.00000
10 c	-0.15844	2.91461	3.24016	0.00367	0.00000	0.00000
11 c	0.22515	2.89408	2.87534	0.00543	0.00000	0.00000
12 c	-0.06613	2.84446	3.21802	0.00366	0.00000	0.00000
13 c	-0.15780	2.93276	3.22126	0.00378	0.00000	0.00000
14 c	-0.26158	2.94569	3.31230	0.00358	0.00000	0.00000
15 c	0.41548	2.79132	2.78585	0.00735	0.00000	0.00000
16 c	-0.18985	2.86411	3.32237	0.00336	0.00000	0.00000
17 c	-0.15860	2.91451	3.24043	0.00367	0.00000	0.00000
18 c	0.22506	2.89410	2.87542	0.00543	0.00000	0.00000
19 o	-0.88298	3.65867	5.21994	0.00437	0.00000	0.00000
20 n	-0.67991	3.29483	4.38160	0.00348	0.00000	0.00000
21 c	0.35445	2.79705	2.84123	0.00727	0.00000	0.00000
22 c	0.08600	2.81645	3.09294	0.00460	0.00000	0.00000

23 c	-0.22206	2.93710	3.28128	0.00367	0.00000	0.00000
24 c	-0.24511	2.94256	3.29890	0.00364	0.00000	0.00000
25 c	-0.20297	2.94793	3.25126	0.00378	0.00000	0.00000
26 c	-0.27549	2.94757	3.32431	0.00361	0.00000	0.00000
27 o	-0.86741	3.63720	5.22663	0.00358	0.00000	0.00000
28 o	-0.88298	3.65865	5.21996	0.00438	0.00000	0.00000
29 n	-0.67989	3.29468	4.38173	0.00348	0.00000	0.00000
30 c	0.35442	2.79709	2.84123	0.00727	0.00000	0.00000
31 c	0.08595	2.81644	3.09302	0.00460	0.00000	0.00000
32 c	-0.22192	2.93709	3.28115	0.00367	0.00000	0.00000
33 c	-0.24510	2.94257	3.29889	0.00364	0.00000	0.00000
34 c	-0.20290	2.94794	3.25118	0.00378	0.00000	0.00000
35 c	-0.27545	2.94756	3.32429	0.00361	0.00000	0.00000
36 h	0.22533	0.77463	0.00004	0.00000	0.00000	0.00000
37 h	0.21915	0.78081	0.00004	0.00000	0.00000	0.00000
38 h	0.21878	0.78118	0.00004	0.00000	0.00000	0.00000
39 h	0.21875	0.78121	0.00004	0.00000	0.00000	0.00000
40 h	0.22532	0.77464	0.00004	0.00000	0.00000	0.00000
41 h	0.21916	0.78080	0.00004	0.00000	0.00000	0.00000
42 h	0.23583	0.76413	0.00004	0.00000	0.00000	0.00000
43 h	0.24035	0.75961	0.00004	0.00000	0.00000	0.00000
44 h	0.23543	0.76453	0.00004	0.00000	0.00000	0.00000
45 h	0.21891	0.78105	0.00004	0.00000	0.00000	0.00000
46 h	0.23579	0.76417	0.00004	0.00000	0.00000	0.00000
47 h	0.24035	0.75961	0.00004	0.00000	0.00000	0.00000
48 h	0.23541	0.76455	0.00004	0.00000	0.00000	0.00000

49 h	0.21897	0.78100	0.00004	0.00000	0.00000	0.00000
50 h	0.23650	0.76346	0.00004	0.00000	0.00000	0.00000
51 h	0.23199	0.76797	0.00004	0.00000	0.00000	0.00000
52 h	0.23211	0.76785	0.00004	0.00000	0.00000	0.00000
53 h	0.23685	0.76311	0.00004	0.00000	0.00000	0.00000
54 h	0.23648	0.76348	0.00004	0.00000	0.00000	0.00000
55 h	0.23201	0.76795	0.00004	0.00000	0.00000	0.00000
56 h	0.23212	0.76784	0.00004	0.00000	0.00000	0.00000
57 h	0.23686	0.76310	0.00004	0.00000	0.00000	0.00000
58 n	0.78535	2.98334	3.20971	0.02160	0.00000	0.00000
59 o	-0.53085	3.73502	4.78929	0.00653	0.00000	0.00000
60 o	-0.58206	3.73979	4.83595	0.00633	0.00000	0.00000
61 o	-0.31540	3.71882	4.58823	0.00835	0.00000	0.00000
62 n	0.78538	2.98331	3.20971	0.02160	0.00000	0.00000
63 o	-0.53112	3.73498	4.78961	0.00653	0.00000	0.00000
64 o	-0.58172	3.73975	4.83564	0.00633	0.00000	0.00000
65 o	-0.31562	3.71890	4.58838	0.00835	0.00000	0.00000
66 al	1.88726	4.38003	6.69370	0.03431	0.00470	0.00000
67 al	1.88715	4.37995	6.69391	0.03430	0.00469	0.00000