ELECTRONIC SUPPLEMENTARY INFORMATION

A fluorescent sensor for Cu^{2+} and Fe^{3+} based on multiple mechanisms

Wei He* and Zheng Liu*

School of Chemistry and Chemical Engineering, University of Jinan, Jinan 250022, China.

*Corresponding author:
Wei He
Zheng Liu
School of Chemistry and Chemical Engineering, University of Jinan
Jinan 250022, China
E-mail address: chm_hew@ujn.edu.cn (W. He)
liuzhengbeyond@163.com (Z. Liu)

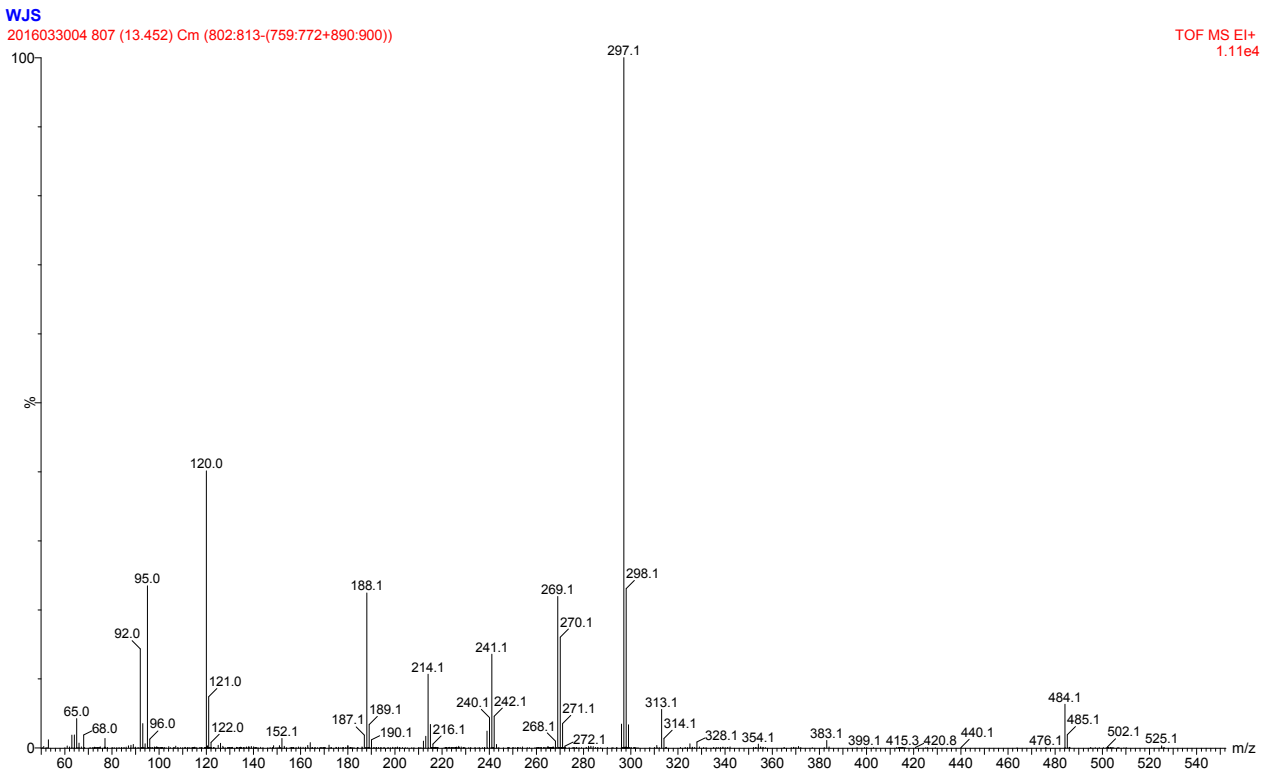


Figure S1. ESI mass spectrum of **L**.

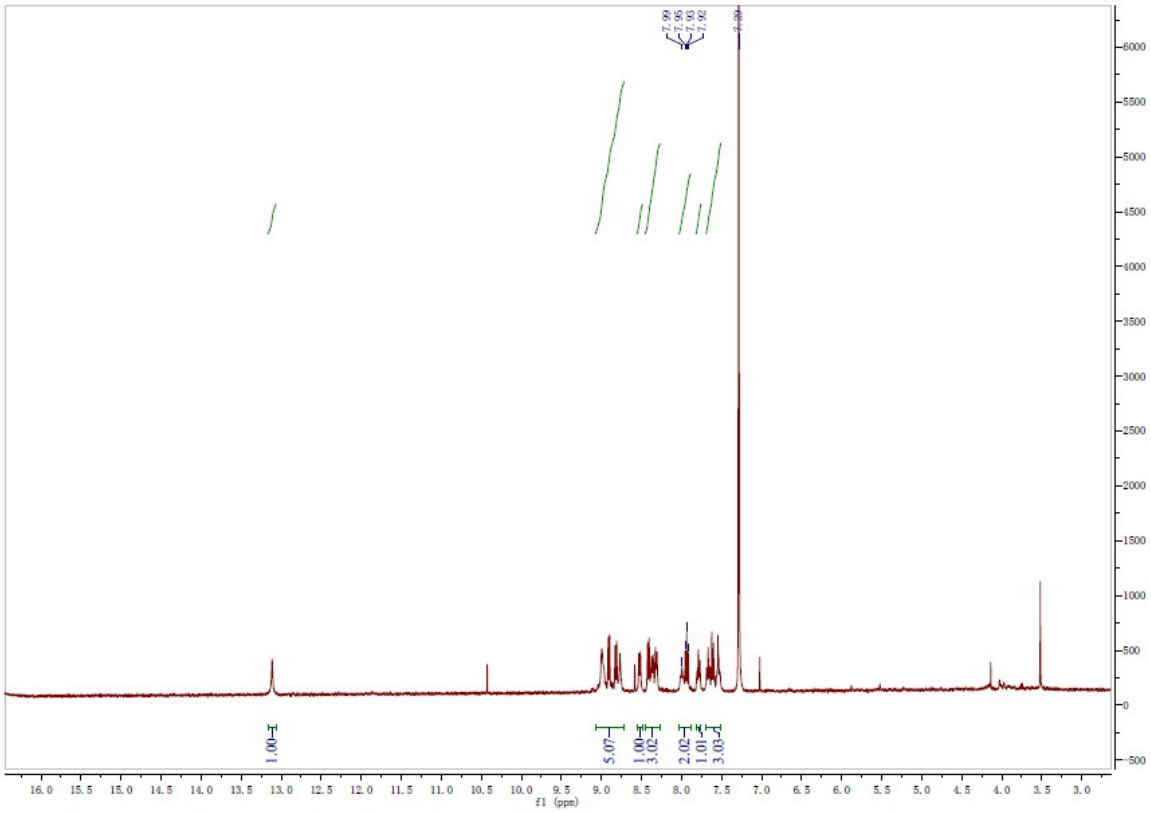


Figure S2. ^{1}H NMR spectra of **L** in $CDCl_3$.

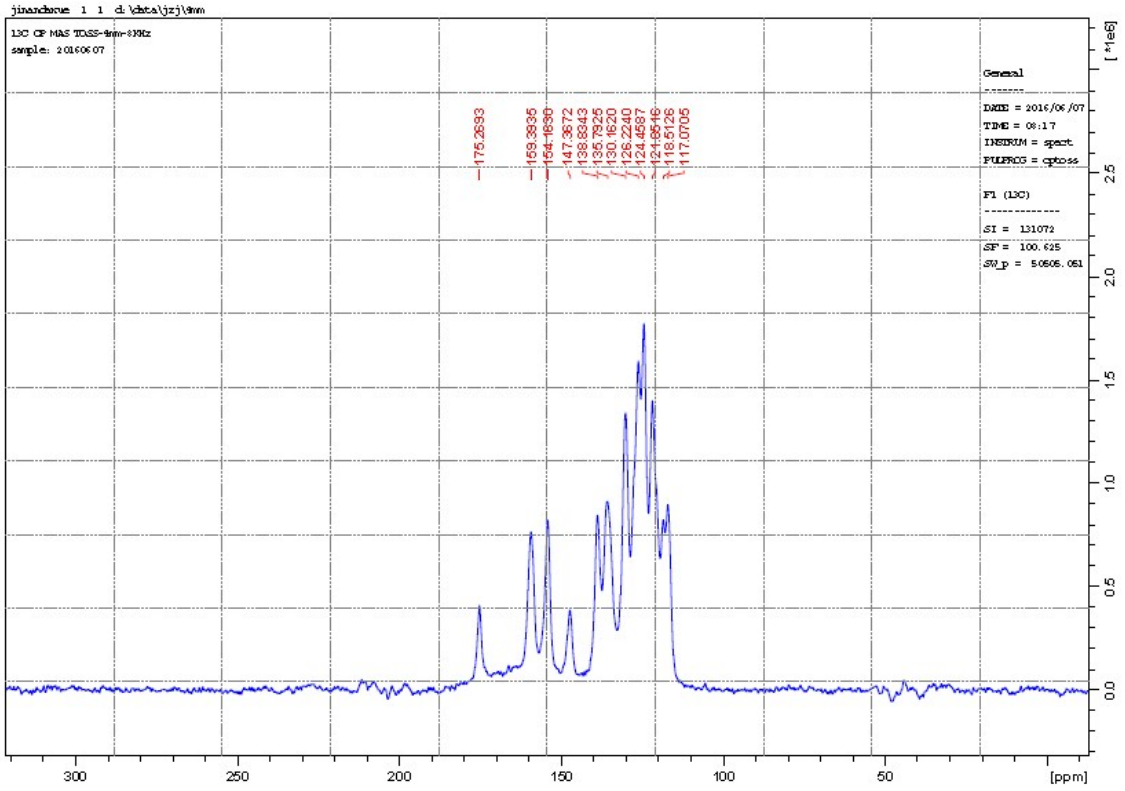
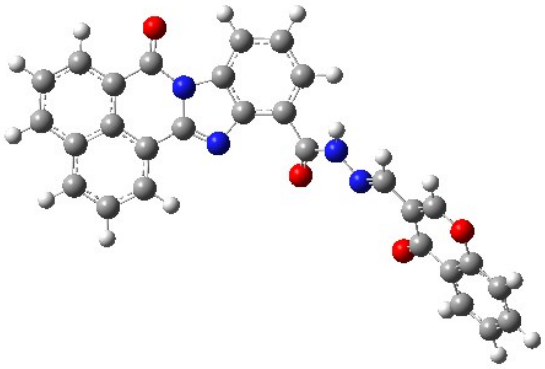


Figure S3. ^{13}C CP/MAS NMR spectra of **L**.

Table S1. XYZ coordination of the optimized structure of **L**.

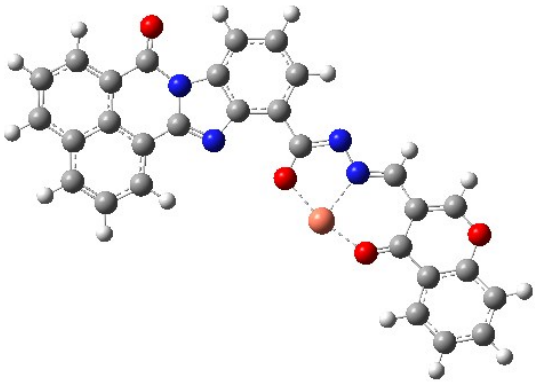


Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000953	0.000001894	-0.000001508
2	6	-0.000001640	0.000001653	0.000000263
3	6	-0.000000605	0.000001283	-0.000001314
4	6	-0.000000533	0.000001630	-0.000000786
5	6	-0.000001456	0.000001693	-0.000000543
6	6	-0.000001190	0.000000694	-0.000000602
7	1	-0.000000918	0.000000796	-0.000000544
8	6	-0.000000939	0.000000941	0.000000132
9	6	-0.000000681	0.000001546	-0.000000423
10	1	-0.000001408	0.000001892	-0.000000858
11	1	-0.000001392	0.000001730	-0.000000872
12	6	-0.000000459	0.000001412	-0.000000879
13	6	-0.000000220	0.000001440	-0.000000358
14	1	-0.000001013	0.000001823	-0.000000640
15	1	-0.000000224	0.000001421	-0.000000463
16	1	0.000000228	0.000000794	-0.000000316
17	6	0.000008918	-0.000005073	0.000000290
18	6	0.000001610	0.000000970	-0.000001289
19	7	-0.000000867	0.000001814	0.000001353
20	7	-0.000005473	0.000006361	0.000000056
21	6	0.000003030	-0.000002398	-0.000003842
22	6	-0.000002870	-0.000000864	0.000002651
23	6	-0.000001178	-0.000002826	-0.000002198
24	6	0.000002323	0.000001880	-0.000000675
25	6	0.000000542	0.000000387	0.000005003
26	6	0.000001411	-0.000000912	-0.000002548
27	1	0.000001507	-0.000000920	-0.000000091

28	1	0.000001908	-0.000000745	0.000000408
29	1	0.000001082	-0.000000232	-0.000000075
30	6	0.000001212	0.000005794	-0.000000214
31	8	0.000000988	-0.000002453	-0.000001577
32	8	-0.000000021	0.000000050	0.000000284
33	7	-0.000000515	-0.000004721	-0.000002845
34	7	0.000000946	-0.000002579	0.000004951
35	6	0.000002352	0.000014928	-0.000002011
36	6	-0.000000532	-0.000001505	0.000000736
37	6	0.000000200	-0.000001741	0.000000216
38	6	-0.000000912	-0.000001052	0.000001061
39	6	-0.000000500	-0.000000781	0.000000631
40	6	-0.000000771	-0.000000882	0.000000470
41	6	0.000000588	-0.000001015	-0.000000093
42	1	-0.000000756	-0.000002011	0.000000940
43	1	-0.000000580	-0.000001635	0.000000546
44	1	-0.000000392	-0.000000657	0.000000132
45	1	-0.000000066	0.000000059	0.000000238
46	6	-0.000000037	-0.000004706	0.000001883
47	6	0.000000345	-0.000003442	0.000002465
48	1	0.000000172	-0.000000775	-0.000000039
49	1	-0.000000589	-0.000007337	0.000001915
50	6	0.000000585	-0.000000785	0.000000944
51	8	-0.000000239	-0.000000680	-0.000000542
52	8	0.000000150	-0.000000982	-0.000000593
53	1	-0.000000166	-0.000001177	0.000001171

Table S2. XYZ coordination of the optimized structure of **L**+Cu^{2+}.

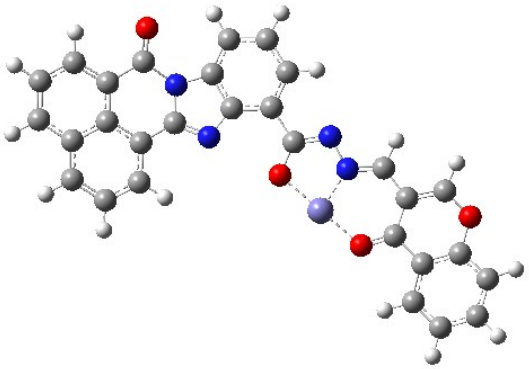


Standard orientation:

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001097	0.000002847	-0.000003076
2	6	-0.000000336	-0.000001092	-0.000000895
3	6	0.000000936	-0.000004023	0.000001642
4	6	-0.000000263	0.000003642	-0.000000819
5	6	0.000003394	-0.000002125	0.000001650
6	6	-0.000002773	-0.000000573	0.000000809
7	1	-0.000000183	-0.000000867	-0.000000022
8	6	-0.000004469	0.000001968	-0.000000858
9	6	0.000000464	-0.000001659	0.000001049
10	1	-0.000000975	-0.000000669	-0.000000727
11	1	0.000001165	0.000000001	0.000000998
12	6	-0.000000228	0.000000455	0.000001465
13	6	0.000003271	0.000000461	0.000000111
14	1	-0.000000194	-0.000000814	0.000000629
15	1	-0.000000127	0.000000182	0.000000273
16	1	-0.000000696	0.000000167	0.000001567
17	6	0.000011054	0.000002166	0.000003007
18	6	0.000003421	-0.000003832	0.000012812
19	7	-0.000005392	-0.000003713	-0.000008939
20	7	-0.000014373	-0.000005496	-0.000002758
21	6	0.000001379	0.000019106	0.000002099
22	6	0.000009690	-0.000005636	0.000005702
23	6	-0.000019697	0.000007377	0.000005279
24	6	-0.000002026	-0.000004640	-0.000006953
25	6	-0.000005428	0.000006789	0.000000504
26	6	0.000005041	-0.000004570	0.000001669
27	1	-0.000001117	0.000000238	0.000000810

28	1	-0.000000977	0.000001499	-0.000000372
29	1	-0.000000007	0.000001388	0.000002106
30	6	0.000007378	0.000012117	-0.000007584
31	8	0.000000685	-0.000026516	0.000007665
32	8	-0.000001737	0.000002943	-0.000002271
33	7	-0.000006243	0.000005305	0.000000629
34	7	0.000008679	0.000020783	-0.000005415
35	6	0.000010198	-0.000035954	-0.000005612
36	6	-0.000004106	-0.000006920	0.000000694
37	6	-0.000000642	0.000000443	-0.000001753
38	6	-0.000004307	-0.000000366	-0.000001074
39	6	-0.000000027	0.000001473	-0.000001070
40	6	-0.000001051	0.000003538	-0.000000020
41	6	-0.000000342	-0.000000950	-0.000000885
42	1	0.000000557	0.000000923	0.000000092
43	1	0.000001328	0.000000857	-0.000001767
44	1	-0.000000186	-0.000000424	-0.000001274
45	1	0.000000021	-0.000000863	-0.000002067
46	6	-0.000005508	0.000012786	-0.000004127
47	6	-0.000005402	-0.000009361	0.000006639
48	1	0.000002109	0.000000440	0.000003779
49	6	0.000016755	0.000013041	0.000001506
50	8	-0.000009040	-0.000009337	0.000006911
51	8	-0.000000728	0.000007255	-0.000008698
52	1	-0.000001247	0.000000376	0.000000955
53	29	0.000011207	-0.000000166	-0.000004019

Table S3. XYZ coordination of the optimized structure of **L**+Fe^{3+}.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.710625	-2.614225	-0.198848
2	6	0	-4.353769	-1.339945	-0.143292
3	6	0	-5.784302	-1.258018	-0.005716
4	6	0	-6.548672	-2.463539	0.034522
5	6	0	-5.872117	-3.696307	-0.059579
6	6	0	-4.466438	-3.768480	-0.170035
7	1	0	-2.630817	-2.648250	-0.284536
8	6	0	-6.437035	-0.020719	0.106475
9	6	0	-7.955430	-2.385146	0.174734
10	1	0	-6.446942	-4.618192	-0.046107
11	1	0	-3.990580	-4.740047	-0.237855
12	6	0	-8.587956	-1.147595	0.287923
13	6	0	-7.837343	0.027187	0.260949
14	1	0	-8.543178	-3.297578	0.193671
15	1	0	-9.665244	-1.100867	0.399626
16	1	0	-8.315931	0.995808	0.358359
17	6	0	-3.634373	-0.136280	-0.209909
18	6	0	-5.679018	1.254951	0.083075
19	7	0	-4.284510	1.086158	-0.287524
20	7	0	-2.276920	0.006274	-0.124788
21	6	0	-2.048323	1.313985	-0.097615
22	6	0	-3.289753	2.065068	-0.162116
23	6	0	-0.780703	2.027533	-0.021873
24	6	0	-3.348945	3.435519	-0.120786
25	6	0	-0.866892	3.415436	0.030974
26	6	0	-2.101529	4.095025	-0.006578
27	1	0	0.043579	3.997285	0.091765

28	1	0	-2.093894	5.179210	0.043769
29	1	0	-4.280350	3.984251	-0.157249
30	6	0	0.520233	1.316311	-0.017658
31	8	0	0.580325	0.034125	-0.070856
32	8	0	-6.127150	2.357858	0.300097
33	7	0	1.622421	2.101634	0.037740
34	7	0	2.711530	1.311741	0.013418
35	6	0	3.925651	1.850878	0.049617
36	6	0	7.639241	-0.207404	0.029570
37	6	0	8.924650	-0.725666	0.105812
38	6	0	9.063503	-2.113054	0.175355
39	6	0	7.937508	-2.953803	0.155920
40	6	0	6.660751	-2.417976	0.083331
41	6	0	6.482741	-1.016102	0.025535
42	1	0	9.777430	-0.057449	0.117007
43	1	0	10.056566	-2.542293	0.248184
44	1	0	8.068577	-4.028783	0.198652
45	1	0	5.788346	-3.059721	0.070861
46	6	0	5.140521	1.076346	0.024380
47	6	0	6.361081	1.769065	0.023218
48	1	0	3.970824	2.938019	0.089680
49	6	0	5.175674	-0.398361	-0.013810
50	8	0	4.123012	-1.131203	-0.085062
51	8	0	7.516741	1.177213	-0.044688
52	1	0	6.446313	2.850819	0.071320
53	26	0	2.365163	-0.569420	-0.075633
