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Supporting Information

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[1] Li Yan and Zhongkui Li contribute equally to the article.

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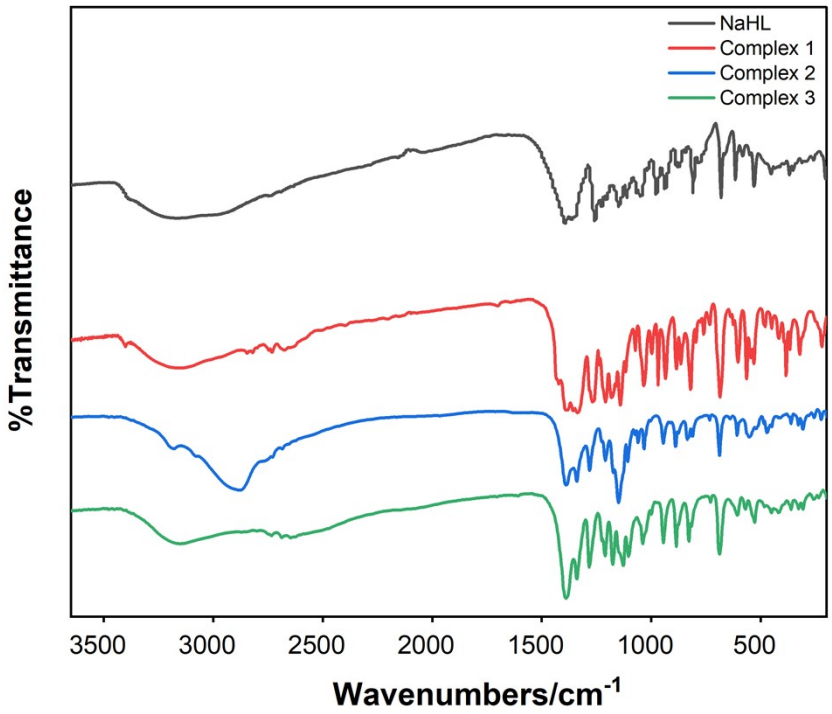

Fig S1. FT-IR spectra of **NaHL**, **1**, **2**, and **3.**

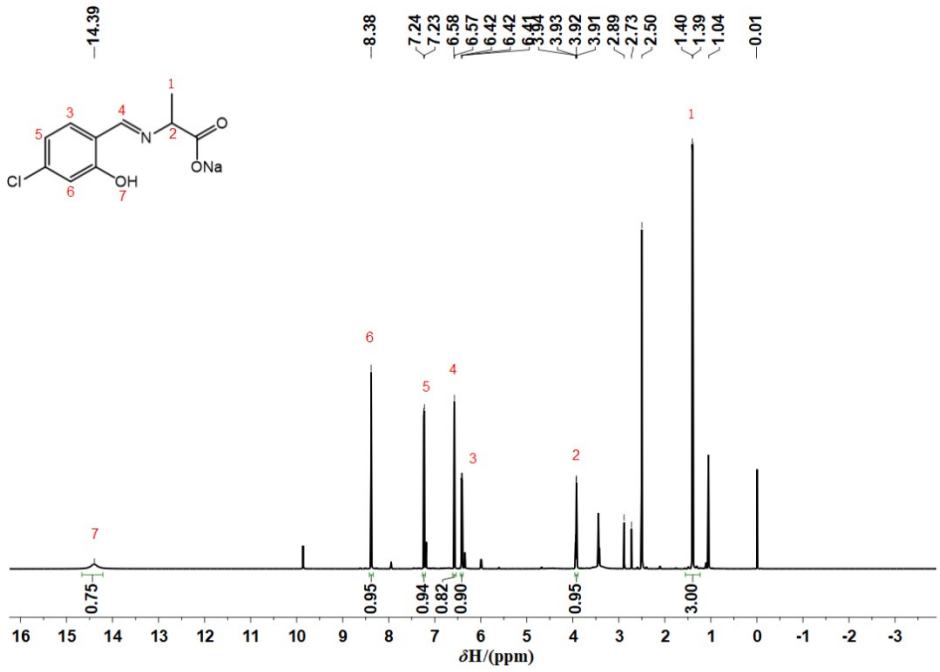

Fig S2. ^{1}H NMR spectrum (700 MHz, 298K) of **NaHL** in DMSO-d_6.

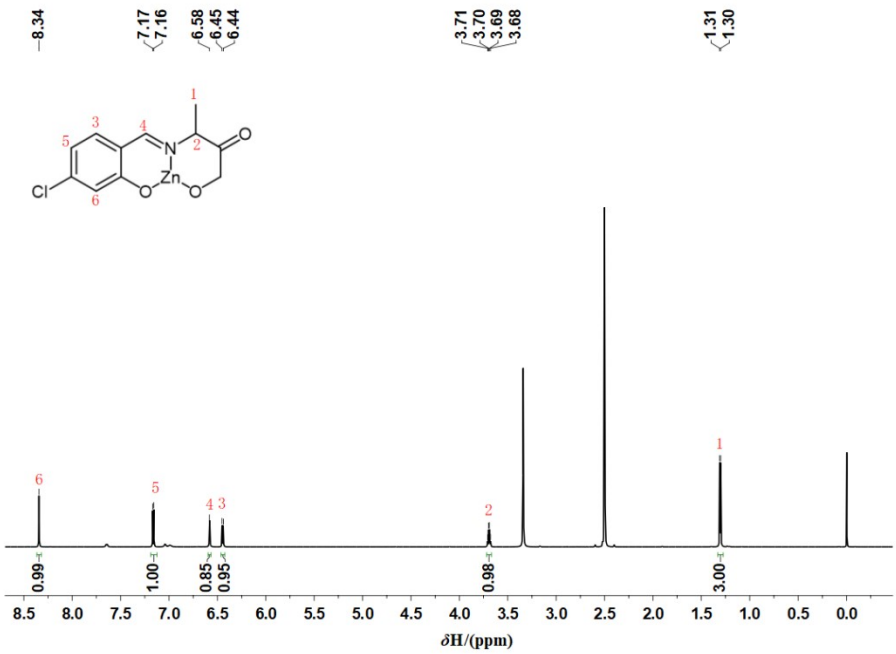

Fig S3. [1]H NMR spectrum (700 MHz, 298K) of **1** and **2** in DMSO-d_6.

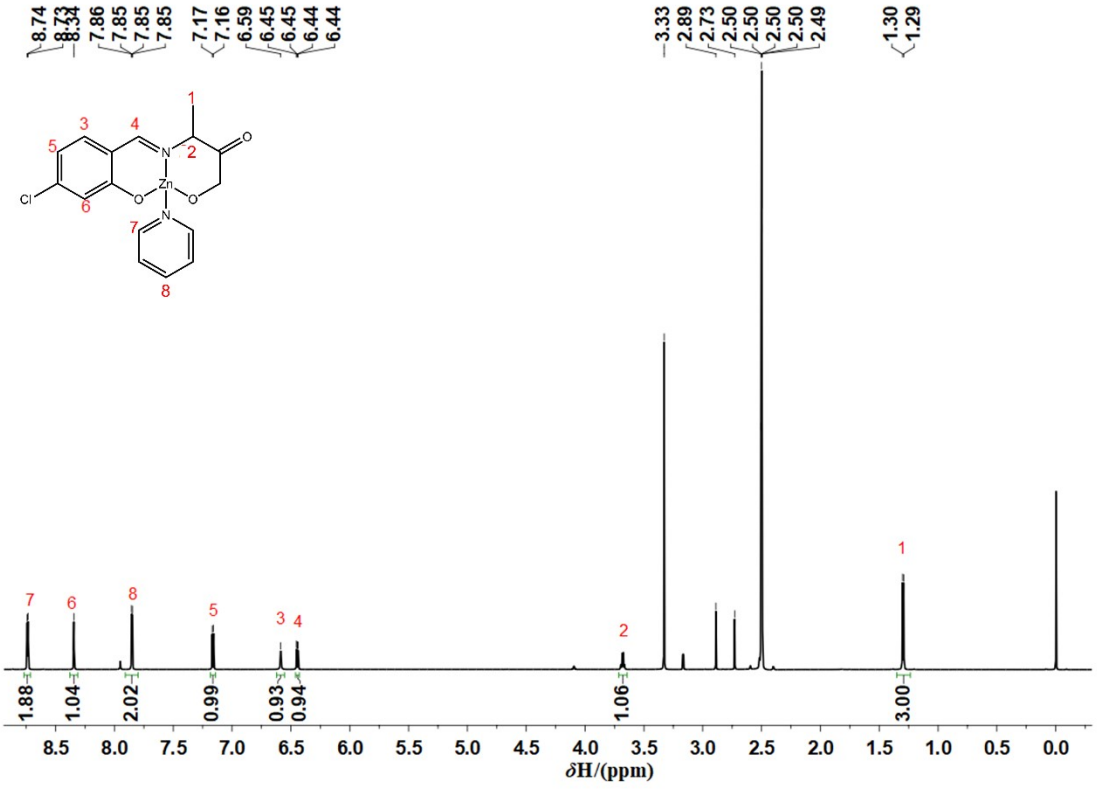

Fig S4. [1]H NMR spectrum (700 MHz, 298K) of **3** in DMSO-d_6.

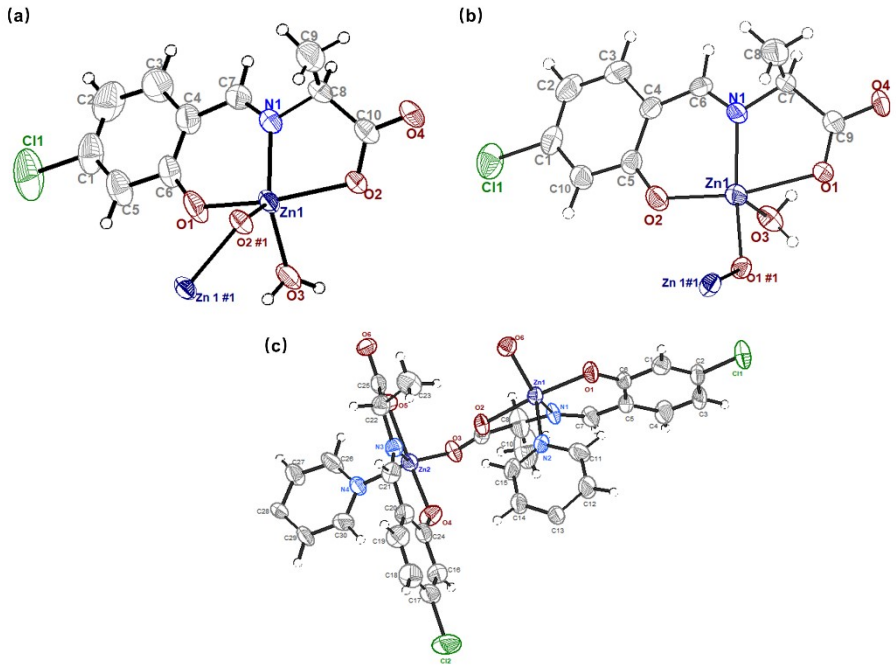

Fig S5. Oak Ridge thermal ellipsoid plot (ORTEP) views of **1** (a), **2** (b), and **3** (c)with 50% thermal ellipsoid probability.

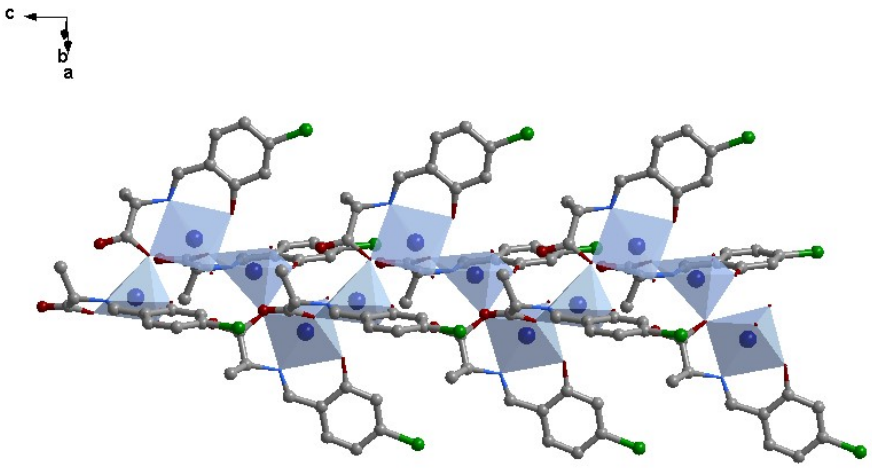

Fig S6. One-dimensional helix chain structure of **1.**

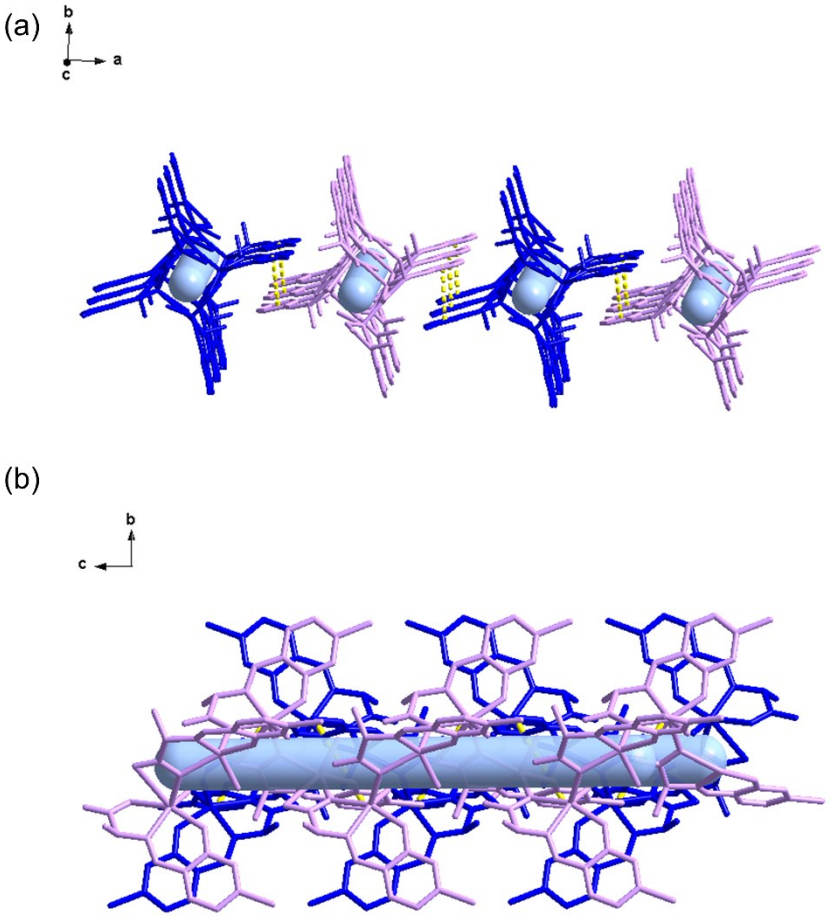

Fig S7. 2D structure of **1** viewed from *c* axis (a) and *a* axis (b).

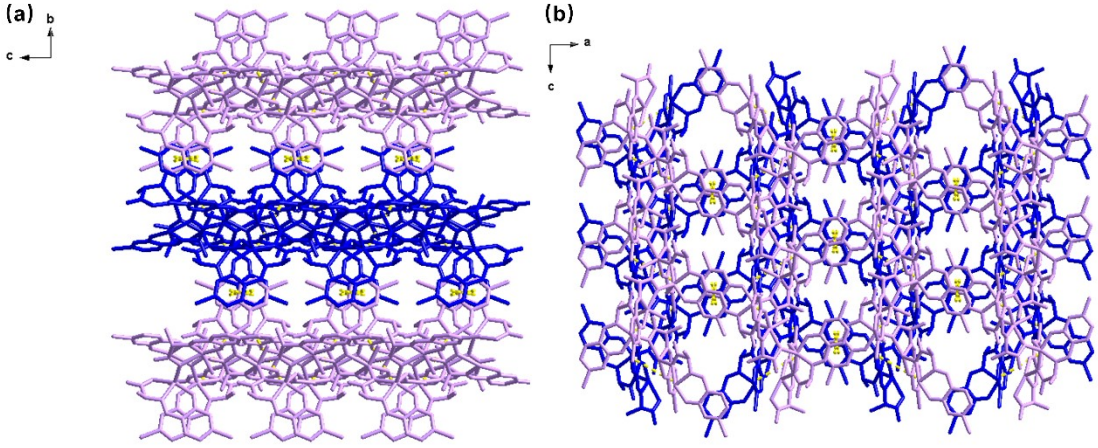

Fig S8. 3D structure of **1** viewed from *a* axis (a) and *b* axis (b).

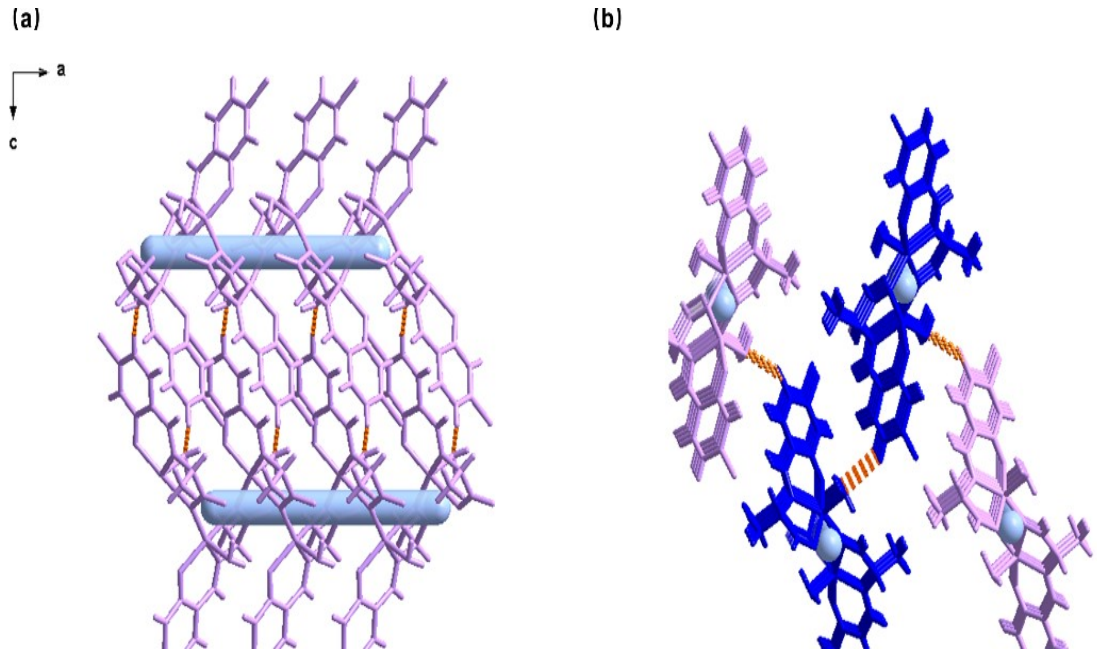

Fig S9. 2D structure of **2** viewed from *b* axis (a); 3D structure of **2** viewed from *a* axis (b).

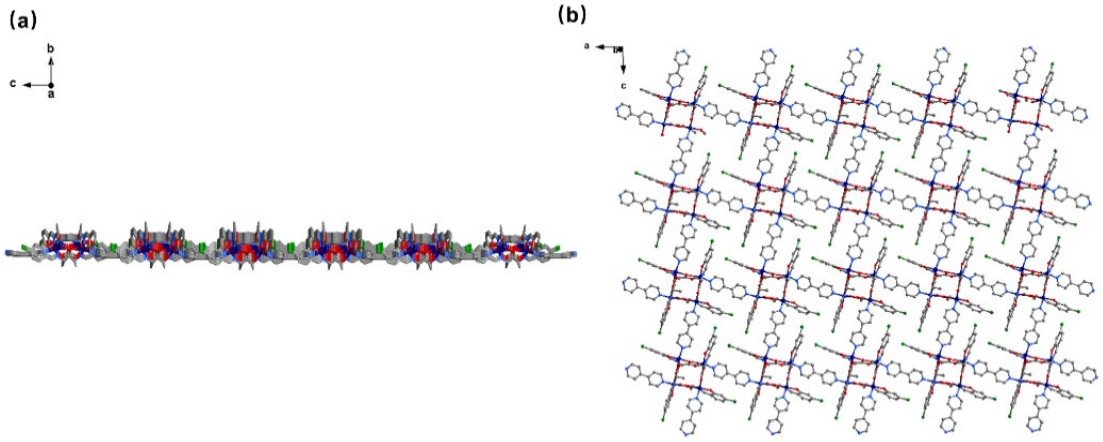

Fig S10. 2D structure of **3** viewed from *a* axis (a); 2D layered structure of **3** viewed from *b* axis (b).

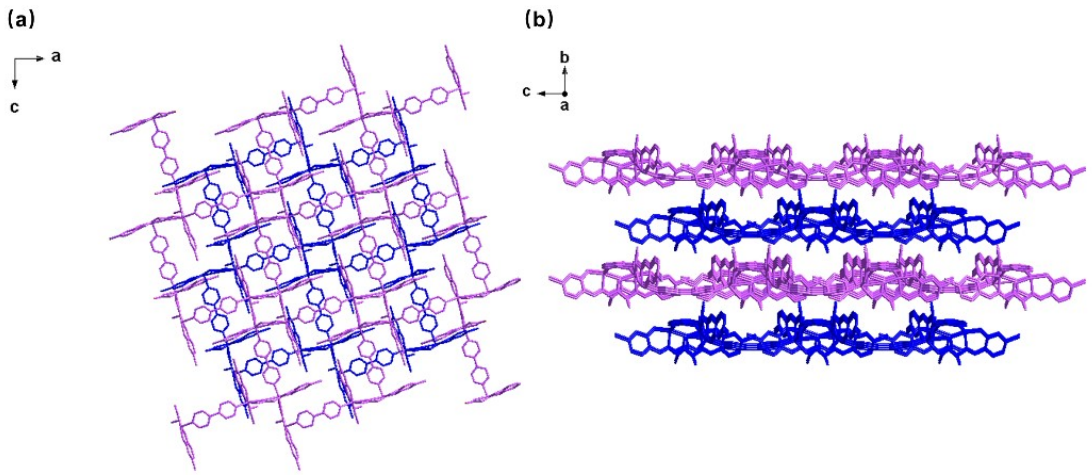

Fig S11. 3D structure of **3** viewed from *b* axis (a), from *c* axis (b).

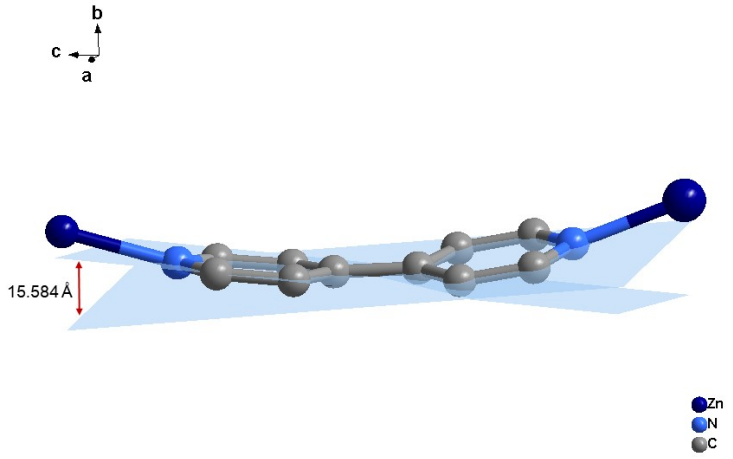

Fig S12. The bending angle between the pyridine ligand benzene ring and the benzene ring is 15.584°.

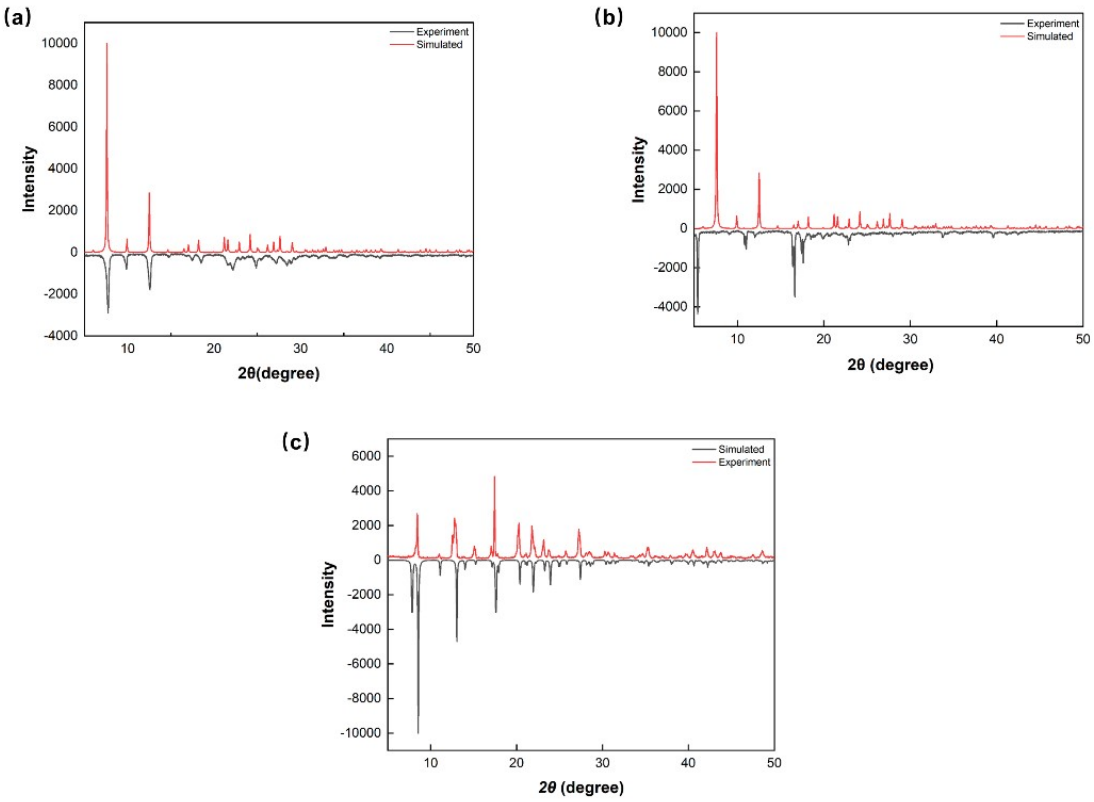

Fig S13. PXRD spectra of **1** (a), **2** (b) and **3** (c).

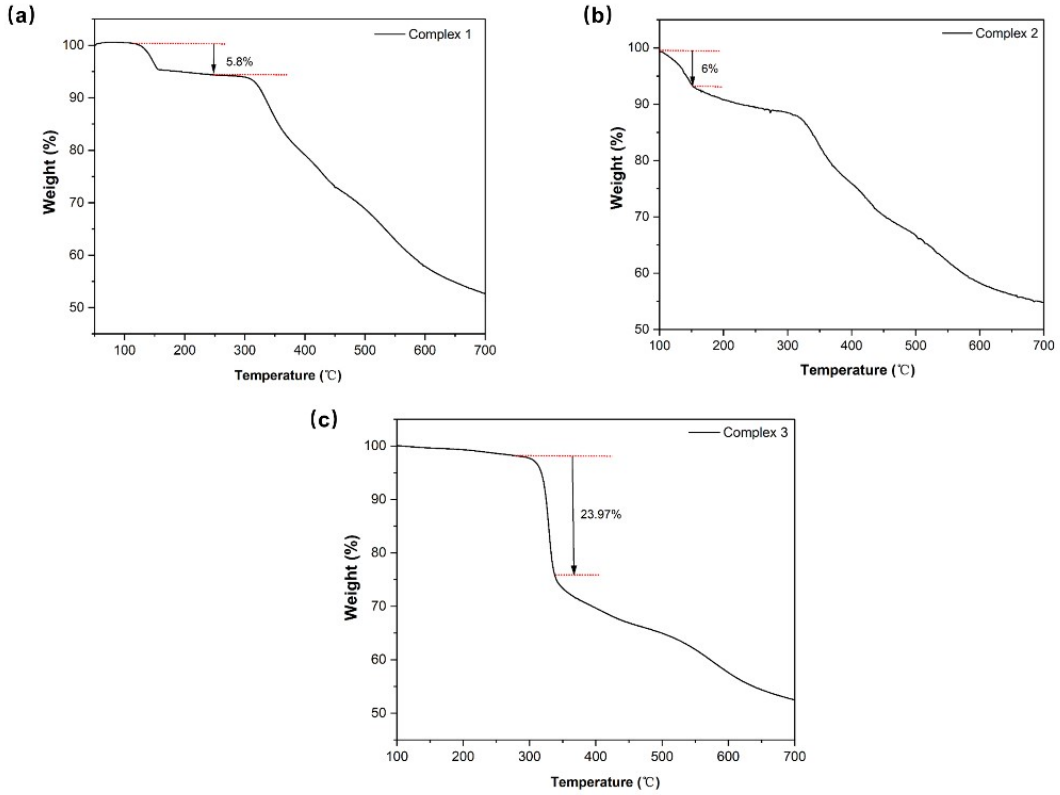

Fig. S14. TG curves of **1**, **2** and **3**. The losses of **1**, **2**, **3** in the first stage were 5.8%, 23.97 % and 6 % respectively.

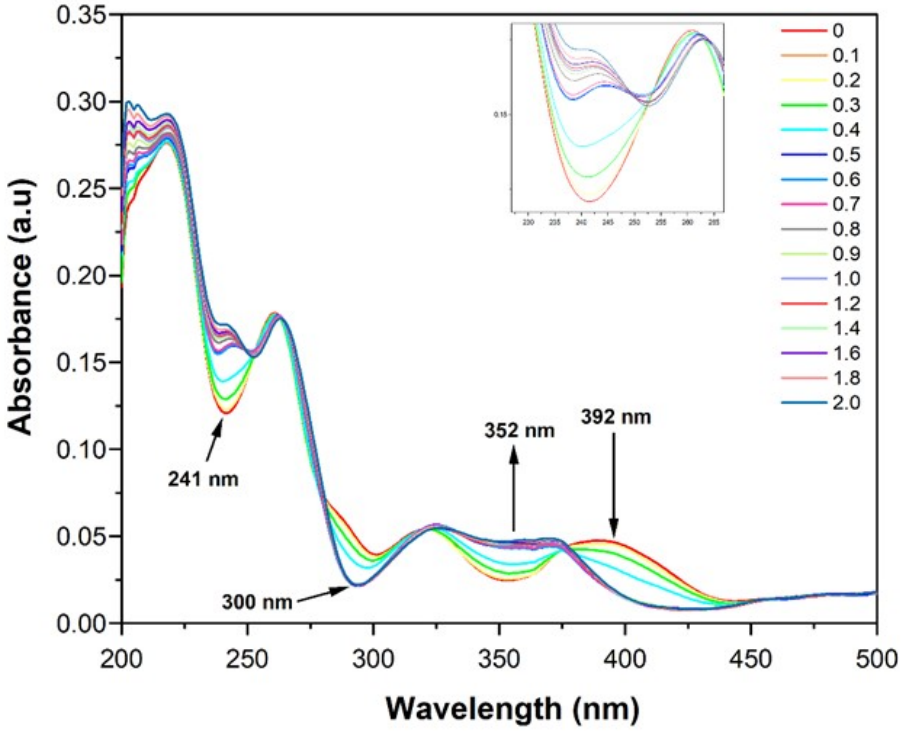

Fig S15. UV−vis spectra changes of **NaHL** (1×10^{-5} mol L^{-1}) after addition of Zn^{2+} (0–2.0 equiv) in ethanol.

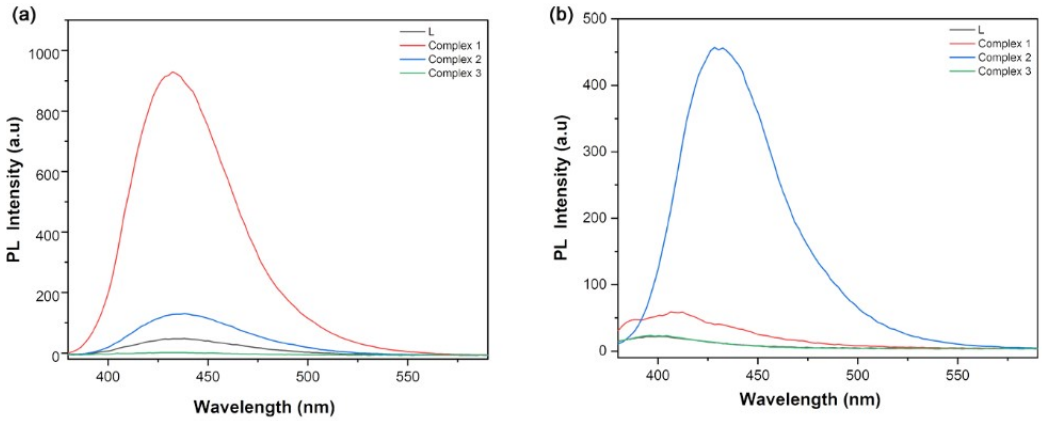

Fig S16. Fluorescence spectra of **NaHL, 1**, **2**, and **3** in CH_3CN (a) and CH_2Cl_2 (b) (E_x = 360 nm and concentration of 2.5×10^{-5} mol L^{-1}).

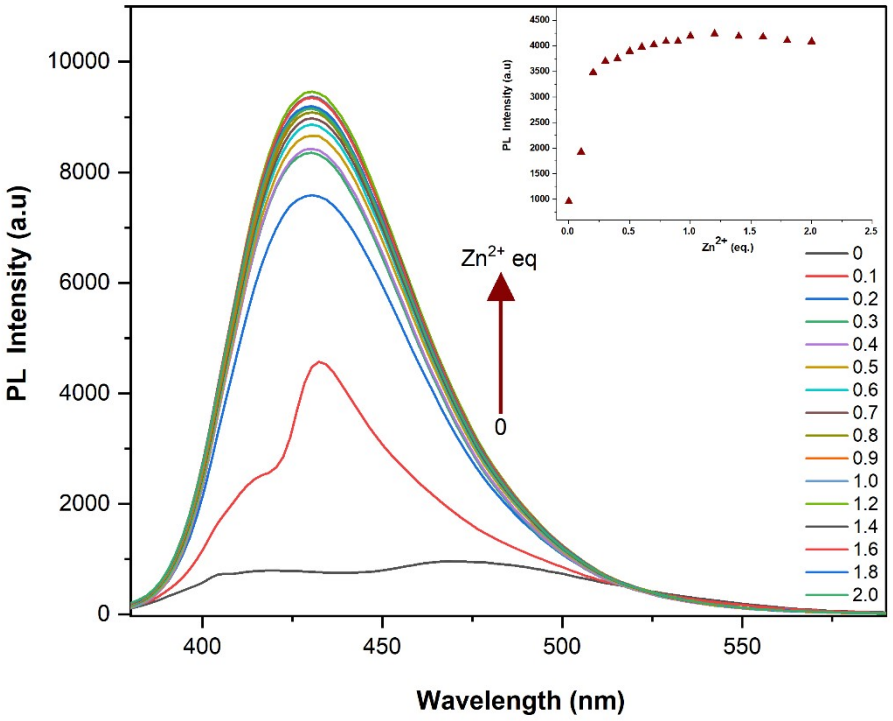

Fig S17. Fluorescence spectrum changes of **NaHL** (The concentration of 2.5×10^{-5} mol L^{-1}) upon addition of Zn^{2+} (The concentration of 2.5×10^{-3} mol L^{-1}) in ethanol (Ex = 360 nm, pass widths 2.5 nm).

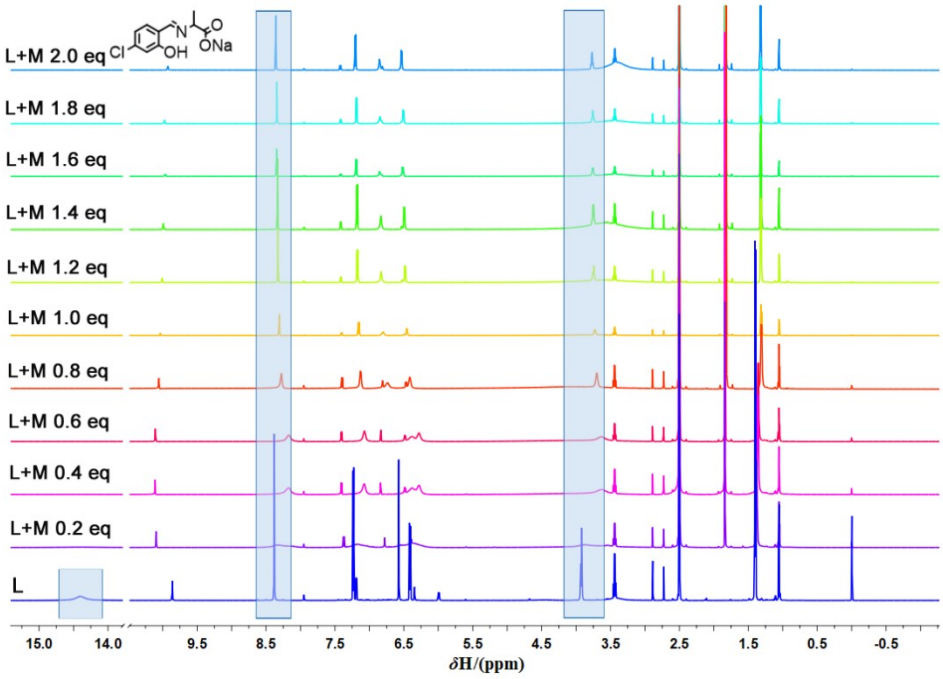

Fig S18. ^{1}H NMR (DMSO-*d6*, 700 MHz) spectra changes of **NaHL** upon addition of Zn^{2+}(0–2 eq).

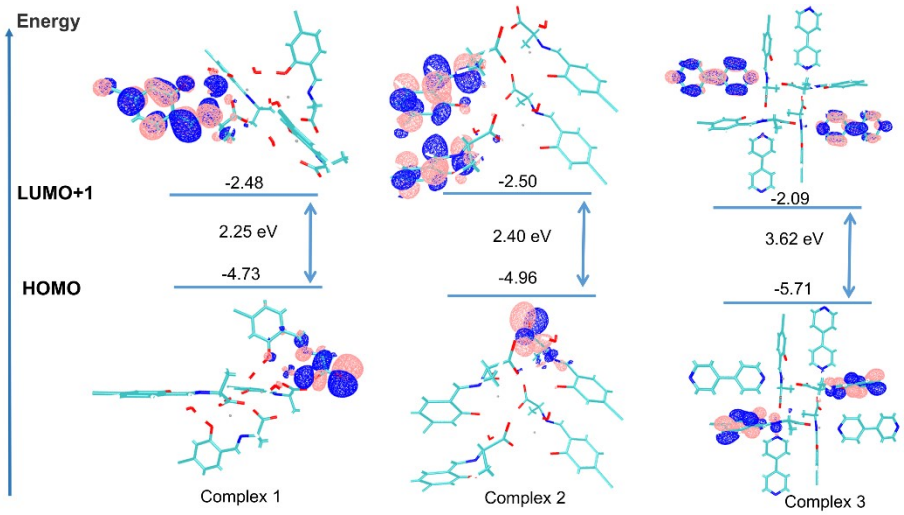

Fig S19. Primary orbitals which contribute to the calculated transitions of **NaHL** and complex **1-3** (iso=0.01).

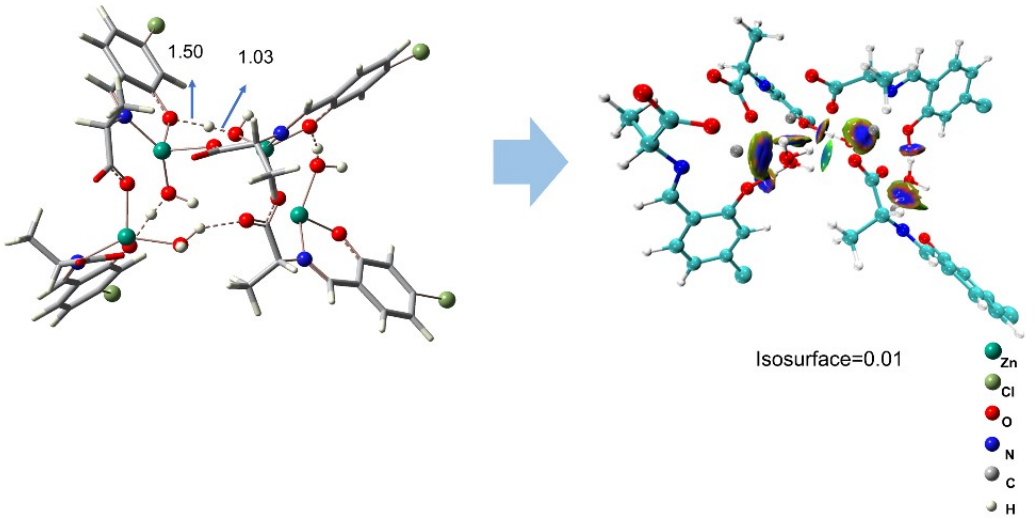

Fig S20. Optimized corresponding structure of complex **1** at the B3LYP(D3BJ)/6-31G(d)/SDD level (distances in Å) and the Color-filled (a) Reduced density gradient (RDG).

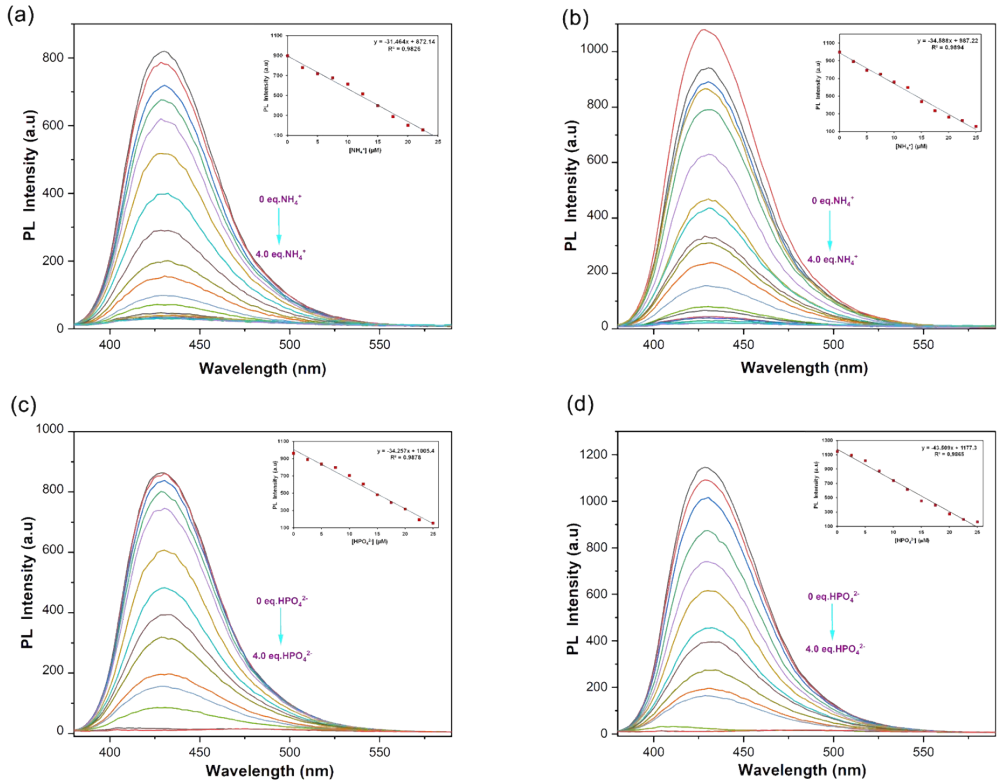

Fig S21. Fluorescence titration curves of complex **1** (a, c) and complex **2** (b, d) in the presence of different concentrations of NH_4^+/HPO_4^{2-}. The linear correlation for the **1**/**2** and NH_4^+/HPO_4^{2-} concentration at low concentration range (insert).

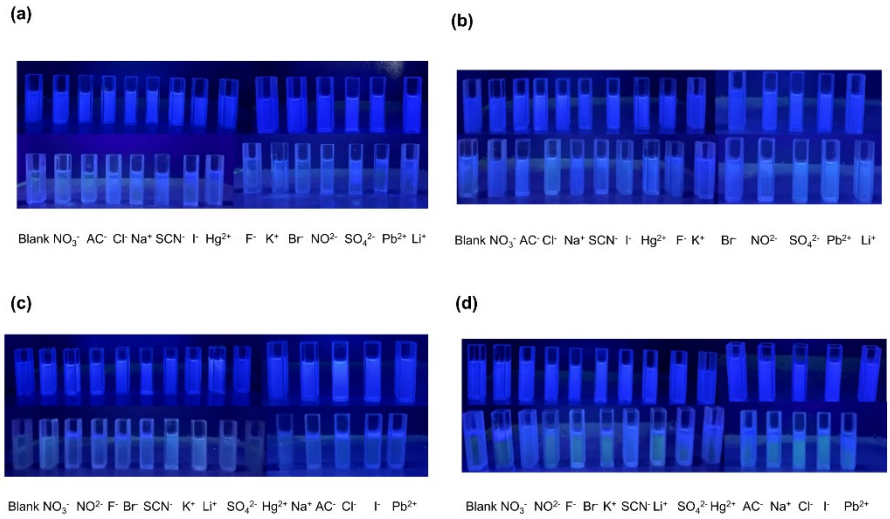

Fig S22. selectivity of NH_4^+ /HPO_4^{2-}(4.0 equiv.) to other competing ions of **1** under UV lamp (365 nm) (a) and (b); (c) and (d) Selectivity of NH_4^+ /HPO_4^{2-}(4 .0 equiv.) to other competing ions of **2** under UV lamp (365 nm).

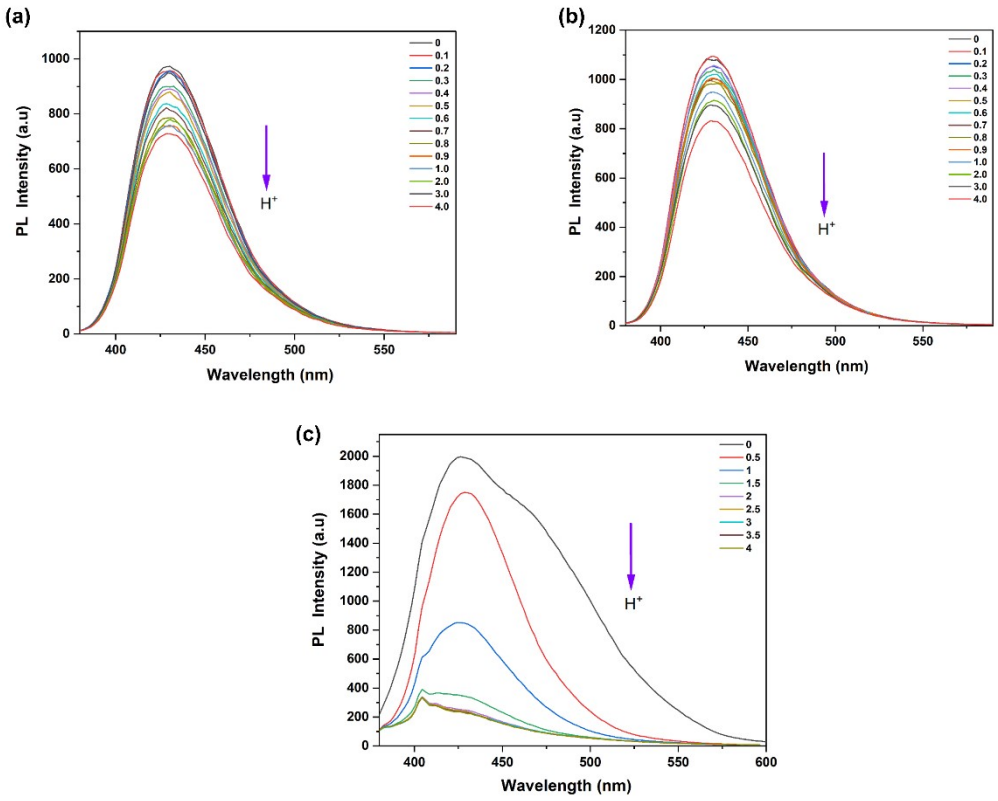

Fig S23 (a) and (b) Fluorescence spectra changes of 1,2 (2.5×10^{-5} mol L-1) up addition of H^+ (0–4.0 equiv) in ethanol. (c) Fluorescence spectra changes of NaHL (2.5×10^{-5} mol L^{-1}) up addition of H^+ (4.0 eq, 1.0×10^{-4} mol L^{-1}) in ethanol, E_x=2.5 nm. E_m=2.5 nm.

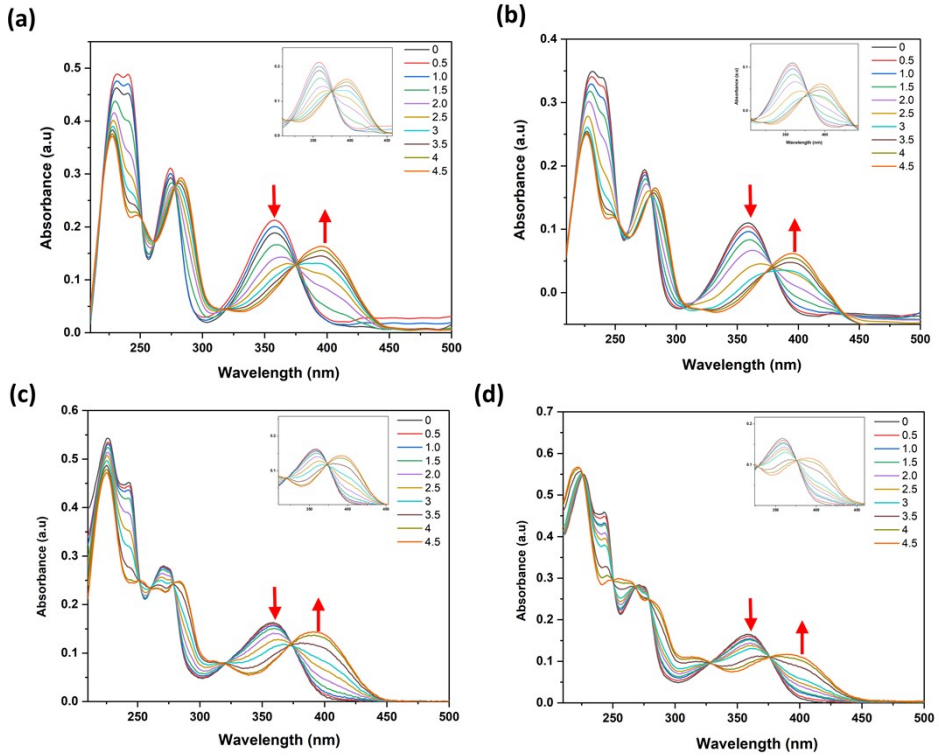

Fig S24 (a) and (b) UV−vis spectra changes of **1** (2.5×10^{-5} mol L^{-1}) up addition of NH_4^+ /HPO_4^{2-} (0–4.5 equiv) in ethanol. (c) and (d) UV−vis spectra changes of **2** (2.5×10^{-5} mol L^{-1}) up addition of NH_4^+ /HPO_4^{2-} (0–4.5 equiv) in ethanol.

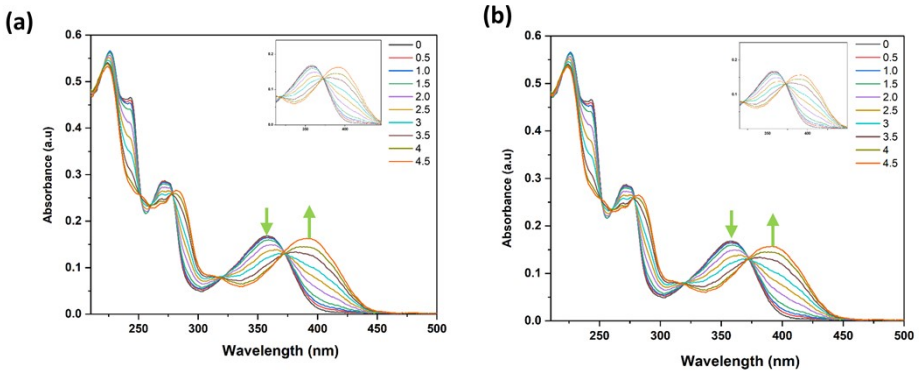

Fig S25 (a) and (b) UV−vis spectra changes of **1** and **2** (2.5×10^{-5} mol L^{-1}) up addition of PO_4^{3-} (0–4.5 equiv) in ethanol.

Table S1 The pH values of **1**, **2**, NH_4^+, HPO_4^{2-}, and **1** or **2** with the addition of NH_4^+ or HPO_4^{2-} in aqueous solution. (The concentration of the aqueous solution of **1** and **2** are 2.5×10^{-5} mol L^{-1}, and the concentration of NH_4^+ and HPO_4^{2-} are 2.5×10^{-5} mol L^{-1}).

	1	**2**	NH_4^+	HPO_4^{2-}	1+NH_4^+ or HPO_4^{2-}	2+$NH4^+$ or HPO_4^{2-}
pH	6.10	6.15	5.98	7.09	5.1 or 5.45	6.01 or 5.6

Table S2 Selected bond distances (Å) and angles (°) for complex **1**.

Atom-Atom	Length	Atom-Atom	Length
Zn1-O1	1.997(3)	N1-C8	1.478(5)
Zn1-O3	2.005(3)	C10-C8	1.507(6)
Zn1-O2[1]	2.018(2)	C6-C4	1.398(6)
Zn1-N1	2.029(3)	C6-C5	1.416(5)
Zn1-O2[1]	2.187(2)	C8-C9	1.507(6)
Cl1-C1	1.743(5)	C4-C3	1.398(6)
O2-C10	1.300(4)	C4-C7	1.463(6)
O4-C10	1.216(5)	C5-C1	1.355(6)
O1-C6	1.300(5)	C3-C2	1.371(7)
N1-C7	1.265(5)	C1-C2	1.373(8)

[1]5/4-Y, -1/4+X, -1/4+Z

Atom-Atom-Atom	Angle	Atom-Atom-Atom	Angle
O1-Zn1-O3	90.96(14)	O4-C10-C8	119.5(3)
O1-Zn1-O2[1]	94.30(11)	O2-C10-C8	117.0(3)
O3-Zn1-O2[1]	98.29(12)	O1-C6-C4	123.8(3)
O1-Zn1-N1	88.70(12)	O1-C6-C5	118.5(4)
O3-Zn1-N1	143.20(14)	C4-C6-C5	117.7(4)
O21-Zn1-N1	118.43(12)	N1-C8-C9	112.3(4)
O1-Zn1-O2	151.70(11)	N1-C8-C10	110.0(3)
O3-Zn1-O2	87.06(10)	C9-C8-C10	111.8(4)
O21-Zn1-O2	113.93(12)	C6-C4-C3	118.8(4)
N1-Zn1-O2	76.48(11)	C6-C4-C7	122.9(4)
C10-O2-Zn1[2]	116.4(2)	C3-C4-C7	118.3(4)
C10-O2-Zn1	113.2(2)	N1-C7-C4	126.9(4)
Zn1[2]-O2-Zn1	128.81(12)	C1-C5-C6	121.1(5)
C6-O1-Zn1	130.2(2)	C2-C3-C4	122.6(5)
C7-N1-C8	117.5(3)	C5-C1-C2	121.9(5)
C7-N1-Zn1	126.4(3)	C5-C1-Cl1	119.5(4)
C8-N1-Zn1	115.1(3)	C2-C1-Cl1	118.6(4)
O4-C10-O2	123.4(4)	C3-C2-C1	117.8(4)

[1]5/4-Y,-1/4+X,-1/4+Z; [2]1/4+Y,5/4-X,1/4+Z

Table S3. Selected bond distances (Å) and angles (°) for complex **2.**

Atom-Atom	Length/Å	Length/Å
Zn1-O1	2.280(3)	1.466(4)
Zn1-O11	2.048(2)	1.409(5)
Zn1-O2	2.000(2)	1.425(5)
Zn1-O3	2.067(3)	1.525(5)
Zn1-N1	2.025(3)	1.432(5)
Cl1-C1	1.747(4)	1.532(6)
O1-C9	1.276(5)	1.384(5)
O2-C5	1.325(4)	1.361(6)
O4-C9	1.243(5)	1.418(5)
N1-C6	1.290(4)	1.373(6)

Atom-Atom-Atom	Angle	Atom-Atom-Atom	Angle
O2-Zn1-O1	168.00(10)	C4-C5-C00D	117.7(3)
O2-Zn1-O1[1]	98.28(9)	O4-C9-O1	124.4(4)
O3-Zn1-O1	87.23(10)	C7-C9-O1	118.8(3)
O3-Zn1-O1[1]	99.54(11)	C7-C9-O4	116.8(3)
O3-Zn1-O2	99.15(12)	C4-C6-N1	127.4(4)
N1-Zn1-O1	77.56(10)	C9-C7-N1	109.8(3)
N1-Zn1-O1[1]	156.99(11)	C8-C7-N1	111.1(3)
N1-Zn1-O2	91.31(11)	C8-C7-C9	108.8(3)
N1-Zn1-O3	99.50(12)	C00D-C1-Cl1	119.3(3)
C9-O1-Zn1	111.2(2)	C2-C1-Cl1	118.7(3)
C9-O1-Zn1[2]	118.7(2)	C2-C1-C00D	122.0(4)
C5-O2-Zn1	124.7(2)	C1-C00D-C5	121.2(4)
C6-N1-Zn1	123.1(3)	C6-C4-C5	124.5(3)
C7-N1-Zn1	118.0(2)	C3-C4-C5	117.8(4)
C7-N1-C6	118.2(3)	C3-C4-C6	117.7(4)
C00D-C5-O2	118.8(3)	C2-C3-C4	123.1(4)
C4-C5-O2	123.4(3)	C3-C2-C1	118.2(4)

[1]-1/2+X,1/2-Y,1-Z; [2]1/2+X,1/2-Y,1-Z

Table S4. Selected Hydrogen bond for complex **2.**

	D-H	H…A	D…A	<(DHA)
O3-H3D-O2	0.86	1.78	2.6261(16)	168

Table S5 Selected bond distances (Å) and angles (°) for complex **3.**

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Zn1-O1	2.007(5)	N3-C22	1.473(10)
Zn1-O6	2.014(5)	C24-C16	1.411(10)
Zn1-N1	2.077(7)	C24-C20	1.423(12)
Zn1-O2	2.126(5)	C6-C5	1.435(11)
Zn1-N2	2.134(6)	C28-C27	1.350(10)
Zn2-O4[1]	1.988(5)	C28-C29	1.370(10)
Zn2-O3	2.013(5)	C28-C28[1]	1.515(14)
Zn2-N3[1]	2.047(7)	C13-C14	1.343(10)
Zn2-O5[1]	2.116(5)	C13-C12	1.385(10)
Zn2-N4	2.122(6)	C13-C13[3]	1.503(14)
Cl1-C2	1.766(8)	C14-C15	1.343(10)
Cl2-C17	1.749(8)	C9-C8	1.556(11)
O2-C9	1.235(9)	C7-C5	1.433(10)
O5-C25	1.247(9)	C3-C4	1.355(11)
O1-C6	1.298(8)	C3-C2	1.369(12)
O4-C24	1.306(8)	C21-C20	1.416(11)
O3-C9	1.237(9)	C12-C11	1.382(11)
O6-C25	1.270(9)	C5-C4	1.395(10)
N2-C15	1.319(9)	C27-C26	1.333(11)
N2-C11	1.359(10)	C16-C17	1.404(12)
N4-C30	1.312(9)	C29-C30	1.368(11)
N4-C26	1.344(9)	C23-C22	1.528(11)
N1-C7	1.271(9)	C22-C25	1.529(10)
N1-C8	1.454(10)	C18-C17	1.355(14)
C1-C2	1.370(10)	C18-C19	1.357(12)
C1-C6	1.405(9)	C19-C20	1.408(11)
N3-C21	1.276(9)	C8-C10	1.441(15)

[1]1-X,+Y,1-Z; [2]-X,+Y,1-Z; [3]1-X,+Y,-Z

Atom-Atom-Atom	Angle	Atom-Atom-Atom	Angle/
O1-Zn1-O1	92.5(2)	C27-C28-C29	115.9(7)
O1-Zn1-N1	89.8(2)	C27-C28-C28[2]	123.1(8)
O6-Zn1-N1	135.3(2)	C29-C28-C28[2]	121.0(8)
O1-Zn1-O2	168.2(2)	C14-C13-C12	115.6(7)
O6-Zn1-O2	96.2(2)	C14-C13-C13[3]	125.2(8)
N1-Zn1-O2	78.5(2)	C12-C13-C13[3]	119.2(8)
O1-Zn1-N2	95.0(2)	C15-C14-C13	122.8(7)
O6-Zn1-N2	112.1(2)	O2-C9-O3	125.3(7)
N1-Zn1-N2	112.1(3)	O2-C9-C8	117.7(7)
O2-Zn1-N2	89.0(2)	O3-C9-C8	116.9(7)

O4[1]-Zn2-N2	97.0(2)	N1-C7-C5	127.6(7)
O4[1]-Zn2-N3[1]	90.2(2)	N2-C15-C14	123.0(7)
O3-Zn2-N3[1]	140.1(2)	C4-C3-C2	117.7(8)
O4[1]-Zn2-O5[1]	168.7(2)	N3-C21-C20	127.8(8)
O3-Zn2-O5[1]	90.3(2)	C1-C2-C3	122.4(7)
N3[1]-Zn2-O5[1]	78.7(2)	C1-C2-Cl1	118.1(7)
O4[1]-Zn2-N4	95.8(2)	C3-C2-Cl1	119.5(6)
O3-Zn2-N4	108.6(2)	C11-C12-C13	119.9(7)
N3[1]-Zn2-N4	109.6(3)	C4-C5-C6	118.8(7)
O5[1]-Zn2-N4	89.9(2)	C4-C5-C7	117.7(7)
C9-O2-Zn1	116.7(5)	C6-C5-C7	123.4(6)
C25-O5-Zn2[1]	116.1(5)	C26-C27-C28	121.6(8)
C6-O1-Zn1	127.0(5)	C3-C4-C5	123.3(8)
C24-O4-Zn2[1]	127.1(5)	C27-C26-N4	123.8(7)
C9-O3-Zn2	107.8(5)	C17-C16-C24	119.9(9)
C25-O6-Zn1	106.6(5)	C30-C29-C28	118.9(7)
C15-N2-C11	116.5(7)	N3-C22-C25	108.6(7)
C15-N2-Zn1	124.4(5)	N3-C22-C23	110.9(6)
C11-N2-Zn1	118.1(5)	C25-C22-C23	112.1(6)
C30-N4-C26	114.2(7)	O5-C25-O6	123.2(7)
C30-N4-Zn2	120.6(6)	O5-C5-C22	119.9(7)
C26-N4-Zn2	123.1(5)	O6-C5-C22	116.8(7)
C7-N1-C8	123.4(7)	C17-C18-C19	118.7(8)
C7-N1-Zn1	123.7(5)	C18-C17-C16	122.2(8)
C8-N1-Zn1	112.9(5)	C18-C17-Cl2	120.4(7)
C2-C1-C6	121.2(7)	C16-C17-Cl2	117.3(8)
C21-N3-C22	119.5(7)	C18-C19-C20	122.7(9)
C21-N3-Zn2[1]	124.0(6)	C19-C20-C21	117.5(8)
C22-N3-Zn2[1]	116.1(5)	C19-C20-C24	119.0(7)
O4-C24-C16	117.9(7)	C21-C20-C24	123.5(7)
O4-C24-C20	124.7(7)	N2-C11-C12	121.8(7)
C16-C24-C20	117.4(7)	N4-C30-C29	125.2(8)
O1-C6-C1	118.9(7)	C10-C8-N1	119.3(9)
O1-C6-C5	124.7(6)	C10-C8-C9	115.3(8)
C1-C6-C5	116.4(7)	N1-C8-C9	109.5(7)

[1]1-X,+Y,1-Z; [2]-X,+Y,1-Z; [3]1-X,+Y,-Z

Table S6 Excited state atomic coordinate information of **NaHL**.

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
17	0	5.070608	-0.23705	0.001405
1	0	2.865976	-1.94539	0.530894
6	0	3.350652	0.042528	-0.06406
6	0	2.499009	-0.96173	0.253276
6	0	2.902041	1.289029	-0.42843
6	0	1.096705	-0.76295	0.239769
6	0	1.547378	1.494752	-0.46435
1	0	3.599553	2.07883	-0.6893
6	0	0.62416	0.5041	-0.11406
8	0	0.325063	-1.76453	0.542285
1	0	1.163455	2.472302	-0.75007
6	0	-0.7981	0.838107	-0.15002
7	0	-1.76571	0.07807	0.144067
1	0	-0.98157	1.892226	-0.43372
6	0	-3.13297	0.623171	0.000948
6	0	-3.59306	1.344966	1.241406
6	0	-4.08554	-0.47547	-0.39181
1	0	-3.16989	1.338926	-0.84137
1	0	-3.54864	0.679811	2.110431
1	0	-4.61032	1.737206	1.14214
1	0	-2.90934	2.178768	1.425091
8	0	-5.25065	-0.20762	-0.61026
8	0	-3.58756	-1.66959	-0.52701
1	0	-0.60605	-1.43449	0.497405

Table S7 Excited state atomic coordinate information of **1.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	3.484359	1.447999	0.808895
2	30	0	-2.1447	-1.44349	0.2266
3	30	0	-4.03095	1.486082	-1.27316
4	30	0	1.55096	-1.48237	-0.62792
5	17	0	-0.35535	-5.06151	5.896847
6	17	0	-2.37312	4.891554	4.566184
7	8	0	2.128738	0.450586	-0.58753
8	8	0	-3.8426	-0.44758	-0.72516
9	8	0	-0.58311	-1.76304	-1.01201
10	8	0	0.413423	0.957972	-1.89551
11	8	0	-1.98389	-1.75622	-2.72895
12	8	0	-1.27934	-2.33592	1.790347

13	8	0	-3.27527	2.199119	0.432784
14	8	0	3.394008	-2.19484	-0.3359
15	8	0	4.287636	-0.35666	1.155833
16	8	0	-1.60347	0.361487	0.913411
17	8	0	-2.25865	1.700836	-2.18715
18	8	0	1.123211	-1.69683	1.319793
19	1	0	-0.8111	0.663455	0.449979
20	1	0	-1.45554	1.172958	-2.03738
21	1	0	1.760972	-2.26009	1.77545
22	7	0	3.181863	2.840259	-0.63362
23	7	0	-3.61735	-2.83756	0.304909
24	7	0	-5.76828	2.444693	-0.85125
25	7	0	1.513547	-2.44223	-2.4149
26	6	0	1.417352	1.281007	-1.29003
27	6	0	-4.70543	-1.27883	-1.23184
28	6	0	-0.86378	-1.88743	-2.2761
29	6	0	-1.72195	-3.27773	2.569751
30	6	0	-3.75137	3.085447	1.255236
31	6	0	4.066483	-3.08249	-1.00689
32	6	0	1.917882	2.698955	-1.38853
33	6	0	-4.67061	-2.69527	-0.72218
34	6	0	0.2679	-2.27107	-3.19341
35	1	0	2.132802	2.857025	-2.45485
36	1	0	-5.64647	-2.85675	-0.24281
37	1	0	-0.01803	-3.24468	-3.61517
38	6	0	5.354325	3.947933	-0.50668
39	6	0	-2.93468	-3.94415	2.372118
40	6	0	-5.01641	3.668622	1.123652
41	6	0	3.614854	-3.66516	-2.1945
42	6	0	4.03423	3.668135	-1.07067
43	6	0	-3.81859	-3.66451	1.241211
44	6	0	-5.94694	3.310576	0.055197
45	6	0	2.342249	-3.30759	-2.81987
46	1	0	3.759482	4.325188	-1.90362
47	1	0	-4.75233	-4.24367	1.239541
48	1	0	-6.8848	3.884589	0.059603
49	1	0	2.107536	-3.87519	-3.73041
50	6	0	-0.9445	-3.64622	3.694783
51	6	0	-2.94475	3.503711	2.340476
52	6	0	5.32401	-3.49982	-0.50628
53	1	0	-0.01032	-3.1207	3.862965
54	1	0	-1.96998	3.040685	2.454605
55	6	0	-3.33292	-4.90954	3.300549
56	6	0	-5.40598	4.647438	2.041907

57	6	0	4.402445	-4.64428	-2.80847
58	1	0	-4.28599	-5.41227	3.149154
59	1	0	-6.38563	5.106182	1.923822
60	1	0	4.037488	-5.10487	-3.72402
61	6	0	-1.36208	-4.61325	4.544999
62	6	0	-3.38557	4.433167	3.22202
63	6	0	6.062374	-4.4297	-1.15796
64	6	0	-2.55901	-5.26681	4.374401
65	6	0	-4.61838	5.026408	3.097743
66	6	0	5.625335	-5.02281	-2.3186
67	1	0	-2.88312	-6.03033	5.071178
68	1	0	-4.9516	5.775157	3.806591
69	1	0	6.223835	-5.77234	-2.82198
70	6	0	0.874525	3.693259	-0.94887
71	6	0	-4.51327	-3.69067	-1.8437
72	6	0	0.430415	-1.28576	-4.3222
73	1	0	-0.0519	3.546342	-1.51169
74	1	0	-0.52554	-1.17618	-4.83975
75	1	0	1.227677	4.715523	-1.1126
76	1	0	-4.59743	-4.71585	-1.46662
77	1	0	1.181315	-1.63791	-5.03706
78	1	0	0.652728	3.579747	0.118191
79	1	0	-3.54501	-3.5647	-2.33545
80	1	0	0.735452	-0.30696	-3.94198
81	1	0	4.03737	-1.13761	0.547851
82	1	0	-2.28446	1.115143	0.809472
83	1	0	-2.53314	1.548288	-3.1075
84	1	0	0.182213	-1.98468	1.597301
85	8	0	5.218786	2.340154	1.243368
86	8	0	-4.95037	1.765228	-3.23729
87	1	0	5.243377	-0.33509	1.296057
88	6	0	-6.84072	2.273028	-1.85495
89	8	0	-5.54818	-0.95532	-2.04552
90	6	0	6.148724	4.914354	-1.13015
91	6	0	5.856662	3.281552	0.615221
92	1	0	5.676209	-3.06174	0.421925
93	17	0	7.620623	-4.88666	-0.5251
94	1	0	-5.29811	-3.51411	-2.58259
95	6	0	-6.24417	1.889273	-3.18368
96	1	0	-7.32244	3.249776	-2.00781
97	6	0	-7.8896	1.287913	-1.4059
98	1	0	5.75682	5.408312	-2.01488
99	6	0	7.385586	5.271219	-0.65866
100	6	0	7.143336	3.651322	1.077734

101	8	0	-6.96965	1.757666	-4.14976
102	1	0	-8.62369	1.184827	-2.20838
103	1	0	-8.39412	1.628333	-0.49353
104	1	0	-7.44003	0.30703	-1.22663
105	1	0	7.974364	6.038662	-1.14726
106	6	0	7.859023	4.618035	0.454975
107	1	0	7.534385	3.128817	1.943462
108	17	0	9.424085	5.066844	1.080373

Table S8 Excited state atomic coordinate information of **2.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	7.425689	-0.01345	1.638865
2	1	0	5.261562	0.21	2.212194
3	1	0	2.735961	-4.17802	2.529732
4	6	0	2.797309	0.732922	2.261079
5	6	0	0.284869	-3.62307	2.599545
6	1	0	3.029277	-0.31996	2.457122
7	1	0	0.512833	-4.67394	2.806295
8	1	0	4.921268	-4.36122	1.986822
9	6	0	2.775041	1.530197	3.568305
10	6	0	0.2626	-2.8258	3.906771
11	1	0	2.0329	1.110675	4.253262
12	1	0	-0.52236	-3.21743	4.558353
13	1	0	3.757707	1.496417	4.048431
14	1	0	1.22562	-2.91838	4.420456
15	1	0	2.521388	2.575327	3.367188
16	1	0	0.081917	-1.76877	3.698952
17	17	0	9.819642	2.363406	-1.78604
18	8	0	4.918752	2.990147	-0.70264
19	6	0	6.025377	2.313542	-0.42291
20	6	0	8.395792	1.974391	-0.85105
21	6	0	7.199052	2.601956	-1.14749
22	1	0	7.134583	3.330783	-1.94702
23	6	0	6.106218	1.335989	0.60977
24	6	0	7.366894	0.740204	0.85922
25	6	0	8.497558	1.050545	0.142606
26	1	0	9.440439	0.560825	0.355893
27	17	0	-4.03997	7.658754	1.008496
28	1	0	-1.83777	5.844551	1.22598
29	30	0	3.070049	2.39132	-0.23154
30	30	0	0.557608	-1.96467	0.106922
31	17	0	7.307202	-1.99259	-1.44757
32	8	0	1.151385	1.626646	0.734879

33	8	0	-1.36106	-2.72935	1.073345
34	8	0	2.406312	-1.36585	-0.36417
35	8	0	2.84201	0.890722	-1.63535
36	8	0	0.329569	-3.46527	-1.29688
37	8	0	0.591516	-0.08453	2.046973
38	8	0	-1.92093	-4.44052	2.385439
39	7	0	3.770754	1.294298	1.319204
40	7	0	1.258314	-3.0617	1.65767
41	6	0	3.512937	-2.04245	-0.08445
42	6	0	1.40152	0.76504	1.642082
43	6	0	-1.11092	-3.59095	1.980548
44	6	0	4.999605	0.911218	1.413127
45	6	0	2.487165	-3.44478	1.751593
46	6	0	5.883353	-2.3816	-0.51258
47	6	0	4.686611	-1.75404	-0.80902
48	1	0	4.636848	-1.01879	-1.60428
49	6	0	3.593778	-3.02001	0.948236
50	6	0	4.854454	-3.61579	1.197686
51	6	0	5.985118	-3.30545	0.481072
52	1	0	6.927828	-3.79433	0.697535
53	1	0	2.239353	0.97998	-2.38379
54	1	0	-0.50175	-3.11166	-1.70668
55	1	0	2.625431	0.009076	-1.18267
56	1	0	0.035513	-4.30036	-0.90073
57	30	0	-0.72498	1.676022	-0.0833
58	30	0	-3.23742	-2.67997	0.255163
59	17	0	-6.55241	3.302759	1.346962
60	8	0	-0.48353	-0.46719	-0.82378
61	8	0	-2.99596	-4.82319	-0.48531
62	8	0	-1.10733	3.619527	0.190249
63	8	0	-3.61977	-0.73647	0.528715
64	8	0	-1.80934	0.901222	1.497301
65	8	0	-4.32178	-3.45477	1.835767
66	8	0	-1.76427	-1.94722	-1.88791
67	7	0	-2.12656	1.557896	-1.53963
68	7	0	-4.639	-2.7981	-1.20117
69	6	0	-2.26571	4.206398	-0.08251
70	6	0	-4.77815	-0.1496	0.25596
71	6	0	-1.41252	-0.78258	-1.63953
72	6	0	-3.92496	-5.13857	-1.30106
73	6	0	-3.08105	2.416651	-1.67052
74	6	0	-5.59349	-1.93934	-1.33205
75	1	0	-3.90403	2.16275	-2.3508
76	1	0	-6.40343	-2.1767	-2.03547

77	6	0	-2.18372	0.332444	-2.34267
78	6	0	-4.69616	-4.02355	-2.0042
79	1	0	-3.21493	-0.02598	-2.4361
80	1	0	-5.73579	-4.35368	-2.11015
81	6	0	-3.7216	6.131133	0.222427
82	6	0	-6.23404	1.775138	0.560893
83	6	0	-2.55902	5.444325	0.523474
84	6	0	-5.07146	1.088331	0.86194
85	1	0	-4.3548	1.50477	1.561484
86	6	0	-3.21786	3.673293	-0.99781
87	6	0	-5.7303	-0.6827	-0.65934
88	6	0	-4.38206	4.436347	-1.26025
89	6	0	-6.8945	0.080354	-0.92179
90	1	0	-5.11838	4.030521	-1.95108
91	1	0	-7.62189	-0.32248	-1.6234
92	6	0	-4.63538	5.64712	-0.66183
93	6	0	-7.14782	1.291126	-0.32337
94	1	0	-5.54746	6.189619	-0.88019
95	1	0	-8.0558	1.839592	-0.54614
96	6	0	-1.57304	0.555342	-3.72916
97	6	0	-4.08548	-3.80065	-3.3907
98	1	0	-1.57522	-0.37703	-4.30024
99	1	0	-4.13275	-4.61564	-3.8965
100	1	0	-2.14703	1.308031	-4.27738
101	1	0	-4.62954	-3.00858	-3.92146
102	1	0	-0.54267	0.916729	-3.63645
103	1	0	-3.04793	-3.47486	-3.28488
104	1	0	-1.13945	0.368979	1.965061
105	1	0	-3.55122	-3.9624	2.206741
106	1	0	-2.50362	0.257172	1.176401
107	1	0	-4.87327	-4.14356	1.437813
108	8	0	-4.27671	-6.30321	-1.54945

Table S9 Excited state atomic coordinate information of **3**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-5.12021	8.355522	-0.13771
2	7	0	-1.12453	11.31618	-1.19475
3	6	0	-0.22587	8.6935	-1.49466
4	6	0	0.586932	9.761343	-1.55031
5	1	0	1.658117	9.629429	-1.68397
6	6	0	0.14633	11.01855	-1.38204
7	1	0	0.841635	11.85562	-1.39489
8	6	0	-1.57945	8.974276	-1.39697

9	1	0	-2.32586	8.187646	-1.36875
10	6	0	-1.99934	10.27639	-1.21107
11	1	0	-3.04831	10.51937	-1.07426
12	30	0	1.832334	2.739654	-0.51956
13	17	0	5.120207	-8.35552	-0.13771
14	8	0	-0.14633	2.258973	0.090256
15	8	0	2.374733	0.127218	-0.25034
16	8	0	3.776019	3.206563	-0.68999
17	8	0	1.932543	1.392381	-2.01302
18	7	0	1.124532	4.636621	-1.19475
19	7	0	1.124525	-11.3162	-1.19475
20	6	0	5.835807	4.128093	-0.11465
21	1	0	6.13303	4.033606	-1.15312
22	7	0	3.003005	-2.03093	-1.63307
23	6	0	3.733068	-4.58204	-0.25848
24	6	0	0.22587	7.259292	-1.49466
25	6	0	0.225866	-8.6935	-1.49466
26	6	0	-0.58693	6.191458	-1.55031
27	6	0	-0.58693	-9.76134	-1.55031
28	1	0	-1.65958	6.313139	-1.67547
29	1	0	-1.65812	-9.62943	-1.68397
30	6	0	-0.14633	4.934245	-1.38204
31	6	0	-0.14633	-11.0186	-1.38204
32	1	0	-0.83878	4.097142	-1.36579
33	1	0	-0.84164	-11.8556	-1.39489
34	6	0	3.554929	-3.02693	-2.20842
35	1	0	3.745296	-2.95676	-3.28925
36	6	0	1.579457	6.978532	-1.39698
37	6	0	1.579448	-8.97428	-1.39697
38	1	0	2.330382	7.758843	-1.3709
39	1	0	2.325862	-8.18765	-1.36875
40	6	0	1.344345	-1.21305	-3.27626
41	1	0	1.089852	-0.34769	-3.89177
42	1	0	1.556083	-2.06185	-3.93501
43	1	0	0.486308	-1.46138	-2.64424
44	6	0	2.574862	-0.88537	-2.42178
45	1	0	3.389306	-0.5522	-3.08247
46	6	0	2.266551	0.288785	-1.48245
47	6	0	4.88941	-6.45384	-2.04152
48	1	0	5.351712	-7.16615	-2.71676
49	6	0	4.661962	-6.78168	-0.74563
50	6	0	4.533127	-5.21807	-2.47303
51	1	0	4.698325	-4.94882	-3.51319
52	6	0	3.925529	-4.26574	-1.63172

53	6	0	1.99934	5.676407	-1.21106
54	6	0	1.999341	-10.2764	-1.21107
55	1	0	3.043477	5.414373	-1.08972
56	1	0	3.048305	-10.5194	-1.07426
57	30	0	-1.83233	-2.73965	-0.51956
58	8	0	0.14633	-2.25897	0.090256
59	8	0	-2.37473	-0.12722	-0.25034
60	8	0	-3.77602	-3.20656	-0.68999
61	8	0	-1.93254	-1.39238	-2.01302
62	7	0	-1.12453	-4.63662	-1.19475
63	6	0	-5.83581	-4.12809	-0.11465
64	1	0	-6.13303	-4.03361	-1.15312
65	7	0	-3.00301	2.030932	-1.63307
66	6	0	-3.73307	4.582043	-0.25848
67	6	0	-0.22587	-7.25929	-1.49466
68	6	0	0.586929	-6.19146	-1.55031
69	1	0	1.659583	-6.31314	-1.67547
70	6	0	0.146328	-4.93425	-1.38204
71	1	0	0.838775	-4.09714	-1.36579
72	6	0	-3.55493	3.026931	-2.20842
73	1	0	-3.7453	2.956758	-3.28925
74	6	0	-1.57946	-6.97853	-1.39698
75	1	0	-2.33038	-7.75884	-1.3709
76	6	0	-1.34435	1.21305	-3.27626
77	1	0	-1.08985	0.347691	-3.89177
78	1	0	-1.55608	2.061849	-3.93501
79	1	0	-0.48631	1.461376	-2.64424
80	6	0	-2.57486	0.885371	-2.42178
81	1	0	-3.38931	0.552195	-3.08247
82	6	0	-2.26655	-0.28879	-1.48245
83	6	0	-4.88941	6.453838	-2.04152
84	1	0	-5.35171	7.166149	-2.71676
85	6	0	-4.66196	6.781679	-0.74563
86	6	0	-4.53313	5.218072	-2.47303
87	1	0	-4.69833	4.948818	-3.51319
88	6	0	-3.92553	4.265737	-1.63172
89	6	0	-1.99934	-5.67641	-1.21106
90	1	0	-3.04348	-5.41437	-1.08972
91	17	0	-8.26381	-5.2333	0.277512
92	7	0	-11.2549	-1.31869	1.21649
93	6	0	-8.66228	-0.34848	1.572034
94	6	0	-9.74701	0.455287	1.616841
95	1	0	-9.63913	1.527008	1.760925
96	6	0	-10.9749	-0.01559	1.396995

97	1	0	-11.831	0.655477	1.38221
98	6	0	-8.91672	-1.68961	1.452639
99	1	0	-8.12638	-2.43097	1.421211
100	6	0	-10.2051	-2.10203	1.257237
101	1	0	-10.3976	-3.16571	1.122784
102	30	0	-2.81913	1.837619	0.396517
103	17	0	8.263811	5.233304	0.277512
104	8	0	3.209767	-3.77399	0.623534
105	8	0	-1.39334	1.706564	1.810863
106	7	0	-4.65084	1.150456	1.216486
107	7	0	11.25487	1.318687	1.21649
108	7	0	2.037497	2.672882	1.546251
109	6	0	4.550626	3.682178	0.236805
110	6	0	-7.24343	0.180246	1.572045
111	6	0	8.662277	0.348481	1.572034
112	6	0	-0.31331	2.000368	1.287091
113	6	0	3.006177	3.203218	2.177248
114	1	0	2.978397	3.211167	3.274711
115	6	0	6.324114	4.820818	2.129749
116	1	0	7.00177	5.275379	2.843163
117	6	0	6.672446	4.688907	0.813509
118	6	0	4.203878	3.767852	1.626315
119	6	0	-6.1587	-0.62352	1.616848
120	6	0	9.747014	-0.45529	1.616841
121	1	0	-6.25659	-1.6972	1.747311
122	1	0	9.639133	-1.52701	1.760925
123	6	0	5.10573	4.36286	2.50834
124	1	0	4.822634	4.437114	3.557237
125	6	0	-4.93077	-0.15264	1.396994
126	6	0	10.97494	0.015593	1.396995
127	1	0	-4.07805	-0.82099	1.337058
128	1	0	11.83101	-0.65548	1.38221
129	6	0	4.084586	-5.88167	0.16353
130	1	0	3.915522	-6.15407	1.198261
131	6	0	-6.98899	1.521381	1.452649
132	6	0	8.916724	1.689606	1.452639
133	1	0	-7.77351	2.267253	1.42007
134	1	0	8.126379	2.430972	1.421211
135	6	0	-5.7006	1.933792	1.257234
136	6	0	10.20511	2.10203	1.257237
137	1	0	-5.49641	2.993762	1.126213
138	1	0	10.39763	3.165707	1.122784
139	6	0	0.932869	1.982181	2.216009
140	1	0	1.215764	0.918349	2.248492

141	6	0	0.600596	2.459313	3.626595
142	1	0	-0.30129	1.949218	3.967678
143	1	0	1.404462	2.234624	4.33434
144	1	0	0.409623	3.537888	3.639507
145	30	0	2.819125	-1.83762	0.396517
146	8	0	-3.20977	3.773986	0.623534
147	8	0	1.39334	-1.70656	1.810863
148	7	0	4.650839	-1.15046	1.216486
149	7	0	-2.0375	-2.67288	1.546251
150	6	0	-4.55063	-3.68218	0.236805
151	6	0	7.243428	-0.18025	1.572045
152	6	0	0.313312	-2.00037	1.287091
153	6	0	-3.00618	-3.20322	2.177248
154	1	0	-2.9784	-3.21117	3.274711
155	6	0	-6.32411	-4.82082	2.129749
156	1	0	-7.00177	-5.27538	2.843163
157	6	0	-6.67245	-4.68891	0.813509
158	6	0	-4.20388	-3.76785	1.626315
159	6	0	6.158696	0.623517	1.616848
160	1	0	6.256594	1.697201	1.747311
161	6	0	-5.10573	-4.36286	2.50834
162	1	0	-4.82263	-4.43711	3.557237
163	6	0	4.930774	0.152641	1.396994
164	1	0	4.078053	0.820991	1.337058
165	6	0	-4.08459	5.881668	0.16353
166	1	0	-3.91552	6.154072	1.198261
167	6	0	6.988994	-1.52138	1.452649
168	1	0	7.77351	-2.26725	1.42007
169	6	0	5.700599	-1.93379	1.257234
170	1	0	5.496413	-2.99376	1.126213
171	6	0	-0.93287	-1.98218	2.216009
172	1	0	-1.21576	-0.91835	2.248492
173	6	0	-0.6006	-2.45931	3.626595
174	1	0	0.301285	-1.94922	3.967678
175	1	0	-1.40446	-2.23462	4.33434
176	1	0	-0.40962	-3.53789	3.639507