Supporting Information

A series of coordination compounds containing rigid multi-pyridine based ligand: syntheses, structures and properties†

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All reagents and solvents employed were commercially available and used as received without further purification. Elemental analyses (C, H, and N) were performed on a Perkin-Elmer 240C elemental analyzer. TG analyses were performed on a Perkin-Elmer TG-7 analyzer heated from 30 to 800 °C in a flow of nitrogen at the heating rate of 10 °C min^{-1}. Powder X-ray diffraction (XRD) patterns of the samples were collected on a Rigaku Dmax 2000. ^{1}HNMR spectra were measured on Bruker Avance 500 MHz with tetramethylsilane as the internal standard. The solid state UV-vis absorption spectra were taken on a Cary 500 spectrophotometer while the liquid spectra were recorded on a Hitachi U3010 spectrometer. The emission spectra were recorded using a transient spectrofluorimeter (Edinburgh FLS920).

The preparation of samples:

The synthesized samples were collected, washed with water for six times, and dried overnight.

The synthesis of 2,4,5-Tris(4-pyridinyl)-imidazole[1]

A mixture of 4 g of 4-pyridinecarbaldehyde and 16 g of ammonium acetate was heated to 120 ºC with stirring for 3 h. The reaction mixture was cooled, and then put into the water. The resulted precipitate was filtered off, and washed with water. Yield

2.0 g (50%). ^{1}H NMR spectrum (500 MHz, DMSO-d_6, δ [ppm]): 7.5 (d, J = 6.0 Hz, 4H, C_5H_4N), 8.0 (d, J = 6.0 Hz, 2H, C_5H_4N), 8.6 (s, 4H, C_5H_4N), 8.7 (d, J = 6.0 Hz, 2H, C_5H_4N). Elemental Anal. Calcd for $C_{18}H_{13}N_5$ (%): C, 72.23; H, 4.38; N, 23.39. Found: C, 72.26; H, 4.34; N, 23.36%.

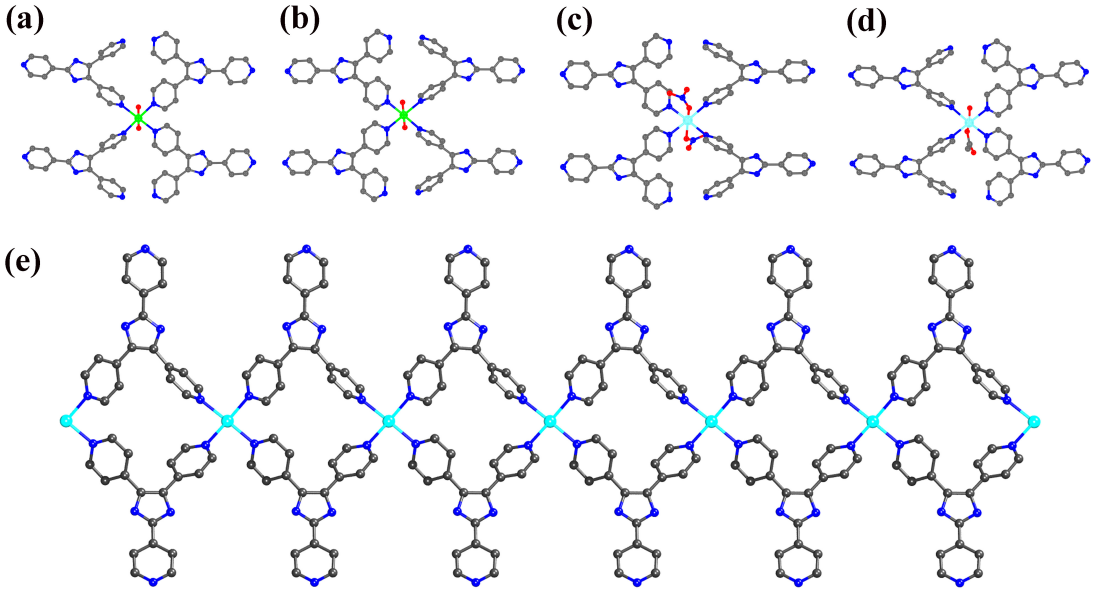

Fig. S1 View of the coordination environments of M centers (Zn^{II} for **2** (a) and **3** (b), Cd^{II} for **4** (c) and **5** (d)). (e) The 1D chain structures. Lattice molecules, coordinated molecules and hydrogen atoms have been omitted for clarity.

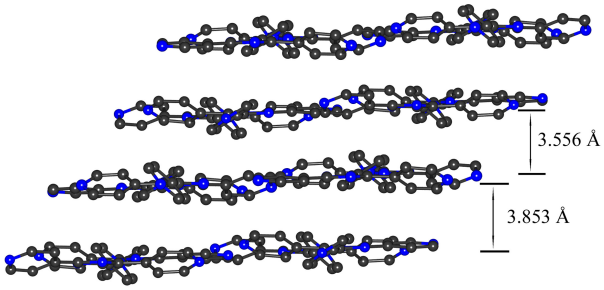

Fig. S2 Crystal packing along *b* axis of compound **1**.

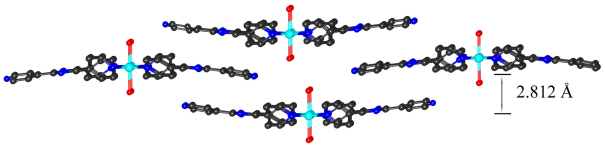

Fig. S3 Crystal packing along *b* axis of compound **2**.

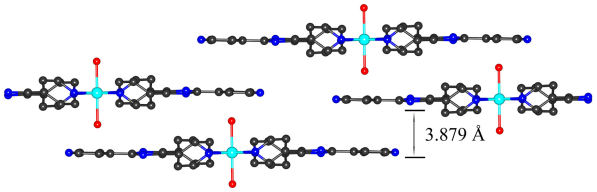

Fig. S4 Crystal packing along *b* axis of compound **3**.

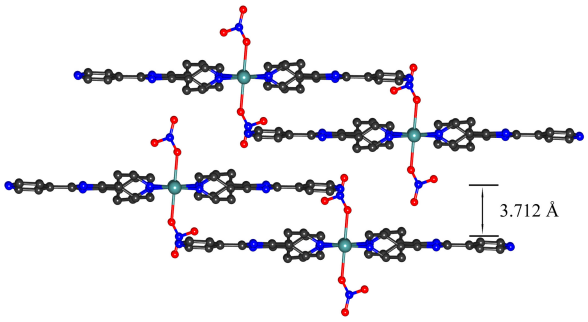

Fig. S5 Crystal packing along *b* axis of compound **4**.

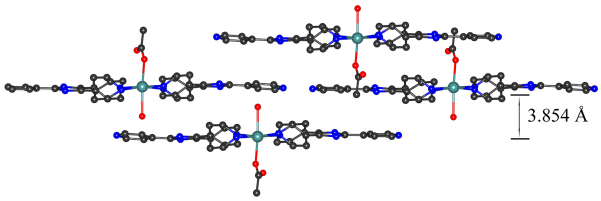

Fig. S6 Crystal packing along *a* axis of compound **5**.

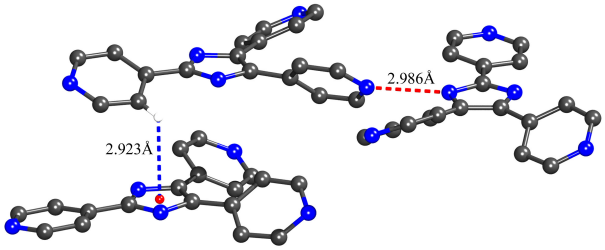

Fig. S7 The intermolecular C-H···π interactions and hydrogen bonds in compound **1**.

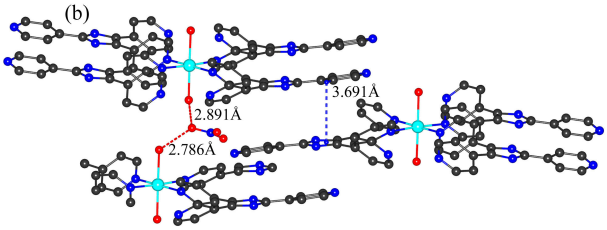

Fig. S8 The intermolecular C-H···π interactions and hydrogen bonds in compound **2**.

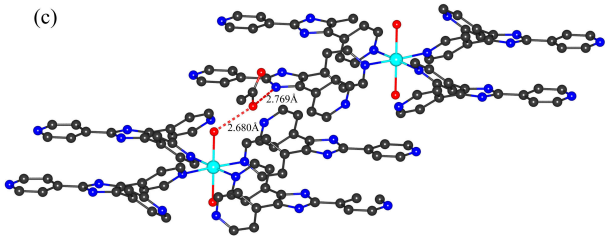

Fig. S9 The intermolecular hydrogen bonds in compound **3**.

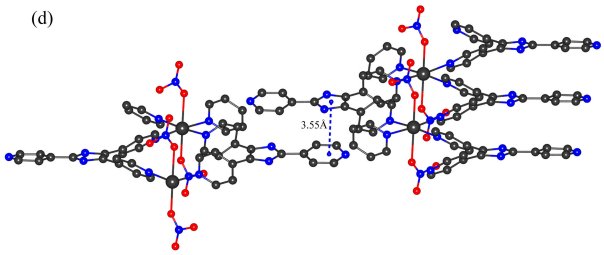

Fig. S10 The intermolecular π···π interaction in compound **4**.

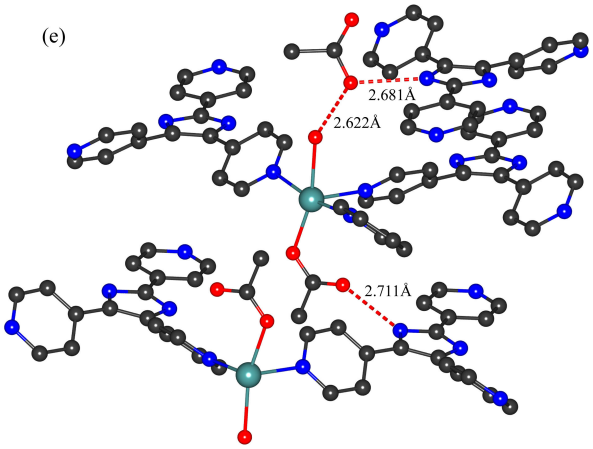

Fig. S11 The intermolecular hydrogen bonds in compound **5**.

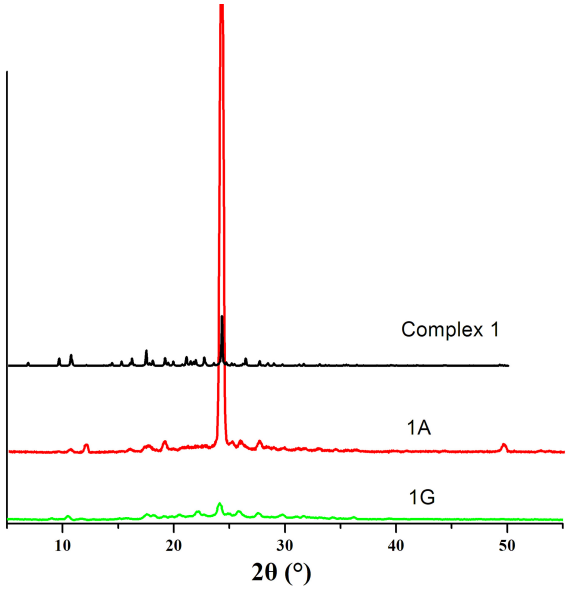

Fig. S12 Power X-ray diffraction patterns of **1A** in different states.

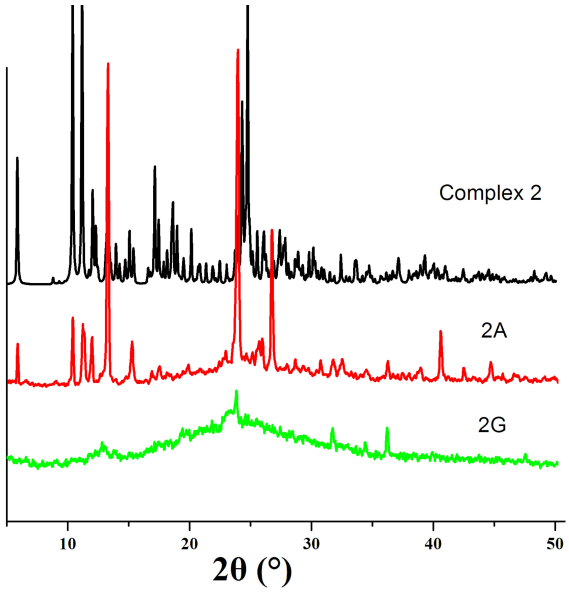

Fig. S13 Power X-ray diffraction patterns of **2A** in different states.

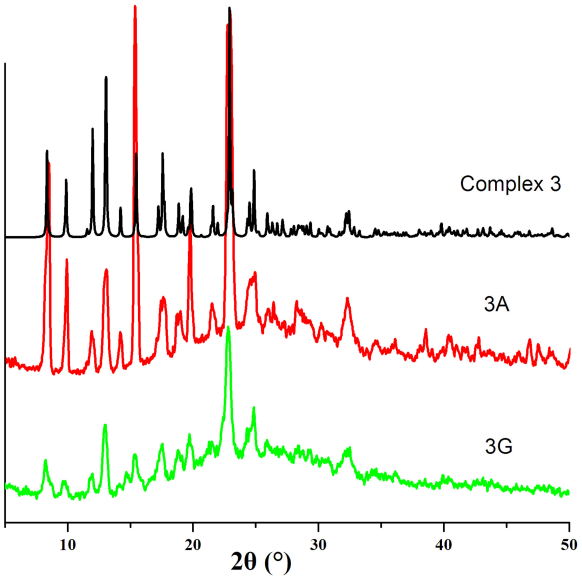

Fig. S14 Power X-ray diffraction patterns of **3A** in different states.

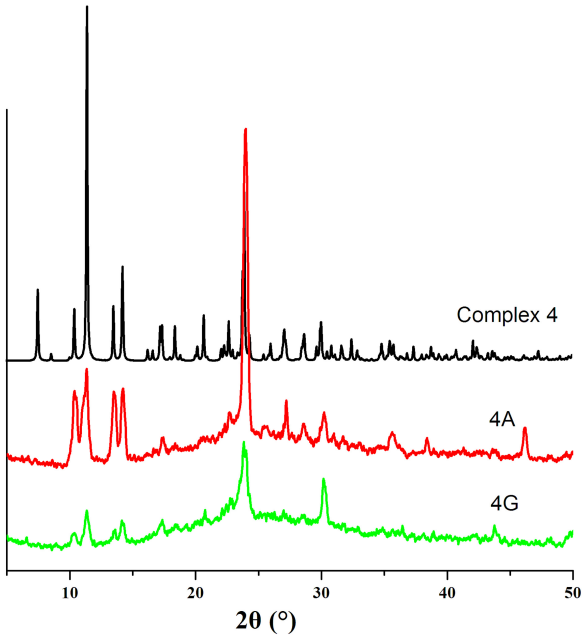

Fig. S15 Power X-ray diffraction patterns of **4A** in different states.

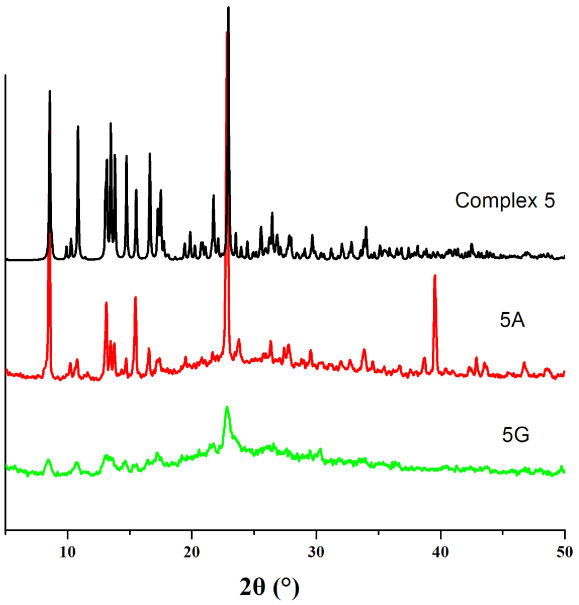

Fig. S16 Power X-ray diffraction patterns of **5A** in different states.

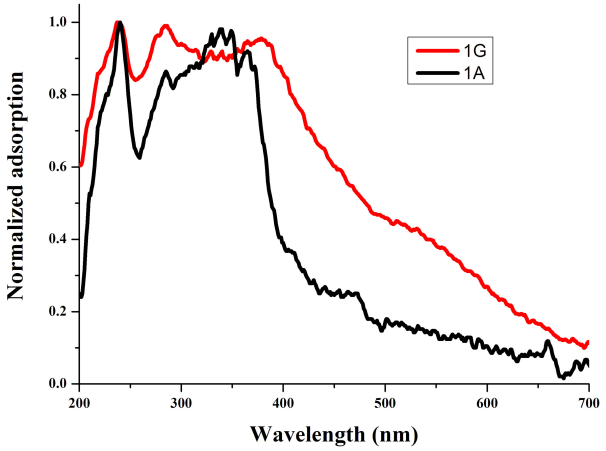

Fig. S17 Solid-state absorption spectra of compound **1** before and after grinding.

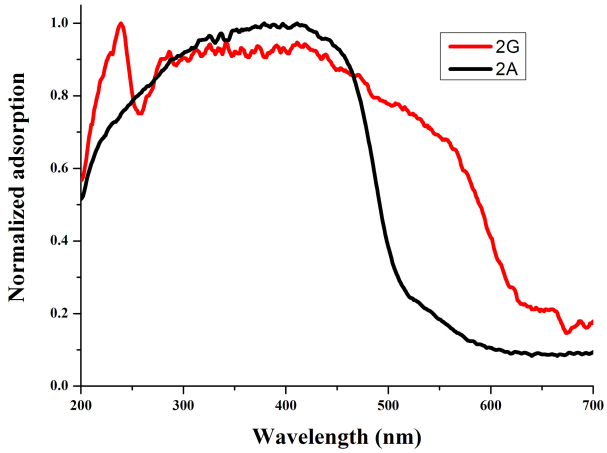

Fig. S18 Solid-state absorption spectra of compound **2** before and after grinding.

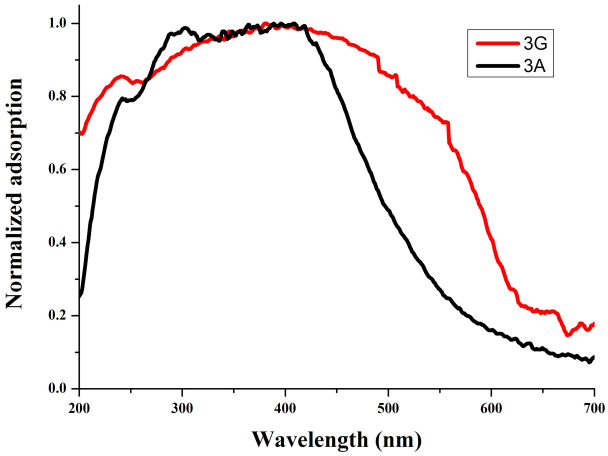

Fig. S19 Solid-state absorption spectra of compound **3** before and after grinding.

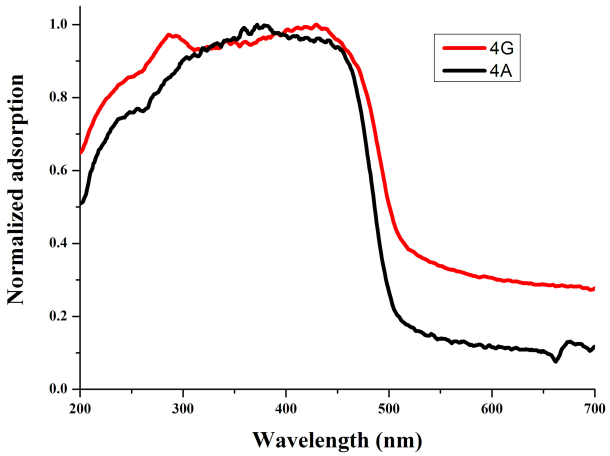

Fig. S20 Solid-state absorption spectra of compound **4** before and after grinding.

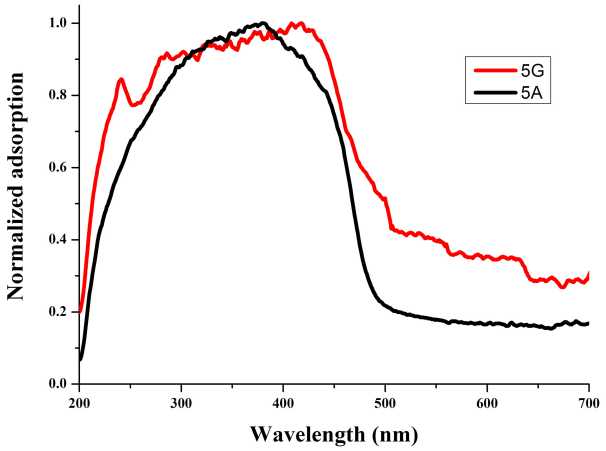

Fig. S21 Solid-state absorption spectra of compound **5** before and after grinding.

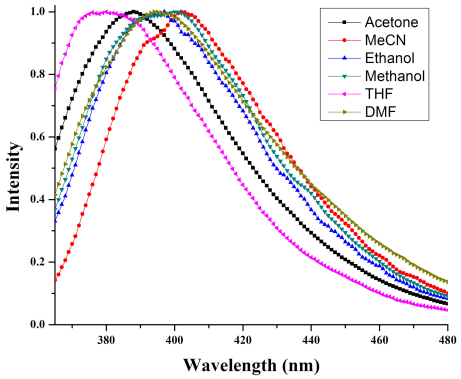

Fig. S22 Normalized emission spectra of **1** in the various solvent at room temperature.

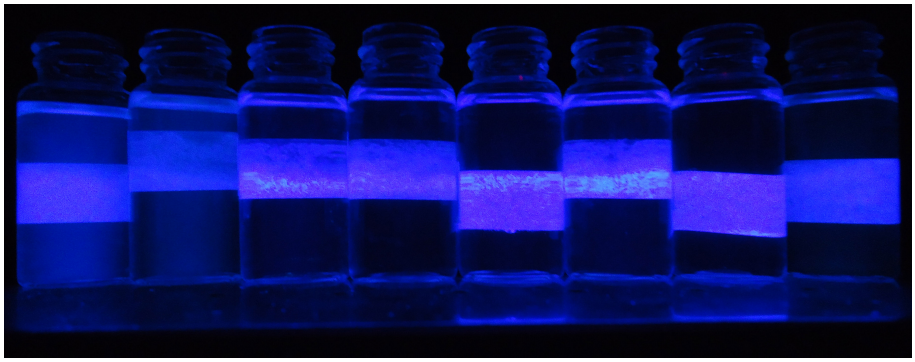

Fig. S23 Luminescent photographs of compound **1** in DMF (3×10^{-5} mol/L) in the presence of different metal ions (1×10^{-4} mol/L) under 365 nm UV-light (left to right: DMF, Hg^{2+}, Zn^{2+}, Cu^{2+}, Co^{2+}, Cd^{2+}, Ni^{2+}, Cr^{3+}).

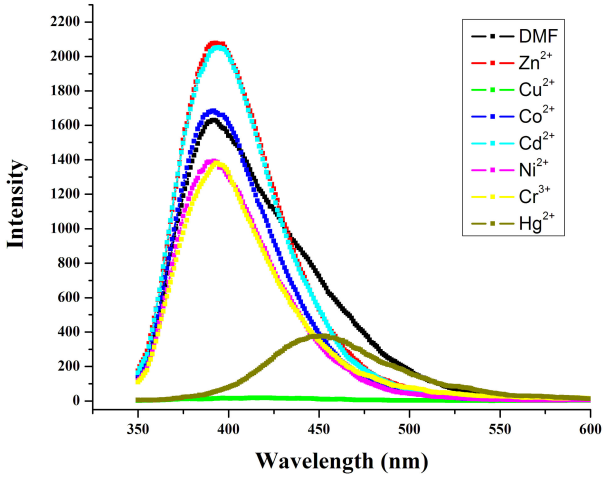

Fig. S24 The emission spectra of compound **1** (3×10^{-5} mol/L) in the DMF solvent containing different metal ions with concentration 1×10^{-4} mol/L at room temperature.

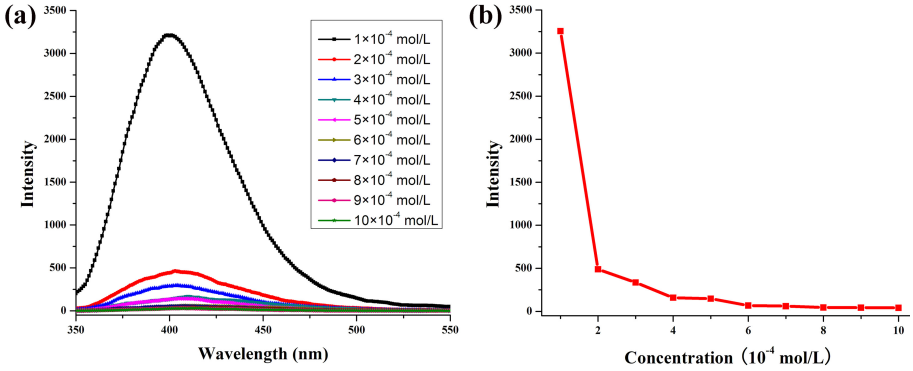

Fig. S25 (a) The emission spectra of **1** (3×10^{-5} mol/L) with $Cu(NO_3)_2$ in DMF. [Cu^{2+}]: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1×10^{-3} mol/L. (b) Fluorescent intensity curve of a series of $Cu(NO_3)_2$ DMF solution in the presence of compound **1**.

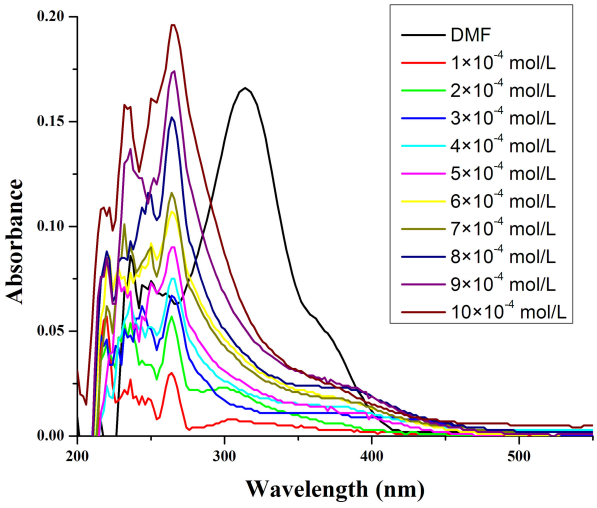

Fig. S26 Absorption of **1** (3×10^{-5} mol/L) in DMF solution with $Cu(NO_3)_2$. [Cu^{2+}]: 0,

0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1×10^{-3} mol/L.

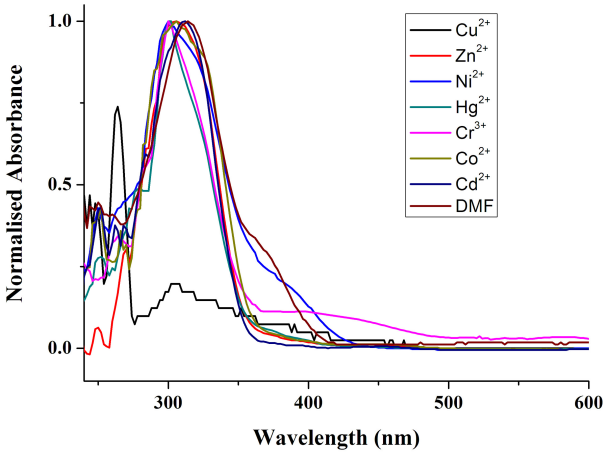

Fig. S27 Normalized absorption of compound **1** in DMF (3×10^{-5} mol/L) in the presence of different metal ions (1×10^{-4} mol/L).

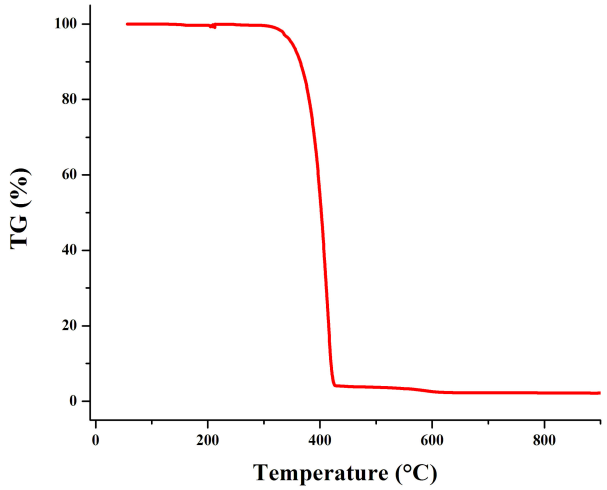

Fig. S28 TG profile of **1**.

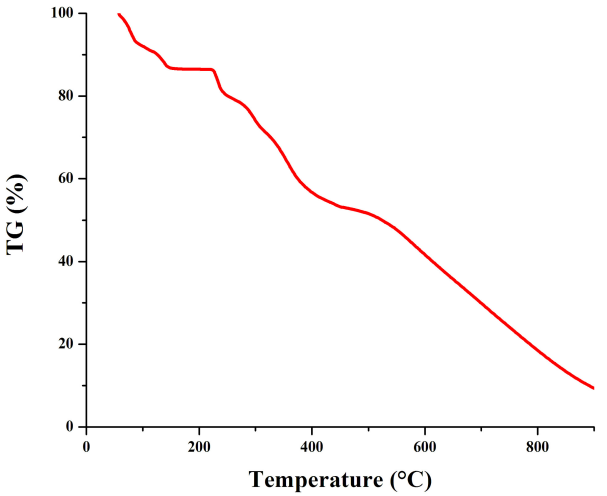

Fig. S29 TG profile of **2**.

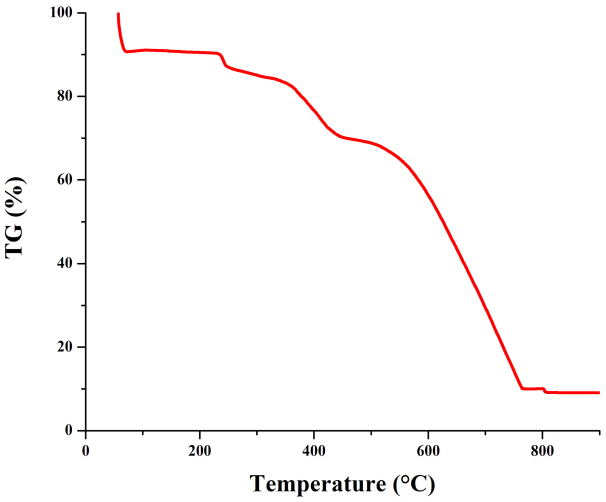

Fig. S30 TG profile of **3**.

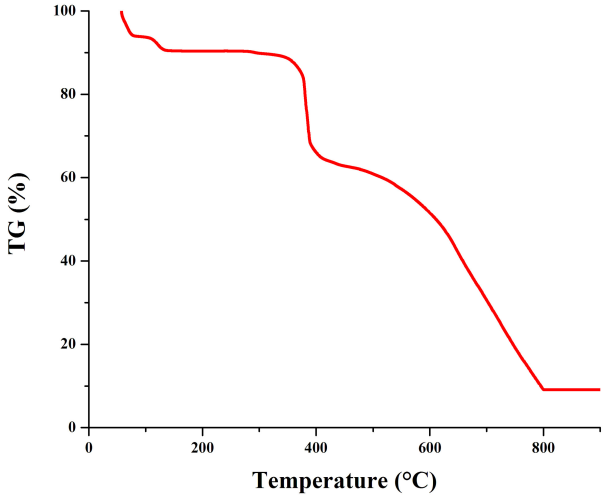

Fig. S31 TG profile of **4**.

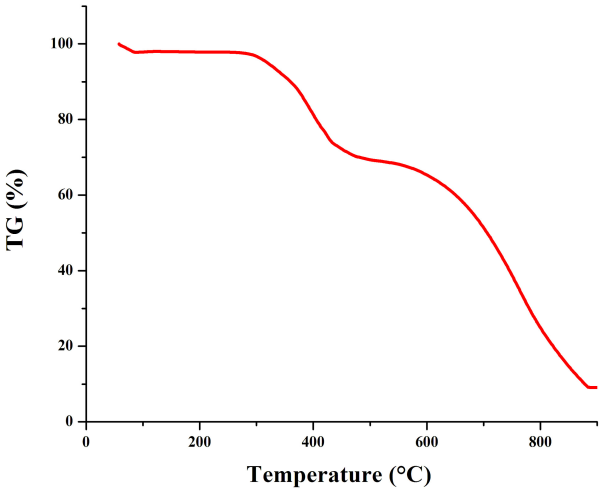

Fig. S32 TG profile of **5**.

(1) Proskurnina, M. V.; Lozinskaya, N. A.; Tkachenko, S. E.; Zefirov, N. S. *Russ. J. Org. Chem.* **2002**, *38*, 1200.