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Supporting information

Pillared metal organic frameworks for luminescence sensing of small molecules and metal ions in aqueous solution

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Table S1 Crystal data and structure refinements for compounds **1** and **2**.

Formula	$C_{15}H_{19}N_7O_6SZn_2$ (**1**)	$C_{22}H_{21}N_7O_5Zn_2$ (**2**)
Formula weight	556.17	594.21
Crystal system	tetragonal	tetragonal
Space group	*I*/4*m*	P4/ncc
a (Å)	13.518(7)	13.642(3)
b (Å)	13.518(7)	13.642(3)
c (Å)	26.420(5)	35.545(11)
α (°)	90.000(5)	90.00
β (°)	90.000(5)	90.00
γ (°)	90.000(5)	90.00
V (Å^3)	4828(3)	6615(3)
Z	8	8
$D_{calcd.}$[gcm^{-3}]	1.241	1.018
F(000)	1784	2032
Reflections collected	13839/2174	31110 /2921
R(int)	0.0399	0.1383
Goodness-of-fit on F^2	1.064	1.019
R_1^a [I>2σ (I)]	0.0691	0.0644
wR_2^b	0.1709	0.1491

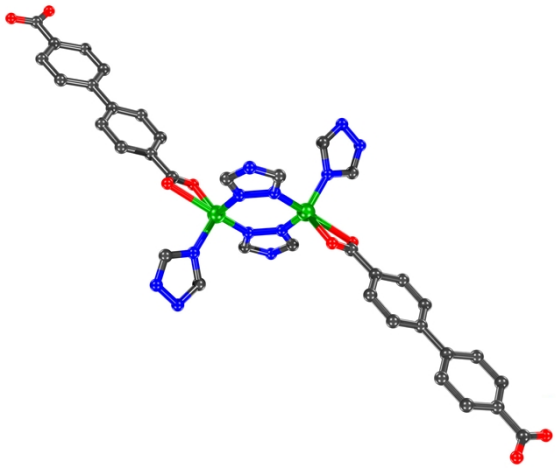

Fig. S1 The coordination environment of the Zn(II) center in **2**. The hydrogen atoms are omitted for clarity (Zn, green; N, blue; C, gray; O, red).

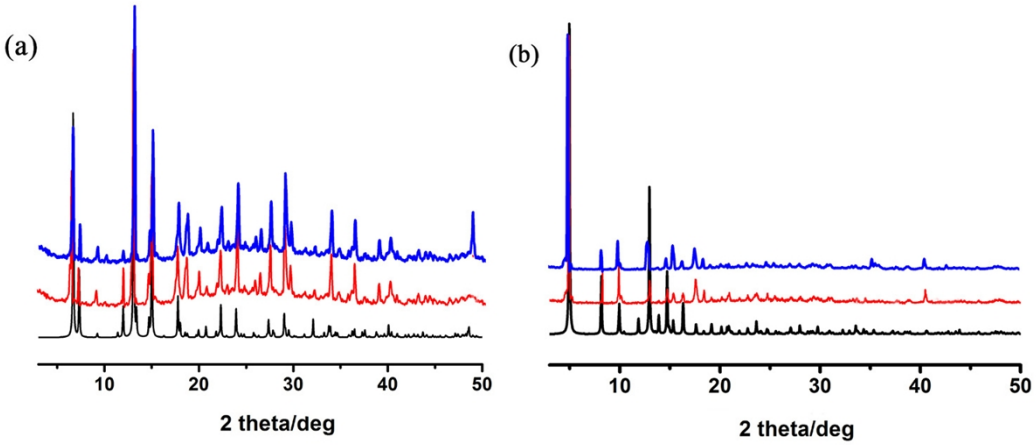

Fig. S2 XRPD patterns of **1** (a) and **2** (b): simulated (black), as-synthesized (red), activated (blue).

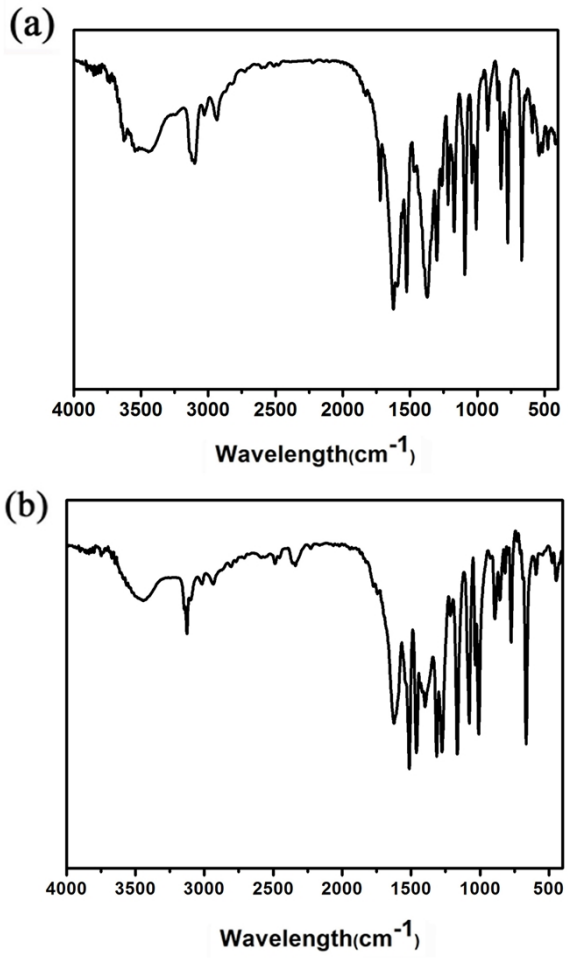

Fig. S3 FT-IR spectra of **1** (a) and **2** (b).

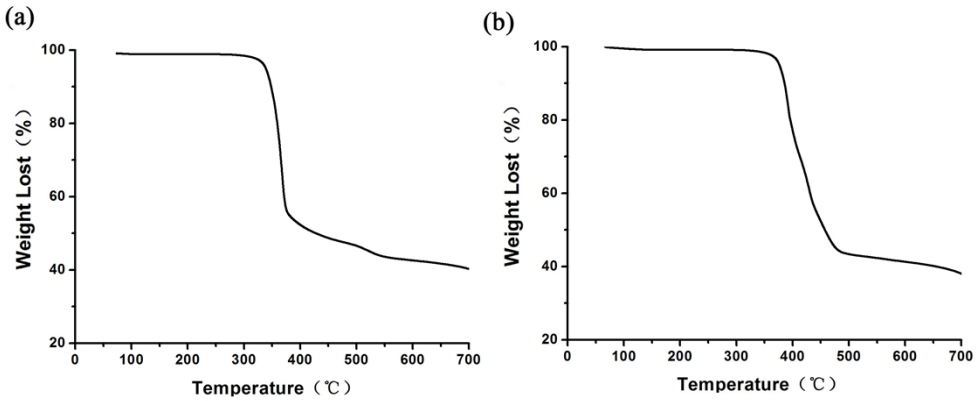

Fig. S4 TGA curves for **1a** (a) and **2a** (b).

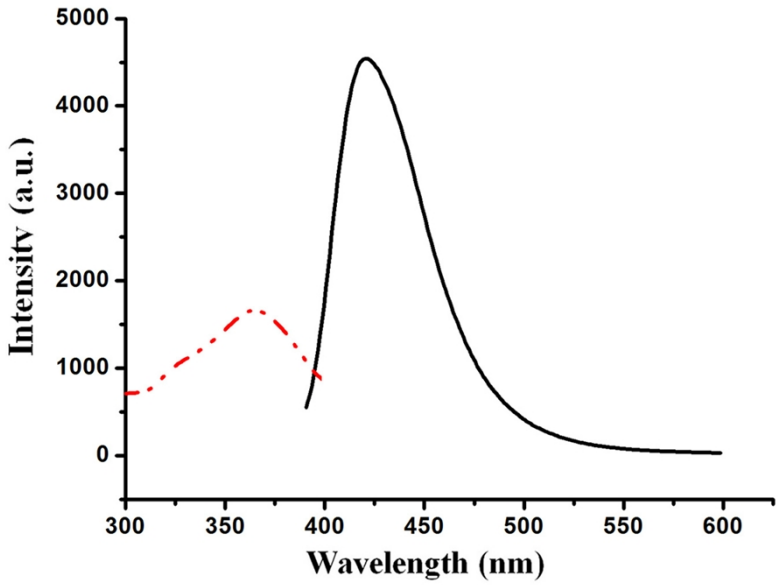

Fig. S5 The excitation (red) and emission (black) spectra of **1**.

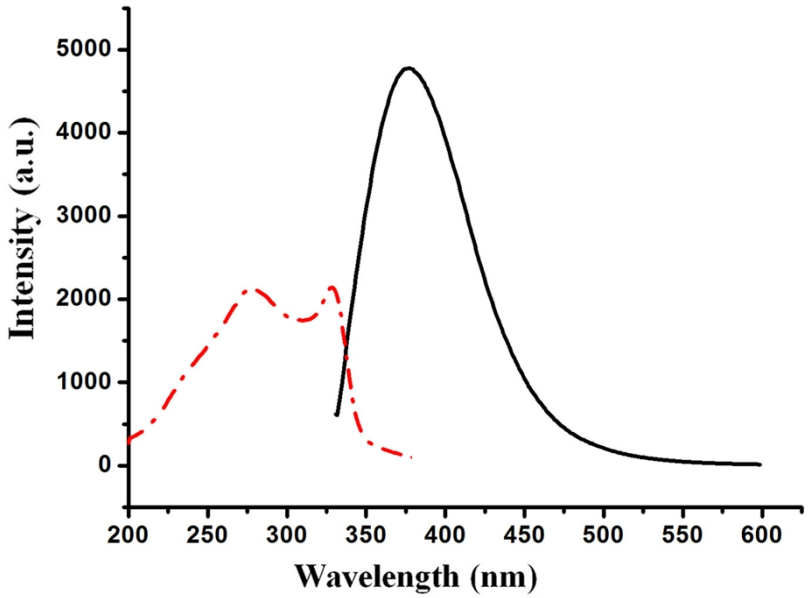

Fig. S6 The excitation (red) and emission (black) spectra of **2**.

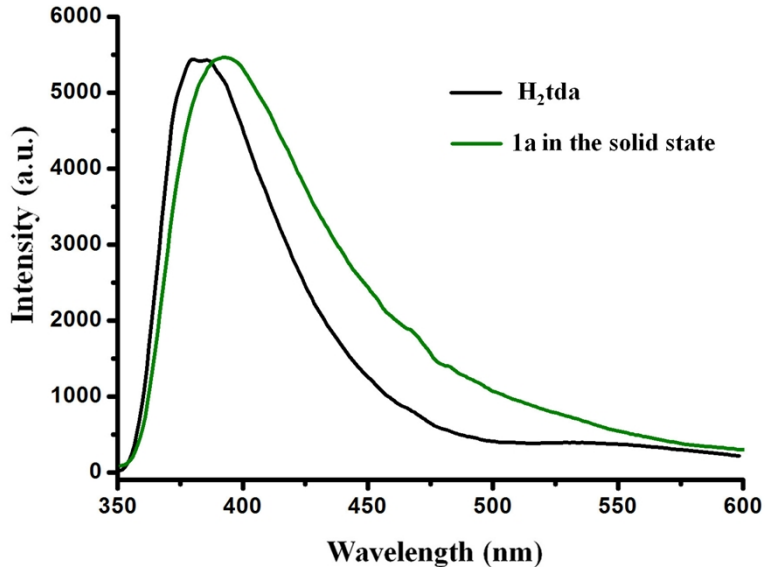

Fig. S7 Luminescent spectra of H_2tda in the solid state (black line) and **1a** in the solid state (green line), λ_{ex} = 313 nm.

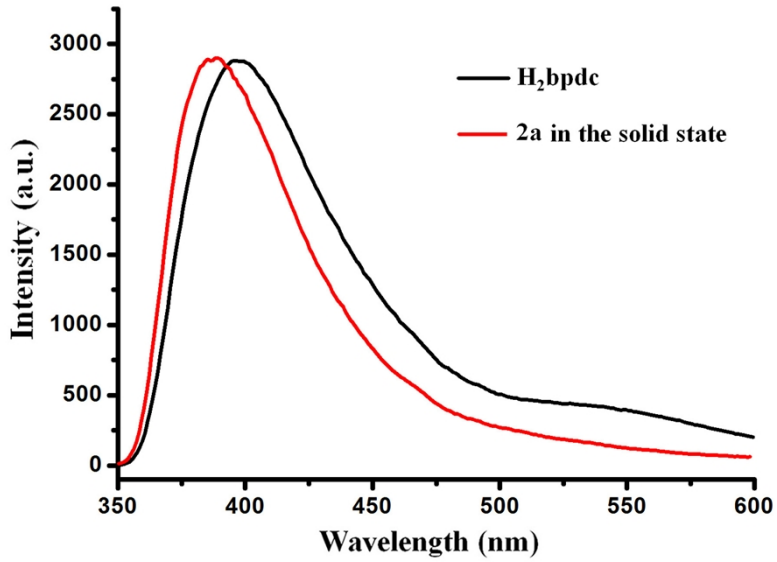

Fig. S8 Luminescent spectra of H_2bpdc in the solid state (black line) and **2a** in the solid state (red line), λ_{ex} = 326 nm.

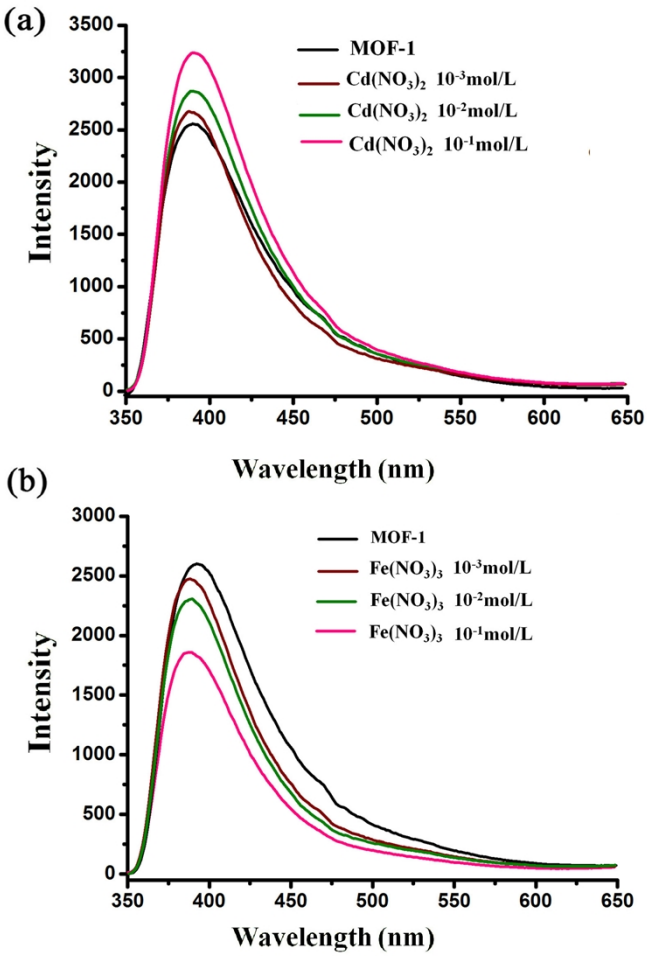

Fig. S9 PL spectra of solid **1a** activated in aqueous solutions of $Cd(NO_3)_2$ and $Fe(NO_3)_3$ at different concentrations.

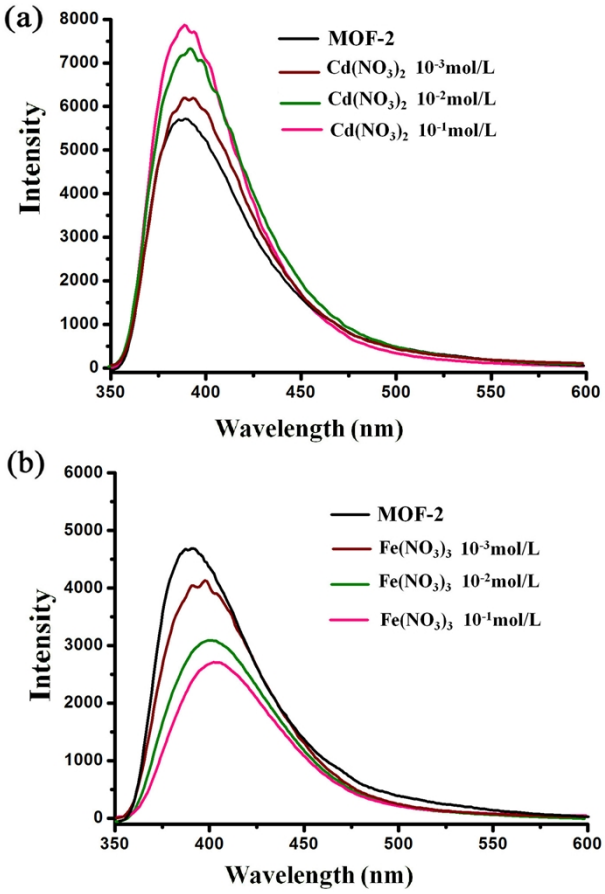

Fig. S10 PL spectra of solid **2a** activated in aqueous solutions of $Cd(NO_3)_2$ and $Fe(NO_3)_3$ at different concentrations.

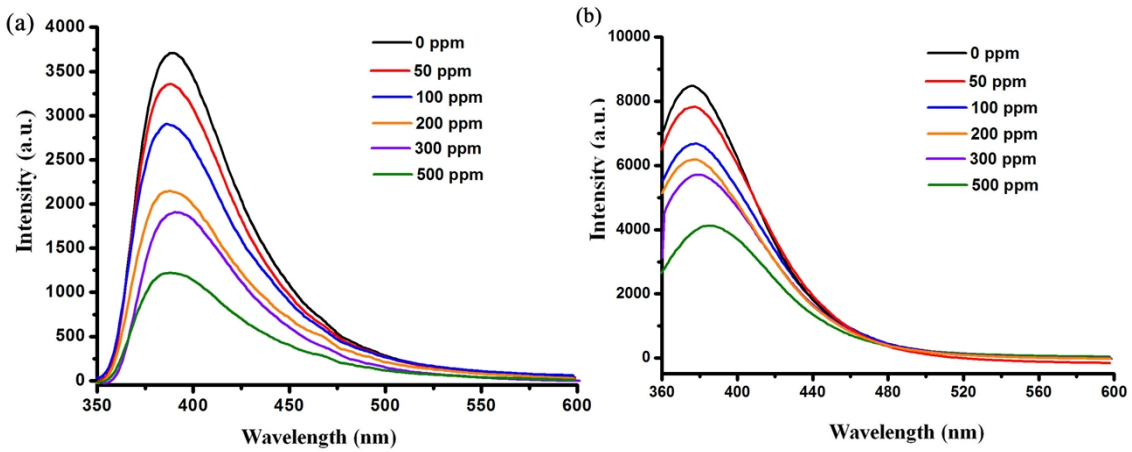

Fig. S11 Emission spectra of (a) **1a** and (b) **2a** at different TNT (trinitrotoluene) concentrations in CH_3OH (excited at 313 nm and 310 nm, respectively).