

Electronic Supporting Information (ESI) for

**The role of terminal coordinated amides in a series of Ca-tatb
frameworks: pore size regulation and fluorescence sensing tunability**

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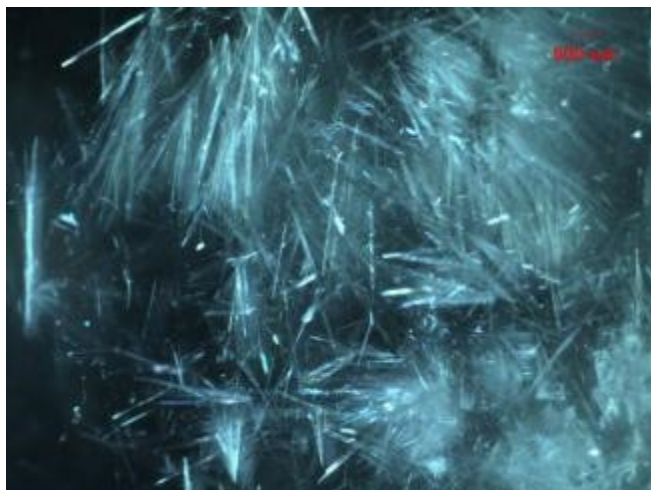


Figure S1 The crystal image of the as-made compound 1.

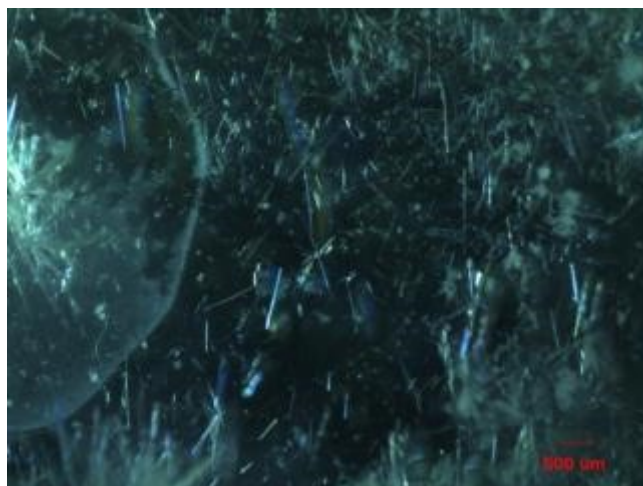


Figure S2 The crystal image of the as-made compound 2.

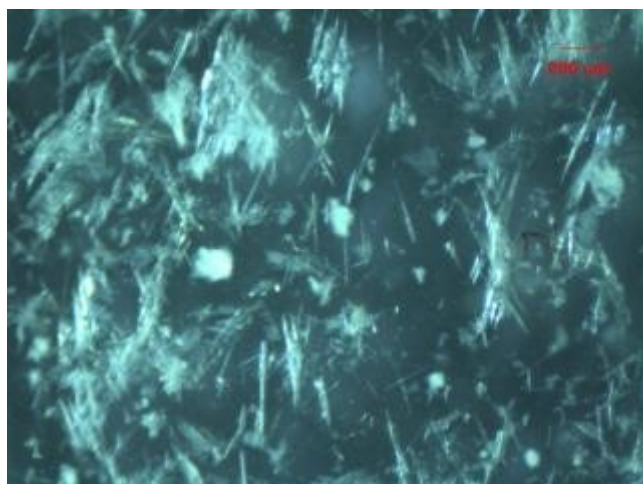


Figure S3 The crystal image of the as-made compound 3.

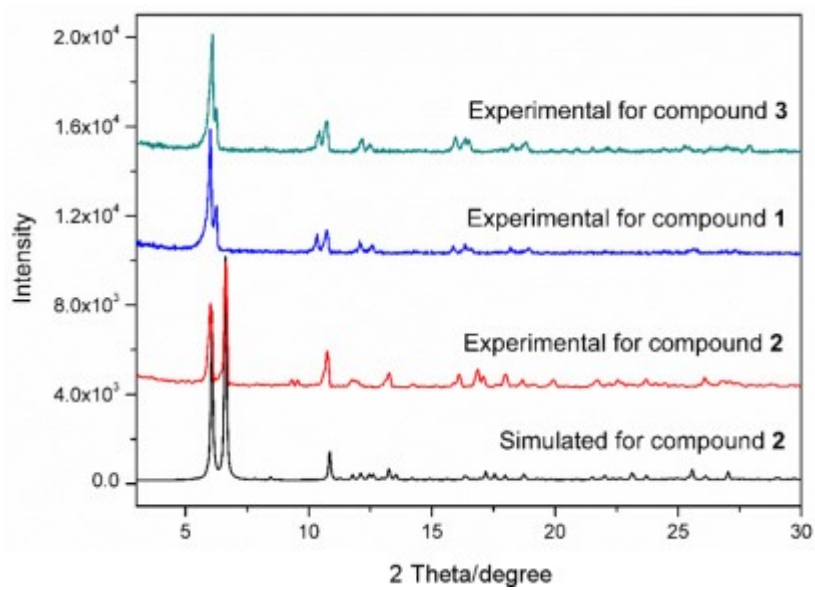


Figure S4 PXRD patterns of the as-made compounds **1**, **2** and **3**. Simulated PXRD pattern of compound **2** is included for comparison.

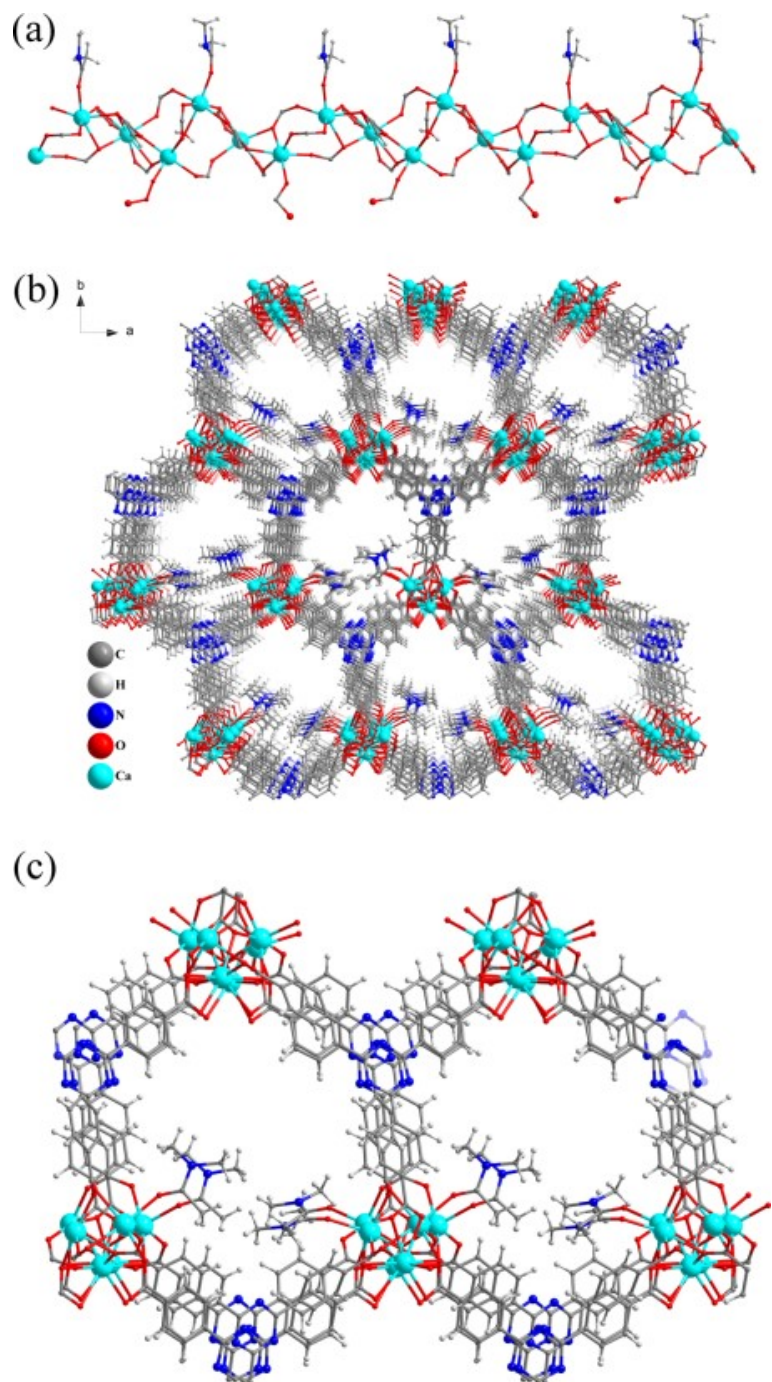


Figure S5 (a) The 1D chain-like SBU in compound **2** with the coordination environment of Ca²⁺. (b) The 3D structure of compound **2** containing DMA solvents viewed along the *a* axis. (c) The channel environment in zoom in mode. The structure figures are depicted according to the single crystal data reported in *Inorg. Chim. Acta*, 2018, **478**, 8.

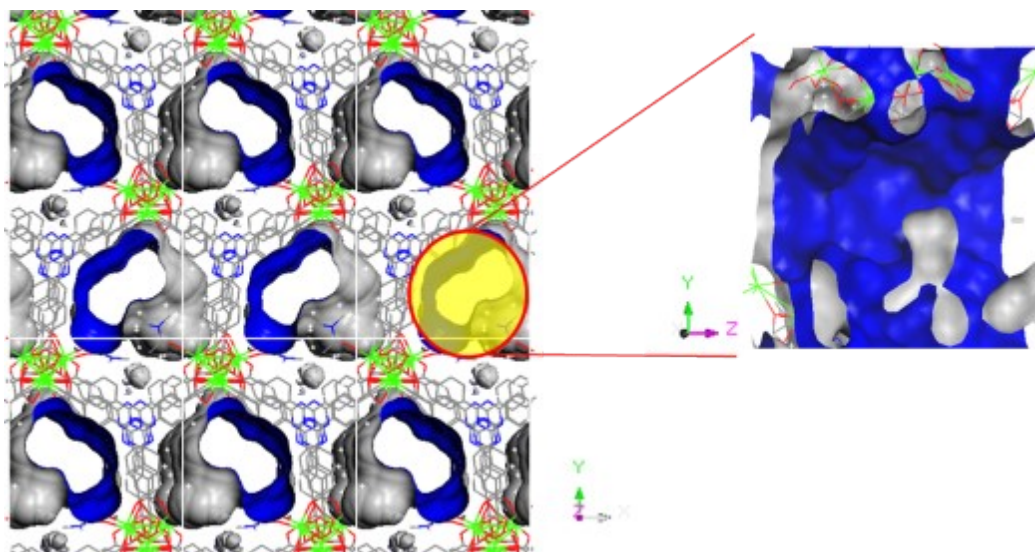


Figure S6 The channel structure of compound **2** that depicted by Material Studio.

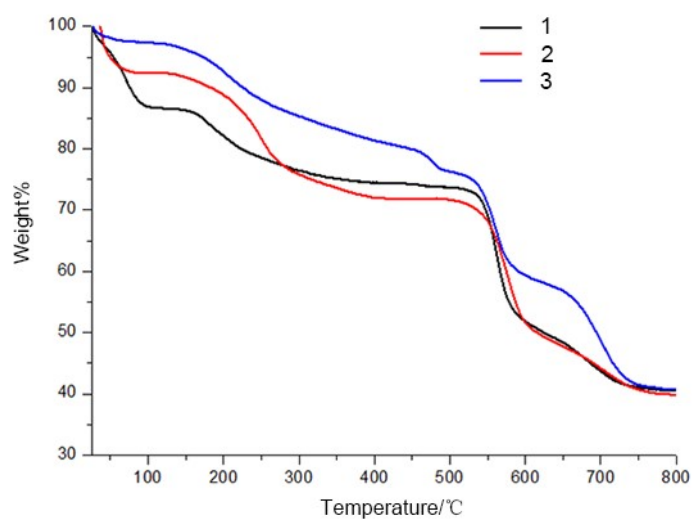


Figure S7 TG curve for the as-made compounds **1**, **2** and **3**.

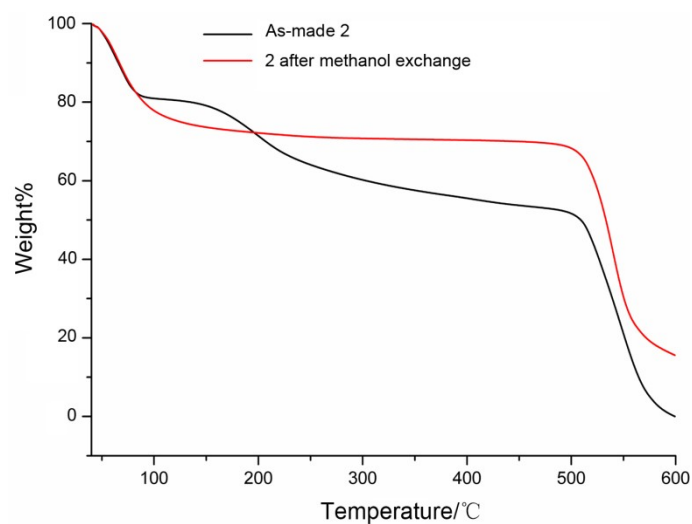


Figure S8 TG curve for compound **2** before and after solvent exchange.

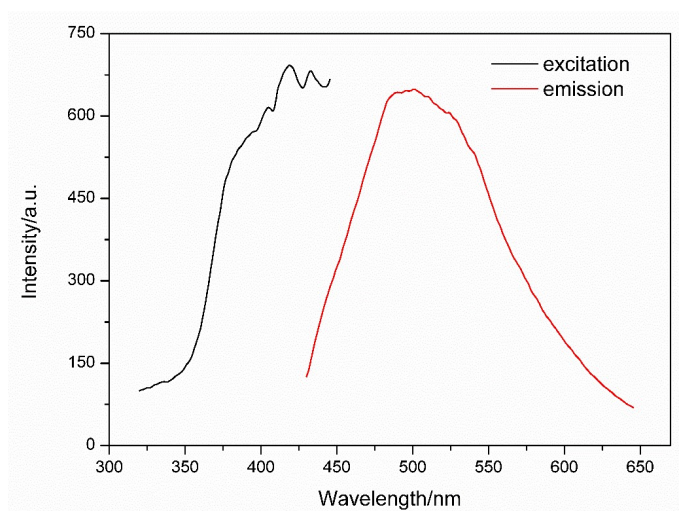


Figure S9 The excitation and emission spectra of H₄tatb ligand at solid state measured at room temperature ($\lambda_{\text{ex}} = 410$ nm and $\lambda_{\text{em}} = 490$ nm).

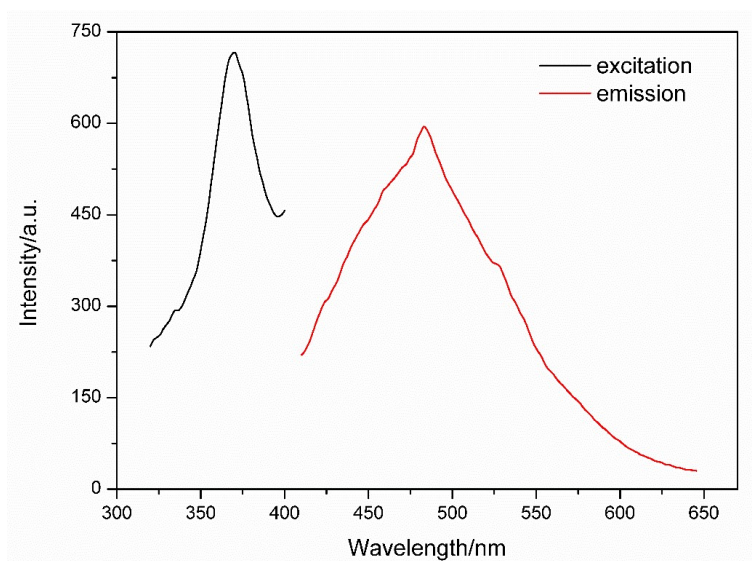


Figure S10 The excitation and emission spectra of compound **1** at solid state measured at room temperature ($\lambda_{\text{ex}} = 370$ nm and $\lambda_{\text{em}} = 480$ nm).

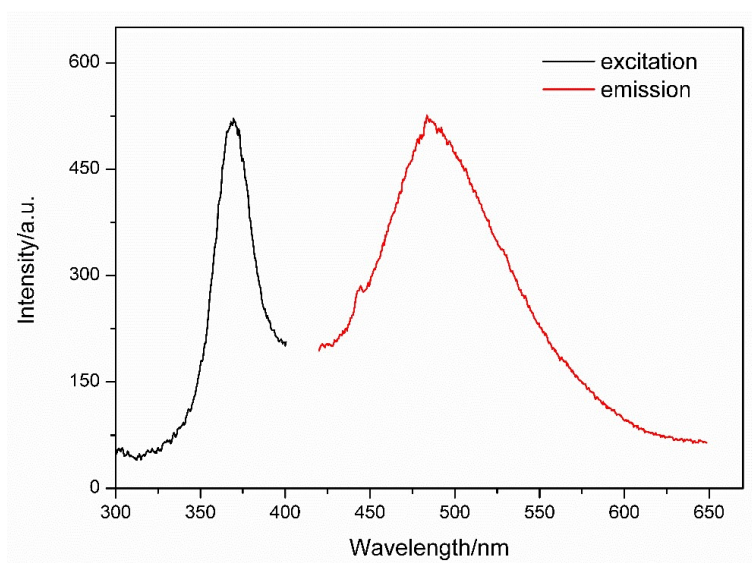


Figure S11 The excitation and emission spectra of compound **2** at solid state measured at room temperature ($\lambda_{\text{ex}} = 370$ nm and $\lambda_{\text{em}} = 480$ nm).

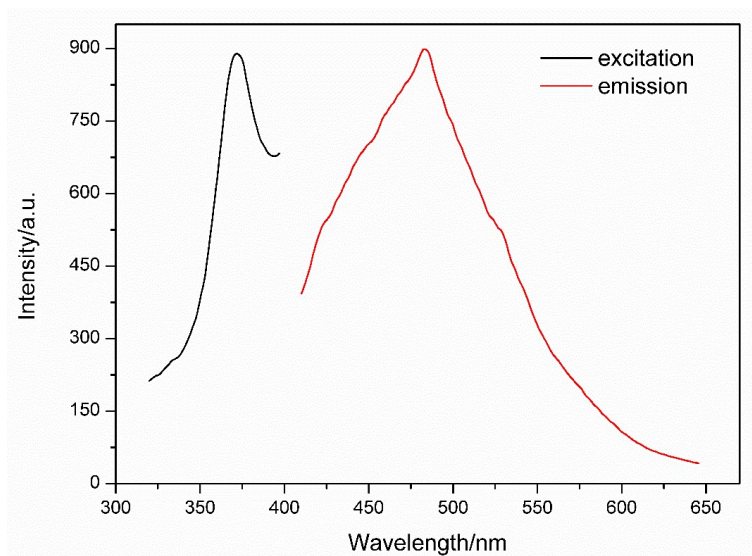


Figure S12 The excitation and emission spectra of compound **3** at solid state measured at room temperature ($\lambda_{\text{ex}} = 370 \text{ nm}$ and $\lambda_{\text{em}} = 480 \text{ nm}$).

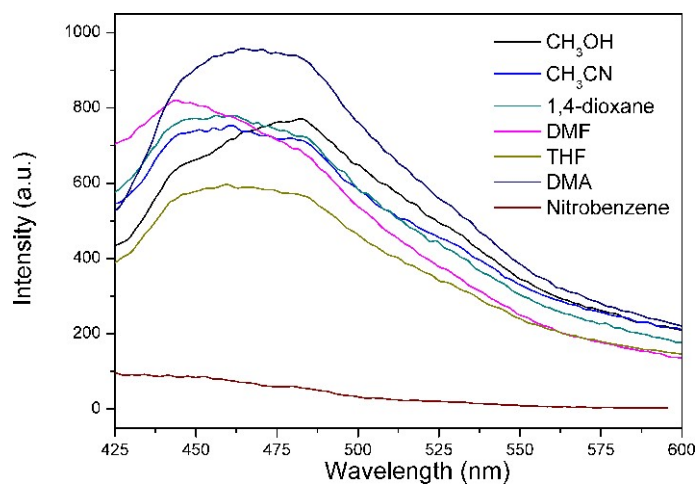


Figure S13 The FL spectra of compound **1** dispersed in solvents and nitrobenzene.

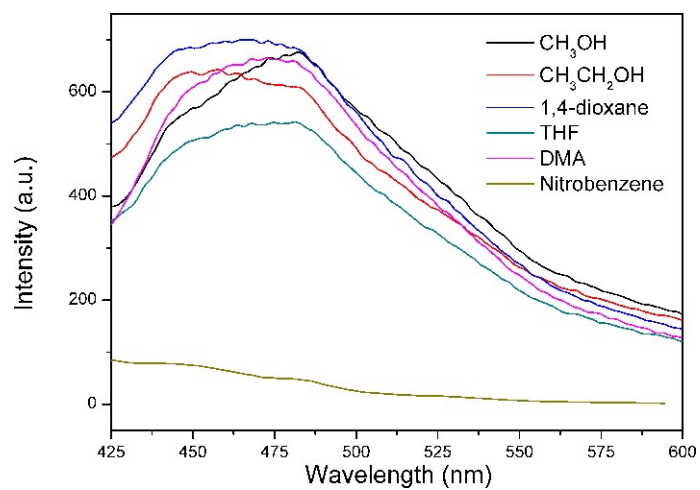


Figure S14 The FL spectra of compound 2 dispersed in solvents and nitrobenzene.

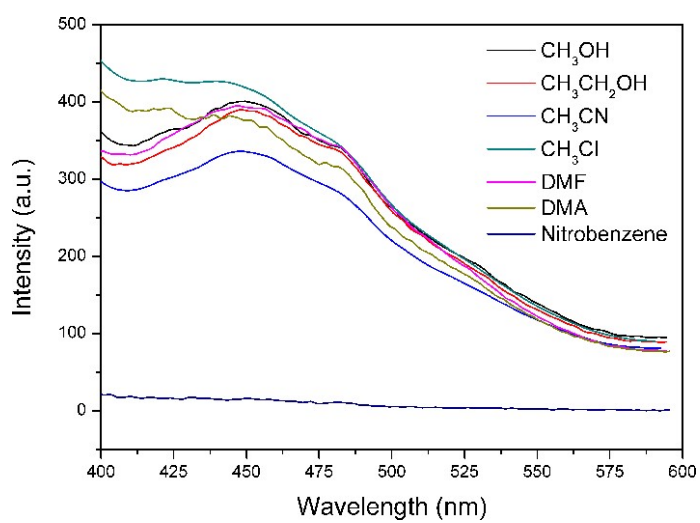


Figure S15 The FL spectra of compound 3 dispersed in solvents and nitrobenzene.

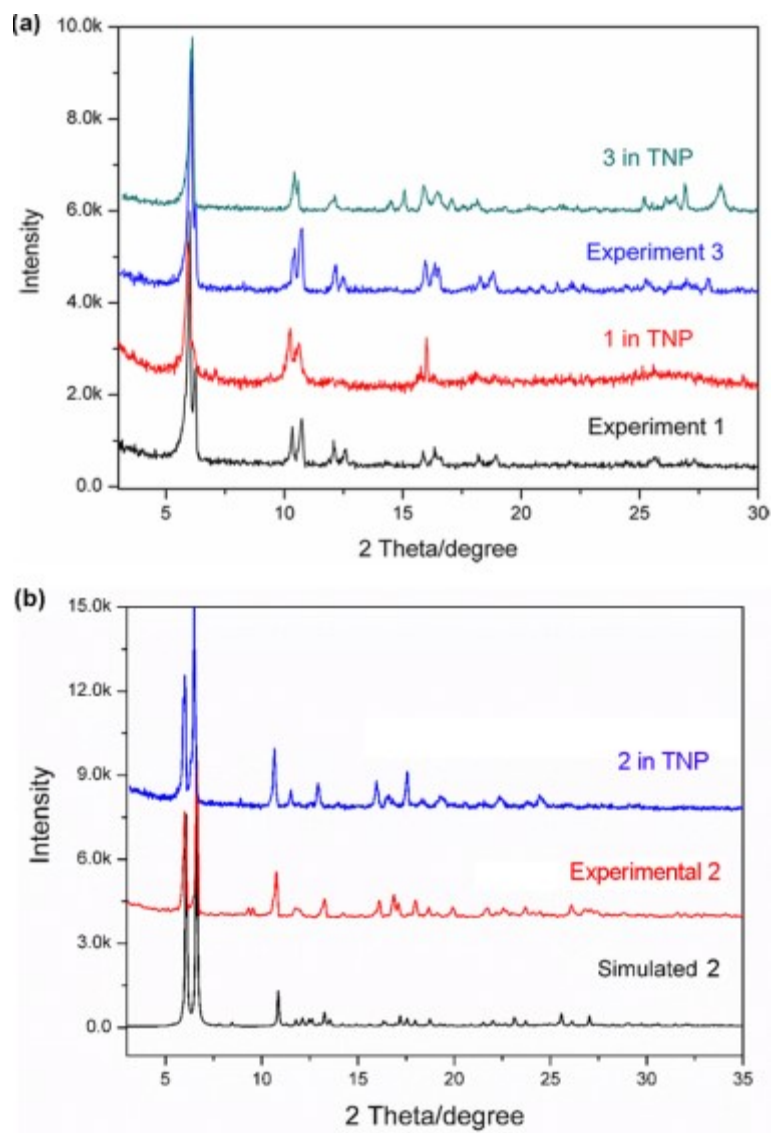


Figure S16 PXRD for the as-made compounds before and after being immersed in 10^{-3} M TNP.

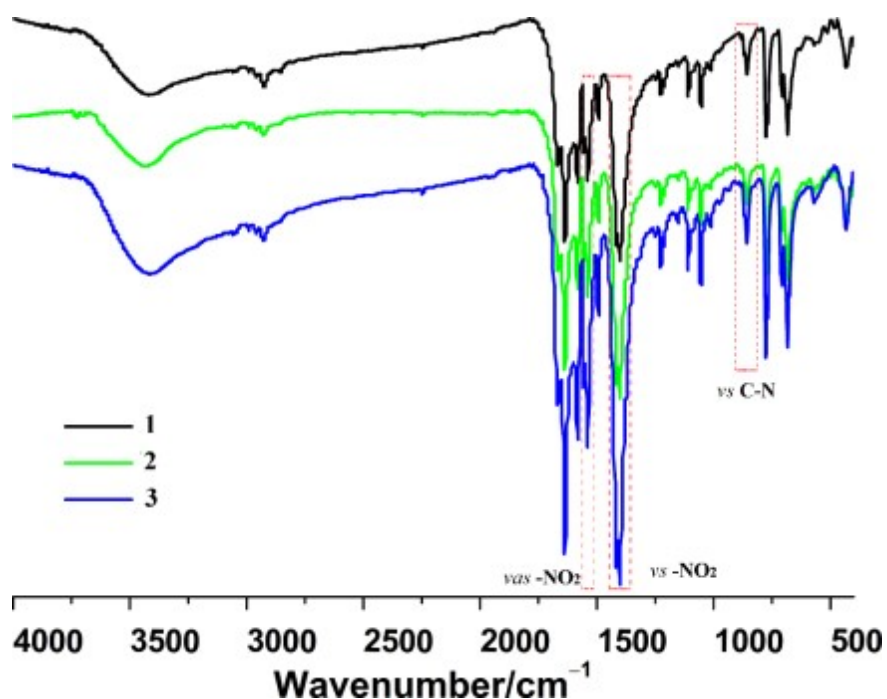


Figure S17 The IR for the as-made compounds before and after being immersed in 10^{-3} M TNP.

Table S1 Selected MOF FL sensors towards TNP.

Compounds	K_{sv} / M^{-1}	Reference
Tb(L)(OH)	7.73×10^{-2}	S1
Eu(BTB)H ₂ O	6.76×10^{-2}	S2
Tb(BTB)H ₂ O	3.25×10^{-2}	
Cd(NDC) _{0.5} (PCA)	3.5×10^4	S3
[(CH ₃) ₂ NH ₂] ₃ [Zn ₄ Na(BPTC) ₃] ₃ ·4CH ₃ OH·2DMF	3.2×10^4	S4
[Zn(NDC)(H ₂ O)] _n	6×10^4	S5
[Cd(NDC)(H ₂ O)] _n	2.385×10^4	
{[Tb(L) _{1.5} (H ₂ O)]·3H ₂ O} _n	7.47×10^4	S6
Zr ₆ O ₄ (OH) ₆ (L) ₆	2.9×10^4	S7
Eu ₃ (L) ₃ (HCOO)(μ ₃ -OH) ₂ (H ₂ O)	2.1×10^4	S8
Zn ₈ (ad) ₄ (BPDC) ₆ O·2Me ₂ NH ₂	4.6×10^4	S9
Zr ₆ O ₄ (OH) ₆ (L) ₆	5.8×10^4	S10
[Cd(NDC)L] ₂ ·H ₂ O	3.7×10^4	S11
Zn ₄ (DMF)(Ur) ₂ (NDC) ₄	10.83×10^4	S12
[{Zn(BINDI) _{0.5} (bpa) _{0.5} (H ₂ O)} ₃ ·4H ₂ O] _n (MOF1)	4.9×10^4	S13
[{Zn(BINDI) _{0.5} (bpe)} ₃ ·3H ₂ O] _n (MOF2)	1.29×10^4	
Cu-CIP	1.07×10^4	S14
{Mn(Tipp)(A) ₂ } _n ·2H ₂ O	11.8×10^4	S15
{(Me ₂ NH ₂) ₄ [Eu ₄ (DDAC) ₃ (HCO ₂)(OH ₂) ₂] ₃ ·8DMF·9H ₂ O} _n	8.6×10^4	S16
[Zn ₃ (TIAB) ₂ (IMDC) ₂] ₃ ·(NO ₃) ₂ ·(DMF) ₂ ·(H ₂ O) ₂	5.68×10^4	S17
[Zn(bipa)(suc)] _n	6.48×10^4	S18

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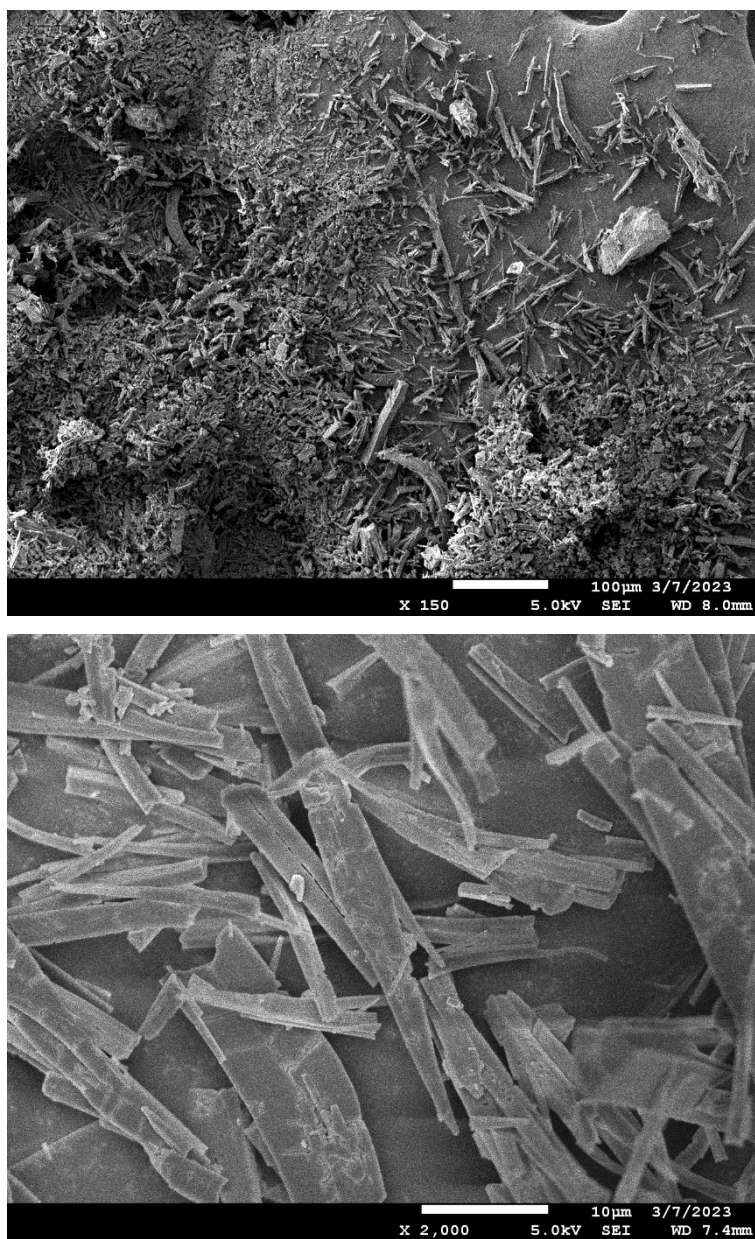


Figure S18 The SEM photographs for the as-made compound **2** before (up) and after (down) immersing treatment in 10^{-3} M TNP.

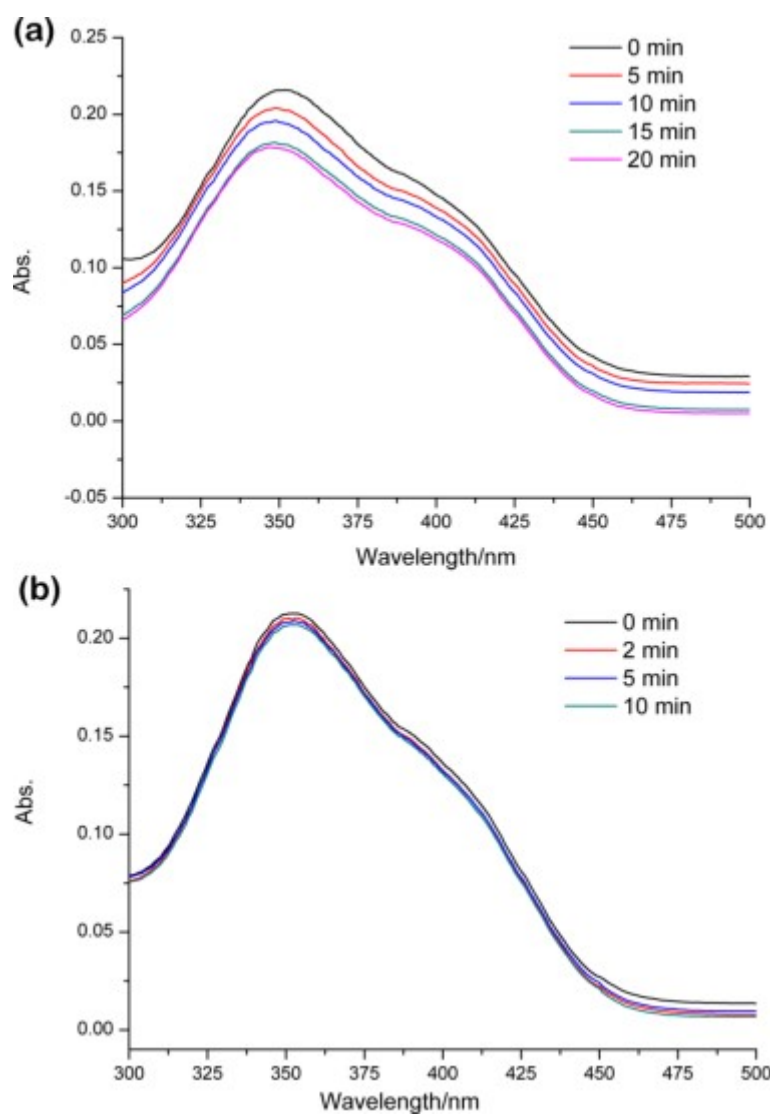


Figure S19 The time-dependent absorption spectra for compounds **1** (a) and **3** (b) that dispersed in 0.5×10^{-4} M TNP.