

Supporting Information

Single-crystal to single-crystal transition from a 7-fold interpenetrated coordination polymer to non-interpenetrated one by photochemical [2+2] polymerization and their sensing properties

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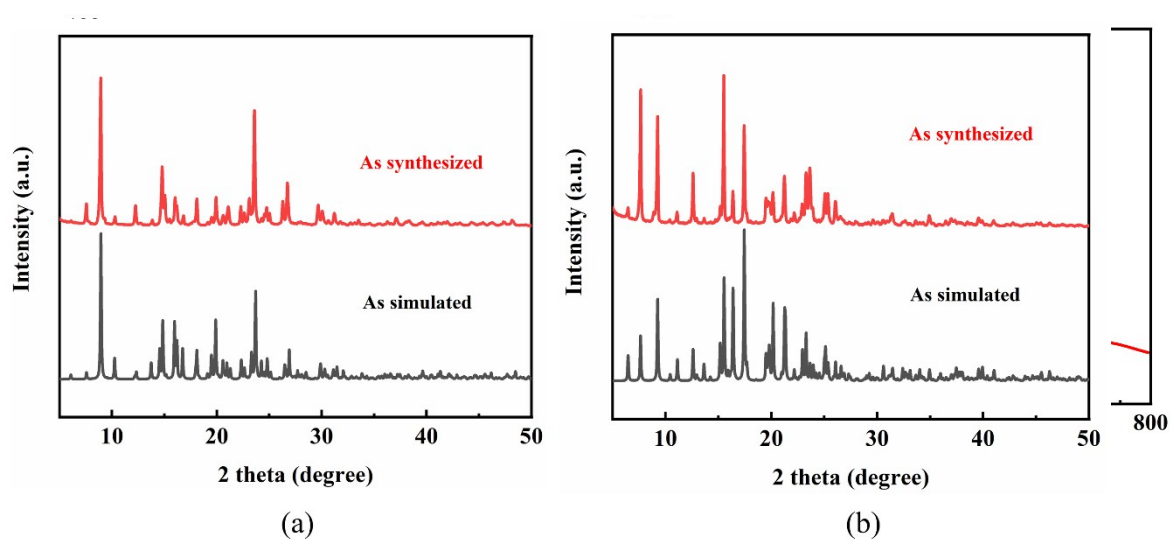
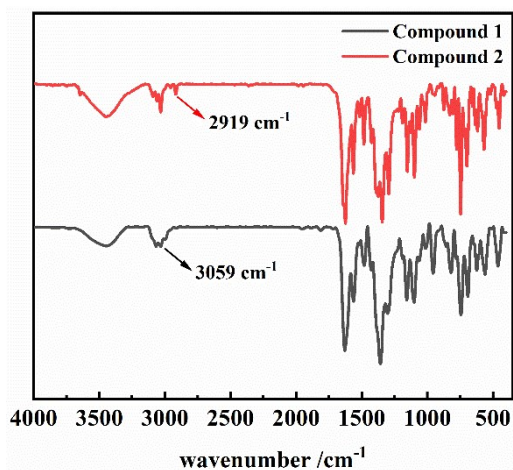
X-ray crystallography

Single-crystal X-ray diffraction data were collected on a Bruker D8 Venture diffractometer with graphite-monochromated Ga K α radiation ($\lambda = 1.34139 \text{ \AA}$). The integration of diffraction data and intensity corrections for the Lorentz and polarization effects were performed by using SAINT program.¹ Semi-empirical absorption corrections were applied using SADABS program.² The structures were solved by direct methods with SHELXT-2014, expanded by subsequent Fourier-difference synthesis, and all the non-hydrogen atoms were refined anisotropically on F² using the full-matrix least-squares technique using the SHELXL-2018 crystallographic software package.^[3,4] The details of crystal parameters, data collection and refinements for **1** and **2** are listed in Table 1, and the selected bond lengths and angles are given in Table S1.

Table S1. Selected bond lengths (Å) and angles (°) for **1** and **2**.^a

| 1 | | | |
|--------------------|-------------|-------------------|-------------|
| Zn(1)-O(1)#1 | 1.972(2) | O(1)-Zn(1)-N(2)#2 | 110.16(8) |
| Zn(1)-O(6) | 1.9330(18) | O(6)-Zn(1)-O(1)#1 | 103.92 (9) |
| Zn(1)-N(1) | 2.022(2) | O(6)-Zn(1)-N(1) | 115.57 (8) |
| Zn(1)-N(2)#2 | 2.036(2) | O(6)-Zn(1)-N(2) | 97.41 (8) |
| O(1)-Zn(1)-N(1) #1 | 106.90(8) | N(1)-Zn(1)-N(2)#2 | 121.49 (9) |
| 2 | | | |
| Zn(1)-O(2)#1 | 1.940(4) | O(2)-Zn(1)-N(1) | 111.83 (18) |
| Zn(1)-O(6) | 1.935(4) | O(6)-Zn(1)-O(2)#1 | 104.46 (17) |
| Zn(1)-N(2)#2 | 2.059(4) | O(6)-Zn(1)-N(2)#2 | 114.27 (17) |
| Zn(1)-N(1)#2 | 2.041(5) | O(6)-Zn(1)-N(1) | 117.77 (17) |
| O(2)-Zn(1)-N(2)#2 | 100.06 (17) | N(1)-Zn(1)-N(2)#2 | 107.06 (17) |

^aSymmetry transformations used to generate equivalent atoms: #1 $-x+5/2, -y+1, z-1/2$; #2 $-x-1, y+1/2, -z+1/2$ for **1**. #1 $-x-3/2, -y+1, z-1/2$; #2 $-x+2, y-1/2, -z+1/2$ for **2**.

**Fig. S1.** (a) PXRD patterns of **1**. (b) PXRD patterns of **2**.**Fig. S3.** FT-IR spectra of compound **1** and **2**.

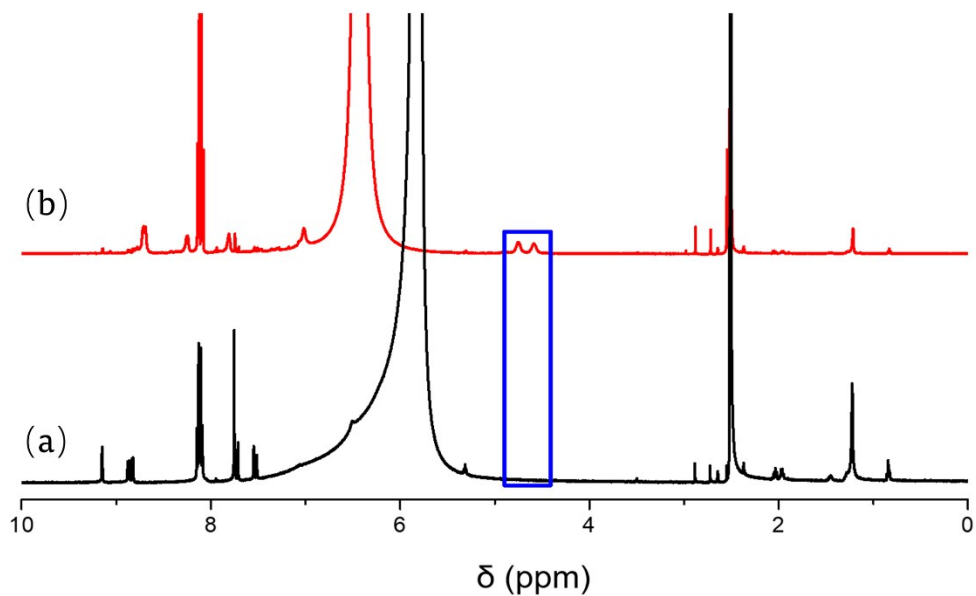


Fig. S4. The ^1H NMR results of **1** (a) and **2** (b) with a drop of HNO_3 in d^6 -DMSO.

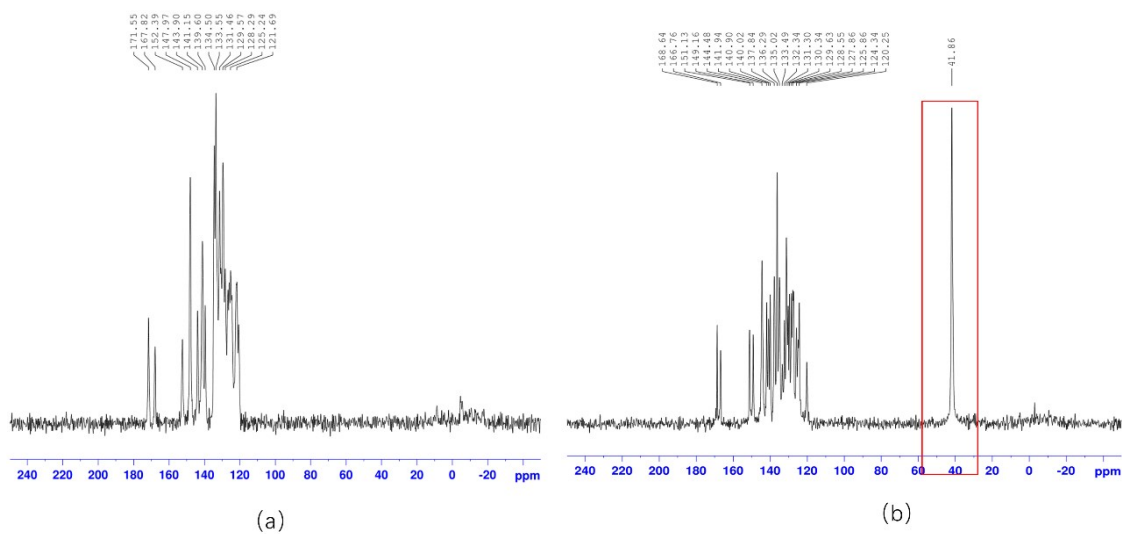


Fig. S5. The ^{13}C solid-state NMR results of **1** (a) and **2** (b).

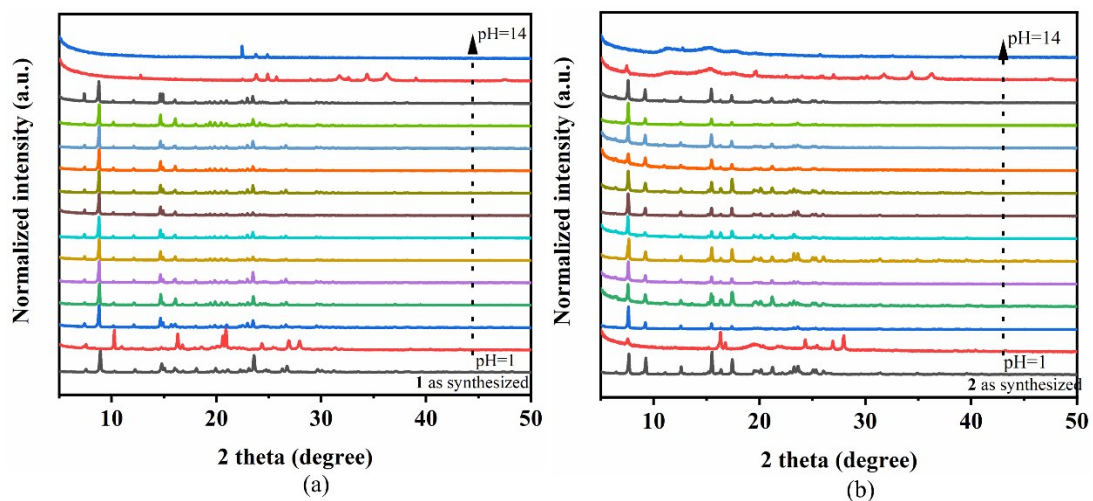


Fig. S6. The pH stability of **1** (a) and **2** (b).

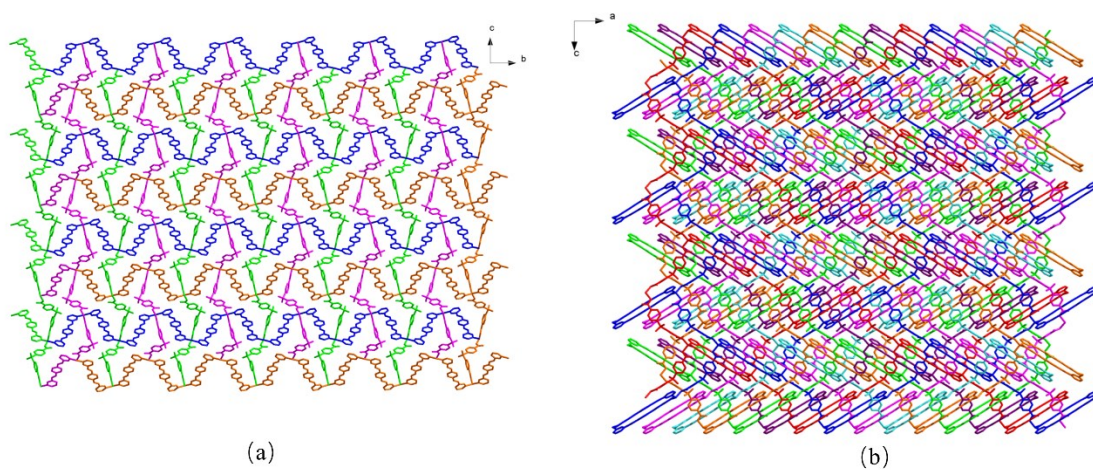


Fig. S7. The final 3D 7-fold interpenetrated frameworks of **1** along a-axis (a) and b-axis (b).

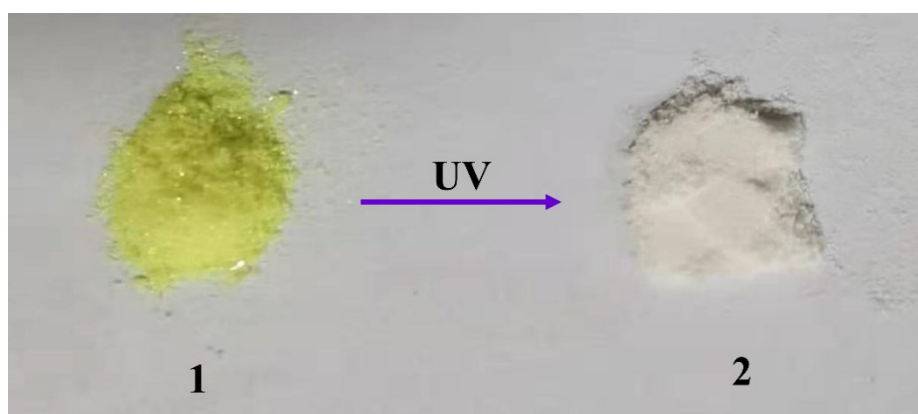


Fig. S8. The picture of Compound **1** and **2**.

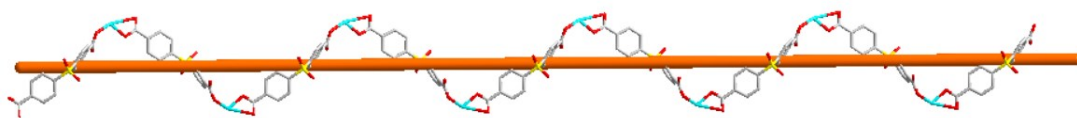


Fig. S9. The supramolecular helices in crystal structure of **1** and **2** composed of Zn (II) cation and sda²⁻.

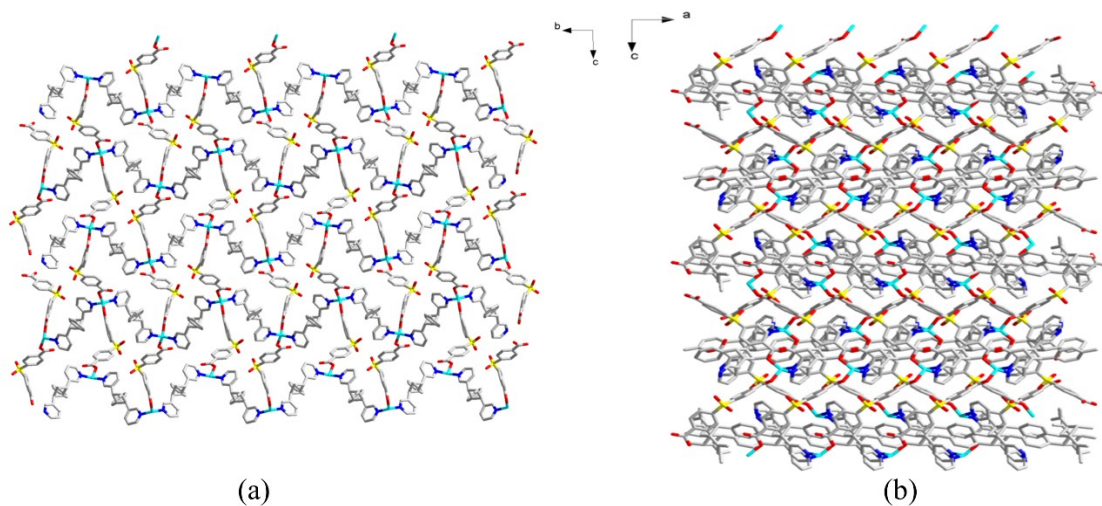


Fig. S10. The final 3D non-interpenetrated frameworks of **2** along with a-axis (a) and b-axis (b).

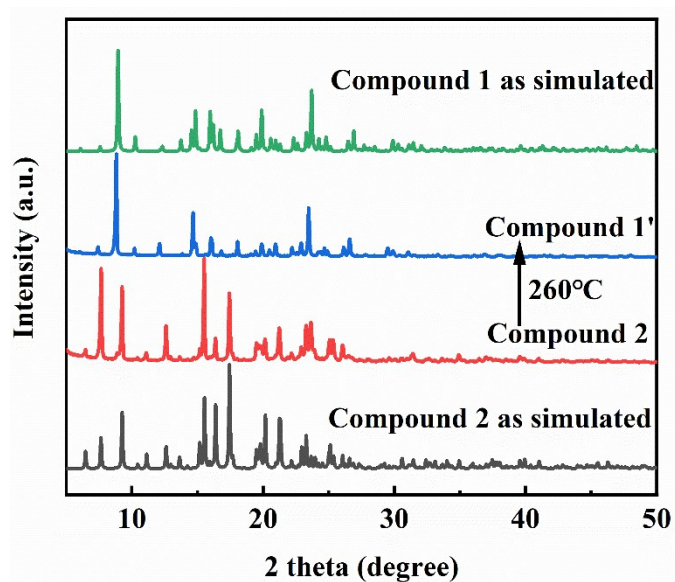


Fig. S11. Changes in the PXRD patterns of compound **2** upon heated at 260 °C.

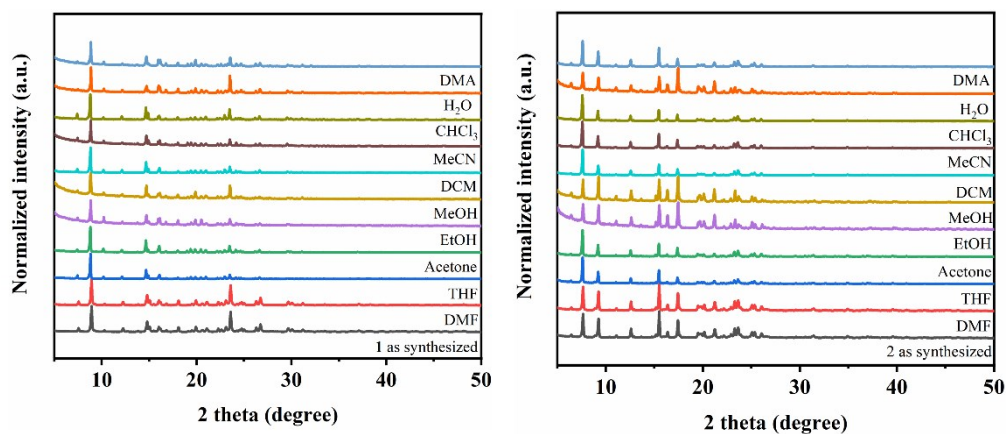


Fig. S12. The stability of **1**(a) and **2**(b) in different solvents.

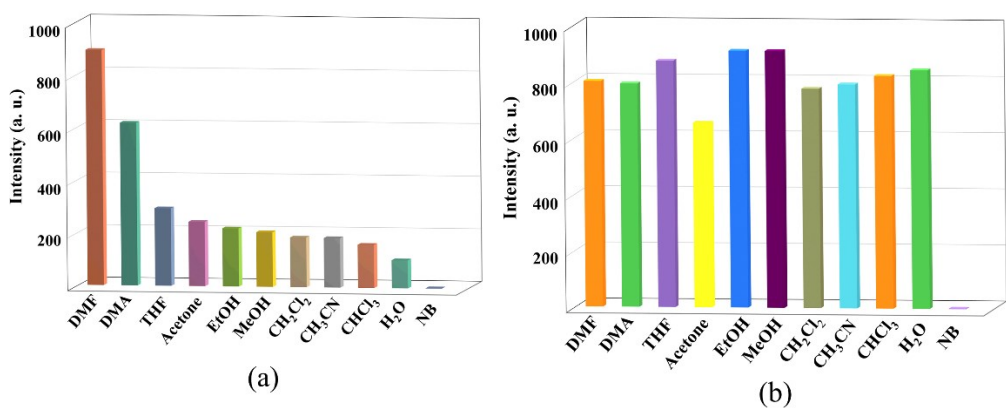


Fig. S13. The fluorescence intensity of **1**(a) and **2**(b) in different solvents.

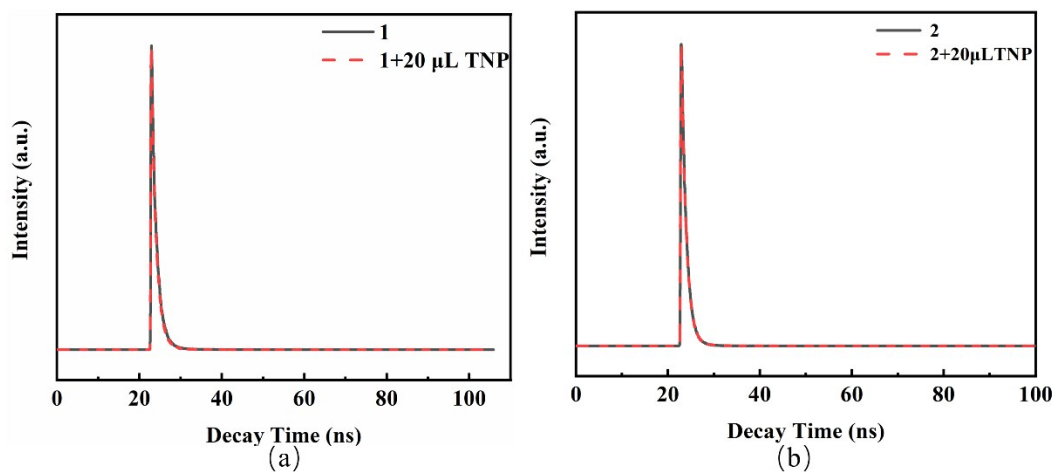
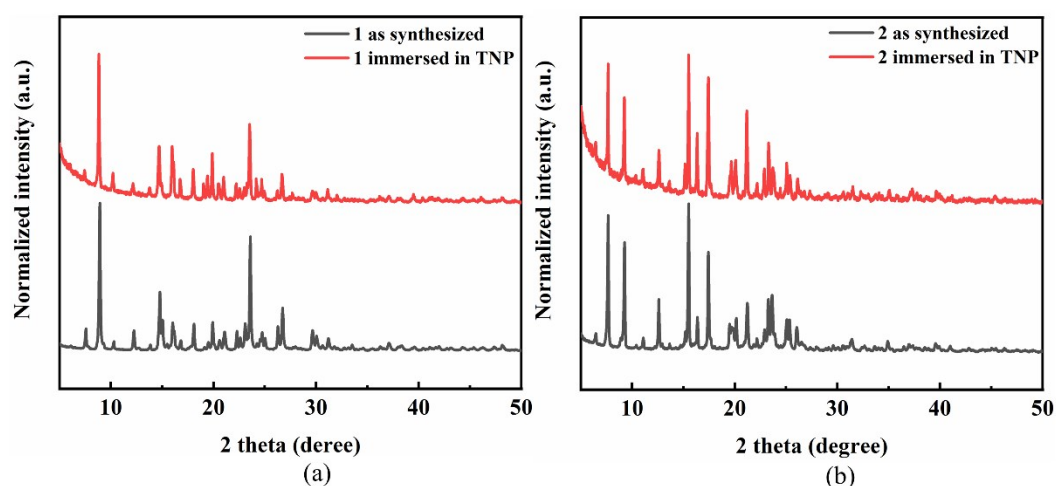


Fig. S14. Lifetimes of **1** (a) and **2** (b) dispersed in DMF before and after the addition of TNP.

Table S2. Standard deviation and detection limit calculation for TNP.

| | 1 | 2 |
|---------------------------------|---------------------------------|---------------------------------|
| 1 | 823.758577 | 822.049487 |
| 2 | 823.463198 | 821.939862 |
| 3 | 824.041157 | 822.175866 |
| 4 | 823.7543107 | 822.055072 |
| Standard deviation(σ) | 0.0964291 | 0.0964291 |
| Slope (m) | $3.5 \times 10^4 \text{M}^{-1}$ | $4.1 \times 10^4 \text{M}^{-1}$ |
| Detection limit ($3\sigma/m$) | $2.0 \times 10^{-5} \text{M}$ | $7.0 \times 10^{-6} \text{M}$ |

**Fig. S15.** PXRD patterns of **1** (a) and **2** (b) before and after soaking in the solution of TNP.

References

- 1 SAINT, *Program for Data Extraction and Reduction*, Bruker AXS, Inc., Madison, WI, 2001.
- 2 G. M. Sheldrick, *SADABS, Program for Empirical Adsorption Correction of Area Detector Data*. University of Gottingen, Gottingen, Germany, 2003.
- 3 G. M. Sheldrick, *SHELXS-2018, Program for the Crystal Structure Solution*, University of Gottingen, Gottingen, Germany, 2018.
- 4 G. M. Sheldrick, *SHELXL-2018, Program for the Crystal Structure Solution*, University of Gottingen, Gottingen, Germany, 2018.