

## One water-stable magnetic coordination polymer material (Fe<sub>3</sub>O<sub>4</sub>@PmPDs-[Co-BT]) as efficient adsorbent for rapidly dye removal

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### The structure of Co-BT

Single-crystal X-ray diffraction analysis result shows that Co-BT crystallizes in orthorhombic space group *Pca2*<sub>1</sub>. The asymmetric unit contains one Co(II) centre, a half bcpo ligand, a tib ligand and two water molecules. There is also a free acetonitrile molecule in the structure. The bond lengths of the Co-O and Co-N bond are 2.048(4)-2.152(3) Å and 2.120(3)-2.136(4) Å, respectively. Each Co(II) centre is in six-coordinate mode, forming an octahedron coordination geometry, three oxygen atoms (O1, O2 and O3) from two individual water molecules and a bcpo ligand, and three N atoms (N1, N4a and N6) from three individual tib ligands (Figure. S1a). The bond angles around Co(II) ions range from 80.10(14) to 178.11(15)°. Each tib ligand is linked to its adjacent six tib ligands by three Co(II) ions to form a reticulated 2D planar structure, and the bcpo ligand is suspended from the network by Co(II) ions (Figure. S1b). Topologically, the framework of Co-BT could be simplified as a 6-connected net with the point symbol of which belongs to the **hxl** topology (Figure. S1c).

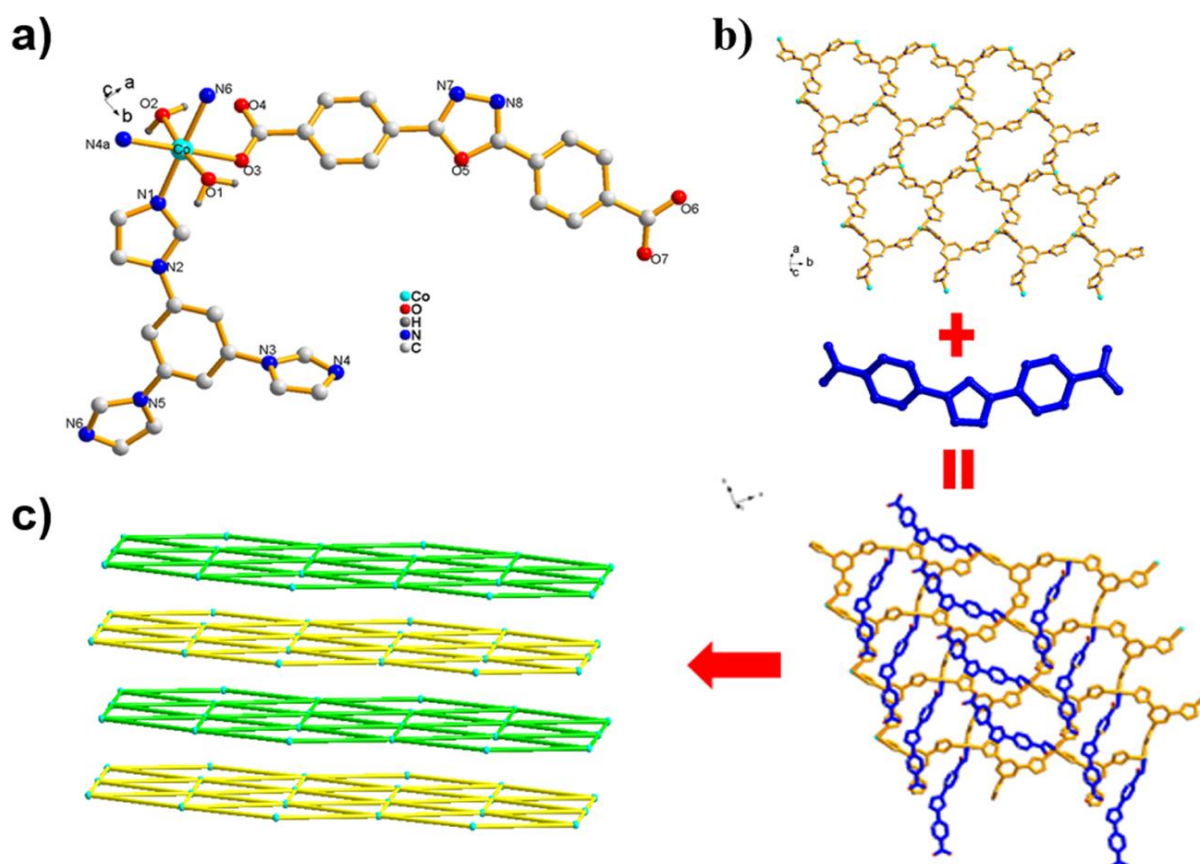


Figure S1. (a) Coordination environment of Co(II) (hydrogen atoms are omitted for clarity) (Symmetry codes: i:  $x+1/2, -y, z$ ; ii:  $x, y+1, z$ ; iii:  $x-1/2, -y, z$ ; iv:  $x, y-1, z$ ); (b) The 2D planar structure of [Co-BT]; (c) [Co-BT] topology of the entire structure.

The structure of the product was confirmed by XRD analysis. The XRD pattern of  $\text{Fe}_3\text{O}_4@\text{PmPDs}-[\text{Co-BT}]$  particles shows a typical characteristic peak, which is in good agreement with the simulated Co-BT crystal structure (Figure. S2b). After modifying  $\text{Fe}_3\text{O}_4$  core with mPDs, the diffraction peaks of Co-BT can still be determined, which indicates that the framework structure of Co-BT is retained. In addition, the microstructure of the synthesized composite was analyzed by FT-IR spectrum (Figure. S2a). As shown in Fig S2a, the peak at  $1618\text{ cm}^{-1}$  is attributed to the C=O vibration of the carboxyl group on Co-BT. On the infrared curve of the composite, the peak position shifted from  $1618\text{ cm}^{-1}$  to  $1602\text{ cm}^{-1}$ . At the same time, after coating Co-BT, the  $-\text{NH}_2$  peak at  $3443\text{ cm}^{-1}$  for  $\text{Fe}_3\text{O}_4@\text{PmPDs}$  becomes the N-H stretching vibration peak ( $3423\text{ cm}^{-1}$ ).

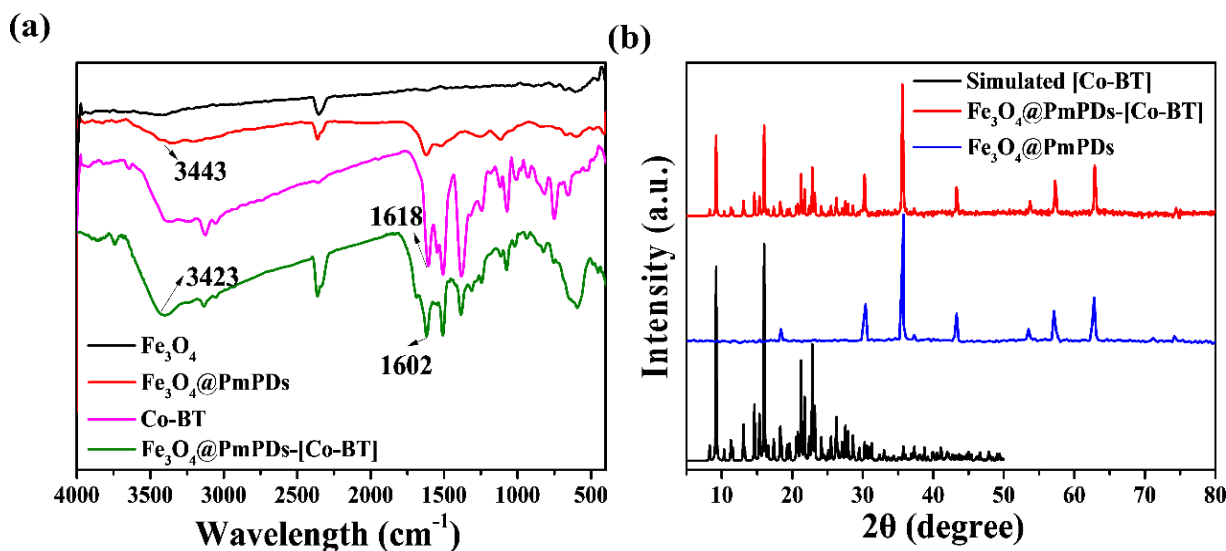


Figure S2. (a) IR spectra of Fe<sub>3</sub>O<sub>4</sub>, Fe<sub>3</sub>O<sub>4</sub>@PmPDs, Co-BT and Fe<sub>3</sub>O<sub>4</sub>@PmPDs-[Co-BT]; (b) Powder XRD spectra of Fe<sub>3</sub>O<sub>4</sub>@PmPDs and Fe<sub>3</sub>O<sub>4</sub>@PmPDs-[Co-BT].

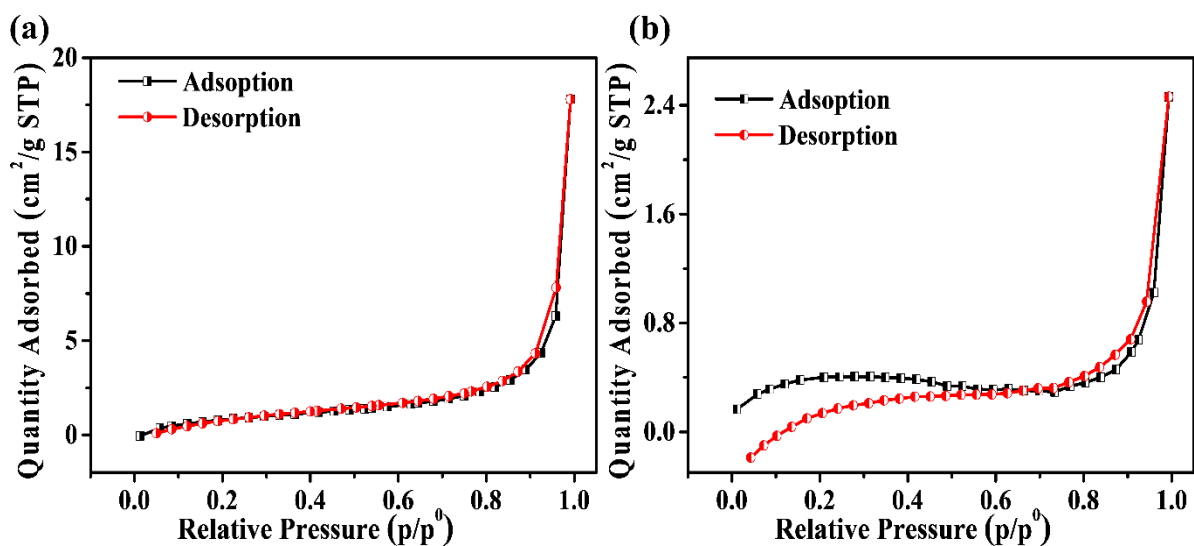


Figure S3 N<sub>2</sub> adsorption-desorption isotherm at 77 K. (a) For Co-BT. (b) For Fe<sub>3</sub>O<sub>4</sub>@PmPDs-[Co-BT].

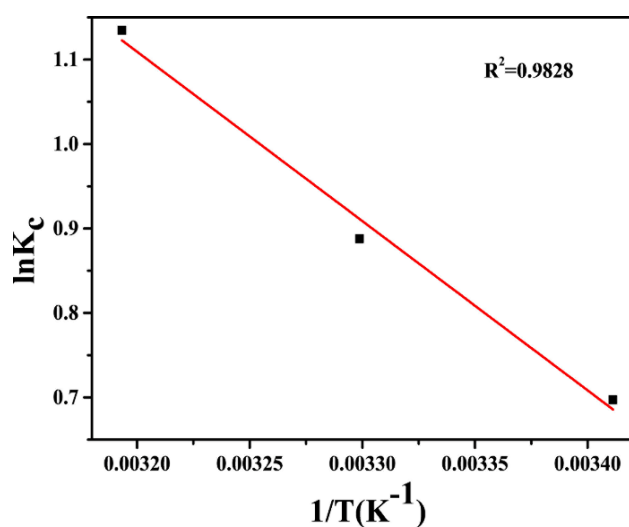


Figure S4. Relationship between lnK<sub>c</sub> and 1/T of CR adsorption by Fe<sub>3</sub>O<sub>4</sub>@PmPDs-[Co-BT].

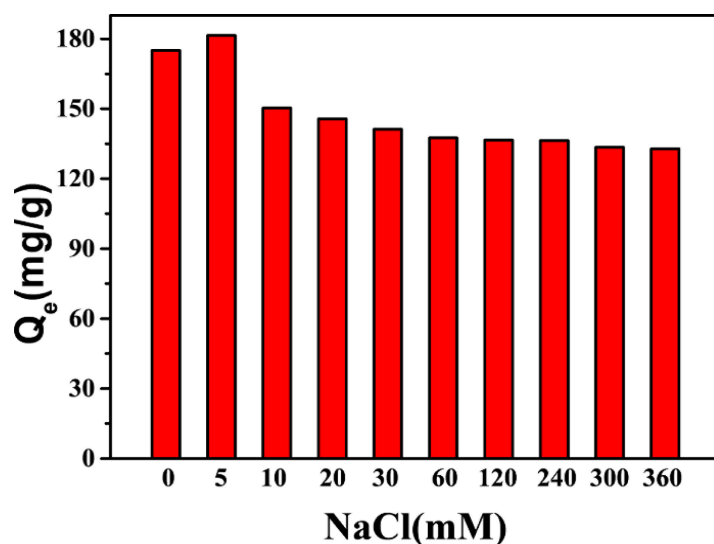


Figure S5. Change of  $\text{Fe}_3\text{O}_4@PmPDs\text{-[Co-BT]}$  adsorption amount as a function of NaCl concentration.

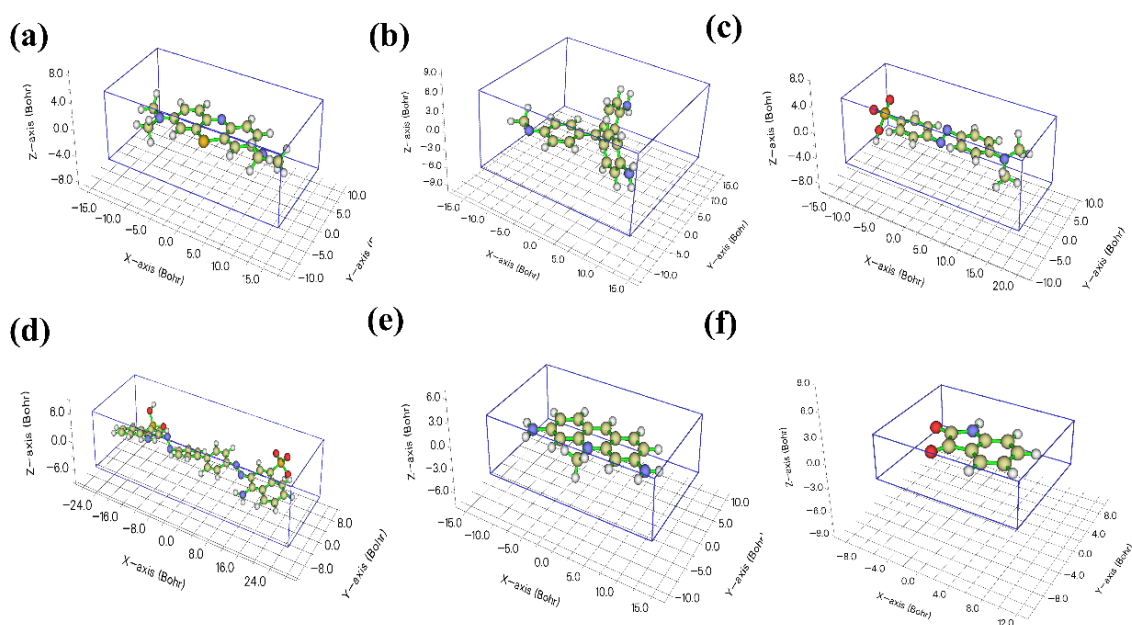


Figure S6. The structural diagrams of the dye molecules of MB(a), MV(b), MO(c), CR(d), AH(e), AR(f) in sequence.

Table S1 Molecular dynamics size and molecular volume of the six selected dyes.

	MB	MV	MO	CR	AH	AR
Molecular size ( $\text{\AA}$ )	$16.50 \times 8.0$ $7 \times 5.46$	$14.46 \times 12.4$ $8 \times 6.71$	$17.21 \times 6.7$ $6 \times 5.42$	$28.08 \times 9.6$ $3 \times 6.32$	$13.80 \times 8.1$ $2 \times 4.00$	$9.56 \times 7.39$ $\times 2.90$
Volume ( $\text{\AA}^3$ )	726.98	1211.30	631.21	1710.16	448.29	204.80