

Electronic Supplementary Material (ESI) for Dalton Trans.
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Supporting Information

Supplementary data

Effective adsorption of Congo red by MOF-based magnetic material

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Materials and instrumentation

All reagents and solvents except BPTP ligand were commercially available and used as received without further purification. The IR absorption spectra of these complexes were recorded in the range of 400-4000 cm⁻¹ by means of a Nicolet (Impact 410) spectrometer with KBr pellets. Element analyses (C, H, N) were carried out on a Perkin-Elmer model 240C analyzer. PXRD measurements were performed on a Bruker D8 Advance X-ray diffractometer using Cu-K α radiation (0.15418 nm), in which the X-ray tube was operated at 40 kV and 30 mA. TG analysis was performed on a Perkin Elmer thermogravimetric analyzer from room temperature to 800 °C with a heating rate of 10 K·min⁻¹ under N₂ atmosphere.

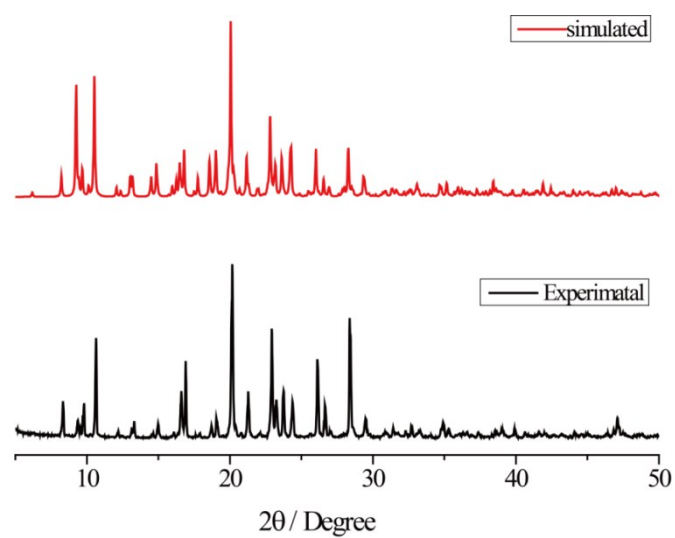


Fig. S1. PXRD of MOF ZTB-1.

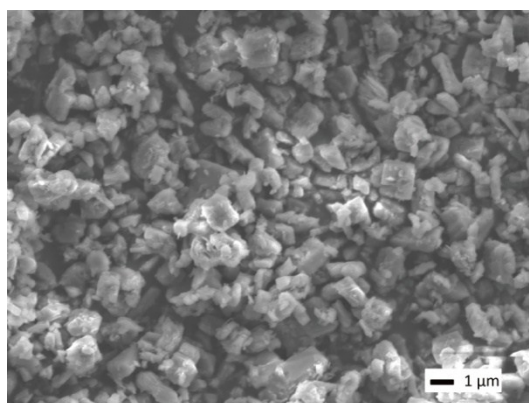


Fig. S2. SEM image of ZTB-1.

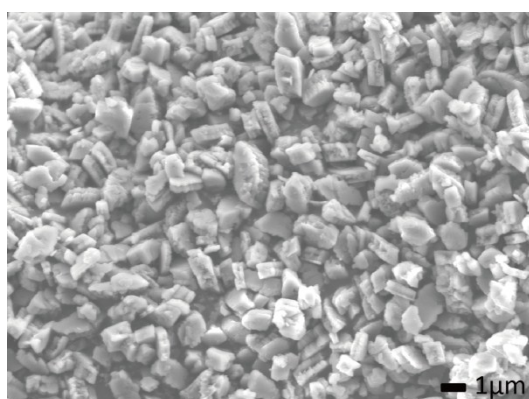


Fig. S3. SEM image of ZTB-1 prepared in the presence of CTAB surfactant.

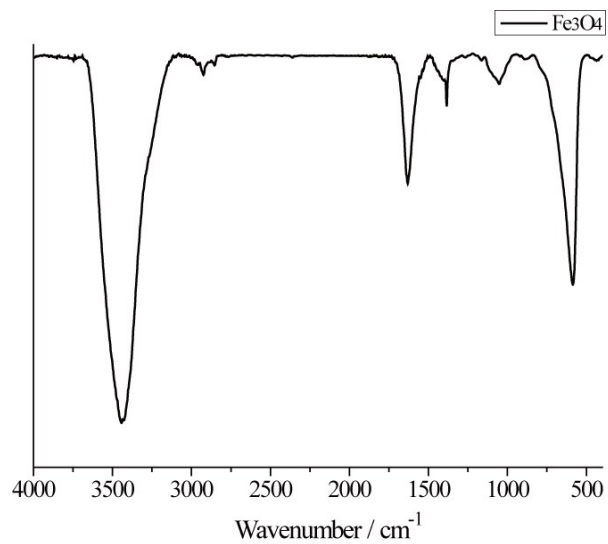


Fig. S4. FT-IR spectroscopy of Fe₃O₄.

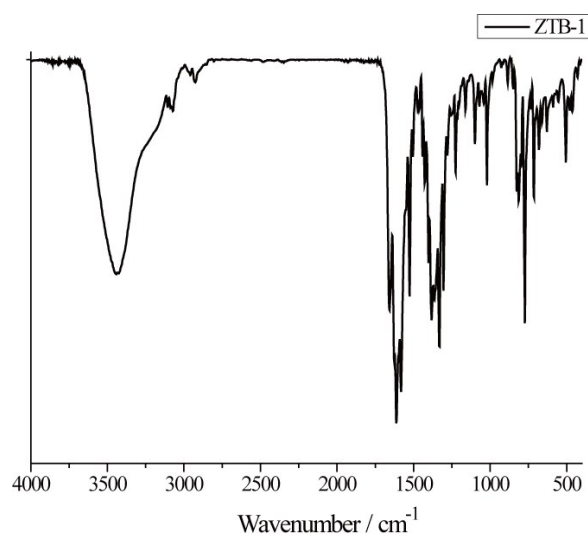


Fig. S5. FT-IR spectroscopy of MOF ZTB-1.

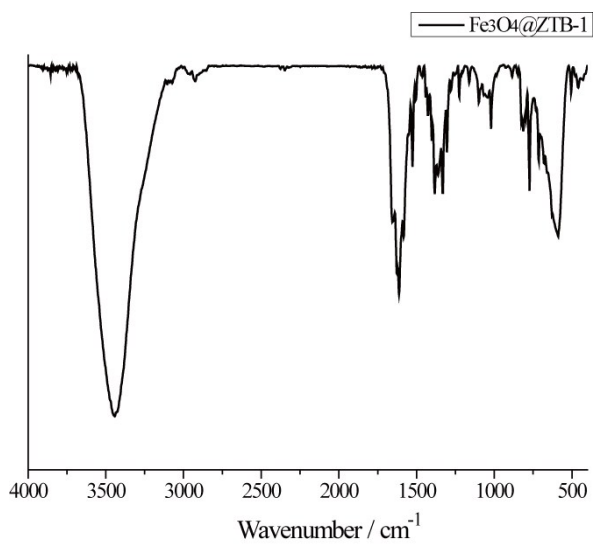


Fig. S6. FT-IR spectroscopy of Fe₃O₄@ZTB-1.

Table S1. Crystal data and structure refinement for ZTB-1.

ZTB-1	
Empirical formula	C ₃₈ H ₂₆ N ₄ O ₁₀ S ₄ Zn ₂
Formula weight	957.61
Crystal color	Yellow
Crystal size (mm)	0.15 x 0.15 x 0.12
Crystal system	Monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	9.228
<i>b</i> (Å)	21.487
<i>c</i> (Å)	19.316
α (deg)	90
β (deg)	98.624
γ (deg)	90
Volume (Å ³)	3787.0
<i>Z</i>	4
d_{calcd} (g/cm ³)	1.683
μ (mm ⁻¹)	1.553
<i>F</i> (000)	1952
λ (Å)	0.71073
Temperature	293(2) K
θ range (deg)	1.43 to 25.00
<i>h</i> , <i>k</i> , <i>l</i> range	-10 ≤ <i>h</i> ≤ 10 -25 ≤ <i>k</i> ≤ 14 -22 ≤ <i>l</i> ≤ 22
Reflections collected / unique	21050 / 6650 [<i>R</i> (int) = 0.0261
Completeness to θ	100.0 % ($\theta = 25$)
Data / restraints / parameters	6650 / 87 / 560
Goodness-of-fit on <i>F</i> ²	1.038
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^b	<i>R</i> ₁ = 0.0253 <i>wR</i> ₂ = 0.0608
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0330 <i>wR</i> ₂ = 0.0644
Largest diff. Peak and hole (e ⁻ ·Å ⁻³)	0.294 and -0.236

^b $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$; $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (°) for ZTB-1.

Zn(1)-O(4)	1.9744(15)
Zn(1)-O(5)#1	1.9851(17)
Zn(1)-O(8)	2.071(5)
Zn(1)-N(3)#2	2.0742(18)
Zn(1)-O(9')	2.112(13)
Zn(1)-O(8')	2.346(12)
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O(4)-Zn(1)-O(5)#1	113.06(7)
O(4)-Zn(1)-O(8)	92.42(13)
O(5)#1-Zn(1)-O(8)	95.26(18)
O(4)-Zn(1)-N(3)#2	104.17(7)
O(5)#1-Zn(1)-N(3)#2	118.31(7)
O(8)-Zn(1)-N(3)#2	131.04(19)
O(4)-Zn(1)-O(9')	105.0(2)
O(5)#1-Zn(1)-O(9')	126.1(2)
N(3)#2-Zn(1)-O(9')	85.8(3)
O(4)-Zn(1)-O(8')	90.2(3)
O(5)#1-Zn(1)-O(8')	83.2(3)
N(3)#2-Zn(1)-O(8')	144.8(4)

Symmetry transformations used to generate equivalent atoms:

#1: $x, -y+3/2, z-1/2$, #2: $-x+1, y+1/2, -z+3/2$