

Electronic Supplementary Information (ESI)

A multi-responsive MOF-based fluorescent probe for detecting Fe³⁺, Cr₂O₇²⁻ and acetylacetone

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Table S1. Selected bond lengths (Å) and angles (°) for **JXUST-7^a**.

Zn1—O2	1.949(2)	Zn1—N5	2.052(3)
Zn1—O5 ^{#1}	2.010(3)	Zn1—N1 ^{#2}	2.074(3)
Zn1—O4 ^{#1}	2.495(3)		
O2—Zn1—O5 ^{#1}	107.63(11)	O2—Zn1—N1 ^{#2}	96.23(11)
O2—Zn1—N5	105.55(11)	O5 ^{#1} —Zn1—N1 ^{#2}	107.99(11)
O5 ^{#1} —Zn1—N5	135.42(12)	N5—Zn1—N1 ^{#2}	96.99(11)

^aSymmetry codes: #1: $x-1, y, z-1$; #2: $x+1, y, z$.

Table S2. SHAPE analysis of the Zn^{II} ions in **JXUST-7**.

Ions	Label	Shape	Symmetry	Distortion(τ)
Zn1	PP-5	Pentagon	D_{5h}	26.371
	vOC-5	Vacant octahedron	C_{4v}	4.324
	TBPY-5	Trigonal bipyramid	D_{3h}	6.753
	SPY-5	Spherical square pyramid	C_{4v}	3.461
	JTBPY-5	Johnson trigonal bipyramid J12	D_{3h}	7.625

Table S3. HOMO and LUMO energies for the

tested small organic molecules.

	HOMO	LUMO
MeOH	-0.217269	-0.005182
EG	-0.225601	-0.019567
NPA	-0.21424	0.003898
IPA	-0.215095	0.001167
CHA	-0.17819	0.032718
TMEDA	-0.170949	0.043141
Et ₃ N	-0.175415	0.049403
TMA	-0.174871	0.040364
THF	-0.199818	0.048569
CH ₃ CN	-0.246269	-0.092173
CYH	-0.221497	0.025644
Acetone	-0.19347	-0.113941
CH ₂ Cl ₂	-0.259379	-0.032987
CHCl ₃	-0.263968	-0.062737
CCl ₄	-0.273404	-0.088098
acac	-0.209983	-0.144376

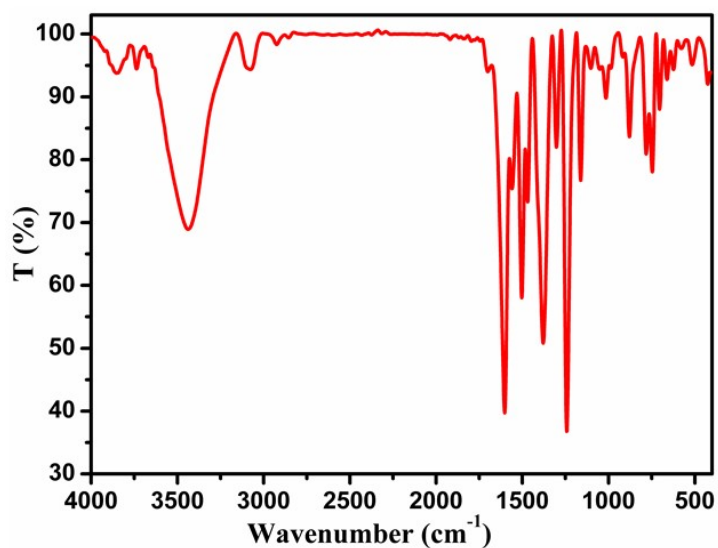


Fig. S1. IR spectrum of JXUST-7 at room temperature.

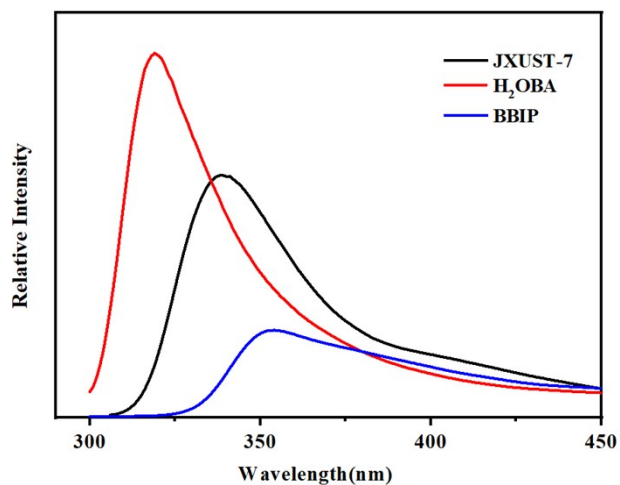


Fig. S2. Solid-state emission spectra of JXUST-7, H₂OBA and BBIP.

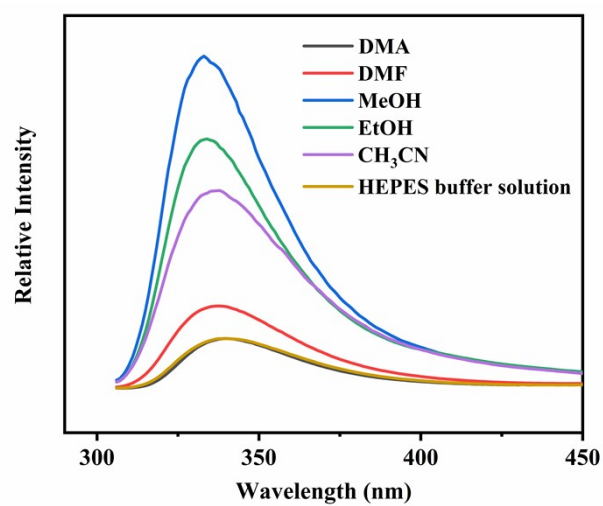


Fig. S3. The emission spectra of JXUST-7 in some common solvents and HEPES buffer solution.

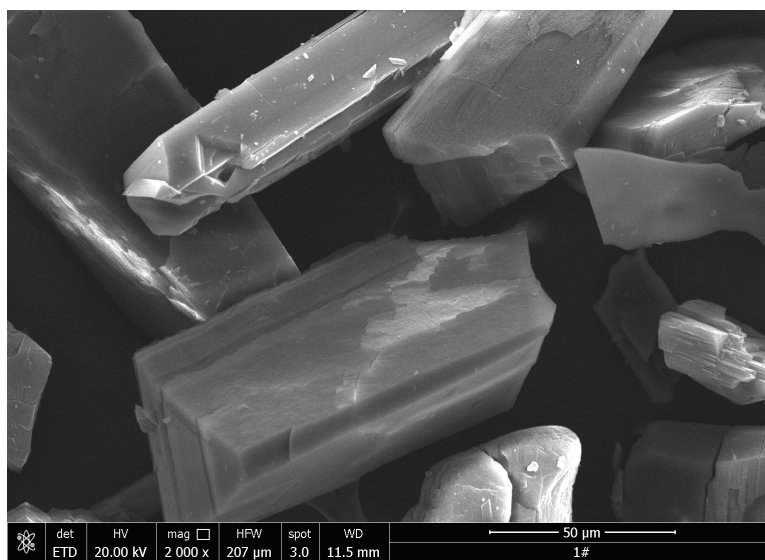
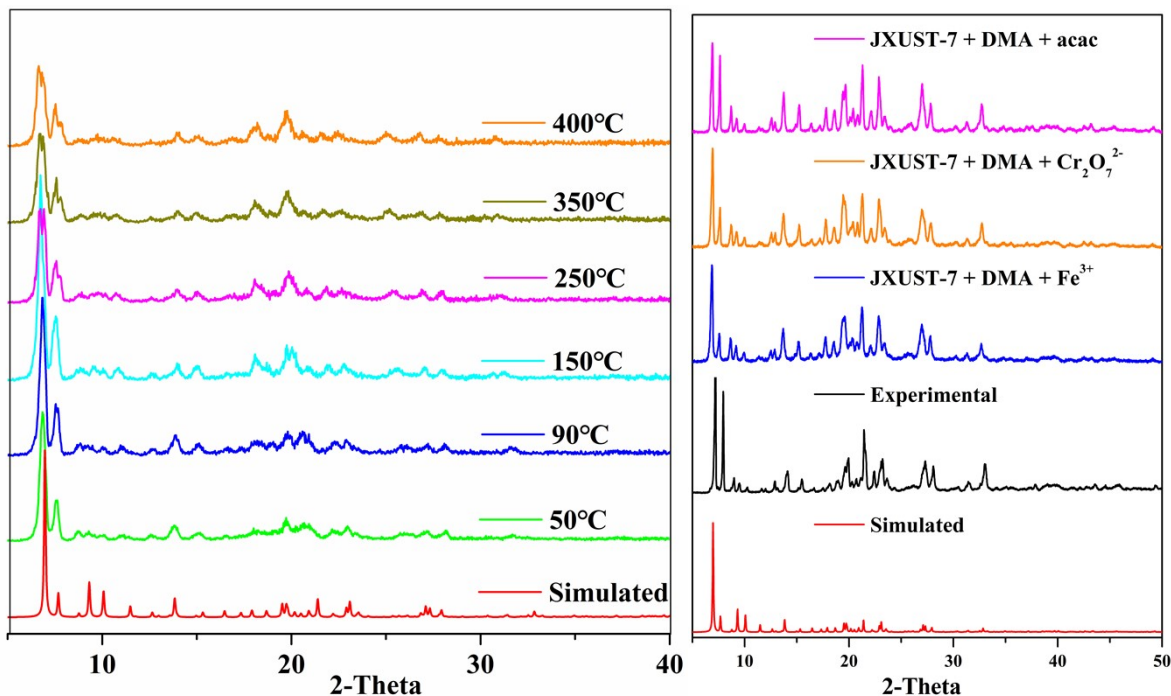
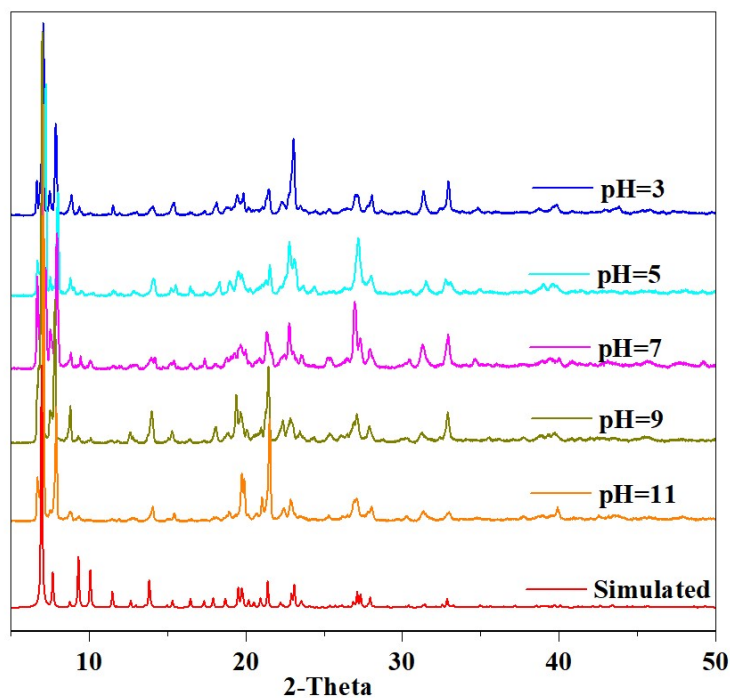


Fig. S4. SEM image of JXUST-7.

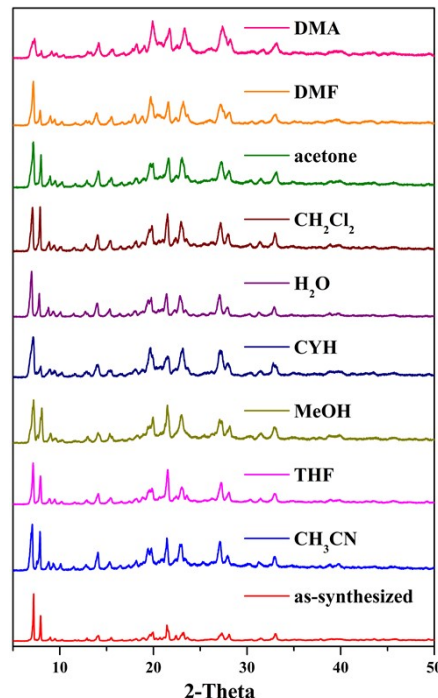


(a)

(b)



(c)



(d)

Fig. S5. (a) The simulated and experimental PXRD patterns of **JXUST-7** at different temperatures; (b) The simulated and experimental PXRD patterns of **JXUST-7** and **JXUST-7** after immersing in DMA solutions containing Fe³⁺, Cr₂O₇²⁻ and acac for 24 h; (c) The simulated and experimental PXRD patterns of **JXUST-7** in aqueous solution with diverse pH. (d) The as-synthesized and experimental PXRD patterns of **JXUST-7** after immersing in common organic solvents for 24 h.

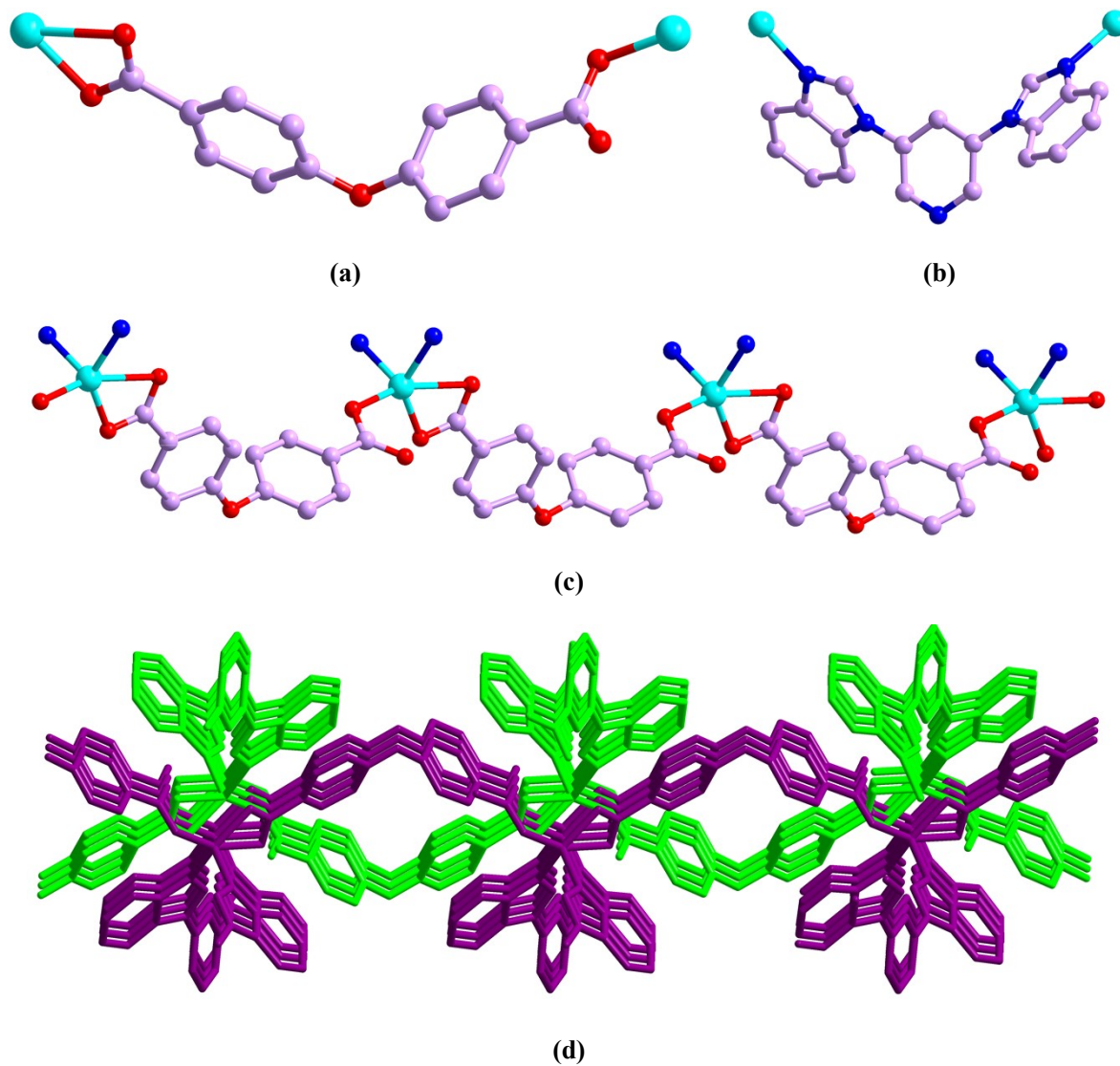


Fig. S6. View of (a) the coordination modes of OBA²⁻ in **JXUST-7**; (b) The coordination mode of BBIP in **JXUST-7**; (c) The 1D Zn^{II}-OBA²⁻ chain in **JXUST-7** and (d) The opposite parallel 2D layers of **JXUST-7**.

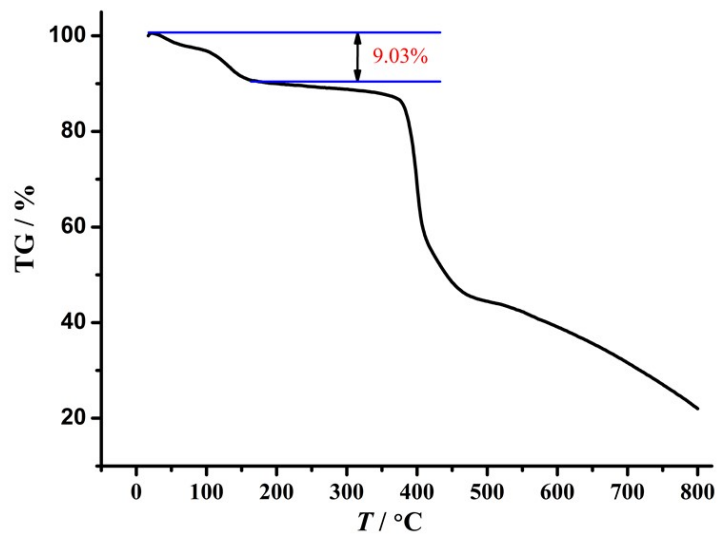


Fig. S7. The TGA curve for JXUST-7.

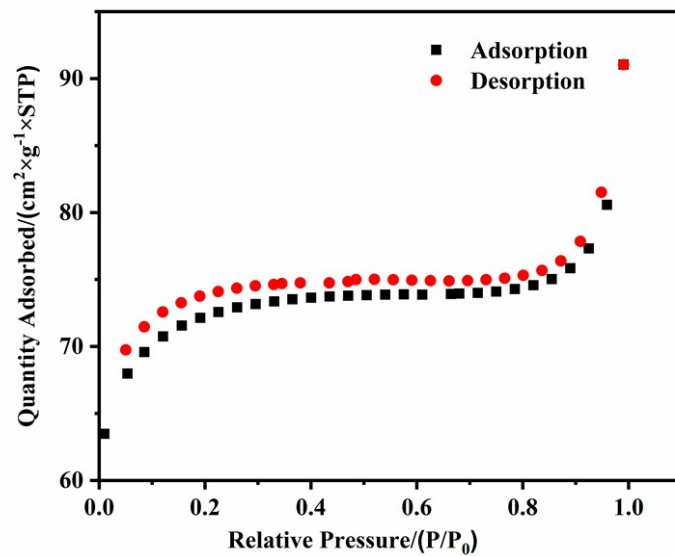


Fig. S8. The N₂ sorption isotherms of JXUST-7 at 77.15 K.

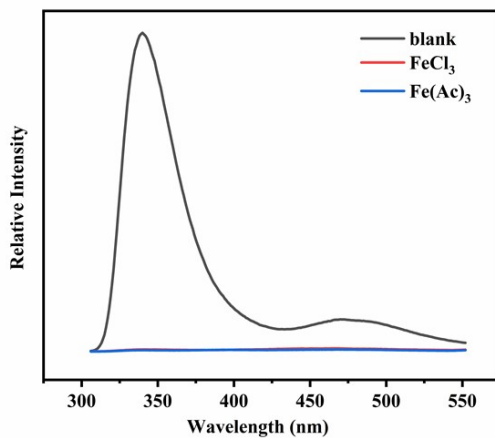


Fig. S9. The competitive experiments of JXUST-7 in sensing Fe^{3+} with the interference of other anion (halide, acetate)-containing Fe^{3+} salts in DMA solutions.

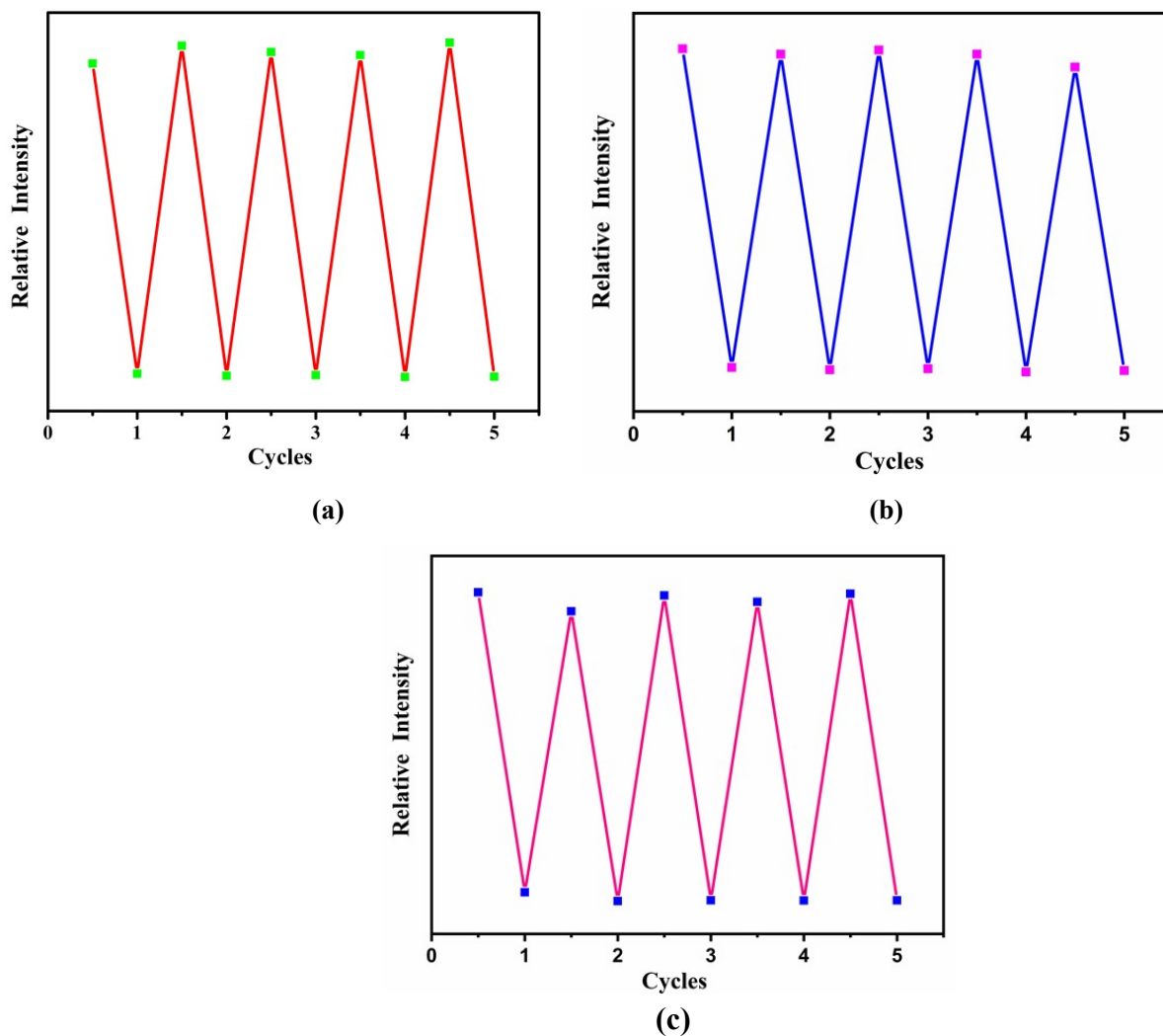


Fig. S10. Relative luminescent intensity of JXUST-7 after five runs of recycling experiments for (a) Fe^{3+} , (b) $\text{Cr}_2\text{O}_7^{2-}$ and (c) acac.

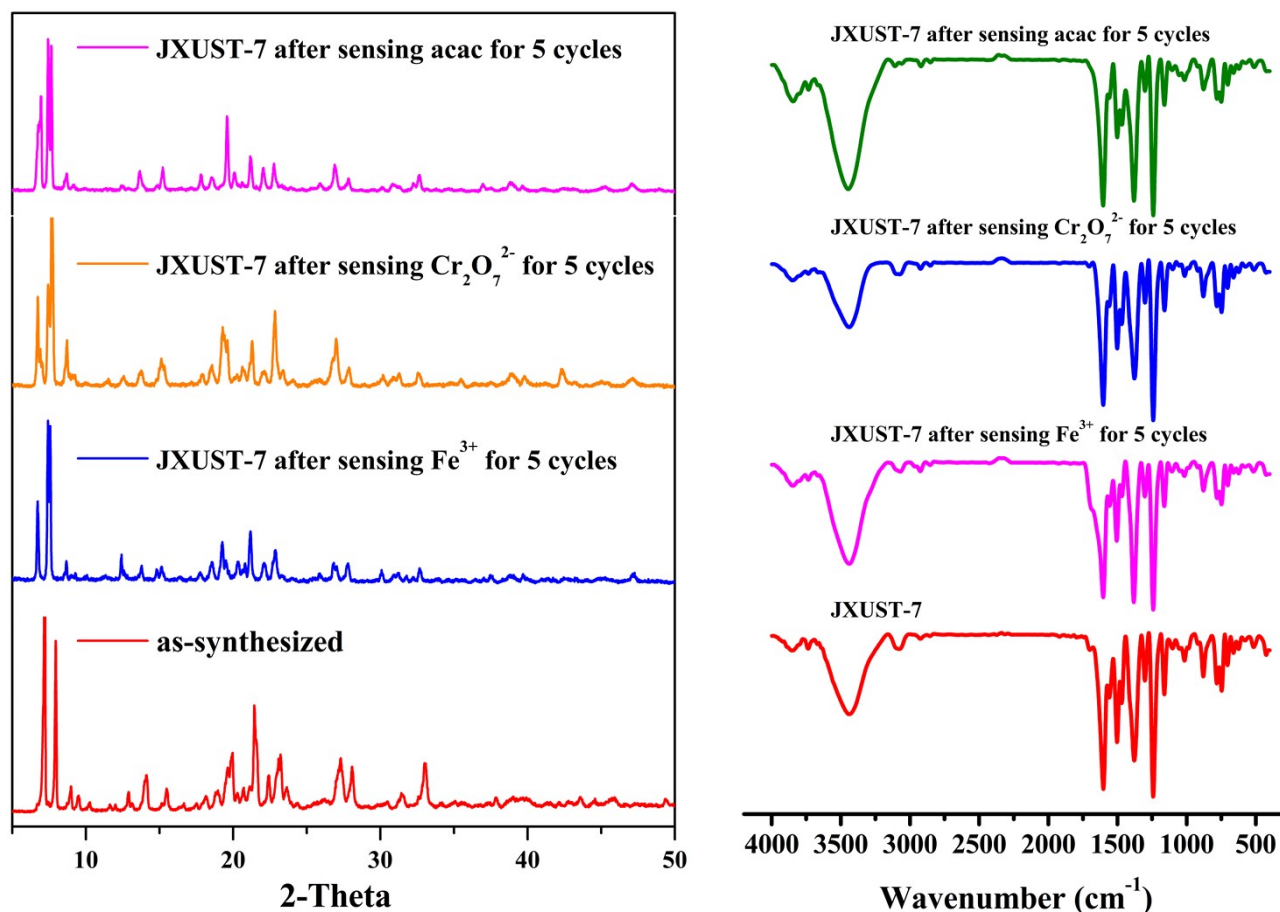


Fig. S11. (a) The as-synthesized and experimental PXRD patterns of JXUST-7 after sensing Fe^{3+} , $\text{Cr}_2\text{O}_7^{2-}$ and acac for 5 cycles; (b) IR spectra of JXUST-7 and JXUST-7 after sensing Fe^{3+} , $\text{Cr}_2\text{O}_7^{2-}$ and acac for 5 cycles, respectively.

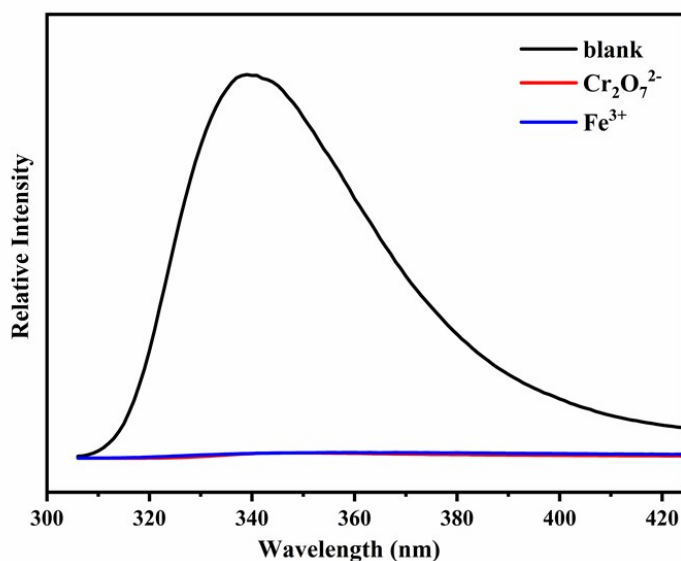


Fig. S12 Emission spectra of JXUST-7 dispersed in HEPES buffer (pH = 7.4) with the addition of Fe^{3+} and $\text{Cr}_2\text{O}_7^{2-}$.

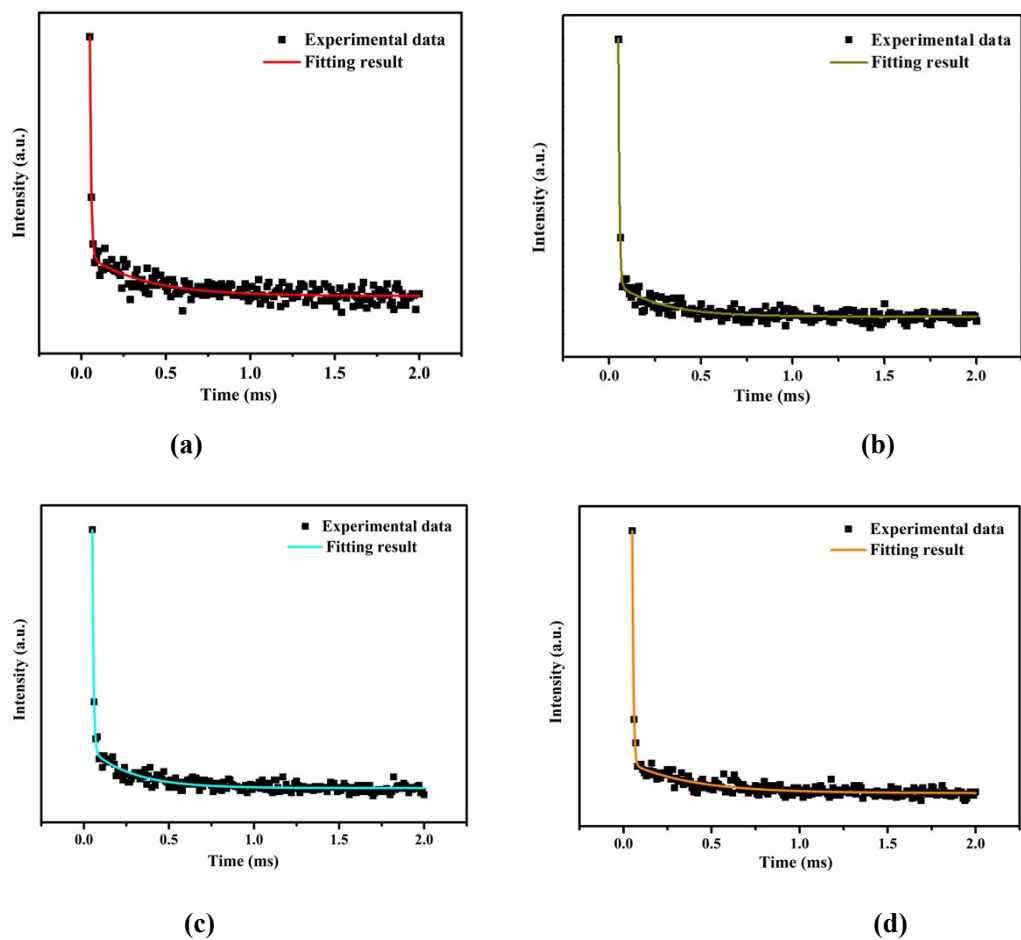


Fig. S13. Time-resolved decay of (a) JXUST-7, (b) JXUST-7@ Fe³⁺, (c) JXUST-7@ Cr₂O₇²⁻ and (d) JXUST-7@ acac.

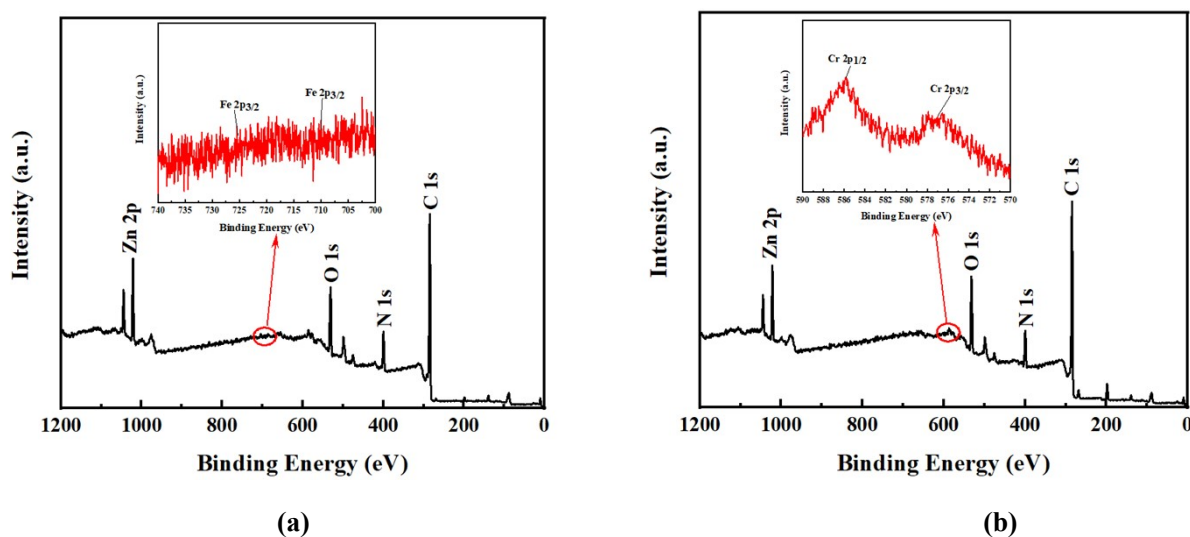


Fig. S14. The XPS patterns of (a) JXUST-7@ Fe³⁺ and (b) JXUST-7@ Cr₂O₇²⁻. (The sample of JXUST-7 was soaked in 5 mM Fe³⁺ or Cr₂O₇²⁻ for 24 h, and then washed with ethanol).

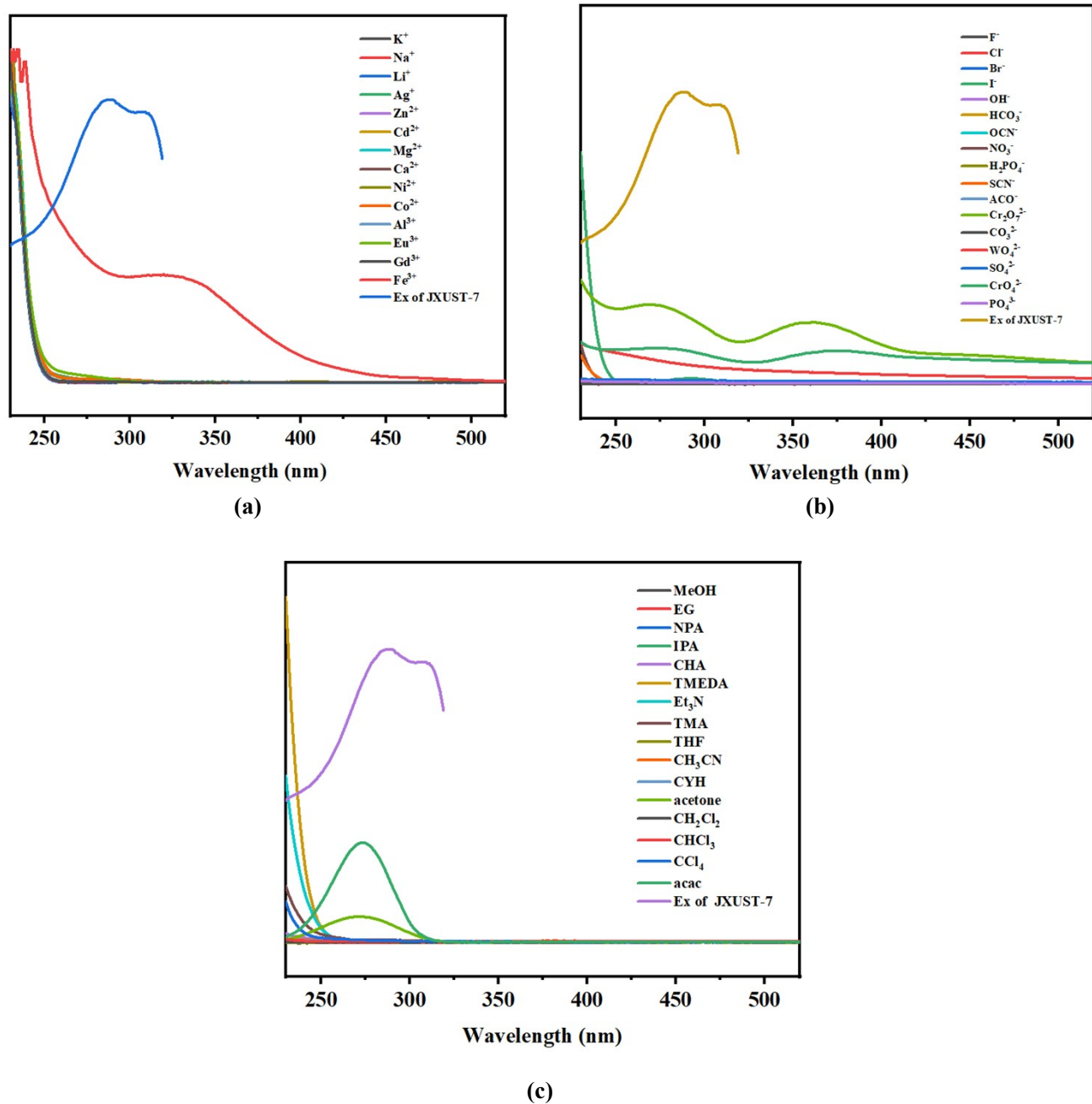


Fig. S15. The excitation spectrum of JXUST-7 and UV-Vis adsorption spectra of different (a) $M(\text{NO}_3)_x$, (b) K_yA and (c) small organic molecules.