

Supporting Information

Tb-MOF: A Naked-eye and Regenerable Fluorescent Probe for Selective and Quantitative Detection of Fe³⁺ and Al³⁺ Ions

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Table S1. Crystal Data and Structure Refinement Summary for compound **1**.

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) for compound **1**.

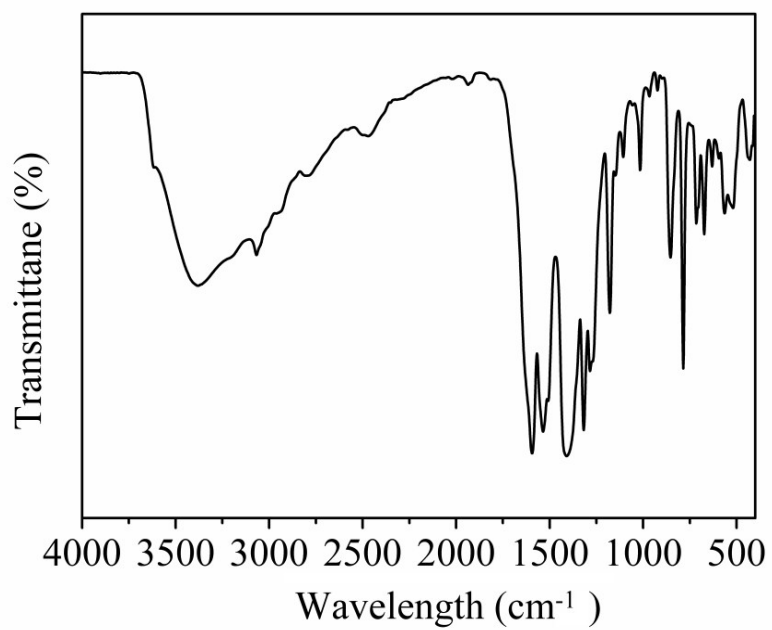


Fig. S1 FT-IR spectra of compound 1.

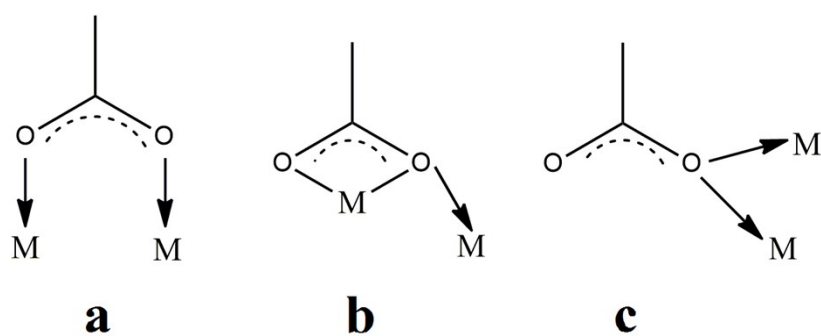


Fig. S2 The coordinated modes of TCA³⁻ ligand in compound 1. a, $\mu_2\text{-}\eta^1\text{:}\eta^1$; b, $\mu_2\text{-}\eta^2\text{:}\eta^1$; c, $\mu_2\text{-}\eta^2$.

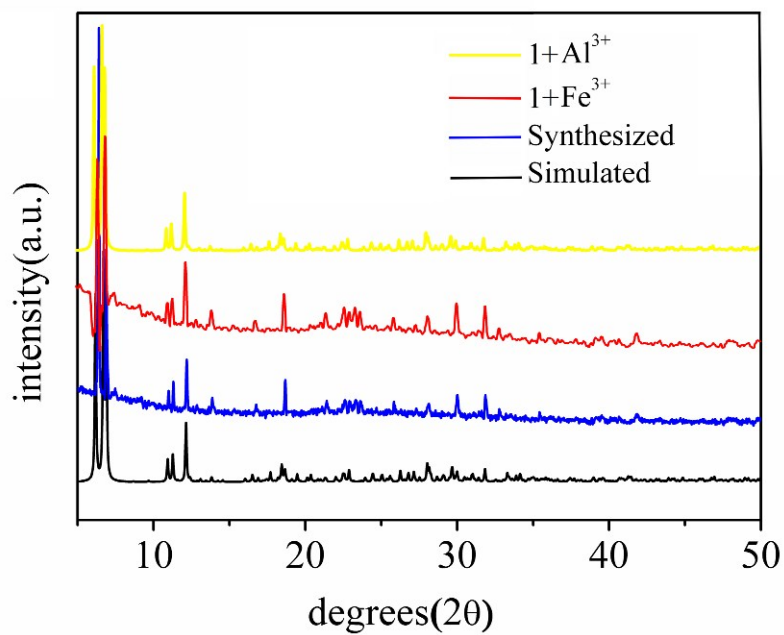


Fig. S3 Powder X-ray diffraction (PXRD) of simulated from the single-crystal data of **1** (black), as-synthesized compound **1** (blue), **1+Fe³⁺** (red) and **1+Al³⁺** (yellow).

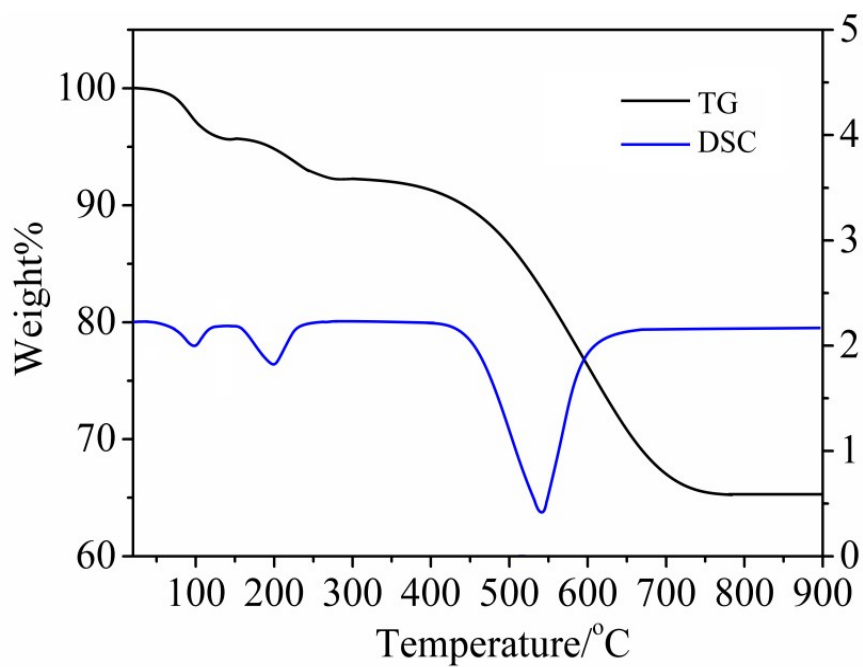


Fig. S4 Typical DSC and TG curves of compound **1**.

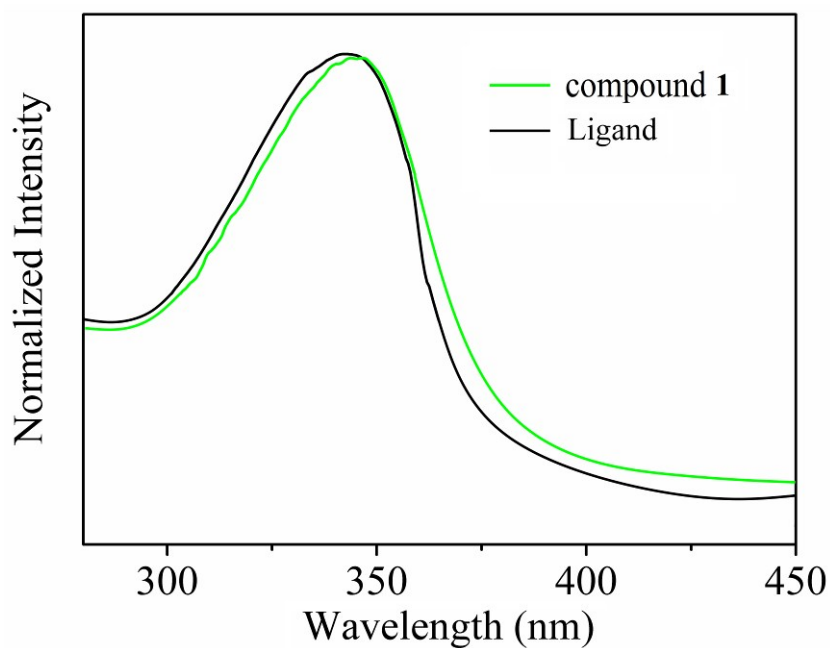


Fig. S5 The UV/vis absorption spectra of the free ligand H_3TCA and its corresponding compounds Tb-MOF were recorded in CH_3OH solution ($c = 1 \times 10^{-5}$ M).

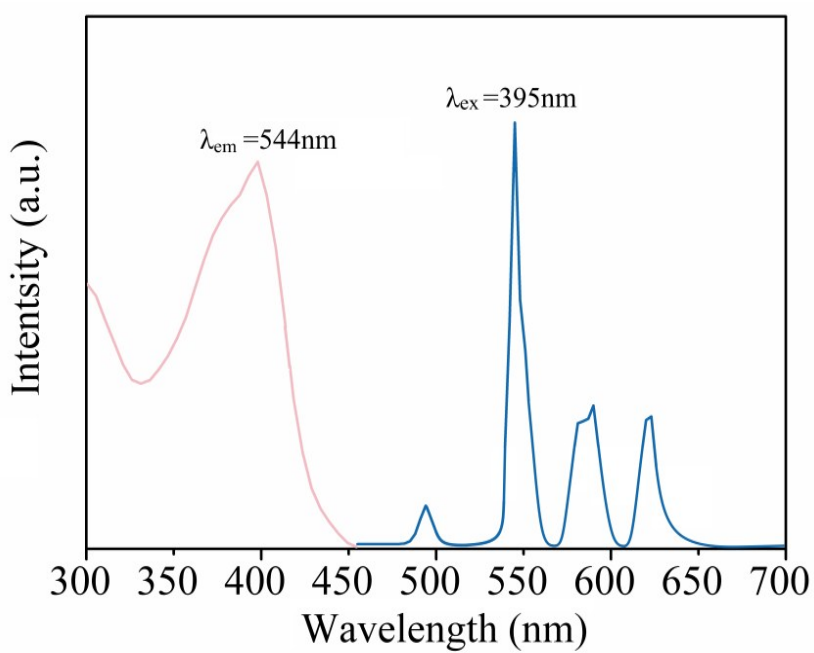


Fig. S6 Solid-state excitation (purple line) and emission (blue line) spectra of compound **1**.

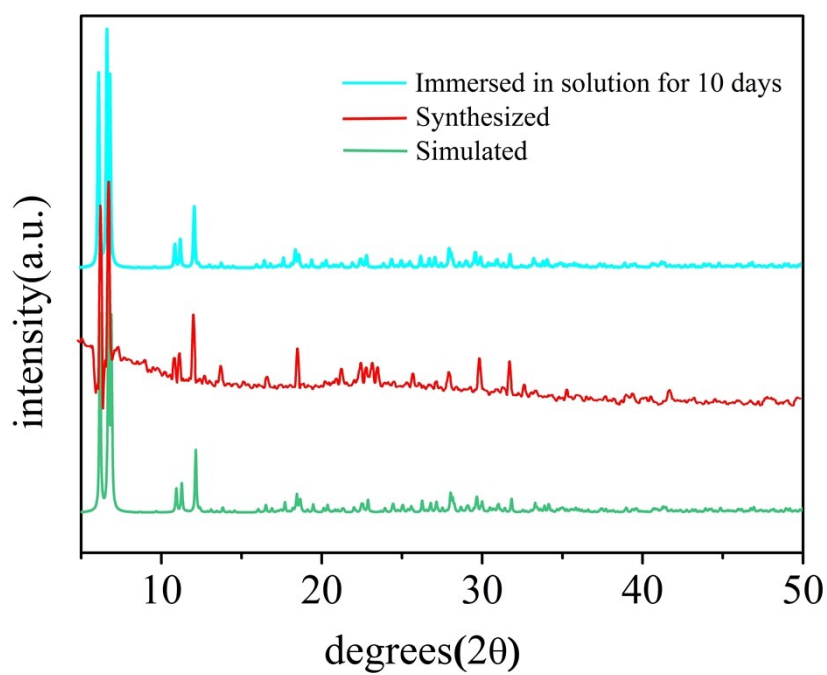


Fig. S7 PXRD patterns of Tb-MOF: the simulated pattern from single crystal analysis, as-synthesized Tb-MOF and immersed in solution for 10 days.

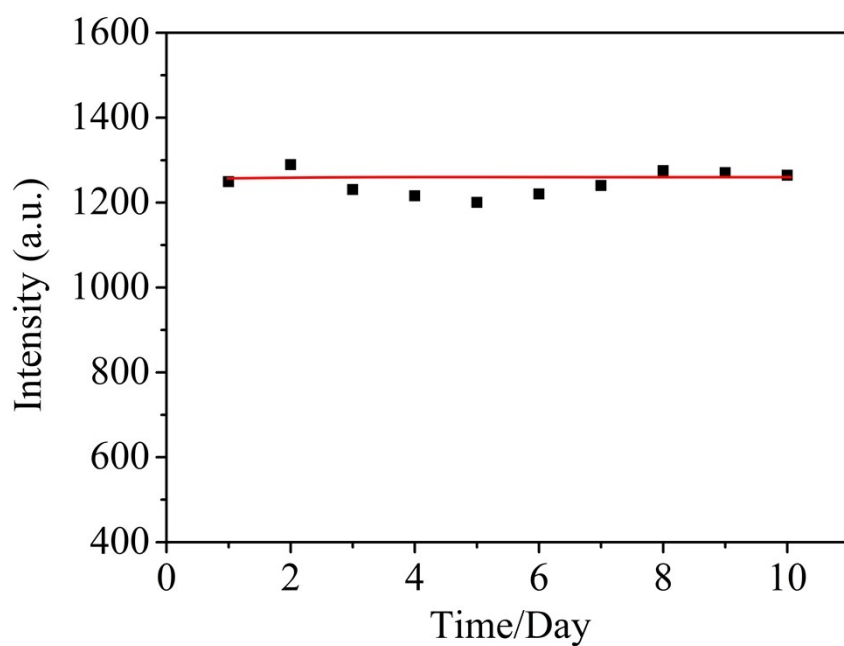


Fig. S8 Day to day fluorescence stability of compound 1 in aqueous solution.

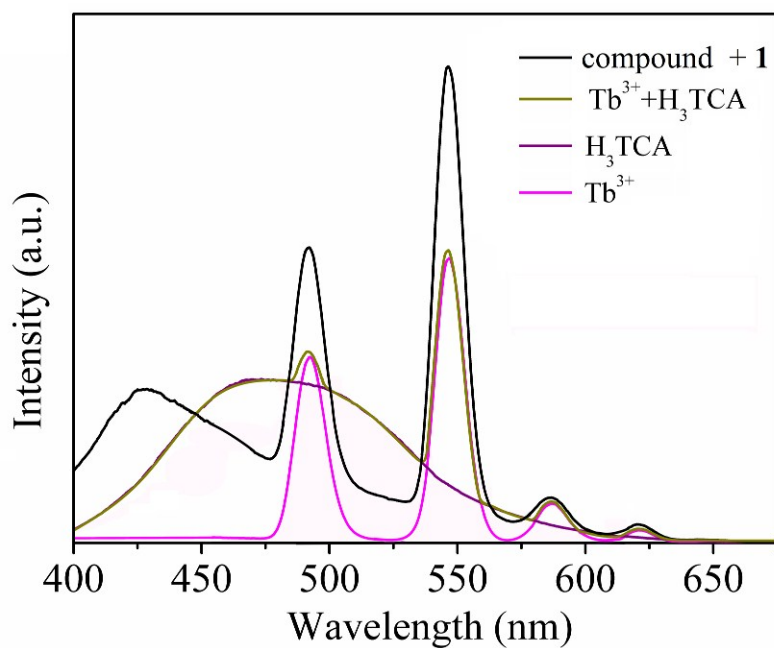


Fig. S8 Comparison of emission spectra of compound **1**, Tb^{3+} and H_3TCA (10^{-3} M) under excitation at 375 nm.

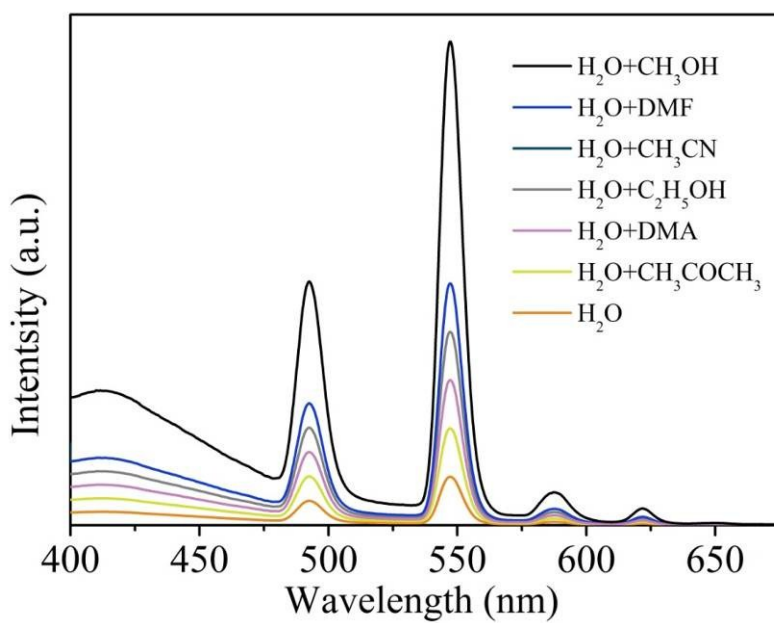


Fig. S10 Optimization of the solvent.

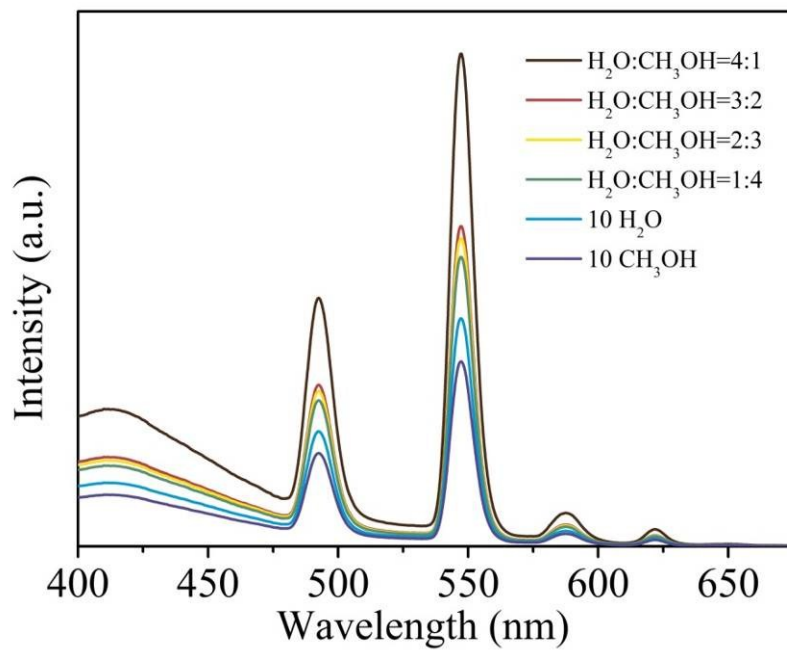


Fig. S11 Optimization of the solvent ratio.

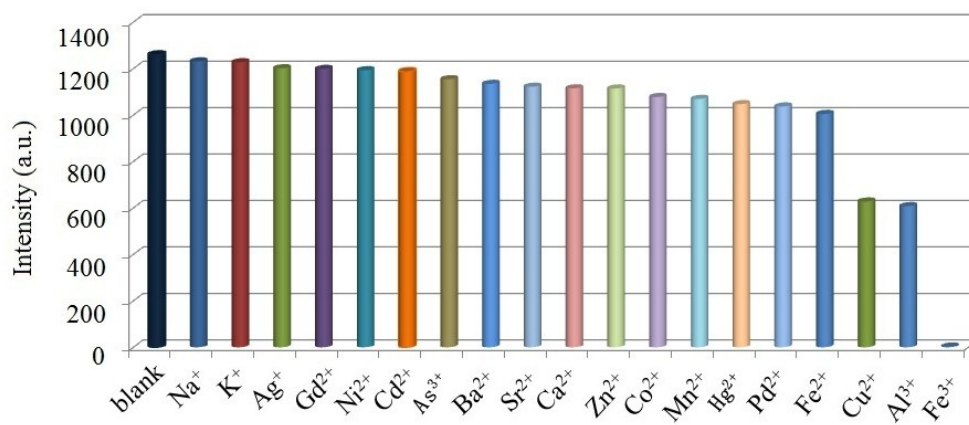


Fig. S12 Comparison of the luminescence intensity at 549 nm of compound **1** in 10^{-3} M different cations.

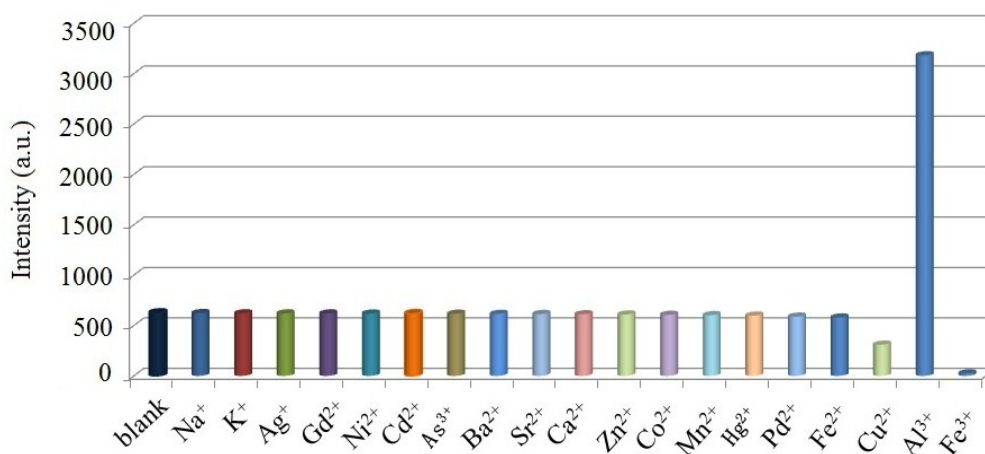


Fig. S13 Comparison of the luminescence intensity at 463 nm of compound **1** in 10^{-3} M different cations.

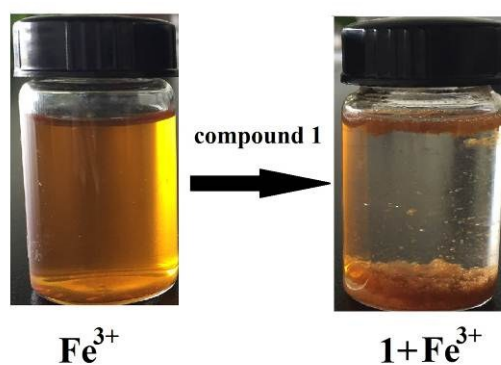


Fig. S14 Photographs showing the visual color change of the Fe^{3+} ions solution before (left) and after (right) add compound **1** about 12h.

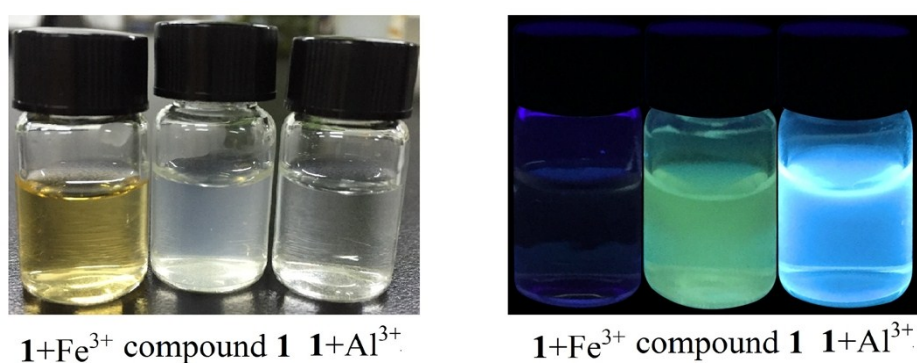


Fig. S15 The visual change on the addition of various $\text{M}(\text{NO}_3)_x$ under the fluorescent lamp (left), laboratory UV light (right, $\lambda_{\text{ex}} = 365$ nm).

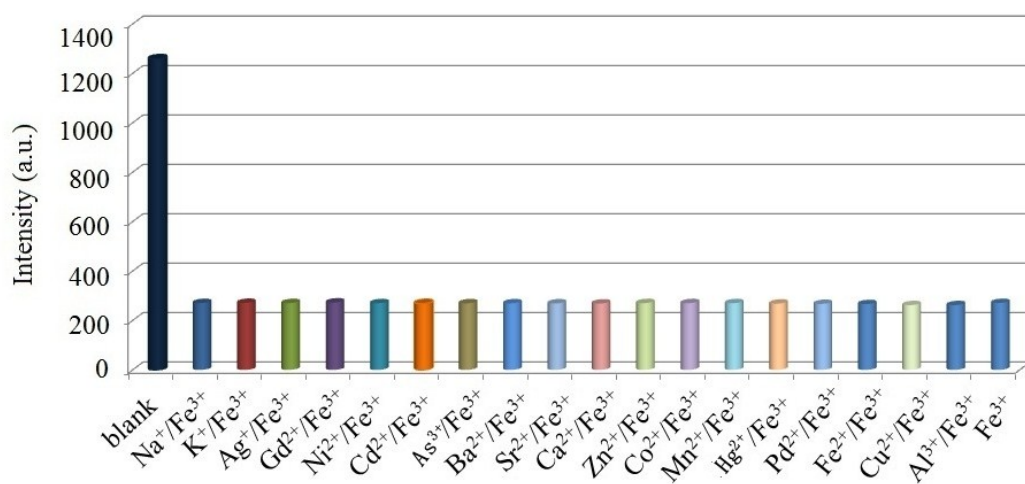


Fig. S16 Comparison of the luminescence intensity of 1+Fe³⁺ with different metal ions at 549 nm (10⁻⁴ M).

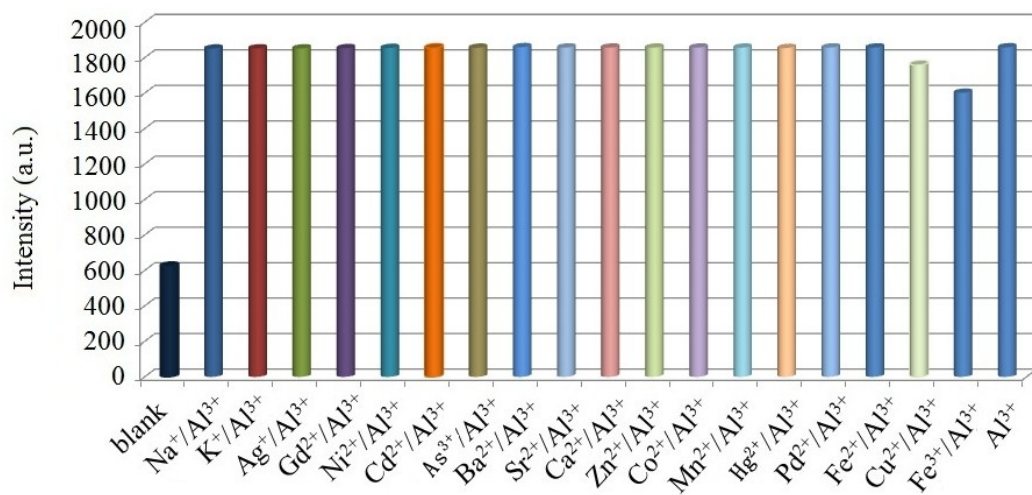


Fig. S17 Comparison of the luminescence intensity of 1+Al³⁺ with different metal ions at 463 nm (10⁻⁴ M).

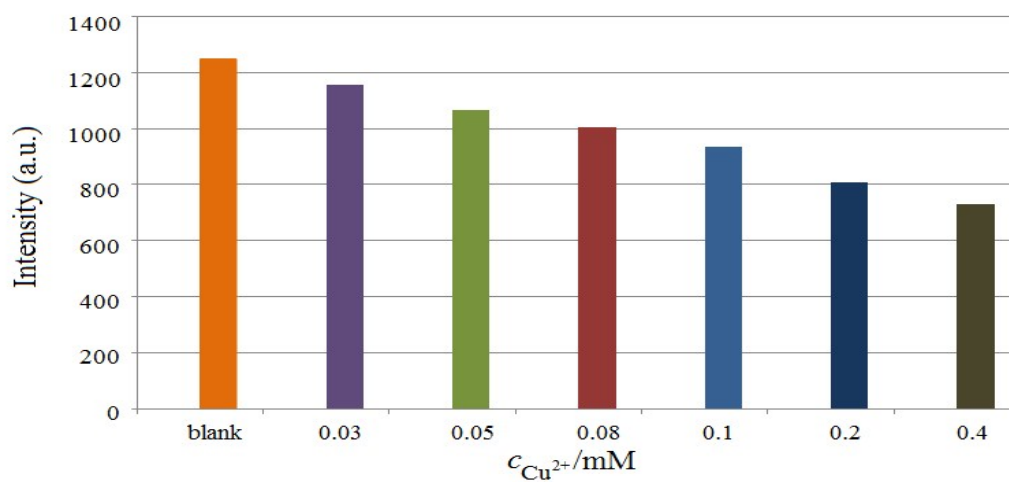


Fig. S18 Fluorescence responses of Tb-MOF in aqueous solutions in the presence of various concentrations of Cu²⁺.

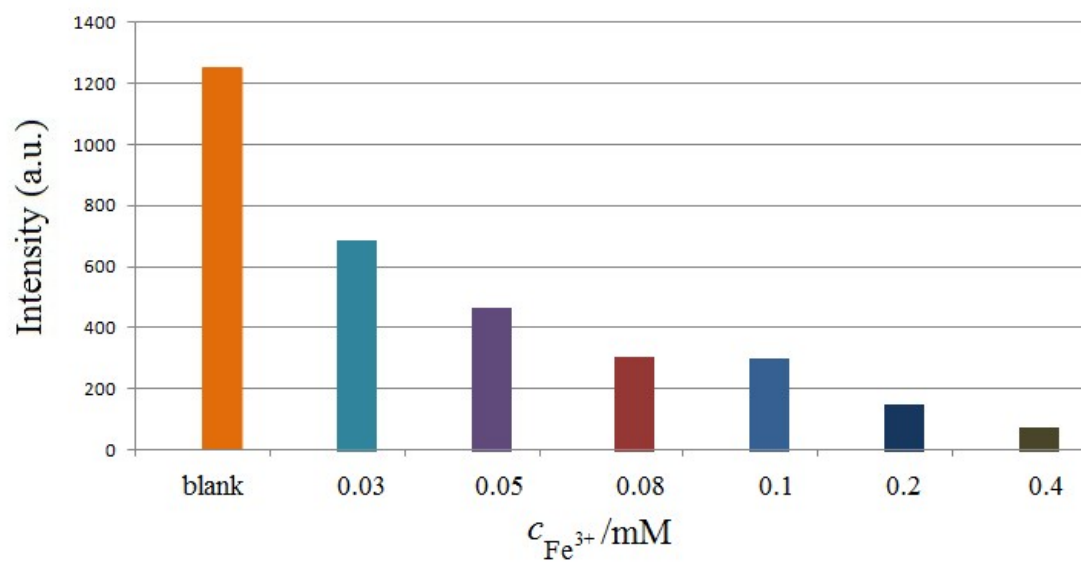


Fig. S19 Fluorescence responses of Tb-MOF in aqueous solutions in the presence of various concentrations of Fe^{3+} .

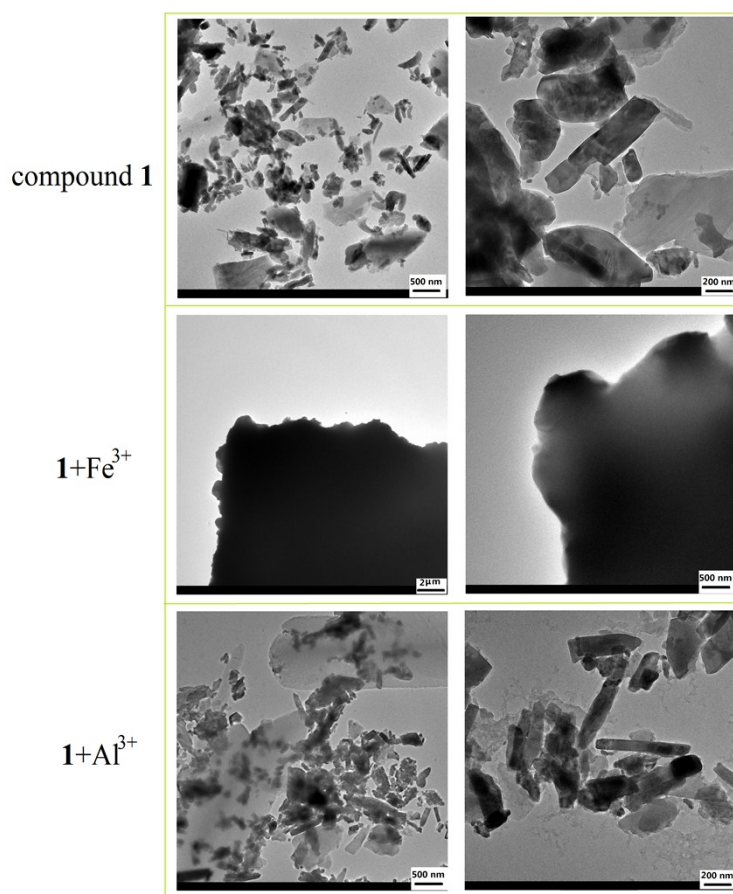


Fig. S20 Low- (right) and high- magnification (left) TEM images of the products.

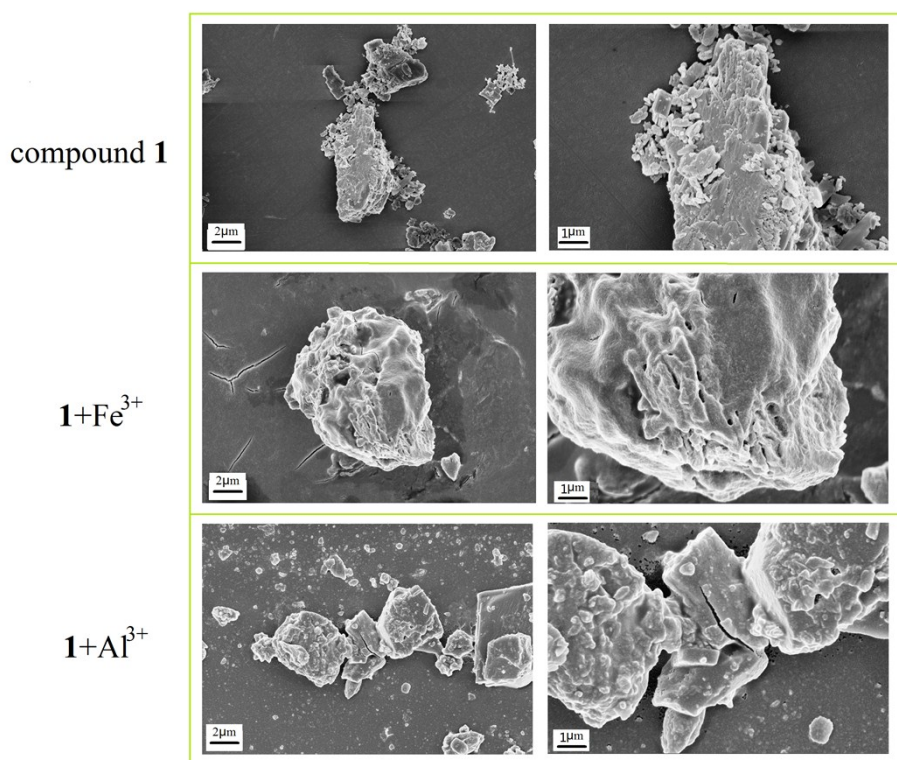


Fig. S21 Low- (right) and high- magnification (left) SEM images of the products.

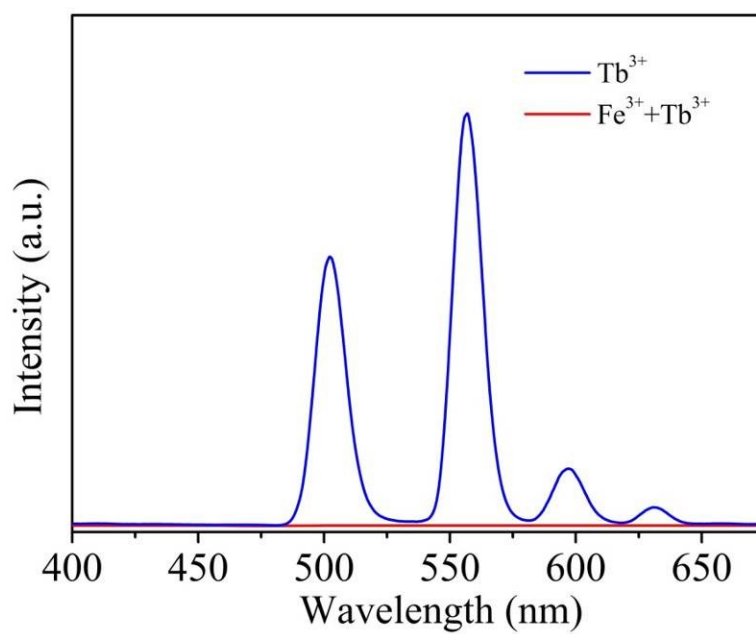


Fig. S22 Comparison of the luminescence intensity of Tb^{3+} under Fe^{3+} (10^{-3} M).

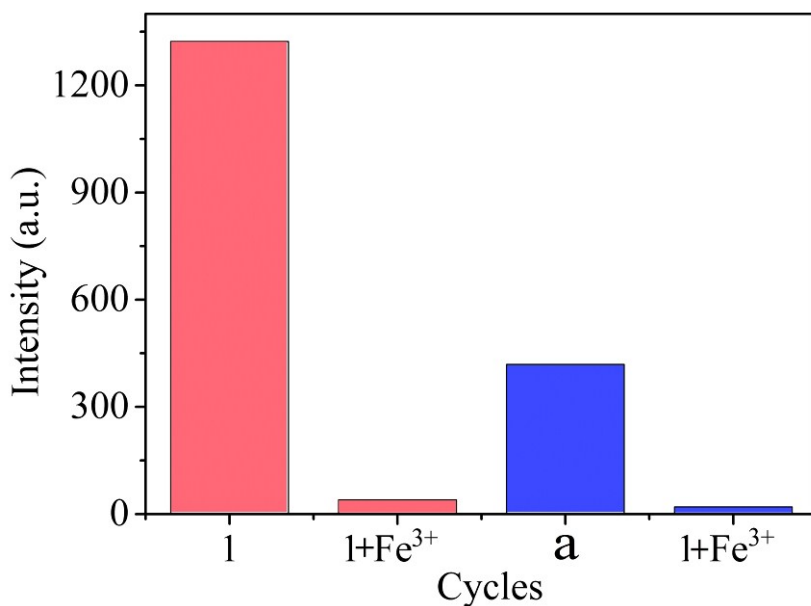


Fig. S23 The luminescence intensity (549 nm) of one recycles (a) after the first recycle.

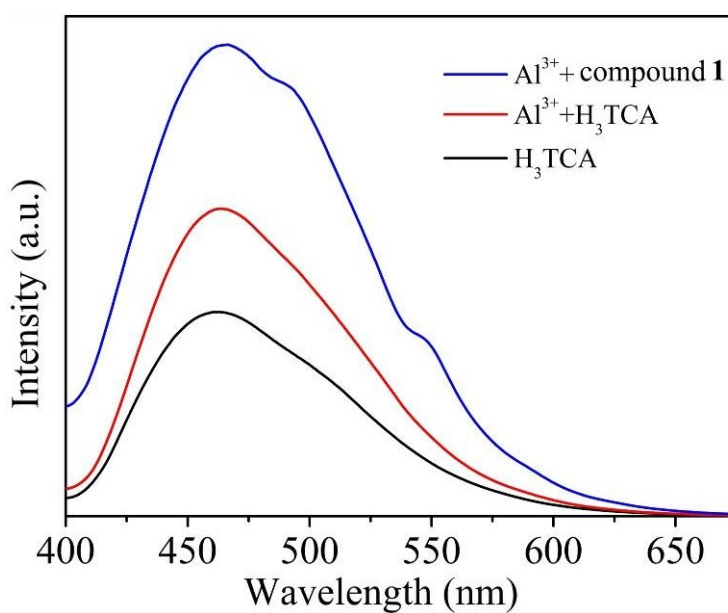


Fig. S24 Comparison of the luminescence intensity of H₃TCA and compound 1 under Al³⁺ (10⁻³ M).

Table S1. Crystal Data and Structure Refinement Summary for compound 1.

	[Tb ₃ (TCA) ₂ (DMA) _{0.5} (OH) ₃ (H ₂ O) _{0.5}]•3H ₂ O
Empirical formula	C ₄₄ H _{38.5} N _{2.5} O ₁₉ Tb ₃
Formula weight	1329.02
Crystal system	Monoclinic
space group	C2/c
<i>a</i> (Å)	29.155(3)
<i>b</i> (Å)	11.0593(13)
<i>c</i> (Å)	31.580(5)

α (deg)	90
β (deg)	115.607(2)
γ (deg)	90
V (Å ³)	9182(2)
Z	8
D_c (mg/m ³)	1.923
μ (mm ⁻¹)	4.643 mm ⁻¹
$F(000)$	5095
Reflections collected/unique	24948/9386
$R(\text{int})$	0.0592
Data / restraints / parameters	9386/42/623
Goodness-of-fit on F^2	1.01
$R1^a$ [$I > 2\sigma(I)$]	0.0422
$wR2^b$ (all data)	0.1097

$$^aR_1 = \Sigma(F_o - F_c)/\Sigma F_o, \quad ^b wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2a}$$

Table S2. Selected Bond Lengths (Å) and Bond Angles (o) for compound **1**.

Tb1-O1 ³	2.772(5)	O14 ² -Tb1-O5 ⁴	156.01(18)
Tb1-O2 ³	2.427(5)	O14 ² -Tb1-O6 ⁴	131.56(18)
Tb1-O3	2.512(5)	O14 ² -Tb1-O9 ¹	99.59(17)
Tb1-O4	2.331(6)	O15 ² -Tb1-O1 ³	131.27(16)
Tb1-O5 ⁴	2.443(6)	O15 ² -Tb1-O2 ³	128.6(2)
Tb1-O6 ⁴	2.427(6)	O15 ² -Tb1-O3	72.30(17)
Tb1-O9 ¹	2.404(5)	O15 ² -Tb1-O5 ⁴	127.27(18)
Tb1-O14 ²	2.390(5)	O15 ² -Tb1-O6 ⁴	138.94(19)
Tb1-O15 ²	2.349(5)	O15 ² -Tb1-O9 ¹	69.68(17)
Tb2-O3 ⁶	2.389(5)	O15 ² -Tb1-O14 ²	66.67(17)
Tb2-O5 ⁷	2.630(6)	O3 ⁵ -Tb2-O5 ⁷	62.15(18)
Tb2-O8	2.314(5)	O3 ⁵ -Tb2-O9 ⁸	81.14(18)
Tb2-O9	2.389(5)	O3 ⁵ -Tb2-O9	77.22(17)
Tb2-O9 ⁸	2.431(5)	O3 ⁵ -Tb2-O10	80.3(2)
Tb2-O10	2.459(6)	O3 ⁵ -Tb2-O13 ⁷	134.79(17)
Tb2-O13 ⁷	2.910(6)	O3 ⁵ -Tb2-O16 ⁷	92.67(19)
Tb2-O15 ⁷	2.349(5)	O8-Tb2-O3 ⁵	128.71(19)
Tb2-O16 ⁷	2.413(6)	O8-Tb2-O5 ⁷	66.60(18)
Tb3-O1 ⁷	2.387(5)	O8-Tb2-O9	83.7(2)
Tb3-O7 ⁷	2.304(5)	O8-Tb2-O9 ⁸	133.38(19)
Tb3-O11 ⁹	2.372(6)	O8-Tb2-O10	140.8(2)
Tb3-O1 ³	2.294(5)	O8-Tb2-O13 ⁷	70.75(19)
Tb3-O14 ¹⁰	2.389(5)	O8-Tb2-O15 ⁷	72.45(19)
Tb3-O14	2.357(5)	O8-Tb2-O16 ⁷	78.0(2)
Tb3-O15	2.325(5)	O9 ⁸ -Tb2-O5 ⁷	128.20(16)
O2 ³ -Tb1-O1 ³	49.70(17)	O9-Tb2-O5 ⁷	69.33(17)

O2 ³ -Tb1-O3	136.63(18)	O9-Tb2-O9 ⁸	67.7(2)
O2 ³ -Tb1-O5 ⁴	76.2(2)	O9 ⁸ -Tb2-O10	68.33(19)
O2 ³ -Tb1-O6 ⁴	92.4(2)	O9-Tb2-O10	133.0(2)
O3-Tb1-O1 ³	149.49(17)	O9 ⁸ -Tb2-O13 ⁷	116.28(16)
O4-Tb1-O1 ³	77.11(19)	O9-Tb2-O13 ⁷	147.36(16)
O4-Tb1-O2 ³	126.3(2)	O9-Tb2-O16 ⁷	146.43(19)
O4-Tb1-O3	92.21(19)	O10-Tb2-O5 ⁷	131.6(2)
O4-Tb1-O5 ⁴	127.82(19)	O10-Tb2-O13 ⁷	70.14(19)
O4-Tb1-O6 ⁴	76.6(2)	O15 ⁷ -Tb2-O3 ⁵	149.56(19)
O4-Tb1-O9 ¹	148.0(2)	O15 ⁷ -Tb2-O5 ⁷	133.30(17)
O4-Tb1-O14 ²	70.51(18)	O15 ⁷ -Tb2-O9 ⁸	69.21(17)
O4-Tb1-O15 ²	78.6(2)	O15 ⁷ -Tb2-O9	85.10(17)
O5 ⁴ -Tb1-O1 ³	100.86(18)	O15 ⁷ -Tb2-O10	94.5(2)
O5 ⁴ -Tb1-O3	63.24(18)	O15 ⁷ -Tb2-O13 ⁷	68.33(16)
O6 ⁴ -Tb1-O1 ³	73.23(18)	O16 ⁷ -Tb2-O5 ⁷	77.60(19)
O6 ⁴ -Tb1-O3	76.53(19)	O16 ⁷ -Tb2-O9 ⁸	143.01(18)
O6 ⁴ -Tb1-O5 ⁴	54.06(18)	O16 ⁷ -Tb2-O10	74.7(2)
O9 ¹ -Tb1-O1 ³	127.72(16)	O16 ⁷ -Tb2-O13 ⁷	47.47(18)
O9 ¹ -Tb1-O2 ³	74.64(16)	O1 ⁷ -Tb3-O14 ¹⁰	72.19(19)
O9 ¹ -Tb1-O3	79.17(18)	O7 ⁷ -Tb3-O17	80.47(19)
O9 ¹ -Tb1-O5 ⁴	72.37(18)	O7 ⁷ -Tb3-O1 ¹⁹	78.4(2)
O9 ¹ -Tb1-O6 ⁴	126.10(18)	O7 ⁷ -Tb3-O14	143.03(18)
O14 ² -Tb1-O1 ³	65.59(17)	O7 ⁷ -Tb3-O14 ¹⁰	136.15(18)
O14 ² -Tb1-O2 ³	80.1(2)	O7 ⁷ -Tb3-O15	76.57(19)
O14 ² -Tb1-O3	137.72(18)		
