

Supporting Information

A terbium (III)-based coordination polymer for selective and sensitive sensing of nitroaromatics and ferric ion: synthesis, crystal structure and photoluminescence properties

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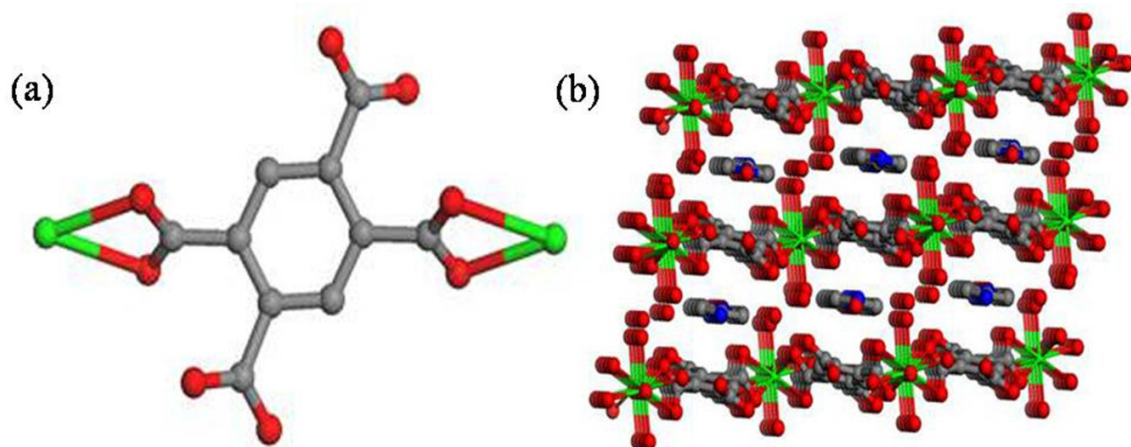


Fig. S1 View of coordination mode of BTEC (a), and interlayer channel (b) in **1**.

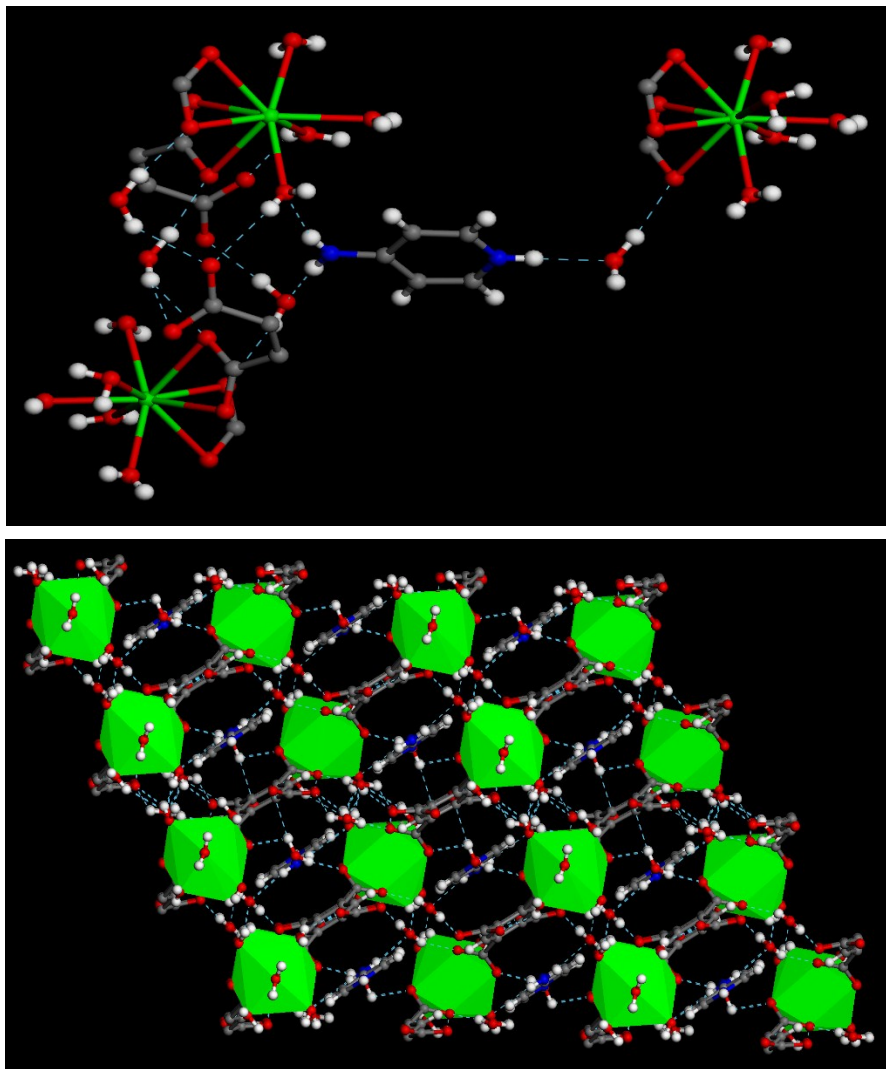


Fig. S2 Hydrogen bonds in **1**.

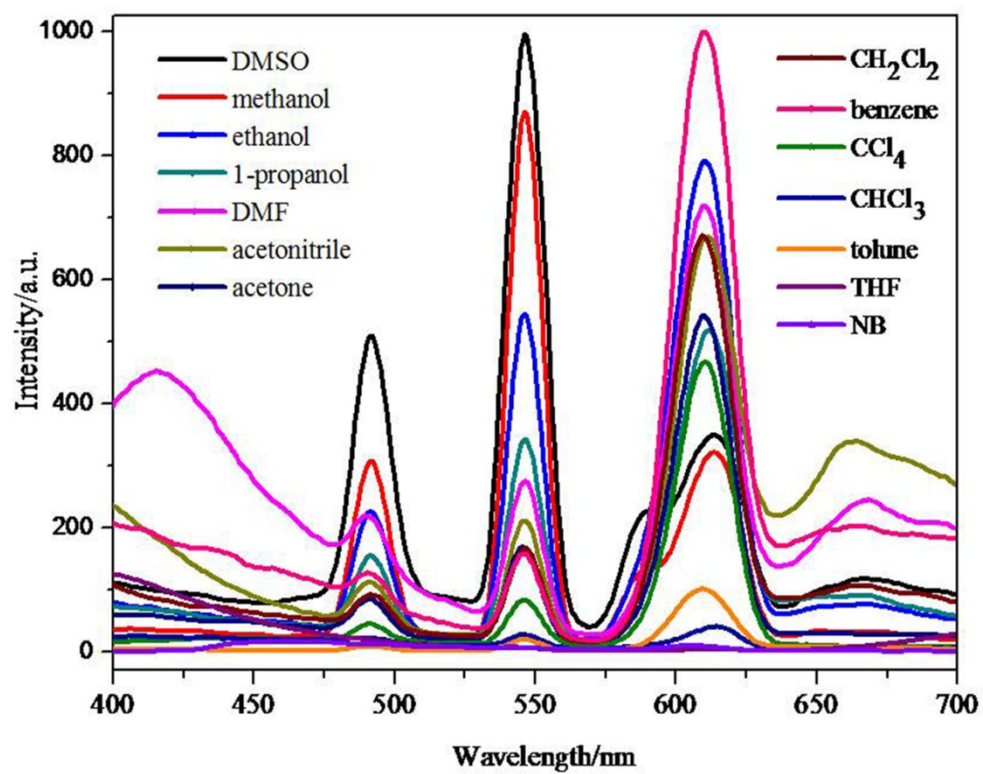


Fig. S3 Luminescence spectra of **1** excited at 290 nm in different organic solvents.

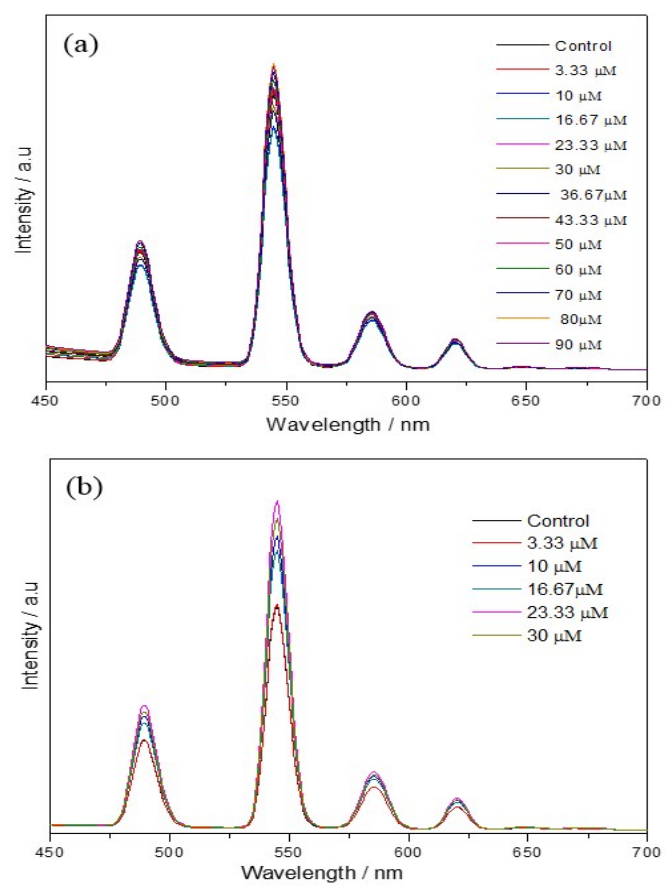


Fig. S4 Photoluminescence spectra of **1** interacting with 2-NP (a) and 3-NP (b).

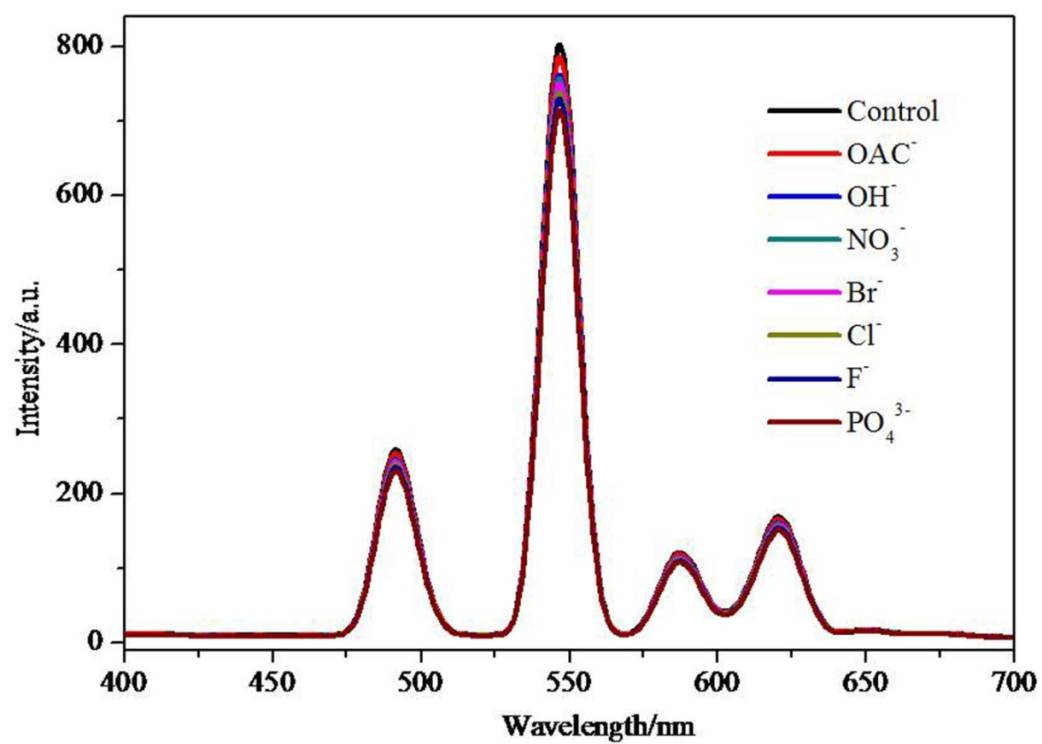


Fig. S5 Luminescence spectra of **1** interacting with different anions under the same conditions.

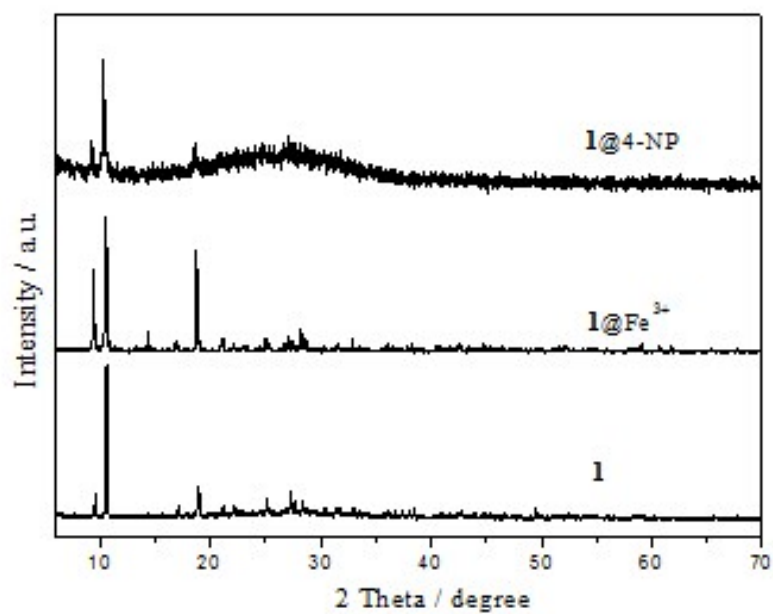


Fig. S6 XRD patterns of **1** before and after treated with 4-NP and Fe³⁺ aqueous solution

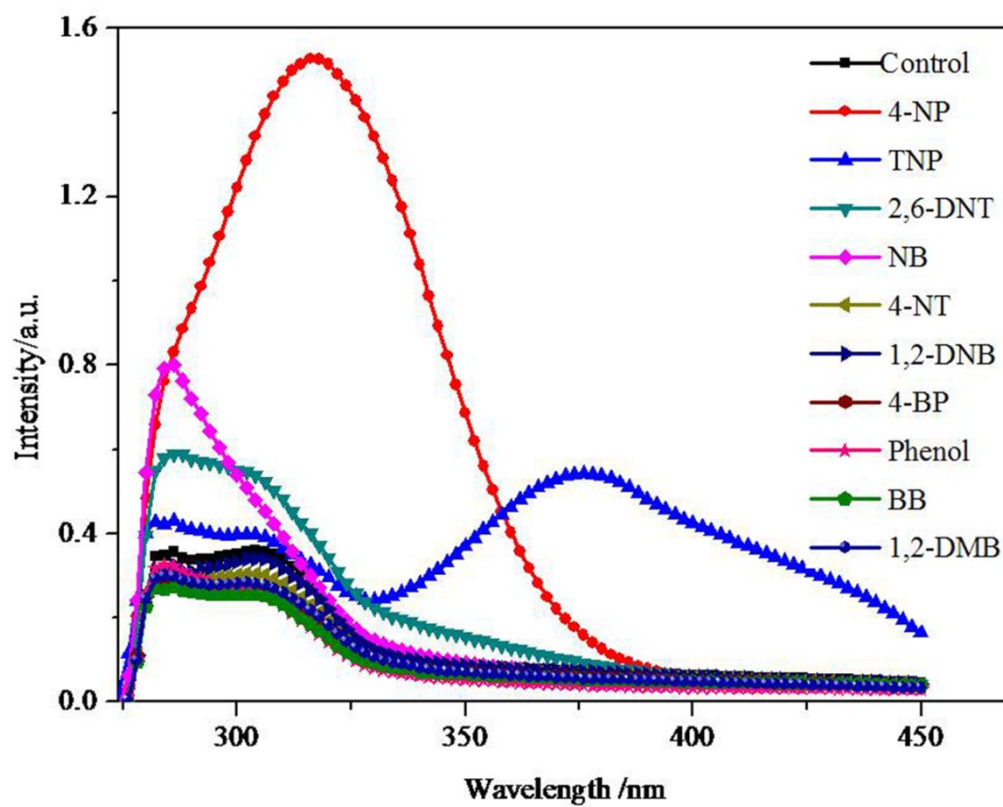


Fig. S7 UV-Vis absorption spectra of **1** after treated with the same volumes (240 μ L) of different compounds (1 mM).

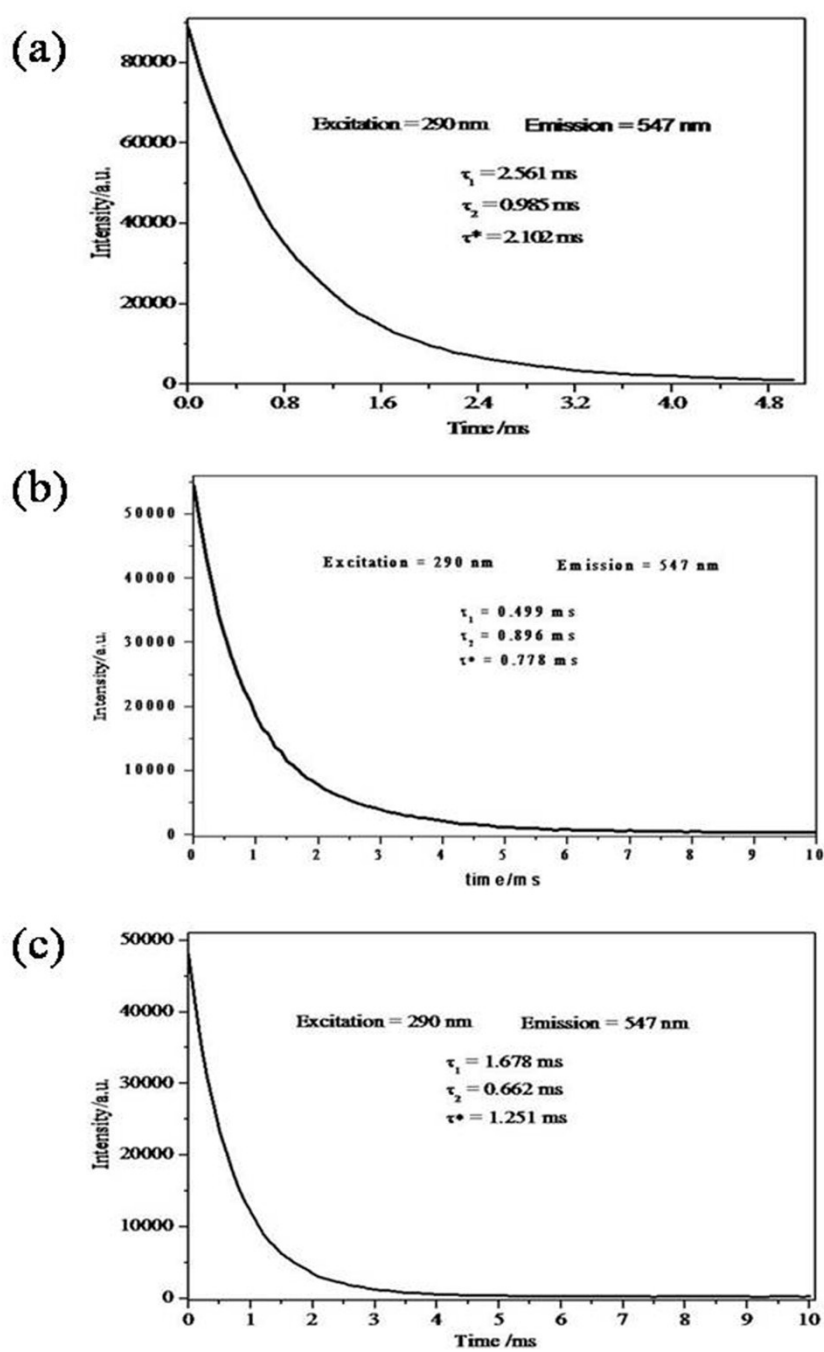


Fig. S8 Fluorescence lifetime curves of **1** dispersed in DMSO (a), after treated with 4-NP (b) and Fe^{3+} aqueous solution (c).

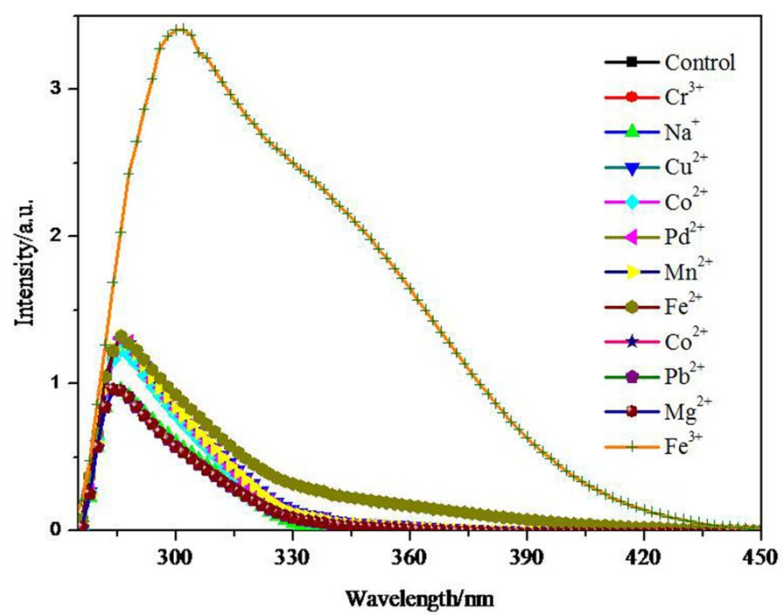


Fig. S9 UV-Vis absorption spectra of **1** after treated with the same volumes (185 μ L) of different metal ions (1 mM).

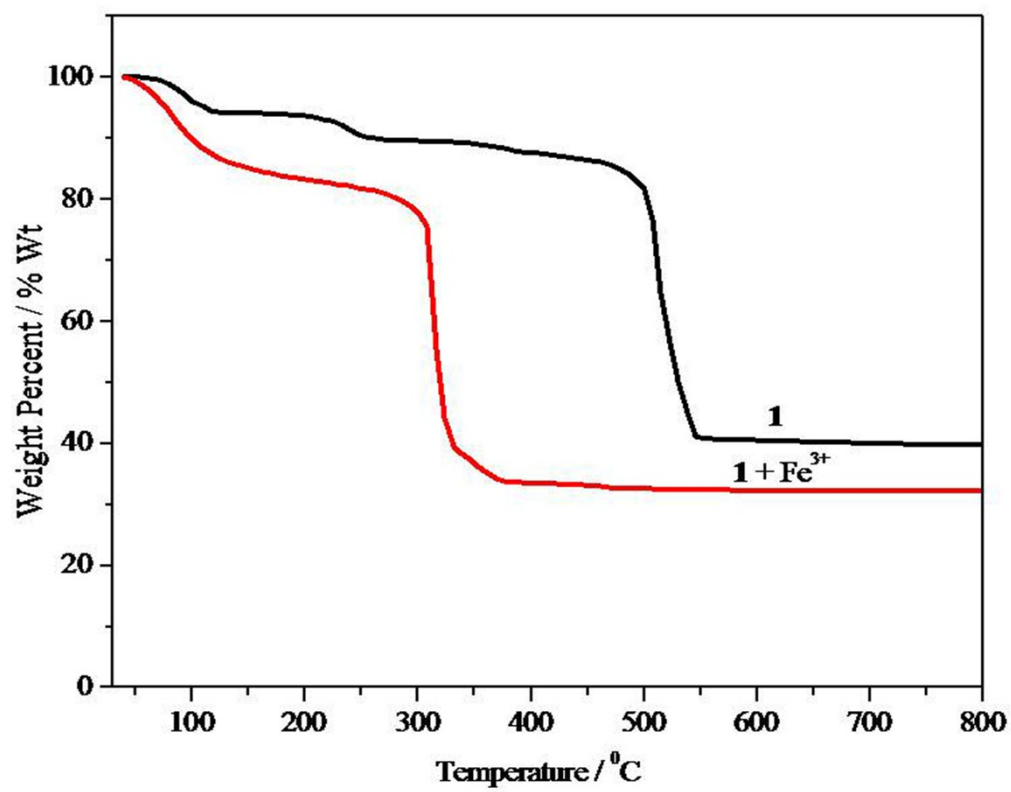


Fig. S10 TGA analysis of **1** before and after immersed in Fe^{3+} aqueous solution.

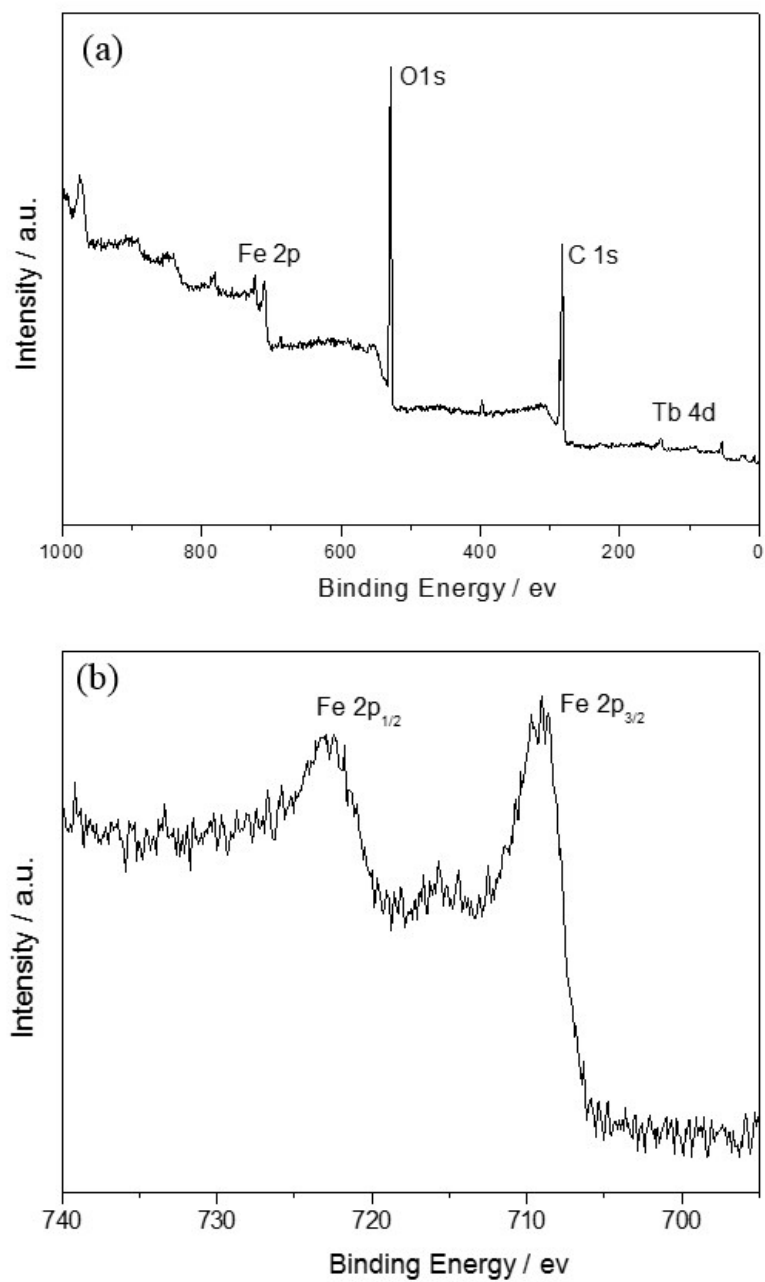


Fig. S11 XPS spectra of compound **1** after immersed in Fe^{3+} aqueous solution.

Table S1 Crystal data and structure refinement for **1**.

Empirical formula	C ₁₅ H ₂₅ N ₂ O ₁₆ Tb
Formula weight	648.30
Crystal system	Monoclinic, <i>P</i> 2(1)/c
<i>a</i> (Å)	13.0587(7)
<i>b</i> (Å)	11.2253(6)
<i>c</i> (Å)	17.2297(8)
<i>α</i> (°)	90
<i>β</i> (°)	120.987
<i>γ</i> (°)	90
Volume (Å ³)	2165.21(19)
<i>Z</i>	4
<i>D</i> _{Calc} (mg/m ³)	1.989
<i>μ</i> (mm ⁻¹)	3.353
<i>F</i> ₍₀₀₀₎	1288
<i>R</i> _{int}	0.0234
GOF on <i>F</i> ²	1.039
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]*	0.0255
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]*	0.0631
<i>R</i> ₁ (all data) *	0.0336
<i>wR</i> ₂ (all data)*	0.0690

* $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; $wR_2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)]^2\}^{1/2}$

Table S2 Selected bond lengths [Å] and angles [°] for **1**.

Tb(1)–O(10)	2.366(2)	O(9)–Tb(1)–O(6)	121.22(7)
Tb(1)–O(13)	2.391(2)	O(1)–Tb(1)–O(6)	77.61(8)
Tb(1)–O(11)	2.390(2)	O(10)–Tb(1)–O(12)	68.98(7)
Tb(1)–O(9)	2.397(2)	O(13)–Tb(1)–O(12)	68.21(7)
Tb(1)–O(1)	2.4332(19)	O(11)–Tb(1)–O(12)	78.55(7)
Tb(1)–O(6)	2.4343(19)	O(9)–Tb(1)–O(12)	79.61(8)
Tb(1)–O(12)	2.470(2)	O(1)–Tb(1)–O(12)	142.46(7)
Tb(1)–O(5)	2.5317(19)	O(6)–Tb(1)–O(12)	139.92(7)
Tb(1)–O(2)	2.5532(19)	O(10)–Tb(1)–O(5)	139.32(7)
O(10)–Tb(1)–O(13)	137.12(8)	O(13)–Tb(1)–O(5)	69.19(7)
O(10)–Tb(1)–O(11)	93.48(8)	O(11)–Tb(1)–O(5)	125.23(7)
O(13)–Tb(1)–O(11)	80.59(8)	O(9)–Tb(1)–O(5)	69.72(7)
O(10)–Tb(1)–O(9)	77.67(8)	O(1)–Tb(1)–O(5)	73.15(7)
O(13)–Tb(1)–O(9)	92.26(8)	O(6)–Tb(1)–O(5)	52.19(6)
O(11)–Tb(1)–O(9)	158.13(9)	O(12)–Tb(1)–O(5)	125.48(6)
O(10)–Tb(1)–O(1)	76.96(7)	O(10)–Tb(1)–O(2)	69.90(7)
O(13)–Tb(1)–O(1)	142.14(7)	O(13)–Tb(1)–O(2)	141.21(7)
O(11)–Tb(1)–O(1)	119.76(7)	O(11)–Tb(1)–O(2)	68.65(6)
O(9)–Tb(1)–O(1)	78.12(7)	O(9)–Tb(1)–O(2)	124.71(7)
O(10)–Tb(1)–O(6)	143.81(7)	O(1)–Tb(1)–O(2)	52.04(6)
O(13)–Tb(1)–O(6)	76.55(7)	O(6)–Tb(1)–O(2)	74.21(6)
O(11)–Tb(1)–O(6)	77.42(7)	O(12)–Tb(1)–O(2)	124.62(6)
O(5)–Tb(1)–O(2)	109.89(7)		