

Supplementary Information for

A Water-stable Terbium–MOF Sensor for Selective, Sensitive, and Recyclable Detection of Al³⁺ and CO₃²⁻ Ions

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Table S1. The selected bond lengths [Å] and angles [°] for **1**.

Compound 1			
Tb(1)-O(1)	2.378(5)	Tb(1)-O(2)#2	2.437(5)
Tb(1)-O(9)	2.383(6)	Tb(1)-O(4)#3	2.453(5)
Tb(1)-O(8)	2.383(5)	Tb(1)-O(3)#3	2.453(5)
Tb(1)-O(7)#1	2.422(5)	Tb(1)-O(1)#2	2.613(5)
Tb(1)-O(6)	2.423(5)		
O(1)-Tb(1)-O(9)	85.2(2)	O(7)#1-Tb(1)-O(4)#3	123.32(19)
O(1)-Tb(1)-O(8)	74.50(18)	O(6)-Tb(1)-O(4)#3	72.5(2)
O(9)-Tb(1)-O(8)	77.8(2)	O(2)#2-Tb(1)-O(4)#3	131.38(19)
O(1)-Tb(1)-O(7)#1	140.64(18)	O(1)-Tb(1)-O(3)#3	80.17(18)
O(9)-Tb(1)-O(7)#1	74.5(2)	O(9)-Tb(1)-O(3)#3	126.13(18)
O(8)-Tb(1)-O(7)#1	68.52(18)	O(8)-Tb(1)-O(3)#3	143.42(18)
O(1)-Tb(1)-O(6)	150.78(18)	O(7)#1-Tb(1)-O(3)#3	138.86(18)
O(9)-Tb(1)-O(6)	96.8(2)	O(6)-Tb(1)-O(3)#3	75.16(17)
O(8)-Tb(1)-O(6)	134.52(18)	O(2)#2-Tb(1)-O(3)#3	82.73(17)
O(7)#1-Tb(1)-O(6)	66.58(17)	O(4)#3-Tb(1)-O(3)#3	53.35(17)
O(1)-Tb(1)-O(2)#2	115.07(17)	O(1)-Tb(1)-O(1)#2	64.4(2)
O(9)-Tb(1)-O(2)#2	148.54(19)	O(9)-Tb(1)-O(1)#2	140.8(2)
O(8)-Tb(1)-O(2)#2	84.6(2)	O(8)-Tb(1)-O(1)#2	70.85(18)
O(7)#1-Tb(1)-O(2)#2	74.84(19)	O(7)#1-Tb(1)-O(1)#2	113.37(17)
O(6)-Tb(1)-O(2)#2	77.27(19)	O(6)-Tb(1)-O(1)#2	121.95(19)
O(1)-Tb(1)-O(4)#3	80.28(19)	O(2)#2-Tb(1)-O(1)#2	50.71(17)
O(9)-Tb(1)-O(4)#3	73.21(19)	O(4)#3-Tb(1)-O(1)#2	121.20(17)
O(8)-Tb(1)-O(4)#3	142.8(2)	O(3)#3-Tb(1)-O(1)#2	74.57(16)
Symmetry transformations used to generate equivalent atoms: #1 -x+3,-y+1,-z #2 -x+2,-y,-z #3 x+1,y,z			

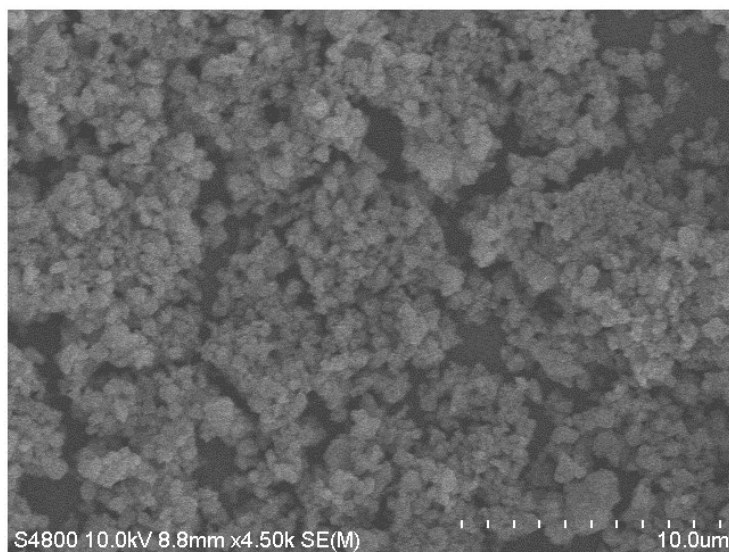


Fig. S1 The SEM image of **1** after grinding.

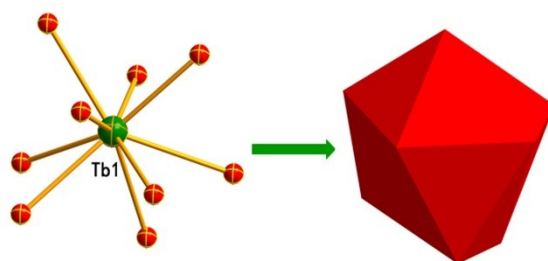


Fig. S2 The monocapped square antiprism coordination geometry of Tb³⁺ ion.

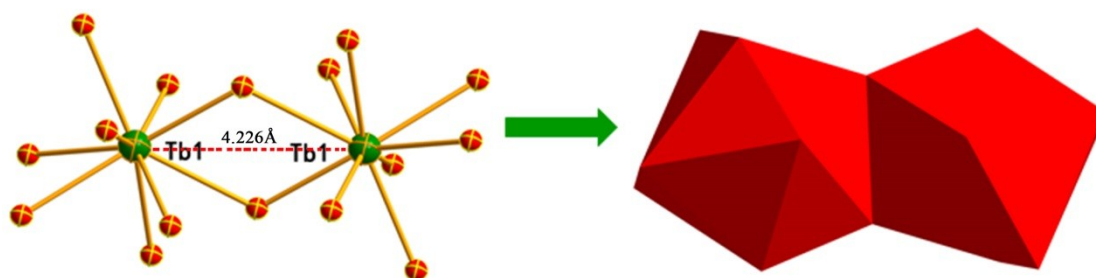


Fig. S3 The binuclear constituted by Tb³⁺ ions.

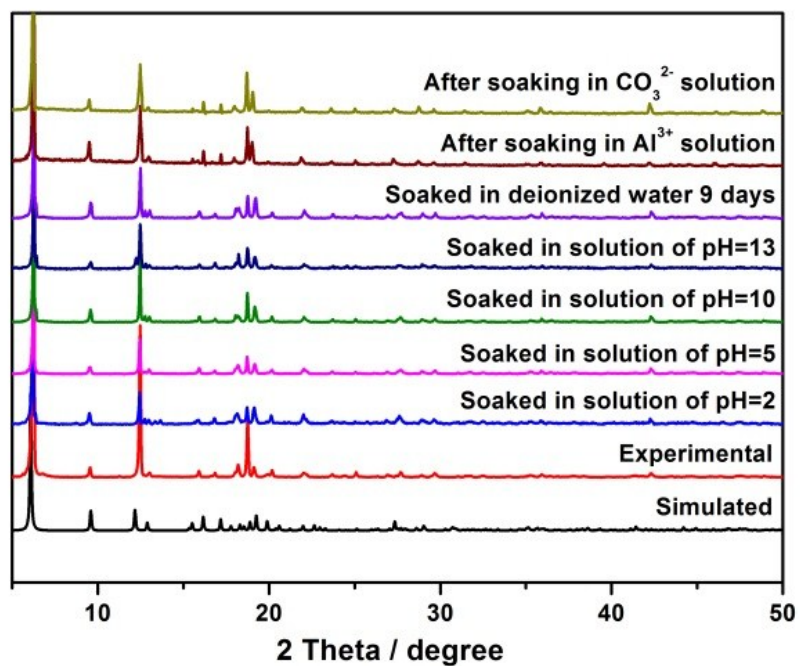


Fig. S4 PXR D patterns of compound **1** simulated from the X-ray single-crystal structure, as-synthesized samples of compound **1**, compound **1** soaked in various solutions, and power X-ray diffraction patterns of **1** after five recyclable experiments.

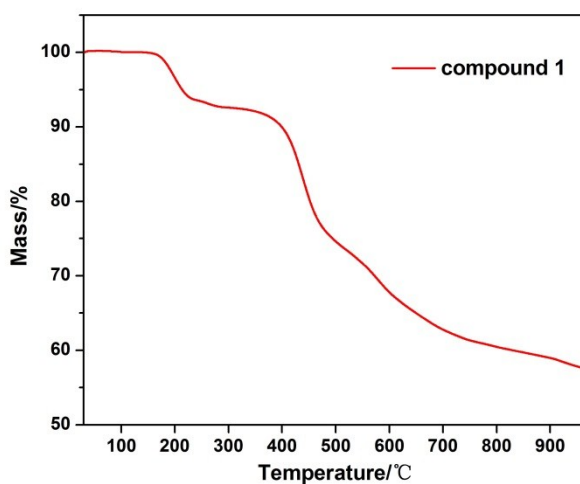


Fig. S5 View of the TG analysis profile of compound **1**.

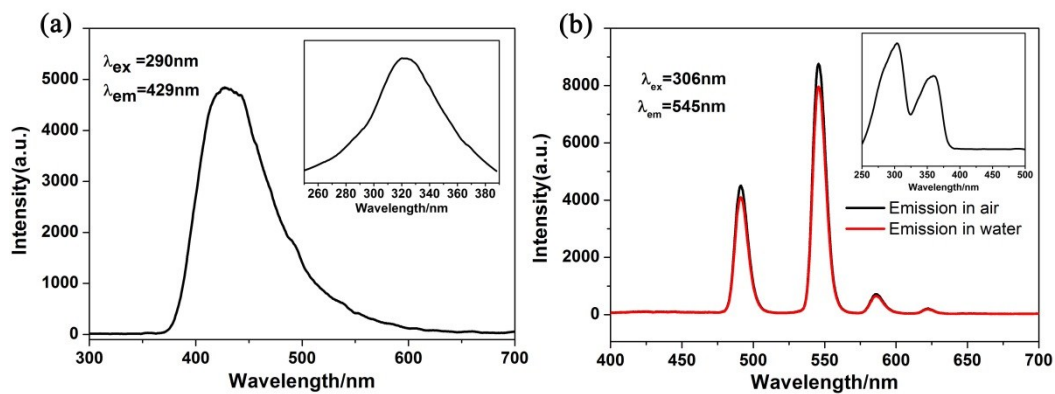


Fig. S6 (a) The emission spectrum of H₂ppda ligand. Insets: The excitation spectrum of H₂ppda ligand; (b) The emission spectra of compound **1** in the solid-state and aqueous suspension, respectively. Insets: The excitation spectrum of compound **1**.

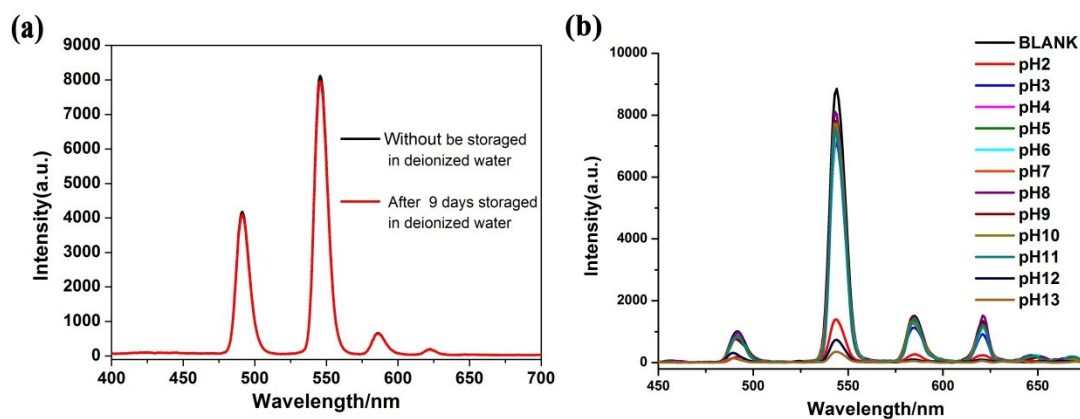


Fig.S7 (a)The emission spectra of **1** without and after 9 days' storage in deionized water; (b)The emission spectra of **1** immersed in acid/base solutions with pH values varied from 2 to 13.

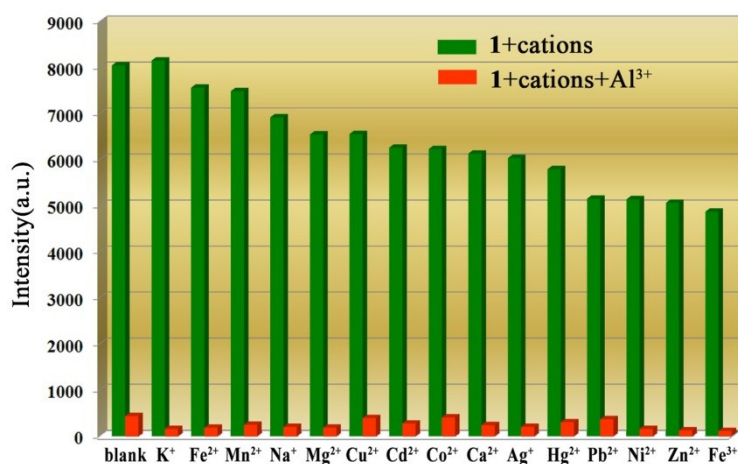


Fig. S8 The fluorescence intensity for **1** exposed to single cation and mixed cations in aqueous solutions.

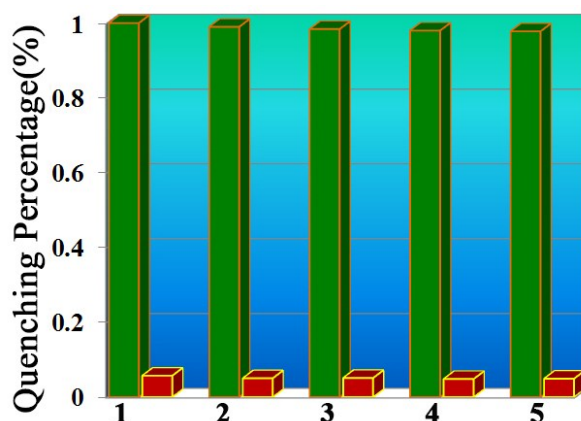


Fig. S9 Quenching and recovery test of **1** in aqueous solution. The green columns represent the initial relative luminescent intensity and the red columns represent the relative intensity on addition of Al^{3+} .

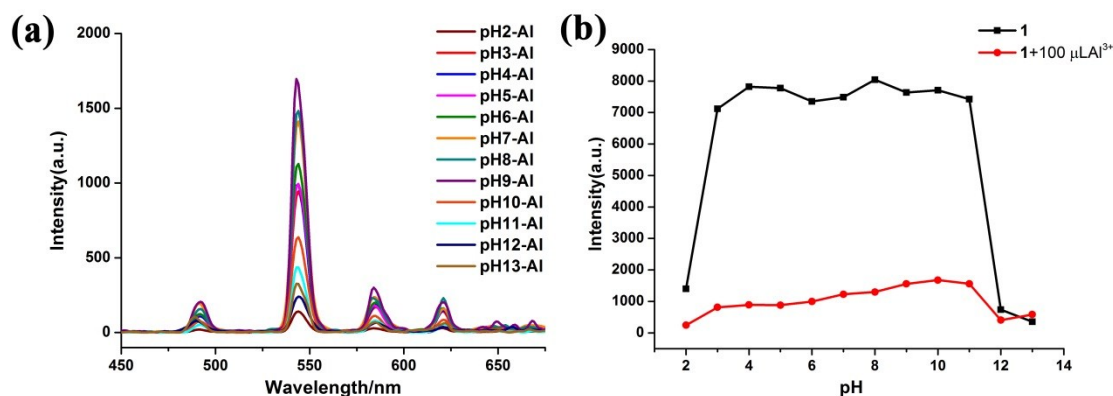


Fig. S10 (a) PL spectra of **1** dispersed in various aqueous solutions (pH 2-13) in presence of $100\mu\text{L Al}^{3+}$ ion; (b) Comparison of fluorescence intensity for **1** dispersed in aqueous solutions of pH 2-13 (black line) and in presence of $100\mu\text{L Al}^{3+}$ ion (red line).

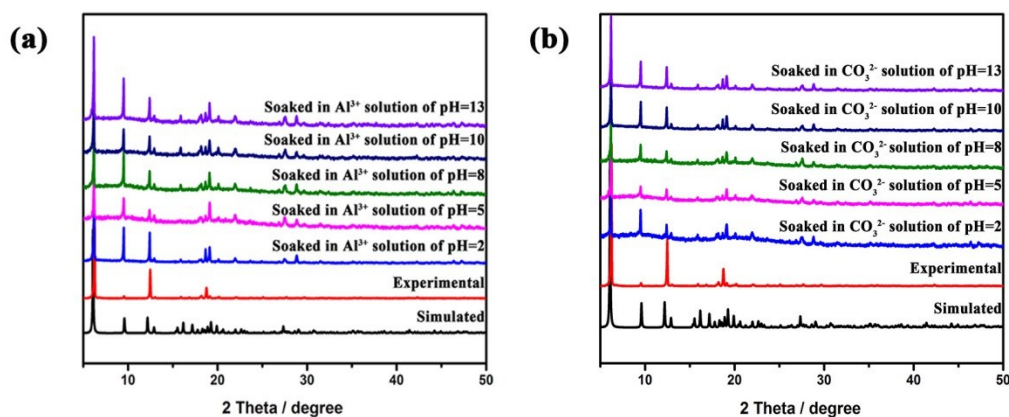


Fig. S11 PXRD patterns of compound **1** simulated from the X-ray single-crystal structure, as-synthesized samples of compound **1**, compound **1** soaked in Al^{3+} (a) and CO_3^{2-} (b) solutions of different pH.

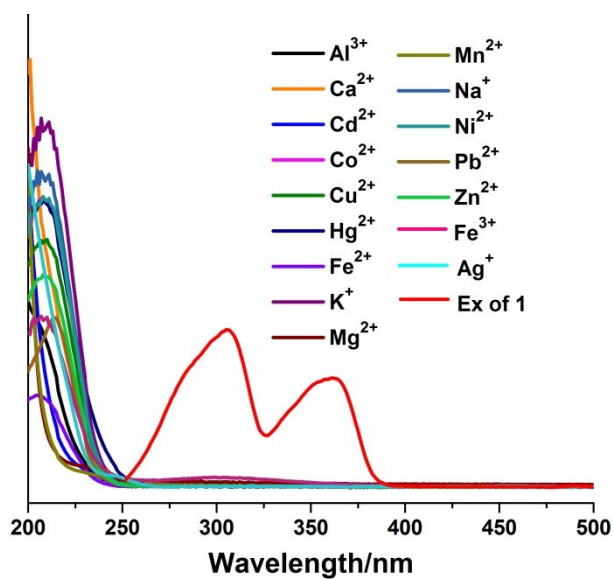


Fig. S12 The UV-Vis adsorption spectra of $M(\text{NO}_3)_X$ aqueous solutions and the excitation spectrum of **1**.

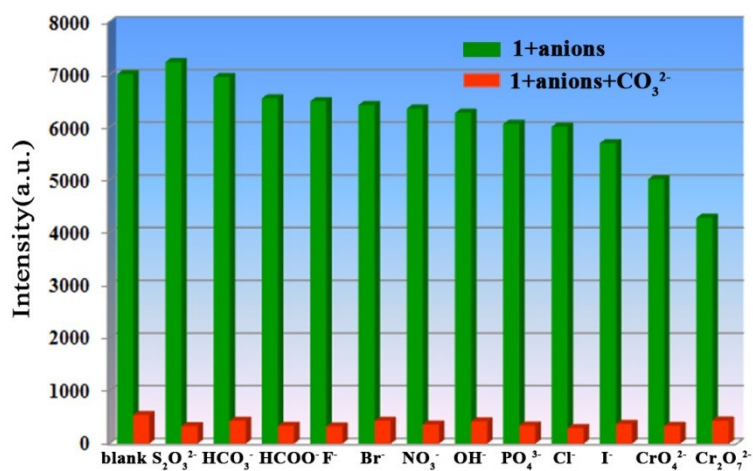


Fig. S13 The fluorescence intensities for **1** exposed to single anion and mixed anions in aqueous solutions.

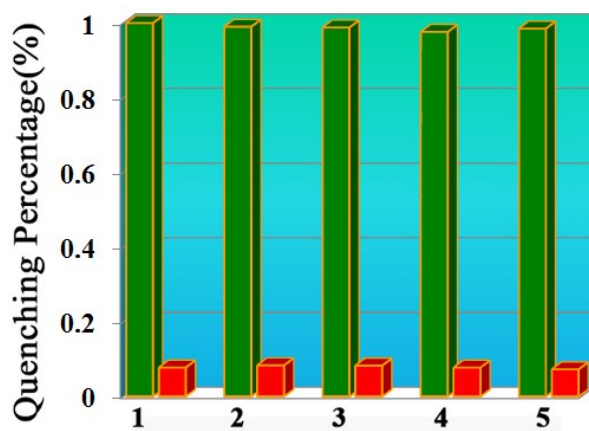


Fig. S14 Quenching and recovery test of **1** in aqueous solution. The green columns represent the initial relative luminescent intensity and the red columns represent the relative intensity on addition of CO₃²⁻.

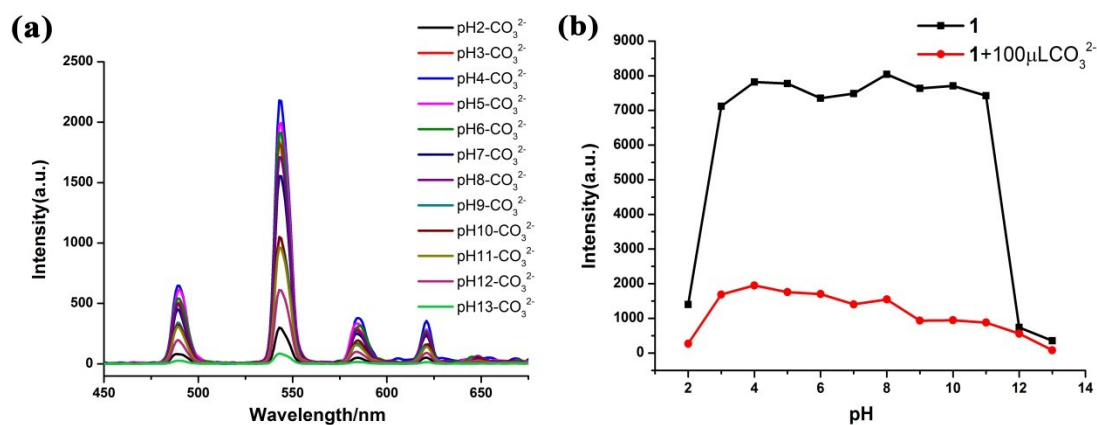


Fig. S15 (a) PL spectra of **1** dispersed in various aqueous solutions of pH = 2-13 in presence of 100 μL CO₃²⁻ ion; (b) Comparison of fluorescence intensity for **1** dispersed in aqueous solutions of pH = 2-13 (black line) and in presence of 100 μL CO₃²⁻ ion (red line).

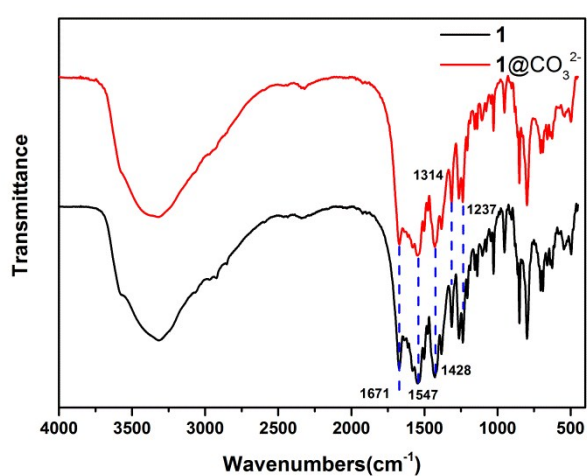


Fig. S16 FT-IR spectra of **1** after immersed in K₂CO₃ aqueous solution and the untreated powder.

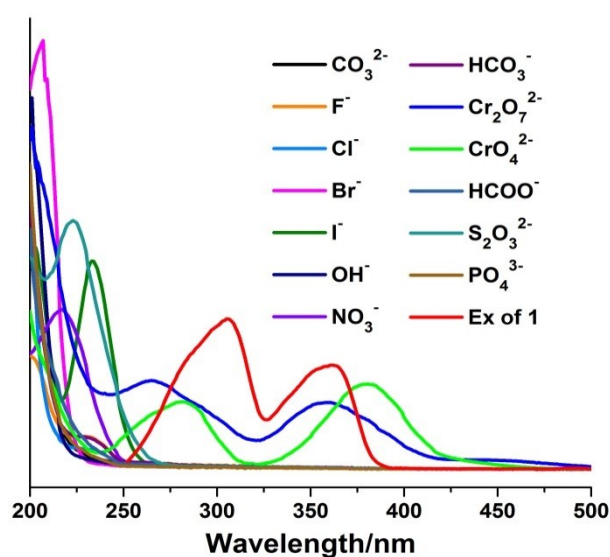


Fig. S17 The UV-Vis adsorption spectra of K(anion)_x aqueous solutions and the excitation spectrum of **1**.

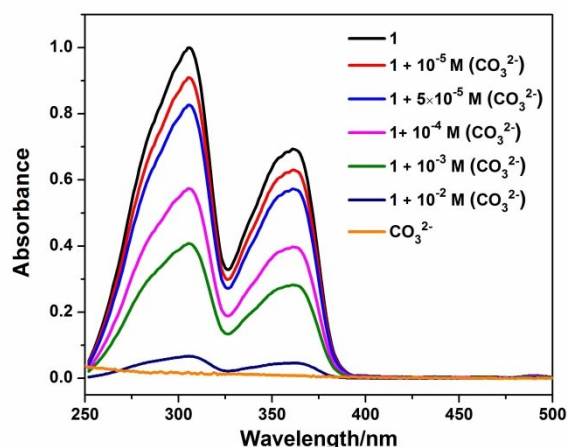


Fig. S18 The UV-Vis adsorption spectra of **1** after adding various concentrations of K_2CO_3 aqueous solutions.

Table S2 Comparison of literature reports for MOFs as sensors of Al^{3+}

MOF	K_{SV} (M^{-1})	Detection Limit	Medium	Ref.
$[Tb(ppda)(ox)_{0.5}(H_2O)_2]_n$ (1)	5.26×10^3	5.66×10^{-6} M (152 ppb)	H_2O	This work
$[\{ Cd_2(syn-dftpmcp)(1,3-BDC)_2 \} \cdot 0.5DMF \cdot H_2O]_n$	/	183 ppb	CH_3CN	1
UiO-66-NH ₂ -SA	/	6.98 μ M	H_2O	2
MOF-LIC-1 (Eu-MOF)	3.79×10^4	/	DMF	3
$[Cd(PAM)(4-bpdb)_{1.5}] \cdot DMF$ (Cd-MOF)	2.3×10^4	5.6×10^{-7} M	H_2O	4
$\{ (Me_2NH_2)[Tb(OBA)_2] \cdot (Hatz) \cdot (H_2O)_{1.5} \}_n$ (1)	3.4×10^4	/	H_2O	5
$[Zn_2(HL)_3]^+ @ MOF-5$	7.478×10^4	/	DMF	6

Table S3 Comparison of literature reports for MOFs as sensors of CO_3^{2-}

MOF	K_{SV} (M^{-1})	Detection Limit	Medium	Ref.
$[Tb(ppda)(ox)_{0.5}(H_2O)_2]_n$ (1)	1.78×10^3	3.76×10^{-7} M (0.38 μ M)	H_2O	This work
$[Eu](Hhpi)_2(OAc)_6$	9.142×10^3	7.8 μ M	DMSO	7
$\{ [Eu(HL)(H_2O)_3] \cdot H_2O \}_n$ (1)	3.78×10^3	10^{-6} M	H_2O	8
$[\{ [Eu(HBPTC)(H_2O)_2] \cdot 2DMF \}_n]$ film	/	10^{-6} M	H_2O	9
(E)-3-(4-methoxyphenyl)-4-[(4-nitrobenzylidene)-amino]-1H-1,2,4-triazole-5(4H)-thione (6)	/	1.91 μ M	EtOH/water (3:7, v/v)	10
$\{ [Zn_2(\mu_3-OH)(cpta)(4,4'-bipy)] \cdot H_2O \}_n$ (1)	9.47×10^3	5.55×10^{-6} M (5.55 μ M)	H_2O	11

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