Supporting Information

Four super water-stable lanthanide-organic frameworks with active uncoordinated carboxylic and pyridyl groups for selective luminescence sensing of Fe³⁺

Yu-Tong Liang^a, Guo-Ping Yang^a, Bo Liu^a, Yang-Tian Yan^a, Zheng-Ping Xi^a and Yao-Yu Wang^{a*}



Fig. S1 Coordination arrangement of Eu centers could be described as a distorted enneahedron.



Fig. S2 PXRD patterns of 1-Eu simulated from the X-ray single-crystal structure and assynthesized samples of 1-Eu, 1-Tb, 1-Nd and 1-Sm. The similar patterns further confirmed the isostructural frameworks of four compounds.



Fig. S3 The TGA curves of four compounds under N_2 environment. For **1-Tb**, the first major weight loss of 9.81% from 30 to 139.00 °C, corresponding to two coordinated water and two guest H_2O molecules per formula unit (calc. 11.33%), the main framework keeps stable to 310.21 °C; For **1-Sm**, the first major weight loss of 9.68% from 30 to 132.27 °C, ascribed to the release of two coordinated water and two guest H_2O molecules per formula unit (calc. 11.26%), the main framework keep stable to 305.12 °C; For **1-Nd**, the first weight loss of 10.05% from 30 to 110.32 °C, corresponding to the loss of two coordinated water and two guest H_2O molecules per unit (calc. 11.60%), the main frameworks keep stable up to 311.14 °C.



Fig. S4 The snapshots of 1-Eu under UV light (365 nm).



Fig. S5 The emission spectra of H_4L (left) and 1-Eu (right) in solid state.



Fig. S6 Luminescence decay curves for 1-Eu (a) and Fe³⁺@1-Eu (b).



Fig. S7 The luminescence spectra of 1-Eu in water.



Fig. S8 The emission spectra of 1-Eu cleaned by water after immersed in Fe³⁺ solution.



Fig. S9 The PXRD patterns of **1-Eu** treated by different $M(NO_3)_x$ ($M = Na^+$, K^+ , Mg^{2+} , Ca^{2+} , Mn^{2+} , Cd^{2+} , Zn^{2+} , Co^{2+} , Cu^{2+} , Al^{3+} , Li^+ , Ni^{2+} , Ba^{2+} , Fe^{3+} and Pb^{2+}) aqueous solutions.



Fig. S10 UV-Vis adsorption spectrum of $M(NO_3)_X$ aqueous solution and the excitation spectrum of 1-Eu.



Fig. S11 X-ray photo-electron spectrum of Fe³⁺@1-Eu.

D-HA	d(D-H) (Å)	d(HA) (Å)	d(DA) (Å)	<(DHA) (°)
O(3)-H(3A)N(1)#4	0.82	1.79	2.574(8)	158.7
O(10)-H(10A)O(11)	0.96	1.80	2.676(10)	149.8
O(10)-H(10B)O(6)#1	0.96	1.81	2.772(6)	175.3
O(9)-H(9B)O(1)#5	0.96	2.07	2.715(6)	123.5
O(9)-H(9A)O(12)#6	0.96	1.84	2.740(12)	154.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+1; #2 x,y+5/2,z+1/2; # 3 x,-y+5/2,z-1/2; #4 x+1,-y+3/2,z+1/2; # 5 -x+2,-y+2,-z+1; #6 x+1,y+1,z

Table. S1 Hydrogen bonds for 1-Eu.

Elem	Line	Units	Avg
Eu	n/a	Ppm	0.0221
Fe	n/a	ppm	0.3790

 Table. S2
 The ICP result of filtrate.