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Supporting Information

A robust 3D In-MOF with imidazole acid ligand as fluorescent sensor for sensitive and selective detection of Fe^{3+} ions

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Contents

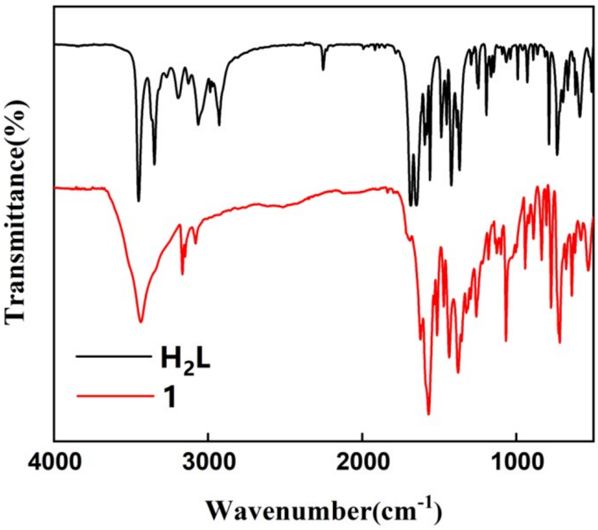

Fig. S1 IR spectra of **1**.

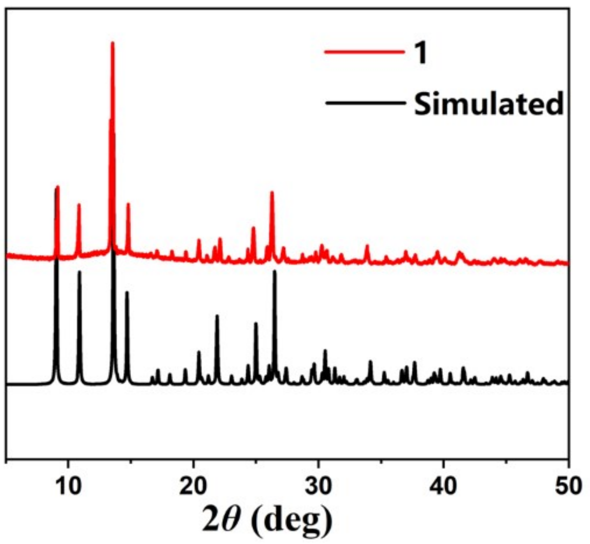

Fig. S2 PXRD pattern of **1**.

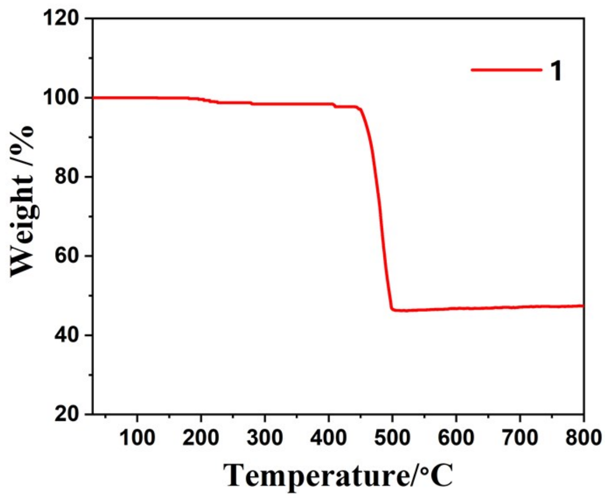

Fig. S3 TG curves of **1**.

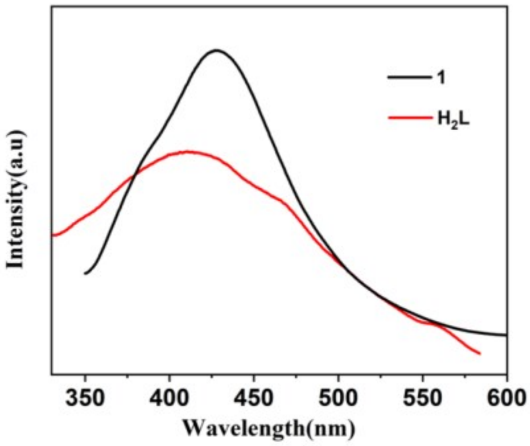

Fig. S4 Solid-state fluorescence emissions recorded at room temperature for free ligand and **1**.

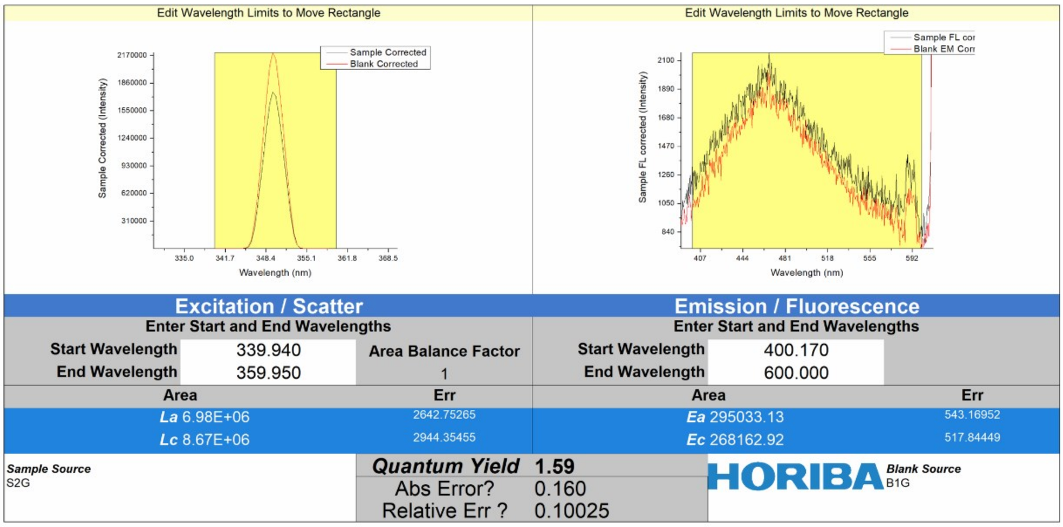

Fig. S5 Solid state quantum yield determination result of **1** at ambient condition.

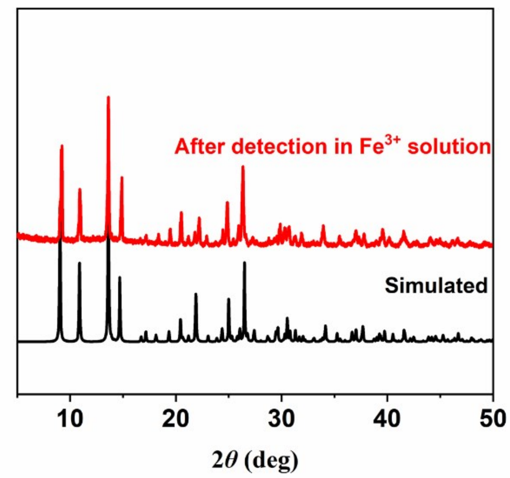

Fig. S6 PXRD patterns of **1** treated by the Fe^{3+} aqueous solution.

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

Compound **1**			
In(1)−O(1)	2.169(3)	In(1)−O(5) #3	2.098(3)
In(1)−O(3)#1	2.175(3)	In(1)−O(5)	2.101(3)
In(1)−O(4) #2	2.198(3)	In(1)−N(2) #4	2.238(3)
O(1)−In(1)−O(3) #1	99.71(10)	C(9)−N(2)−C(11)	105.4(3)
O(1)−In(1)−O(4) #2	96.80(10)	C(11)−N(2)−In(1) #7	128.8(2)
O(1)−In(1)−N(2) #3	178.67(10)	O(5) #4−In(1)−O(5)	162.571(18)
O(3) #1−In(1)−O(4) #2	163.38(10)	O(5)−In(1)−N(2) #3	96.47(12)
O(3) #1−In(1)−N(2) #3	81.56(10)	O(5) #4−In(1)−N(2) #3	100.77(11)
O(4) #2−In(1)−N(2) #3	81.92(11)	C(7)−O(1)−In(1)	127.1(2)
O(5)−In(1)−O(1)	83.98(11)	C(8)−O(3)−In(1) #5	129.2(2)
O(5) #4−In(1)−O(1)	78.73(10)	C(8)−O(4)−In(1) #2	129.0(2)
O(5)−In(1)−O(3) #1	89.10(10)	In(1) #6−O(5)−In(1)	123.67(12)
O(5) #4−In(1)−O(3) #1	95.89(10)	C(9)−N(2)−In(1) #7	125.7(3)
O(5)−In(1)−O(4) #2	94.57(10)	O(5) #4−In(1)−O(4) #2	85.41(10)

Symmetry transformations used to generate equivalent atoms:
#1 +X,1−Y,1/2+Z; #2 3/2−X,3/2−Y,1−Z; #3 1/2+X,3/2−Y,1/2+Z; #4 3/2−X,−1/2+Y,3/2−Z; #5 +X,1−Y,−1/2+Z; #6 3/2−X,1/2+Y,3/2−Z; #7 −1/2+X,3/2−Y,−1/2+Z

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

D−H···A	d(D−H)/Å	d(H···A)/Å	d(D···A)/Å	D−H···A/°
O(5)−H(5)···O(2)	0.86	1.97	2.777(4)	156.3
O(6)−H(6A)···O(2)	0.85	1.95	2.781(5)	165.7
O(7)−H(7)···O(2)#1	0.85	1.84	2.686(16)	172.4

Symmetry transformations used to generate equivalent atoms:
#1 +X,1−Y,−1/2+Z

Table S3. Comparison of detection capacity of **1** towards Fe ion with other materials.

Materials	Solvent	Detection Limit	Ref.
$[Tb(tftba)1.5(phen)(H_2O)]_n$	Water	1.27×10^{-5} M	1
$[Tb(HL)_{1.5}(H_2O)(DMF)]\cdot 2H_2O$	aqueous	$2.0 \times 10^{-5-}$ M	2
$[In(L)(\mu_2\text{-}OH)]\cdot 0.5H_2O$	Water	2.2×10^{-5} M	This work
Eu^{3+}@MIL-53-COOH (Al)	Water	5.0×10^{-5} M	3
BUT-15	Water	8.0×10^{-5} M	4
$[Eu(bpda)_{1.5}]\cdot H_2O_n$	Water	9.0×10^{-5} M	5
$\{[Cd_3(HL)_2(H_2O)_3]\cdot 3H_2O\cdot 2CH_3CN\}_n$	Water	9.06×10^{-5} M	6
$[Zn_5(hfipbb)_4(trz)_2(H_2O)_2]_n$	Water	2.0×10^{-4} M	7
$[(CH_3)_2NH_2]\cdot[Tb(bptc)]$	Ethanol	1.8×10^{-4} M	8

EuL_3	Ethanol	10^{-4} M	9
$Eu(acac)_3 \subset Zn(C_{15}H_{12}NO_2)_2$	DMF	5.0×10^{-3}M	10

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