

Supporting Information

Dual functional fluorescent sensor for selectively detecting acetone and Fe³⁺ based on {Cu₂N₄} substructure bridged Cu(I) coordination polymer

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Table S1 Selected luminescent compound materials for sensing acetone.

No.	luminescent materials	solution	detection limit	ref
1	{[Cd ₃ (L) ₂ (H ₂ O) ₆]·1.5DMF} (H ₃ L=4,4',4''-(methylsilanetriyl)- tribenzoic acid)	aqueous solutions	3 vol%	<i>Chin. Chem. Lett.</i> 2016, 27 , 497
2	[Cd(Tipb)(pta) _{0.5} (H ₂ O)-(NO ₃)]·(DMF) _x (H ₂ O) _y (Tipb=2,4,6-tris[4-(1Himidazole-1- yl)]-benzene, pta = para-phthalate)	acetonitrile	0.084vol% decreased 83%	<i>J. Mater. Chem. A</i> , 2014, 2 , 9469 by
3	[Cd(Tipb)(mta)]·(DMF) _x (H ₂ O) _y (Tipb=2,4,6-tris[4-(1Himidazole-1- yl)]-benzene, mta= meta-phthalate)	acetonitrile	0.075vol% decreased 94%	<i>J. Mater. Chem. A</i> , 2014, 2 , 9469 by
4	{[Tb ₄ (μ ₃ - OH) ₄ (BPDC) ₃ (BPDCA) _{0.5} (H ₂ O) ₆]ClO ₄ ·5H ₂ O (BPDC ²⁻ = 3,3'-dicarboxylate-2,2'- dipyridine anion and BPDCA ²⁻ = biphenyl-4,4'-dicarboxylate anion)	EtOH	21vol%	<i>J. Phys. Chem. C</i> 2014, 118 , 416
5	Ln(FBPT)(H ₂ O)(DMF) (Ln = Eu or Tb, FBPT = 2'-fluoro- biphenyl-3,4',5-tricarboxylate)	DMF	5%	<i>J. Mater. Chem. A</i> 2013, 1 , 11043
6	Tb(BTC)(H ₂ O) ₆ (BTC = benzenetricarboxylate)	aqueous suspension	0.3vol%	<i>J. Mater. Chem.</i> , 2012, 22 , 6819.
7	Cd ₃ (L)(H ₂ O) ₂ (DMF) ₂ ·5DMF (H ₆ L=hexa[4- (carboxyphenyl)oxamethyl]-3- oxapentane acid)	1-propanol	0.1vol%	<i>J. Mater. Chem.</i> , 2012, 22 , 23201.
8	Cd ₃ (L)(dib)·3H ₂ O·5DMA (H ₆ L=hexa[4- (carboxyphenyl)oxamethyl]-3- oxapentane acid, dib = 1,4-bis(1- imidazoly)benzene)	1-propanol	0.1vol%	<i>J. Mater. Chem.</i> , 2012, 22 , 23201.
9	Yb(BPT)(H ₂ O)·(DMF) _{1.5} (H ₂ O) _{1.25} (BPT = biphenyl-3,4',5-tricarboxylate)	2-propanol	0.5vol%	<i>Chem. Commun.</i> 2011, 47 , 5551
10	Eu ₂ (pzdc)(pzdc)(ox)(H ₂ O) ₄ ·8H ₂ O	methanol	0.5vol%	<i>CrystEngComm</i> , 2010, 12 ,

(pzdc = 2,5-pyrazinedicarboxylate,
ox =oxalate)

4372.

11	Eu(BTC) (BTC = benzenetricarboxylate)	DMF	0.3 vol %	<i>Adv. Mater.</i> 2007, 19 , 1693
12	[Cu(tpp)•H ₂ O] _{2n} [Htp = 1-(4-tetrazol-5"-yl)benzyl-3 - (pyraziny-1)pyrazole]	aqueous suspension	0.0842vol%	This work

Table S2 Selected luminescent compound materials for sensing Fe³⁺.

No.	luminescent materials	solution	K _{sv} / detection limit	ref
1	Ba ₅ (ADDA) ₅ (EtOH) ₂ (H ₂ O) ₃ ·5DMF H ₂ ADDA = 3,3'-(anthracene-9,10-diyl) diacrylic acid	methanol (turn-off) acetone (turn-off) THF (turn-on)	1.68 × 10 ⁴ / 10 ⁻⁶ M None/2.1 × 10 ⁻⁷ M -9.09 × 10 ³ / 10 ⁻⁶ M	<i>Inorg. Chem.</i> 2016, 55 , 1782
2	{[Eu(L)(H ₂ O) ₂] · NMP · H ₂ O} _n (NMP = N-methyl-2-pyrrolidone)	DMF HEPES	3.83 × 10 ⁴ / none 2.55 × 10 ⁴ / none	<i>Inorg. Chem.</i> 2016, 55 , 10114
3	{[Cd ₃ (L) ₂ (H ₂ O) ₆] · 1.5DMF} (H ₃ L=4,4',4''-(methylsilanetriyl) tribenzoic acid)	aqueous solutions	None / 1 × 10 ⁻² M	<i>Chin. Chem. Lett.</i> 2016, 27 , 497
4	{[Tb ₄ (OH) ₄ (DSOA) ₂ (H ₂ O) ₈]·(H ₂ O) ₈ } _n Na ₂ H ₂ DSOA=disodium-2,20- disulfonate-4,4'-oxydibenzoic acid	aqueous solutions	3543 / none	<i>J. Mater. Chem. A.</i> 2015, 3 , 641
5	[Tb(BTB)(DMF)]·1.5DMF·2.5H ₂ O (H ₃ BTB = benzene-1,3,5-tribenzoate)	ethanol	None / 10 ⁻⁵ M	<i>Inorg. Chem.</i> 2015, 54 , 4585
6	EuL (L=2-aminoterephthalic acid)	DMF	2.88 × 10 ⁴ / none	<i>J. Mater. Chem. C,</i> 2014, 2 , 6758
7	[H ₂ N(CH ₃) ₂][Eu(H ₂ O) ₂ (BTMIPA)]·2H ₂ O O {H ₄ BTMIPA = 5,5'-methylenebis- (2,4,6-trimethylisophthalic acid)}	DMF	None / 10 ⁻³	<i>Chem. Commun.</i> 2013, 49 , 11557
8	EuL ₃ (L = 4'-(4-carboxyphenyl)-2,2': 6',2''- terpyridine)	aqueous solution	4.1 × 10 ³ / 10 ⁻⁴ M	<i>ACS Appl. Mater.</i> <i>Interfaces</i> 2013, 5 , 1078
9	[Eu(BTPCA)(H ₂ O)]·2DMF·3H ₂ O (H ₃ BTPCA = 1,1',1''-(benzene-1,3,5-	DMF	None / 10 ⁻⁵ M	<i>Inorg. Chem.</i> 2013, 52 , 2799

triy)tripiperidine-4-carboxylic acid

10	MIL-53(AI) (BDC =1,4-benzenedicarboxylic acid)	aqueous solution	None / 0.9×10^{-6} M	<i>Anal. Chem.</i> 2013, 85 , 7441
11	Eu(C ₃₃ H ₂₄ O ₁₂)(H ₂ NMe)(H ₂ O)	HEPES aqueous	None / 10^{-4} M	<i>J. Mater. Chem.</i> 2012, 22 , 16920
12	Eu(acac) ₃ ·Zn(C ₁₅ H ₁₂ NO ₂) ₂	CH ₂ Cl ₂ / MeOH	None / 5×10^{-3} M	<i>Chem. Commun.</i> 2011, 47 , 10731
13	[Cu(tp _p)·H ₂ O] _{2n} [Htp _p = 1-(4-tetrazol-5"-yl)benzyl-3 - (pyraziny-l)pyrazole]	aqueous suspension	$4.6 \times 10^4 / 10^{-5}$ M	This work

Table S3 Selected bond lengths [Å] and angles [°] for **1**.

Bond length	(Å)	Bond angle	(°)
Cu(1)-N(3)	1.976(4)	N(3)-Cu(1)-N(8)	111.62(14)
Cu(1)-N(8)	2.028(4)	N(3)-Cu(1)-N(6)	124.47(15)
Cu(1)-N(6)	2.076(4)	N(8)-Cu(1)-N(6)	107.32(15)
Cu(1)-N(4)	2.130(4)	N(3)-Cu(1)-N(4)	120.93(15)
Cu(2)-N(10)	2.005(4)	N(8)-Cu(1)-N(4)	109.28(14)
Cu(2)-N(16)	2.009(4)	N(6)-Cu(1)-N(4)	78.90(14)
Cu(2)-N(12)	2.088(4)	N(10)-Cu(2)-N(16)	110.79(15)
Cu(2)-N(14)	2.116(3)	N(10)-Cu(2)-N(12)	115.89(15)
		N(16)-Cu(2)-N(12)	113.66(16)
		N(10)-Cu(2)-N(14)	117.27(15)
		N(16)-Cu(2)-N(14)	117.16(15)
		N(12)-Cu(2)-N(14)	78.81(14)

Table S4 Standard deviation calculation and detection limit calculation.

Text 1 Fluorescence intensity	5842.45 a.u.
Text 2 Fluorescence intensity	5842.02 a.u.
Text 3 Fluorescence intensity	5841.25 a.u.
Text 4 Fluorescence intensity	5841.88 a.u.
Text 5 Fluorescence intensity	5842.11 a.u.
Standard Deviation (σ)	0.4402
Slope (m)	1568.14

Detection limit ($3\sigma/m$)	0.0842 vol%
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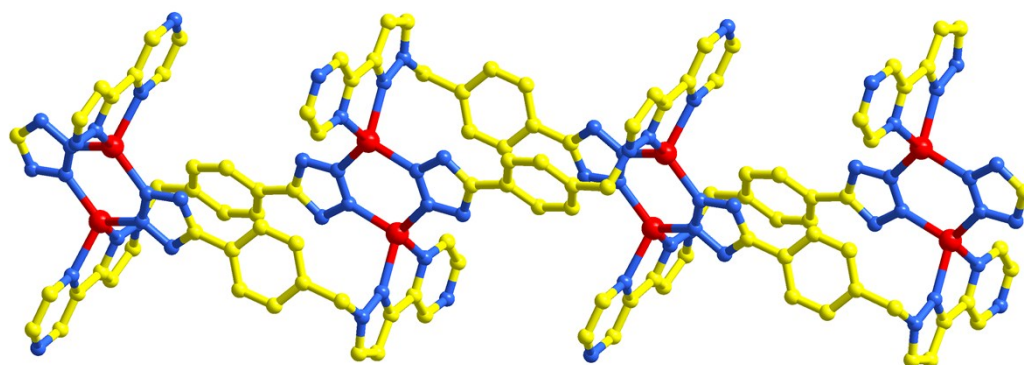


Fig. S1 The 1D chain structure of 1.

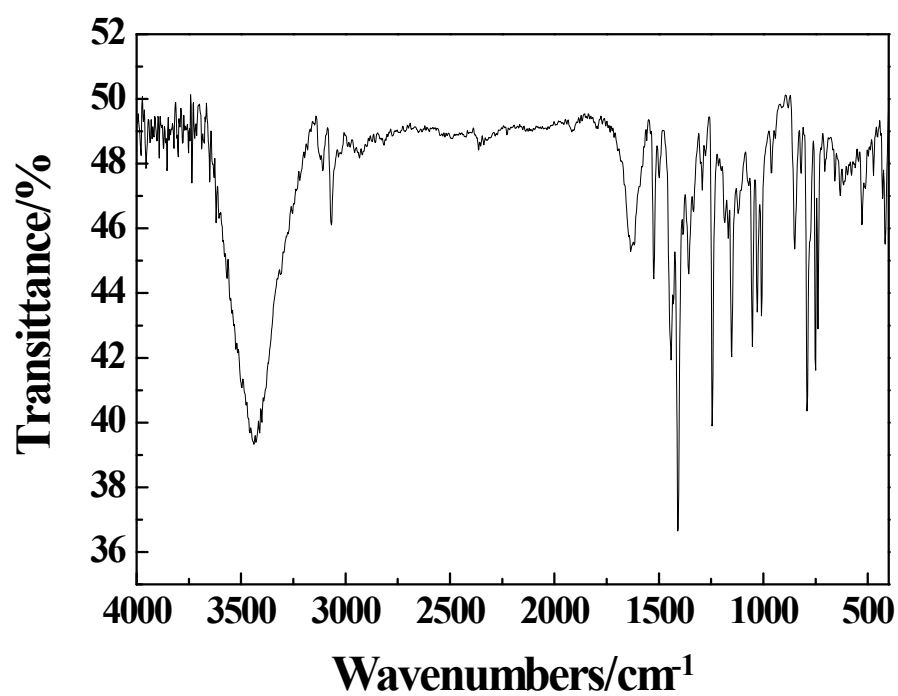


Fig.S2 The IR spectra of 1.

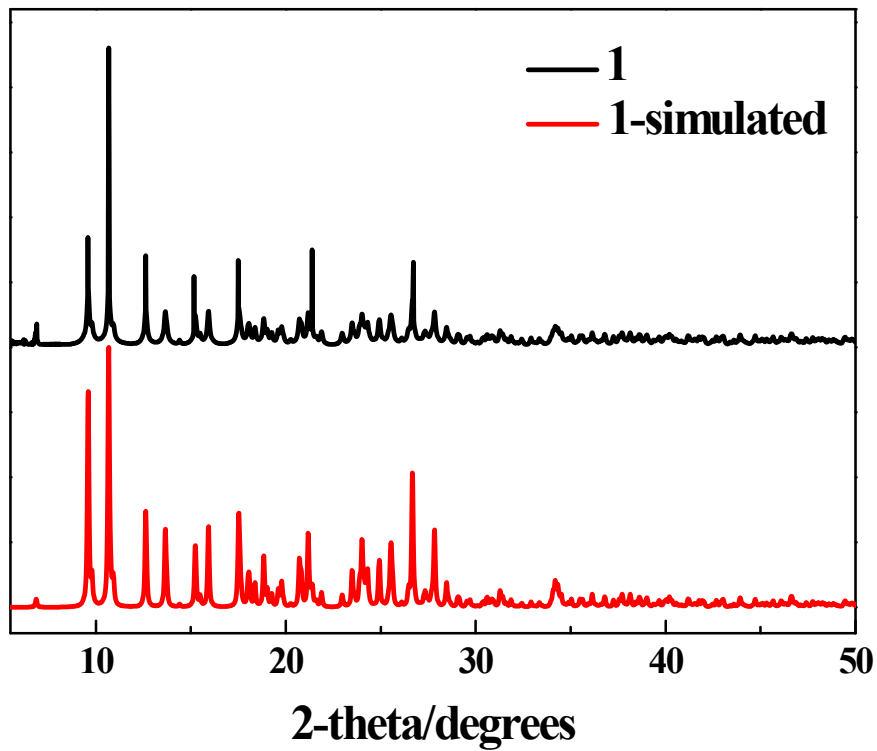


Fig.S3 The PXR D patterns of 1.

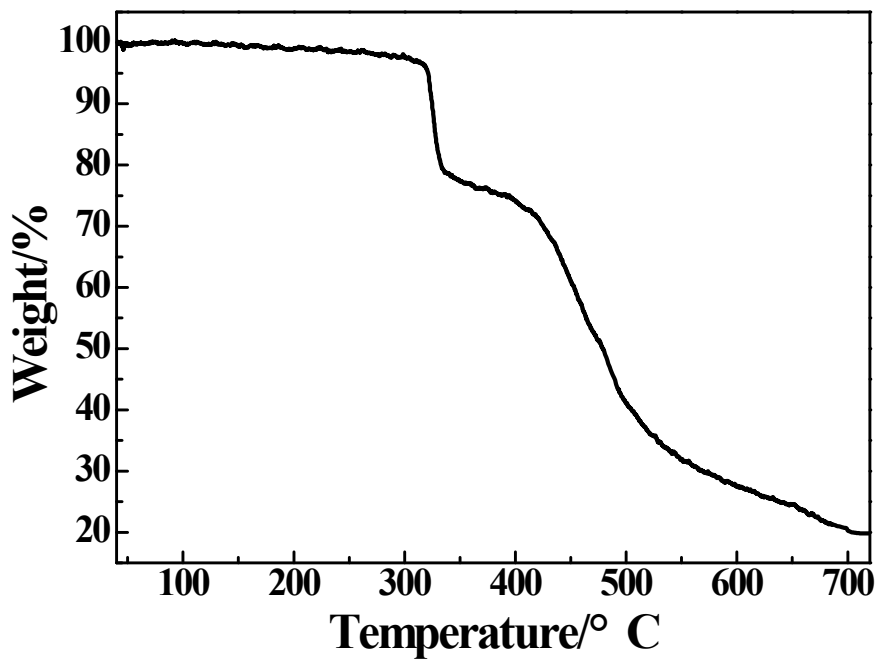


Fig.S4 The TGA curves of compounds 1.

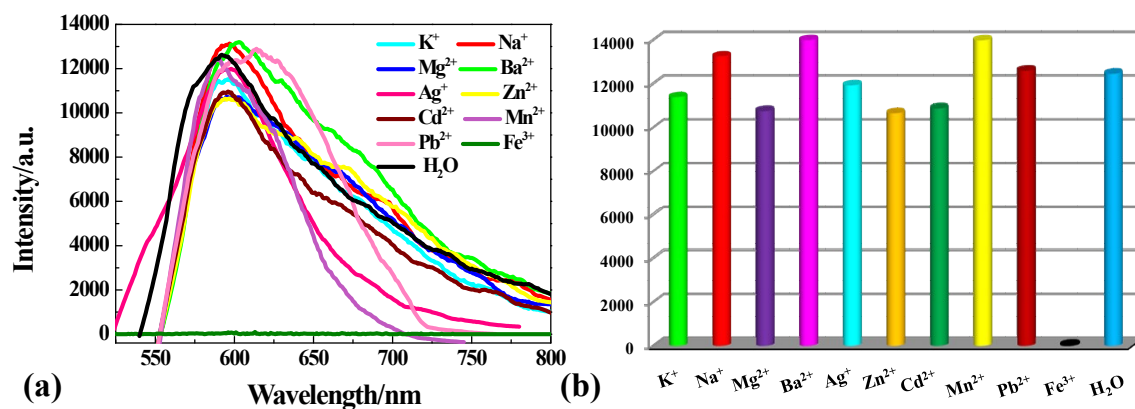


Fig.S5 (a) Fluorescence intensity of compound **1** in different metal ion; (b) Results of the competition experiments between Fe³⁺ and selected other metal ions.

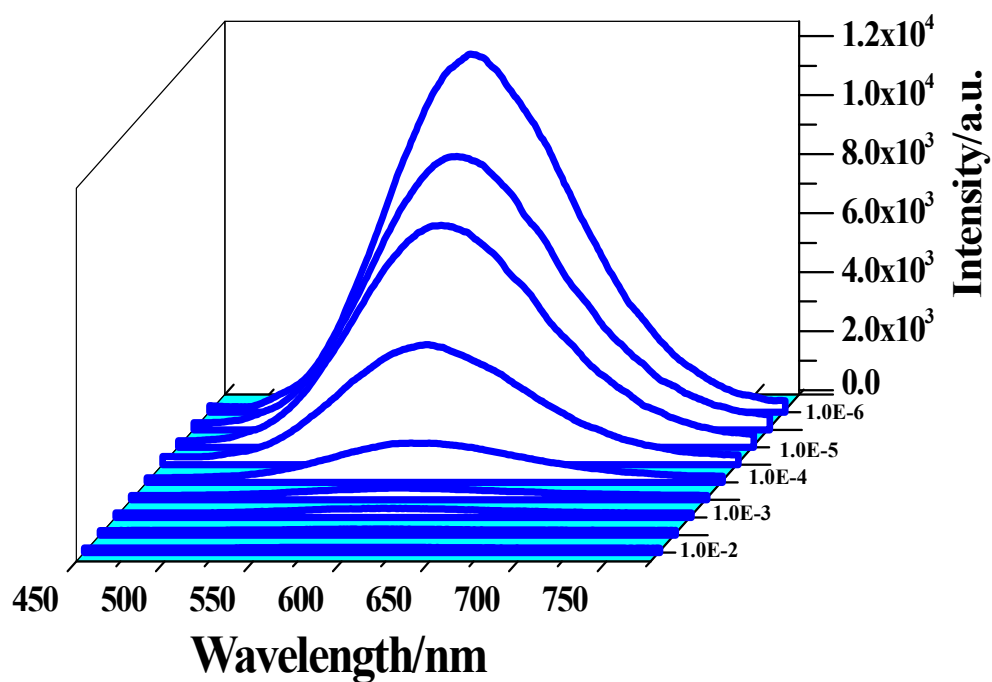


Fig.S6 Fluorescence intensity of compound **1** at 597 nm in different concentrations aqueous solutions of Fe³⁺ (in the range of approximately 10⁻⁶–10⁻² mol/L).