Electronic Supporting Information

A multifuctional Cd(II)-based metal-organic framework with amide groups exhibiting luminescent sensing towards multiple substances

Runzhong Guo, Hao Dong, Peiyuan Li, Yi Sun, Haiying Wang* and Huiyan Liu*

School of Chemistry & Materials Science, Jiangsu Key Laboratory of Green Synthetic Chemistry for Functional Materials, Jiangsu Normal University, Xuzhou 221116, P. R. China



Fig. S1 (a) The coordination environment of Cd(II) atoms in 1; symmetry code: A 1x, -y, -z; B -1+x, y, z; C x, 1+y, -1+z; D x, y, -1+z. (b) The three coordination modes of H_4L in **1**.



Fig. S2 Ball-and-stick representation of 3D framework of 1 showing channels along the a (a), b (b) and c (c) direction, respectively.



Fig. S3 Conformation of L^{4-} linker in **1** in which the two terminal isophthalic moieties are not coplanar with a dihedral angle of about 80.2°.



Fig. S4 The 4,8-connected *flu* network in 1 shown as a stick diagram.



Fig. S5 TGA data of 1.



Fig. S6 PXRD patterns for 1: a simulated PXRD pattern from the single-crystal structure, as-synthesized, water-exchanged and activated samples, respectively.



Fig. S7 Solid-state luminescence spectra of H₄L and 1 at room temperature.



Fig. S8 The Stern-Volmer plots for 1 with Fe^{3+} (a), Cu^{2+} (b) and $Cr_2O_7^{2-}$ (c).



Fig. S9 Experimental XRD patterns of 1 before and after treated with aqueous solution of different ions.



Fig. S10 View for the UV-vis adsorption spectra of some metal ions (a) and anions (b) in water and exaction spectrum for **1**.



Fig. S11 The Stern-Volmer plots for 1 with NB (a), 4-NT (b) and 1,3-DNB (c).



Fig. S12 Simulated and experimental XRD patterns of 1 after treated with different nitroaromatics.

MOFs	analyte	<i>K</i> _{SV} (M ⁻¹)	solvent	reference
${[(CH_3)_2NH_2]_4[Ca_2Zn_4(L)_4] \cdot 4DMF}_n$	Fe ³⁺	4.36×10 ³	H ₂ O	1
[Eu(IMS1) ₂]Cl·4H ₂ O	Fe ³⁺	5.87×10 ³	H ₂ O	2
Zn-TCPP	Fe ³⁺	1.08×10 ⁴	EtOH	3
$\{[Cd_2(L)_2(bpe)_2]\cdot 3DMF\cdot 2.5H_2O\}n$	Fe ³⁺	1.7×104	DMF	4
$[Tb_4(L)_6(H_2O)_8]$	Fe ³⁺	1.88×10 ⁴	$\rm H_2O$	5
Eu-MOF	Fe ³⁺	2.09×10 ⁴	$\rm H_2O$	6
${[Cd(L)(BPDC)] \cdot 2H_2O}n$	Fe ³⁺	3.63×10 ⁴	H ₂ O	7
${[Cd(L)(SDBA)(H_2O)] \cdot 0.5H_2O}n$	Fe ³⁺	3.59×10 ⁴	H_2O	7
([Zn ₂ Na ₂ (TPHC)(4,4-Bipy)(DMF)]· 8H ₂ O) (JLU-MOF71)	Fe ³⁺	5.77×10 ⁴	DMF	8
CPP-16	Cu ²⁺	7.85×10 ³	MeCN	9
Zr ₆ O ₄ (OH) ₄ (TCPPH ₂) ₃ (MOF-525)	Cu ²⁺	4.5×10 ⁵	DMF	10
Eu@3	Cu ²⁺	501.2	DMF	11
$Eu_2(FMA)_2(OX)(H_2O)_4 \cdot 4H_2O$	Cu ²⁺	528.7	H ₂ O	12
(Me ₂ NH ₂) ₂ [Cd ₃ (L) ₂]·7H ₂ O (1)	Fe ³⁺	1.1×10^{4}	H ₂ O	This work
	Cu ²⁺	7.6×10 ³	H ₂ O	This work

Table S1 Summary of some MOF-based sensors for detecting Fe^{3+} and Cu^{2+} ions

MOFs	analyte	K _{SV} (M ⁻¹)	solvent	reference
$\{[(CH_3)_2NH_2]_4[Ca2Zn_4(L)_4] \cdot 4DMF\}_n$	$Cr_2O_7^{2-}$	1.15×10 ³	H ₂ O	1
[Cd3(cpota)2(phen)3]n·5nH2O	$Cr_2O_7^{2-}$	1.21×10 ³	H_2O	13
[Zn(IPA)(3-PN)]n	$Cr_2O_7^{2-}$	1.37×10 ³	H_2O	14
[Cd(IPA)(3-PN)]n	$Cr_2O_7^{2-}$	2.91×10 ³	H_2O	14
[Zn(btz)]n	$Cr_2O_7^{2-}$	3.19×10 ³	H_2O	15
$\{[Zn_2(ttz)H_2O]n\}$	$Cr_2O_7^{2-}$	2.19×10 ³	H_2O	14
$\{[Cd_2(L)2(bpe)_2]\cdot 3DMF\cdot 2.5H_2O\} n$	$Cr_2O_7^{2-}$	3.7×10 ³	DMF	4
$[Tb_4(L)_6(H_2O)_8]$	$Cr_2O_7^{2-}$	4.1×10 ³	H ₂ O	5
${[Cd(L)(BPDC)] \cdot 2H_2O}n$	$Cr_2O_7^{2-}$	6.4×10 ³	H_2O	7
$\{[Cd(L)(SDBA)(H_2O)] \cdot 0.5H_2O\}n$	$Cr_2O_7^{2-}$	4.97×10 ³	H_2O	7
$\{[Zn_2(TPOM)(NH_2\text{-}BDC)_2]\cdot 4H_2O\}n$	$Cr_2O_7^{2-}$	7.59×10 ³	DMF	16
NU-1000	$Cr_2O_7^{2-}$	1.34×10 ⁴	H ₂ O	17
(Me ₂ NH ₂) ₂ [Cd ₃ (L) ₂]·7H ₂ O (1)	$Cr_2O_7^{2-}$	4.8×10 ³	H ₂ O	This work

Table S2 Summary of some MOF-based sensors for detecting $Cr_2O_7^{2-}$ ions

References

- 1 W.-J. Ji, G.-F. Liu, B.-Q. Wang, W.-B. Lu and Q.-G. Zhai, *CrystEngComm*, 2020, **22**, 4710-4715.
- 2 Y.-Q. Huang, H.-Y. Chen, Y. Wang, Y.-H. Ren, Z.-G. Li, L.-C. Li and Y. Wang, *RSC Adv.*, 2018, **8**, 21444-21450.
- 3 Y. Jiang, L. Sun, J. Du, Y. Liu, H. Shi, Z. Liang and J. Li, *Cryst. Growth Des.*, 2017, **17**, 2090-2096.
- 4 Z. Chen, X. Mi, J. Lu, S. Wang, Y. Li, J. Doua and D. Li, Dalton Trans., 2018, 47, 6240-6249.

- 5 X. Wang, J. L. Li, C. Jiang, P. Hu, B. Li, T. Zhang and H. C. Zhou, *Chem. Commun.*, 2018, **54**, 13271-13274.
- 6 J. Wang, M. Jiang, L. Yan, R. Peng, M. Huangfu, X. Guo, Y. Li and P. Wu, *Inorg. Chem.*, 2016, 55, 12660-12668.
- 7 S. Chen, Z. Shi, L. Qin, H. Jia and H. Zheng, Cryst. Growth Des., 2016, 17, 67-72.
- 8 C. Yu, X. Sun, L. Zou, G. Li, L. Zhang and Y. Liu, Inorg. Chem., 2019, 58, 4026-4032.
- 9 W. Cho, H. J. Lee, G. Choi, S. Choi and M. Oh, J. Am. Chem. Soc., 2014, 136, 12201-12204.
- 10 L. Li, S. Shen, R. Lin, Y. Baia and H. Liu, Chem. Commun., 2017, 53, 9986-9989.
- 11 J.-Y. Liang, G.-P. Li, R.-C. Gao, N.-N. Bai, W.-Q. Tong, L. Hou and Y.-Y. Wang, *Cryst. Growth Des.*, 2017, **17**, 6733-6740.
- 12 Y. Xiao, Y. Cui, Q. Zheng, S. Xiang, G. Qian and B. Chen, *Chem. Commun.*, 2010, **46**, 5503-5505.
- 13 S. Li, L. Lu, M. Zhu, C. Yuan and S. Feng, Sensor Actuat. B-Chem., 2018, 258, 970-980.
- 14 B. Parmar, Y. Rachuri, K. K. Bisht, R. Laiya and E. Suresh, *Inorg. Chem.*, 2017, 56, 2627-2638.
- 15 C. Cao, H. Hu, H. Xu, W. Qiao and B. Zhao, CrystEngComm, 2016, 18, 4445-4451.
- 16 R. Lv, J. Wang, Y. Zhang, H. Li, L. Yang, S. Liao, W. Gu and X. Liu, *J. Mater. Chem. A*, 2016, 4, 15494-15500.
- 17 Z.-J. Lin, H.-Q. Zheng, H.-Y. Zheng, L.-P. Lin, Q. Xin and R. Cao, *Inorg. Chem.*, 2017, 56, 14178-14188.