

## Supporting Information

### **A novel Cd-MOF with enhanced thermo-sensitivity: The rational design, synthesis and multipurpose applications**

**Ping Ju,<sup>a</sup> Mengting Li,<sup>a</sup> Hua Yang,<sup>b</sup> Long Jiang,<sup>c</sup> Lian Xia,<sup>a</sup> Rongmei Kong,<sup>a</sup> Ensheng Zhang,<sup>\*a</sup> Fengli Qu<sup>\*a</sup>**

<sup>a</sup> College of Chemistry and Chemical Engineering, Qufu Normal University, Qufu, Shandong, 273165, P. R. China.

<sup>b</sup> Laboratory of New Energy & New Functional Materials, College of Chemistry and Chemical Engineering, Yan'an University, Yan'an, Shaanxi, 716000, P. R. China.

<sup>c</sup> Instrumental Analysis & Research Center, Sun Yat-Sen University, Guangzhou 510275, PR China

E-mail address: sdzes2006@163.com; fengliqun@hotmail.com

**Table S1** Lanthanide metal ions based LMOF thermometers

LMOF thermometers	Metal center	Detection ranges (K)	Reference
Eu <sub>0.0069</sub> Tb <sub>0.9931</sub> -DMBDC	Eu <sup>3+</sup> and Tb <sup>3+</sup>	50-200	1
Tb <sub>0.9</sub> Eu <sub>0.1</sub> PIA	Eu <sup>3+</sup> and Tb <sup>3+</sup>	100-300	2
Tb <sub>0.957</sub> Eu <sub>0.043</sub> cpda	Eu <sup>3+</sup> and Tb <sup>3+</sup>	40-300	3
Tb <sub>0.98</sub> Eu <sub>0.02</sub> (OA) <sub>0.5</sub> (DSTP)·3H <sub>2</sub> O	Eu <sup>3+</sup> and Tb <sup>3+</sup>	77–275	4
{[Eu <sub>2</sub> (L) <sub>3</sub> ·(H <sub>2</sub> O) <sub>2</sub> ·(DMF) <sub>2</sub> ]·16H <sub>2</sub> O} <sub>n</sub>	Eu <sup>3+</sup>	10–150	5
Tb <sub>0.95</sub> Eu <sub>0.05</sub> FTPTC	Eu <sup>3+</sup> and Tb <sup>3+</sup>	25–300	6
Tb <sub>0.80</sub> Eu <sub>0.20</sub> BPDA	Eu <sup>3+</sup> and Tb <sup>3+</sup>	298-318	7
ZJU-88⇨perylene	Eu <sup>3+</sup>	293-353	8

**Table S2.** Selected Bond Lengths (Å) and Bond Angles (°)

Bond	Dist.	Bond	Dist.	Bond	Dist.
Cd(1)-O(1)	2.507(2)	Cd(1)-N(1)	2.430(2)	Cd(1)-O(4W)	2.213(2)
Cd(1)-O(5)	2.518(2)	Cd(1)-O(6)	2.268(2)	Cd(1)-O(3)	2.293(2)
Cd(1)-O(2)	2.537(2)	Cd(2)-O(1W)	2.201(2)	Cd(2)-O(1W)	2.344(3)
Cd(2)-O(4)	2.510(2)	Cd(2)-O(3)	2.326(2)	Cd(2)-O(3W)	2.530(3)
Cd(2)-O(2)	2.312(2)	Cd(2)-O(2W)	2.368(2)	Cd(2)-N(2)	2.343(3)
Angle	(°)	Angle	(°)	Angle	(°)
N(1)-Cd(1)-O(1)	141.44(8)	O(1)-Cd(1)-O(2)	51.14(7)	O(1)-Cd(1)-O(5)	71.80(7)
O(3)-Cd(1)-O(2)	69.69(7)	O(3)-Cd(1)-O(5)	141.11(7)	O(3)-Cd(1)-N(1)	97.91(8)
O(3)-Cd(1)-O(1)	120.60(7)	O(6)-Cd(1)-O(2)	90.01(8)	O(6)-Cd(1)-O(3)	87.76(8)

O(6)-Cd(1)-O(5)	54.51(7)	O(6)-Cd(1)-N(1)	96.53(8)	O(6)-Cd(1)-O(1)	87.50(8)
O(5)-Cd(1)-O(2)	114.37(7)	O(4w)-Cd(1)-O(2)	89.99(9)	O(4w)-Cd(1)-O(3)	102.95(10)
O(4w)-Cd(1)-O(6)	168.56(10)	O(4w)-Cd(1)-O(5)	115.45(10)	O(4w)-Cd(1)-N(1)	86.07(9)
O(4w)-Cd(1)-O(1)	83.61(9)	N(1)-Cd(1)-O(2)	165.81(8)	N(1)-Cd(1)-O(5)	79.59(4)
O(2w)-Cd(2)-O(3w)	77.76(10)	O(2w)-Cd(2)-O(4)	163.70(8)	O(2)-Cd(2)-O(2w)	80.60(8)
O(2)-Cd(2)-O(3w)	102.57(9)	O(2)-Cd(2)-O(3)	73.25(7)	O(2)-Cd(2)-O(4)	115.54(8)
O(2)-Cd(2)-N(2)	84.88(8)	O(3)-Cd(2)-O(2w)	135.41(8)	O(3)-Cd(2)-O(3w)	73.64(9)
O(3)-Cd(2)-O(4)	53.77(7)	O(3)-Cd(2)-N(2)	104.05(8)	O(4)-Cd(2)-O(3w)	95.54(10)
N(2)-Cd(2)-O(2w)	108.91(8)	N(2)-Cd(2)-O(3w)	170.91(10)	N(2)-Cd(2)-O(4)	76.37(8)
O(1w)-Cd(2)-O(2w)	82.00(9)	O(1w)-Cd(2)-O(2)	161.62(8)	O(1w)-Cd(2)-O(3w)	79.39(10)
O(1w)-Cd(2)-O(3)	124.16(8)	O(1w)-Cd(2)-O(4)	82.16(8)	O(1w)-Cd(2)-N(2)	95.23(10)

Symmetry codes: #1 1-x, -1-y, -z; #2 +x, -1-y, 1/2+z; #3 1-x, -y, -z; #4 +x, -1-y, -1/2+z; #5 1/2-x, -1/2-y, -z .

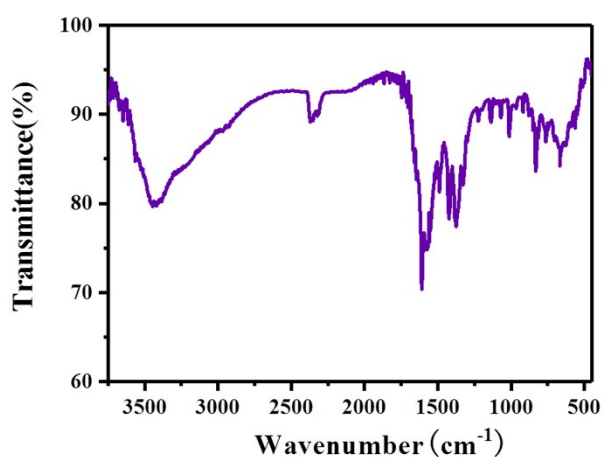
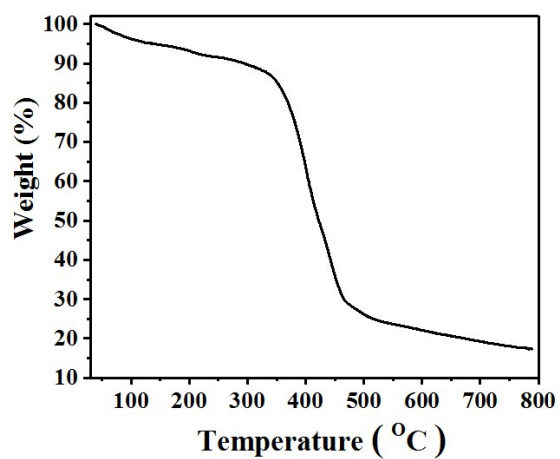
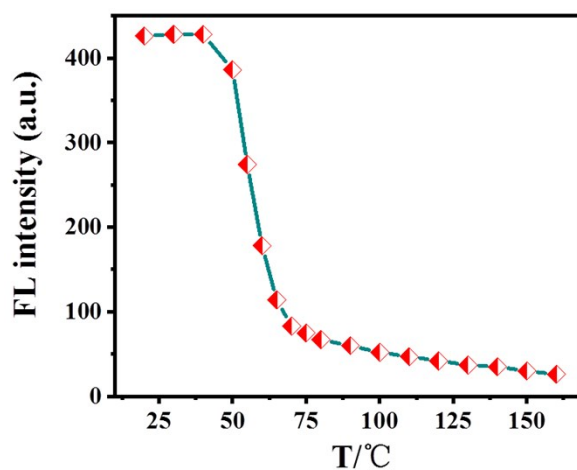


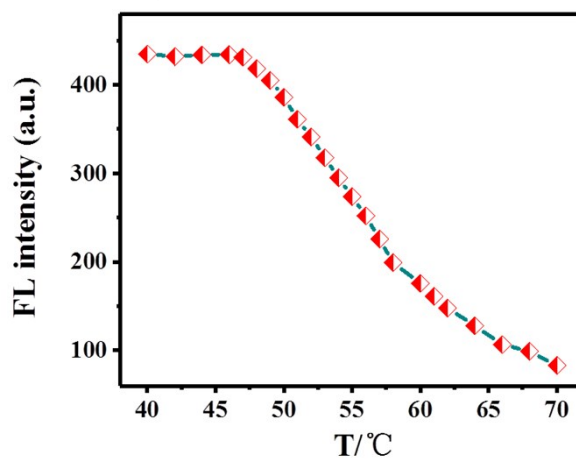
Fig. S1 FT-IR spectrum of complex 1



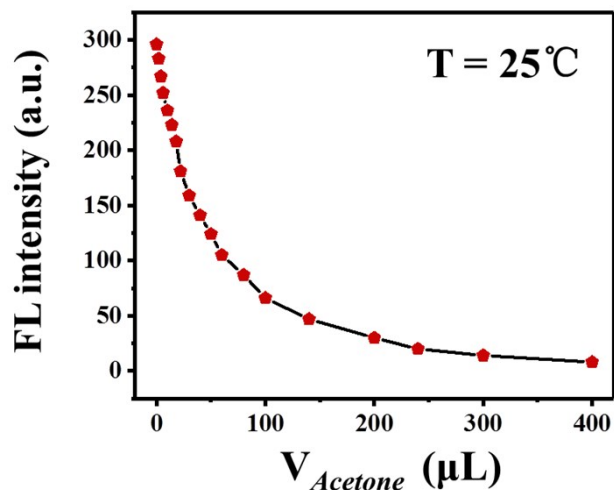
**Fig. S2** TG curve for complex 1.



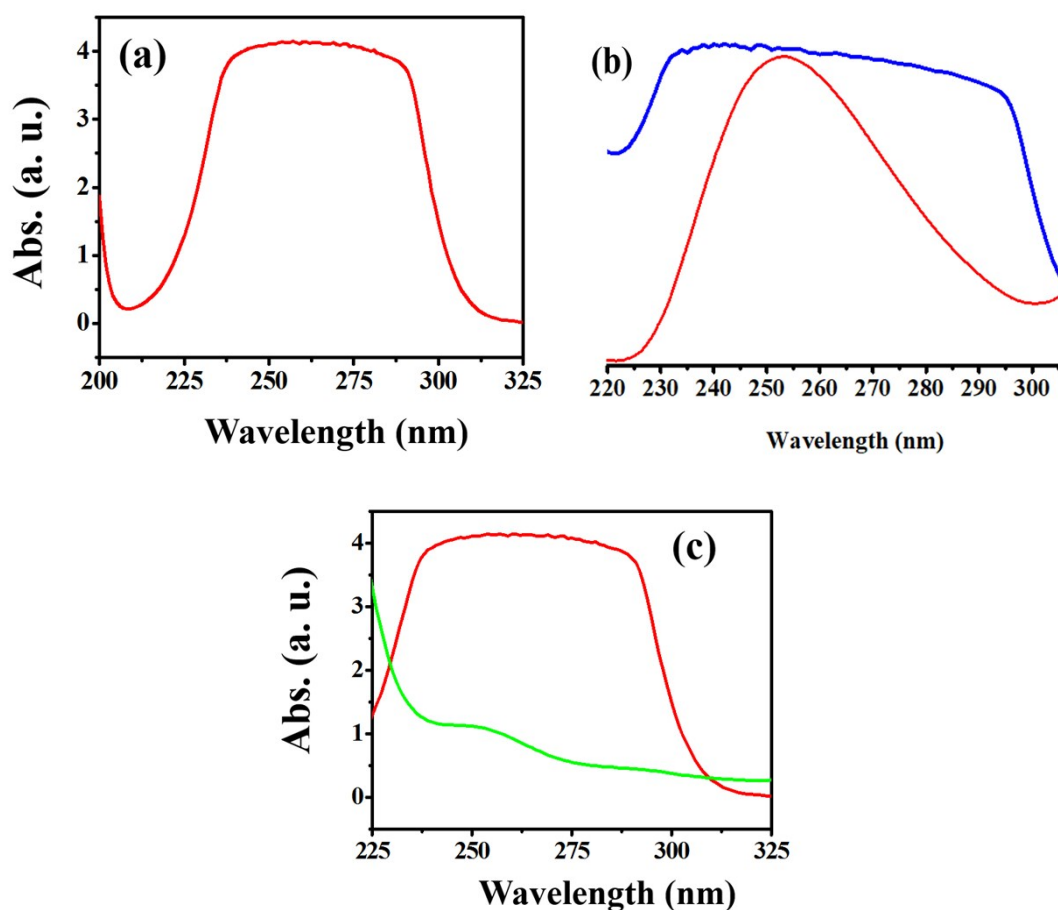
**Fig. S3** Fluorescent intensity of complex 1 with gradually change temperature from 160 °C to 20 °C ( $\lambda_{\text{ex}} = 300 \text{ nm}$ , slits: 2.5 nm/5 nm).



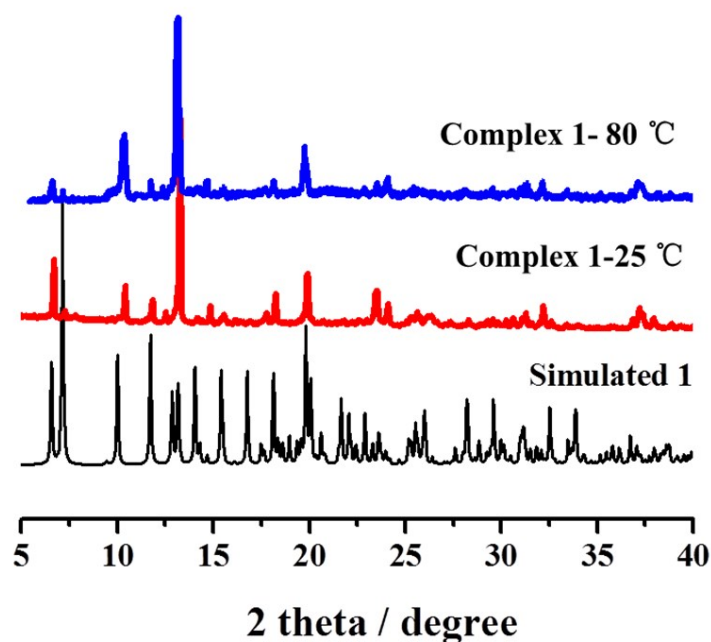
**Fig. S4** Fluorescent intensity of complex 1 with gradually change temperature from 70 °C to 40 °C ( $\lambda_{\text{ex}} = 300 \text{ nm}$ , slits: 2.5 nm/5 nm).



**Fig. S5** Fluorescent intensity of complex **1**-H<sub>2</sub>O suspension after the addition of acetone ( $\lambda_{\text{ex}} = 300 \text{ nm}$ ,  $\lambda_{\text{em}} = 410 \text{ nm}$ , slits: 5 nm/10 nm, all the tests were carried out at 25°C).



**Fig. S6** (a) The UV-vis spectrum of acetone in water; (b) Overlap of absorption spectrum of acetone (the blue line) and fluorescent excitation spectrum of complex **1** (the red line) ; (c) Overlap of absorption spectra of acetone (the red line) and complex **1** (the green line).



**Fig. S7** PXR D patterns of complex 1 at 25 °C and 80 °C.

#### References:

- [1] Y. Cui, H. Xu, Y. Yue, Z. Guo, J. Yu, Z. Chen, J. Gao, Y. Yang, G. Qian, B. Chen, A luminescent mixed-lanthanide Metal-organic framework thermometer, *J. Am. Chem. Soc.*, 2012, **134**, 3979-3982.
- [2] X. T. Rao, T. Song, J. K. Gao, Y. J. Cui, Y. Yang, C. D. Wu, B. L. Chen, G. D. Qian, A highly sensitive mixed lanthanide metal-organic framework self-calibrated luminescent thermometer, *J. Am. Chem. Soc.*, 2013, **135**, 15559-15564.
- [3] Y. Cui, W. Zou, R. Song, J. Yu, W. Zhang, Y. Yang, G. Qian, A ratiometric and colorimetric luminescent thermometer over a wide temperature range based on a lanthanide coordination polymer, *Chem. Commun.*, 2014, **50**, 719-721.
- [4] Y. Wei, R. Sa, Q. Li, K. Wu, Highly stable and sensitive Ln MOF ratiometric thermometers constructed with mixed ligands, *Dalton Trans.*, 2015, **44**, 3067-3074.
- [5] D. Wang, Q. Tan, J. Liu, Z. Liu, A stable europium metal-organic framework as a dual-functional luminescent sensor for quantitatively detecting temperature and humidity, *Dalton Trans.*, 2016, 45, 18450-18454.
- [6] D. Zhao, D. Yue, L. Zhang, K. Jiang, G. Qian, Cryogenic luminescent Tb/Eu-MOF thermometer based on a fluorine-modified tetracarboxylate ligand, *Inorg. Chem.*, 2018, **57**, 12596-12602.
- [7] D. Zhao, X. Rao, J. Yu, Y. Cui, Y. Yang, G. Qian, Design and synthesis of an MOF thermometer with high sensitivity in the physiological temperature range, *Inorg. Chem.*, 2015, **54**, 11193-11199.
- [8] Y. Cui, R. Song, J. Yu, M. Liu, Z. Wang, C. Wu, Y. Yang, Z. Wang, B. Chen, G. Qian, Dual-emitting MOF=Dye composite for ratiometric temperature sensing, *Adv. Mater.*, 2015, **27**, 1420-1425.

