Supporting Information

A photochromic Cd(II)-organic framework showing highly efficient dual-response sensing properties

Jinfang Zhang[a,*], Zhuo Lin[a], Yinlong Yue[a], Qinghan Chen[a], Dejing Yin[b], Chi Zhang[a,c,*]

[a] *International Joint Research Center for Photoresponsive Molecules and Materials, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, P. R. China*

[b] *School of Biotechnology, Jiangnan University, Wuxi 214122, P. R. China*

[c] *School of Chemical Science and Engineering, Tongji University, Shanghai 200092, P. R. China*

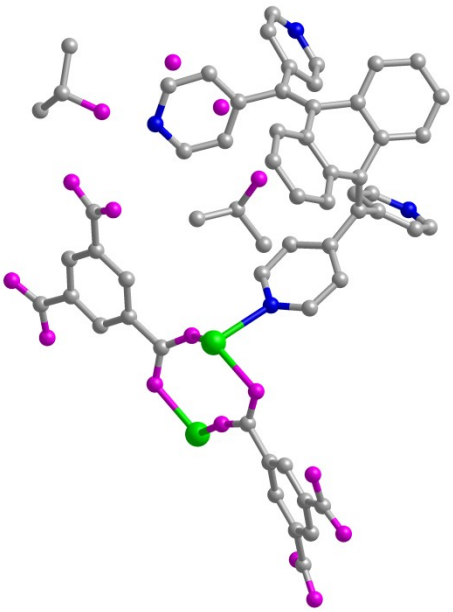

Figure S1. The asymmetric unit of **1** (Cd, green; N, blue; O pink; C, grey; all H atoms are omitted for clarity).

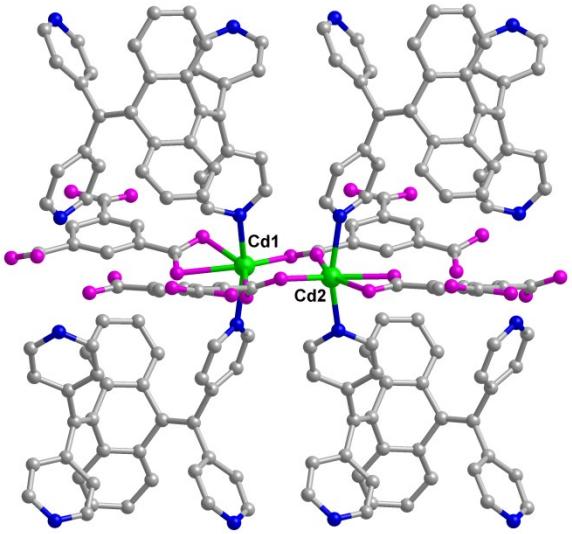

Figure S2. The coordination environment of Cd(II) in **1** (all H atoms are omitted for clarity).

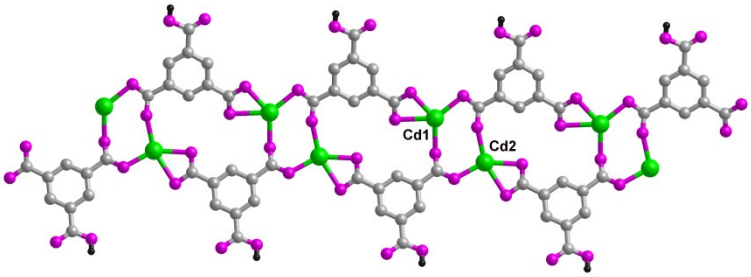

Figure S3. 1-D chain fabricated by $[Cd_2(COO)]^{2+}$ clusters and HBTC double-bridges (Cd, green; O pink; C, grey H, black).

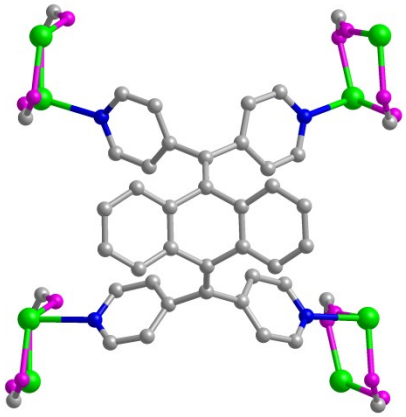

Figure S4. The coordination and connected environment of **L** unit in **1** (Cd, green; N, blue; O pink; C, grey; all H atoms are omitted for clarity).

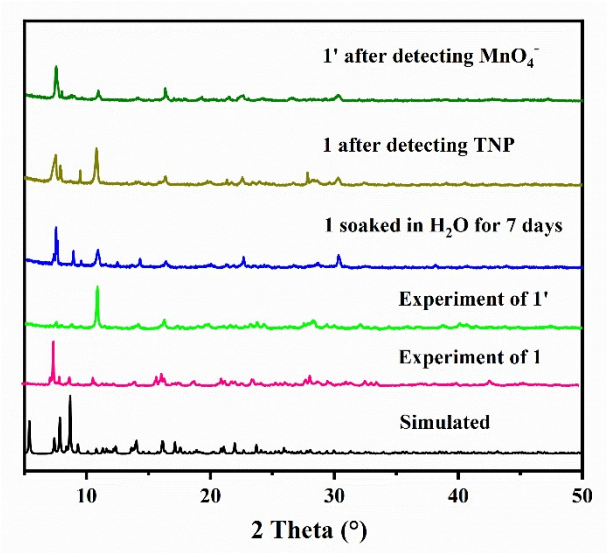

Figure S5. PXRD pattens of **1** and **1'**.

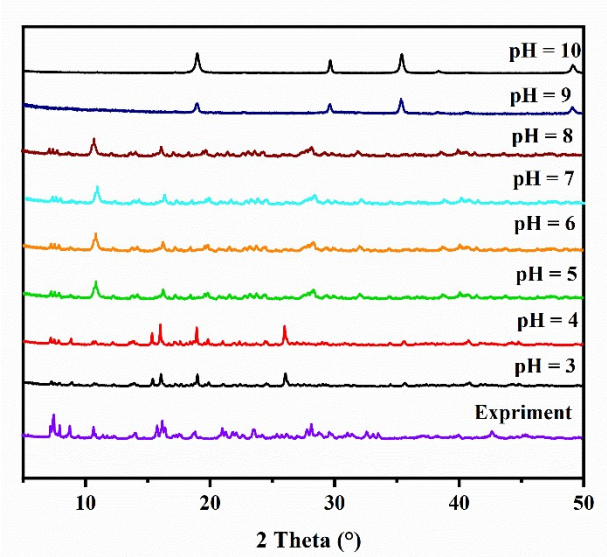

Figure S6. PXRD pattens of **1** in water with different pH values.

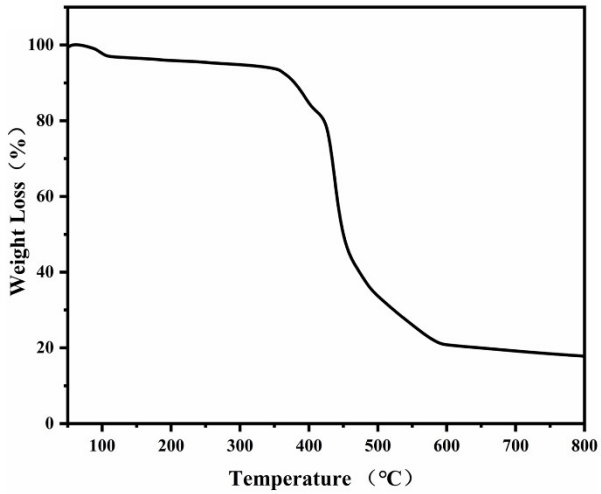

Figure S7. TGA curve of **1**

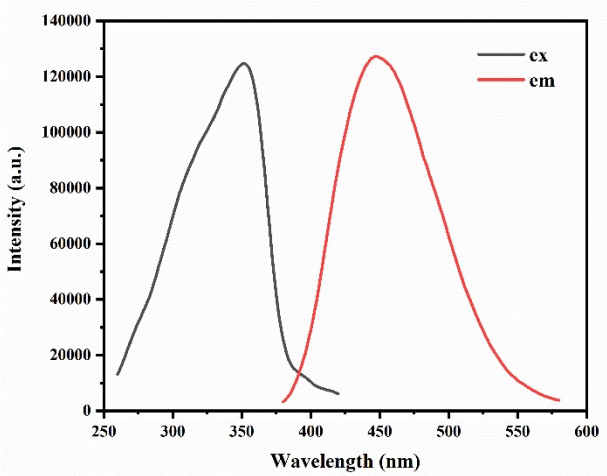

Figure S8. Excitation and emission of **1**.

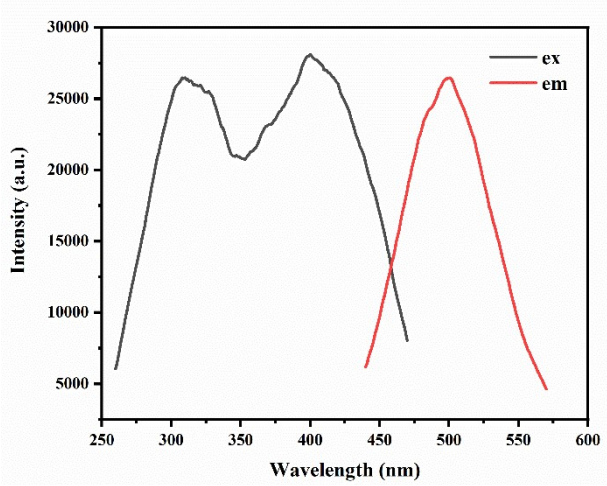

Figure S9. Excitation and emission of **1'**

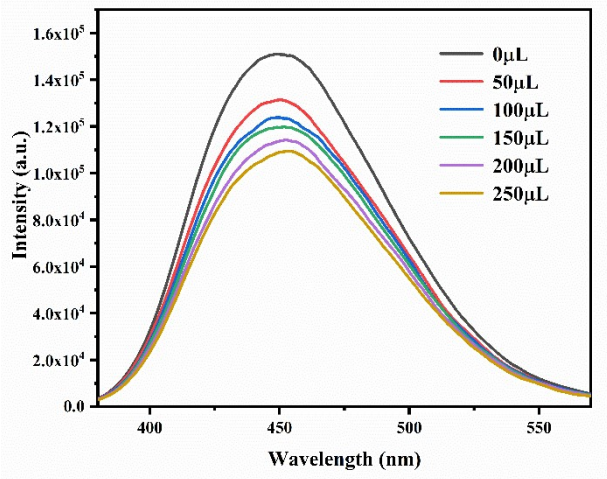

Figure S10. Emission spectra of **1** dispersed in H_2O with the addition of 1,3-DNB solution (1 mM) (λ_{ex} = 350 nm).

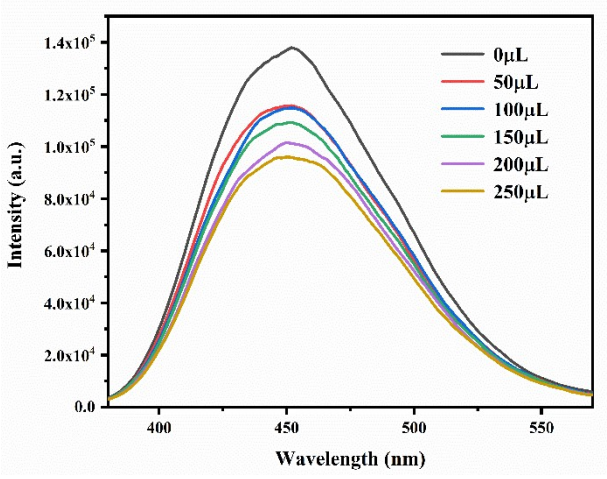

Figure S11. Emission spectra of **1** dispersed in H_2O with the addition of 2,4-DNT

solution (1 mM) (λ_{ex} = 350 nm).

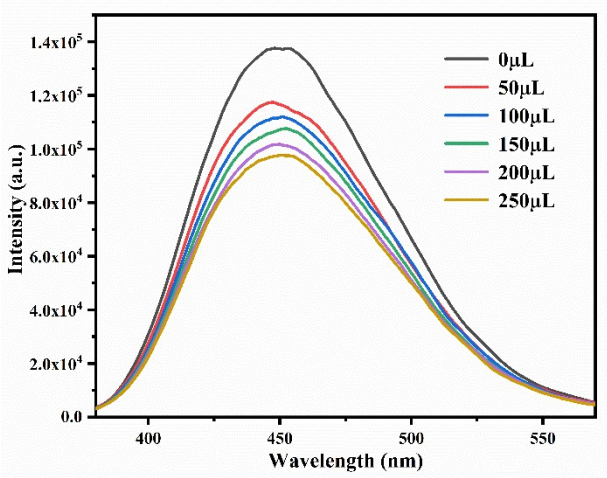

Figure S12. Emission spectra of **1** dispersed in H_2O with the addition of 2,6-DNT solution (1 mM) (λ_{ex} = 350 nm).

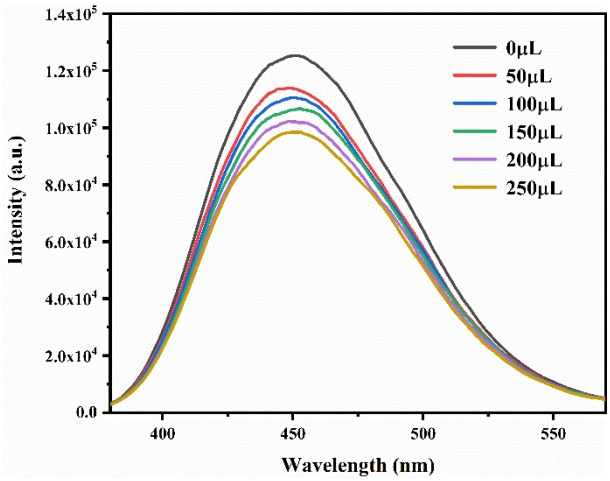

Figure S13. Emission spectra of **1** dispersed in H_2O with the addition of NB solution (1 mM) (λ_{ex} = 350 nm).

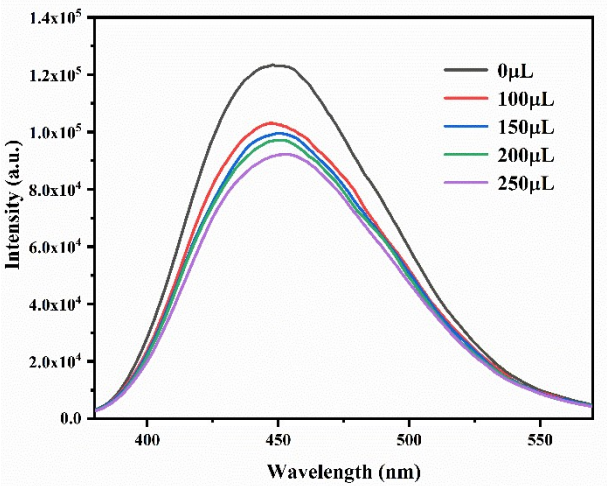

Figure S14. Emission spectra of **1** dispersed in H_2O with the addition of NM

solution (1 mM) (λ_{ex} = 350 nm).

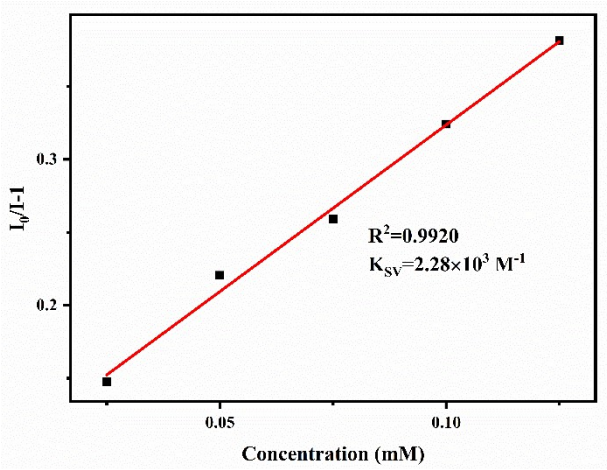

Figure S15. Stern-Volmer plot for 1,3-DNB of **1** in H_2O suspension at the low concentration.

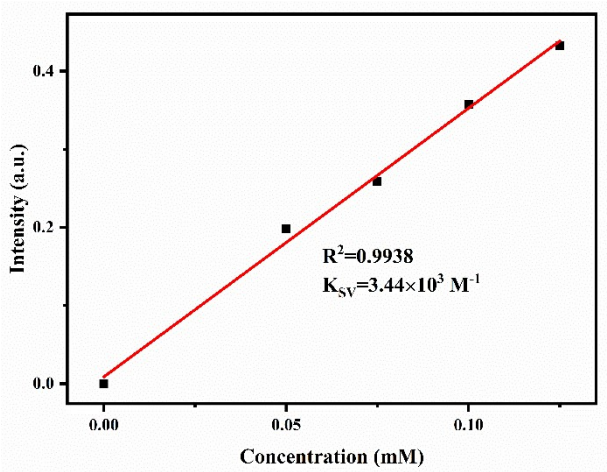

Figure S16. Stern-Volmer plot for 2,4-DNT of **1** in H_2O suspension at the low concentration.

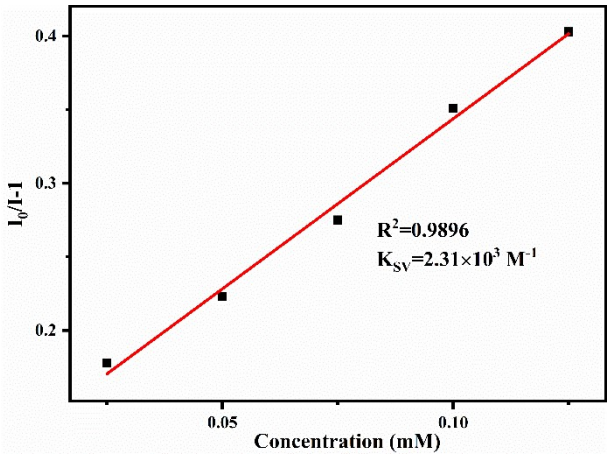

Figure S17. Stern-Volmer plot for 2,6-DNT of **1** in H_2O suspension at the low

concentration.

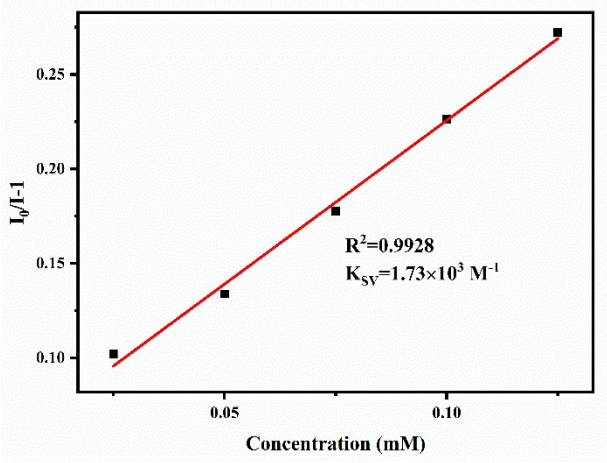

Figure S18. Stern-Volmer plot for NB of **1** in H_2O suspension at the low concentration.

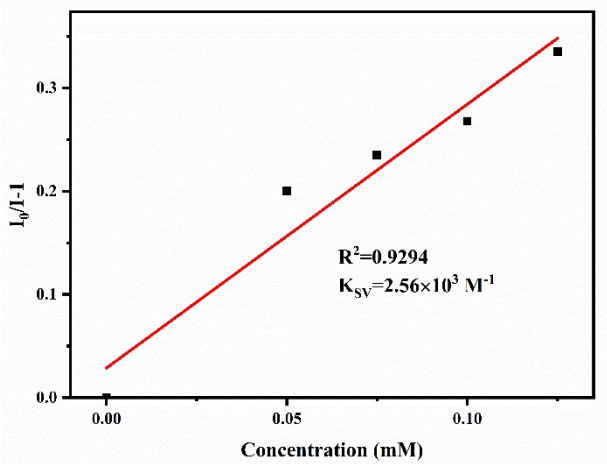

Figure S19. Stern-Volmer plot for NM of **1** in H_2O suspension at the low concentration.

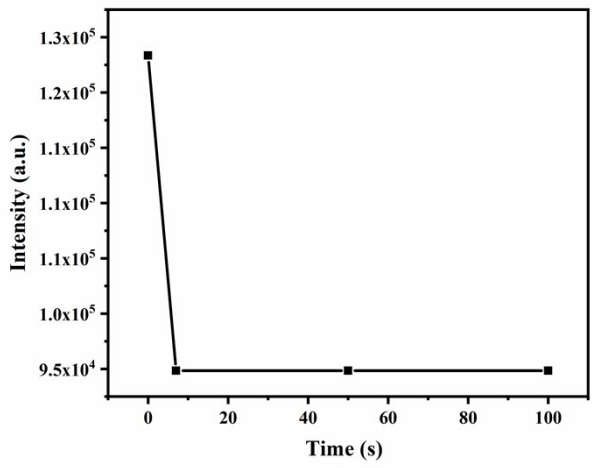

Figure S20. Response time on the Luminescence intensities of **1** after adding 50 μL H_2O solution of TNP (1 mM).

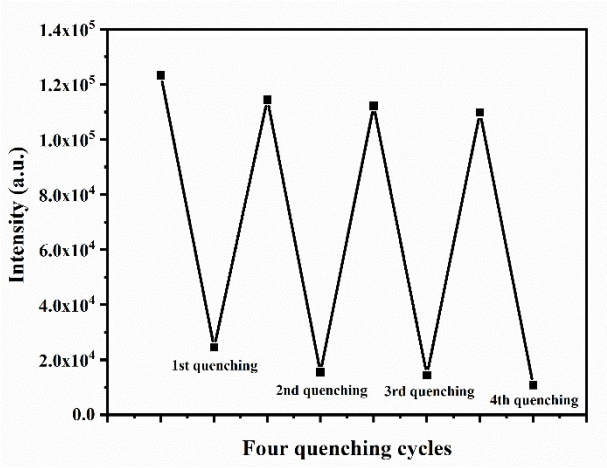

Figure S21. Reproducibility of response capability of **1** for sensing TNP in H_2O.

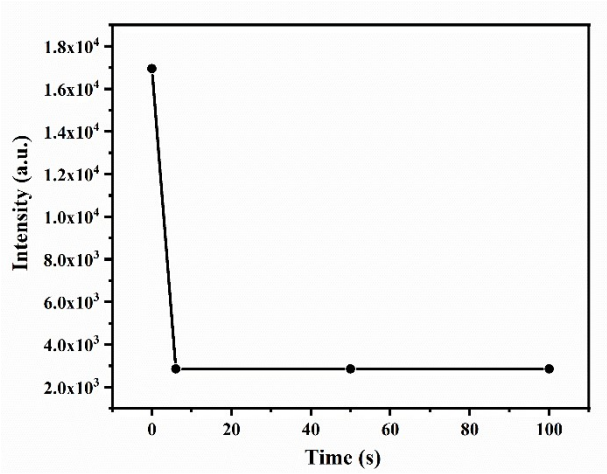

Figure S22. Response time on the Luminescence intensities of **1'** after adding 50 μL H_2O solution of MnO_4^- (2 mM).

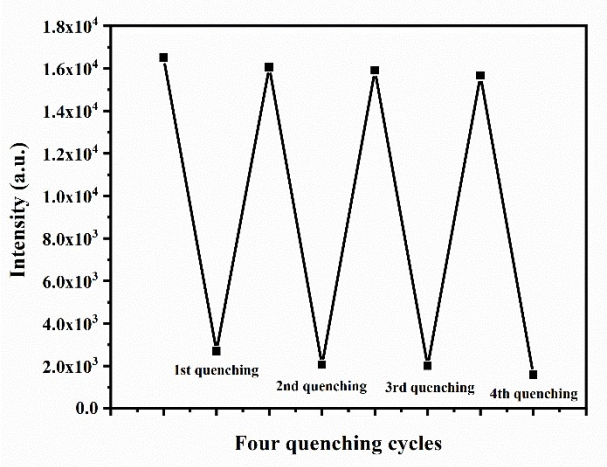

Figure S23. Reproducibility of response capability of **1'** for sensing MnO_4^- in H_2O.

Table S1 Selected bond lengths for **1**.

Bond	Length (Å)	Bond	Length (Å)
Cd(1)-O(4)	2.257(4)	Cd(1)-O(2)	2.310(3)
Cd(1)-O(11)#1	2.319(4)	Cd(1)-N(1)	2.320(4)
Cd(1)-O(12)#1	2.514(3)	Cd(1)-N(4)#2	2.361(4)
N(2)-Cd(2)#3	2.305(4)	Cd(2)-O(3)	2.278(4)
Cd(2)-O(7)#5	2.332(3)	Cd(2)-N(2)#4	2.305(4)
Cd(2)-N(3)#5	2.362(5)	Cd(2)-O(8)#5	2.457(4)

Table S2 Selected bond angles for **1**.

Bond	Angles (°)	Bond	Angles (°)
O(4)-Cd(1)-O(2)	126.82(13)	O(4)-Cd(1)-O(11)#1	93.83(13)
O(2)-Cd(1)-O(11)#1	139.30(12)	O(4)-Cd(1)-N(1)	107.39(15)
O(2)-Cd(1)-N(1)	84.29(13)	O(4)-Cd(1)-N(4)#2	89.57(15)
O(11)#1-Cd(1)-N(1)	85.11(15)	O(11)#1-Cd(1)-N(4)#2	96.87(14)
O(2)-Cd(1)-N(4)#2	83.14(13)	N(1)-Cd(1)-N(4)#2	162.79(15)
O(2)-Cd(1)-O(12)#1	86.40(12)	O(4)-Cd(1)-O(12)#1	143.40(12)
N(1)-Cd(1)-O(12)#1	88.89(14)	O(11)#1-Cd(1)-O(12)#1	54.21(12)
N(4)#2-Cd(1)-O(12)#1	78.65(13)	O(1)-Cd(2)-O(3)	105.62(13)
O(1)-Cd(2)-N(2)#4	109.46(16)	O(3)-Cd(2)-N(2)#4	83.17(15)
O(1)-Cd(2)-O(7)#5	148.37(12)	O(3)-Cd(2)-O(7)#5	104.20(13)
N(2)#4-Cd(2)-O(7)#5	84.30(14)	O(1)-Cd(2)-N(3)#5	90.47(15)
O(3)-Cd(2)-N(3)#5	86.13(15)	N(2)#4-Cd(2)-N(3)#5	159.29(15)
O(7)#5-Cd(2)-N(3)#5	81.20(14)	O(1)-Cd(2)-O(8)#5	94.44(12)
O(3)-Cd(2)-O(8)#5	158.01(13)	N(2)#4-Cd(2)-O(8)#5	98.78(14)
O(7)#5-Cd(2)-O(8)#5	54.60(12)	N(3)#5-Cd(2)-O(8)#5	84.77(14)

Table S3 Hydrogen bonds for **1**.

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	Angle(D-H···A) (°)
C(1)-H(1)···O(3)	0.93	2.52	3.191(7)	128.8
O(5)-H(5A)···O(13)	0.74	1.99	2.691(6)	158.0
C(5)-H(5)···O(12)#1	0.93	2.54	3.229(7)	131.3
C(9)-H(9)···O(2)#3	0.93	2.35	3.203(6)	153.0
O(9)-H(9A)···O(8)#7	0.79	1.90	2.677(5)	166.7
C(10)-H(10)···O(7)#6	0.93	2.39	3.033(7)	126.5
O(14)-H(6)···O(6)	0.905(10)	2.11(5)	2.878(8)	142(7)
O(15)-H(13)···O(13)	0.901(10)	2.09(3)	2.862(7)	143(4)
O(17)-H(17B)···N(2)#8	0.93	2.68	3.505(8)	147.7
C(29)-H(29)···O(2)#6	0.93	2.51	3.092(6)	120.5
C(34)-H(34)···O(10)#8	0.93	2.45	3.207(7)	138.7
C(36)-H(36)···O(15)#7	0.93	2.47	3.254(8)	142.7
C(54)-H(54)···O(1)#9	0.98	2.57	3.406(9)	143.5
O(14)-H(3)···O(13)	0.900(10)	2.204(15)	2.708(8)	114.9(11)

Symmetry transformations used to generate equivalent atoms: #1 x+1, y, z; #2 -x+2, y-1/2, -z+3/2; #3 -x+1, y+1/2, -z+3/2; #4 -x+1, y-1/2, -z+3/2; #5 x-1, y, z; #6 -x+2, y+1/2, -z+3/2; #7 -x+3/2, -y+1, z+1/2; #8 -x+3/2, -y+1, z-1/2; #9 x+1/2, -y+1/2, -z+1.