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An AIE-ligand-based coordination polymer with new wheel-shaped Cd_6 cluster, unique bamboo-like architecture and highly efficient dual-response sensing properties

Jinfang Zhang[a,*], Shunchang Zhao[a], Xingyu Tao[a], Qinghan Chen[a], Dejing Yin[b] and 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*

Materials and methods

H_2L ligand was obtained according to a previously reported procedure.[1] Other purchased chemicals were used without further purification. Powder X-ray diffraction (PXRD) patterns were obtained using Cu $K\alpha_1$ radiation *via* a Bruker D8 X-ray diffractometer. Simulated PXRD patterns were achieved by Mercury 3.3. Thermal analysis was carried out using a TGA/1100SF thermal analyzer between 40 and 1000°C at a heating rate of 20°C min^{-1} under a nitrogen atmosphere at a flow rate of 30 cm^3 min^{-1}. IR spectra (4000-400 cm^{-1}) were obtained from KBr discs using a Nicolet Nexus 470 transform spectrometer. The HITACHI S-4800 field-emission scanning electron microscope was utilized to conduct Energy Dispersive Spectrometer (EDS). Particle size distribution is measured by zeta sizer nano ZS. Luminescent spectra were measured by PTI QM-TM fluorescent spectrometer. Uv-*vis* adsorption spectra were obtained using a TU-1950 spectrophotometer at 293 K.

References

1. Q. Li, X. Wu, X. Huang, X. Xiao, S. Jia, Z. Lin and Y. Zhao, C*rystal Growth & Design*, 2018, **18**, 912-920.

Table S1 Selected bond lengths(Å) for **1**.

Bond	Lengths(Å)	Bond	Lengths(Å)
Cd(1)-O(1)#2	2.290(9)	Cd(2)-O(2)	2.309(10)
Cd(1)-O(2)#2	2.528(9)	Cd(2)-O(3)	2.277(9)
Cd(1)-O(4)#1	2.285(11)	Cd(2)-O(4)	2.506(12)
Cd(1)-O(5)	2.270(9)	Cd(2)-O(6)#3	2.251(10)
Cd(1)-O(6)	2.476(12)	Cd(2)-O(8)#3	2.360(7)
Cd(1)-O(8)	2.360(7)	Cd(2)-O(9)#4	2.499(9)
Cd(1)-O(9)	2.261(9)	Cd(2)-O(10)#4	2.272(9)

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

Bond	Angles(°)	Bond	Angles(°)
O(1)#2-Cd(1)-O(2)#2	53.8(3)	O(2)-Cd(2)-O(4)	97.9(4)
O(1)#2-Cd(1)-O(6)	146.0(4)	O(2)-Cd(2)-O(8)#3	89.9(3)
O(1)#2-Cd(1)-O(8)	137.3(3)	O(2)-Cd(2)-O(9)#4	81.3(3)
O(4)#1-Cd(1)-O(1)#2	88.9(4)	O(3)-Cd(2)-O(2)	94.0(3)
O(4)#1-Cd(1)-O(2)#2	91.1(4)	O(3)-Cd(2)-O(4)	55.2(4)
O(4)#1-Cd(1)-O(6)	81.4(4)	O(3)-Cd(2)-O(8)#3	125.4(3)
O(4)#1-Cd(1)-O(8)	74.3(3)	O(3)-Cd(2)-O(9)#4	146.9(4)
O(5)-Cd(1)-O(1)#2	95.5(3)	O(6)#3-Cd(2)-O(2)	164.2(3)
O(5)-Cd(1)-O(2)#2	147.8(4)	O(6)#3-Cd(2)-O(3)	98.5(4)
O(5)-Cd(1)-O(4)#1	98.4(4)	O(6)#3-Cd(2)-O(4)	81.4(4)
O(5)-Cd(1)-O(6)	54.4(4)	O(6)#3-Cd(2)-O(8)#3	75.0(4)
O(5)-Cd(1)-O(8)	125.3(3)	O(6)#3-Cd(2)-O(9)#4	93.4(4)
O(6)-Cd(1)-O(2)#2	157.7(3)	O(6)#3-Cd(2)-O(10)#4	89.6(4)
O(8)-Cd(1)-O(2)#2	86.9(3)	O(8)#3-Cd(2)-O(4)	70.3(3)
O(8)-Cd(1)-O(6)	70.9(3)	O(8)#3-Cd(2)-O(9)#4	87.5(3)
O(9)-Cd(1)-O(1)#2	98.3(4)	O(9)#4-Cd(2)-O(4)	157.8(3)

O(9)-Cd(1)-O(2)#2	81.6(3)	O(10)#4-Cd(2)-O(2)	98.9(4)
O(9)-Cd(1)-O(4)#1	163.7(4)	O(10)#4-Cd(2)-O(3)	95.5(3)
O(9)-Cd(1)-O(5)	95.5(4)	O(10)#4-Cd(2)-O(4)	147.1(4)
O(9)-Cd(1)-O(6)	100.0(4)	O(10)#4-Cd(2)-O(8)#3	137.5(3)
O(9)-Cd(1)-O(8)	90.7(3)	O(10)#4-Cd(2)-O(9)#4	53.6(3)

Symmetry transformations used to generate equivalent atoms: #1 -x, -x+y, z+1/2; #2 x-y+1, -y+2, z+1/2; #3 -x, -x+y, z-1/2; #4 x-y+1, -y+2, z-1/2

Table S3 Calculated HOMO and LUMO energy levels of **L** from **1** and NACs.

Analytes	HOMO (ev)	LUMO (eV)	Band Gap (eV)
L	-5.779	-2.336	3.443
TNP	-8.237	-3.897	4.340
1,3-DNB	-7.985	-3.431	4.554
2,4-DNT	-7.764	-3.217	4.547
2,6-DNT	-7.644	-3.287	4.357
NB	-7.591	-2.428	5.163
4-NT	-7.654	-2.790	4.864

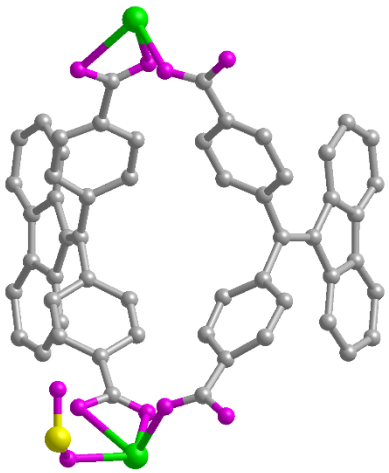

Fig. S1 The asymmetric unit of **1** (C: grey, O: pink, S: yellow and Cd: green, and all H atoms are omitted for clarity).

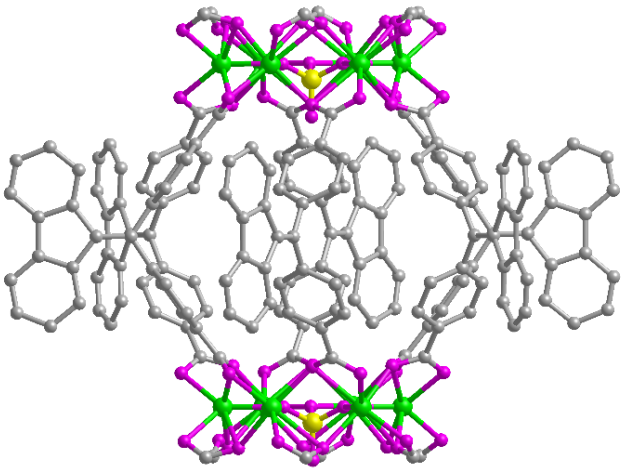

Fig. S2 The angular **L** bridges linking two wheel-shaped $[Cd_6(COO)_{12}SO_4]^{2-}$ hexanuclear clusters (C: grey, O: pink, S: yellow and Cd: green, and all H atoms are omitted for clarity).

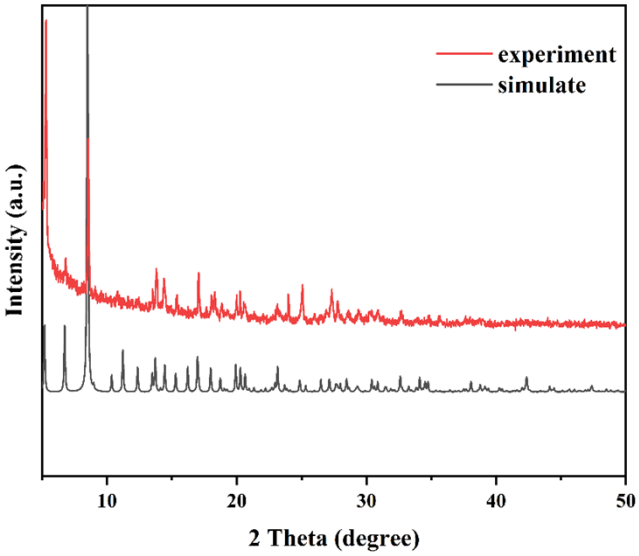

Fig. S3 The PXRD patterns of **1**.

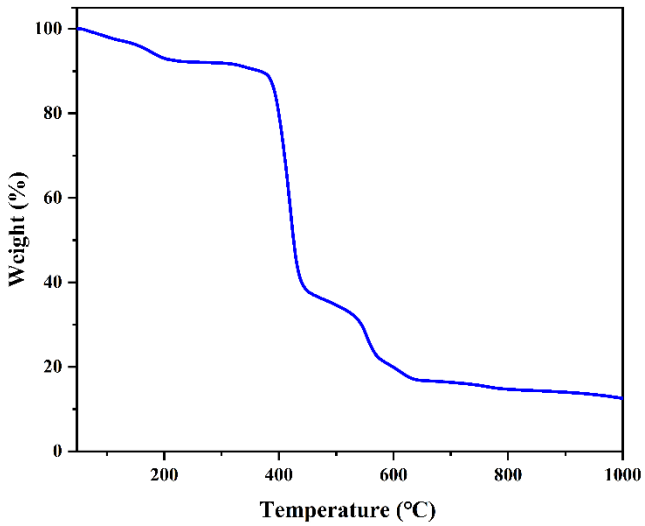

Fig. S4 The TGA curves of **1**.

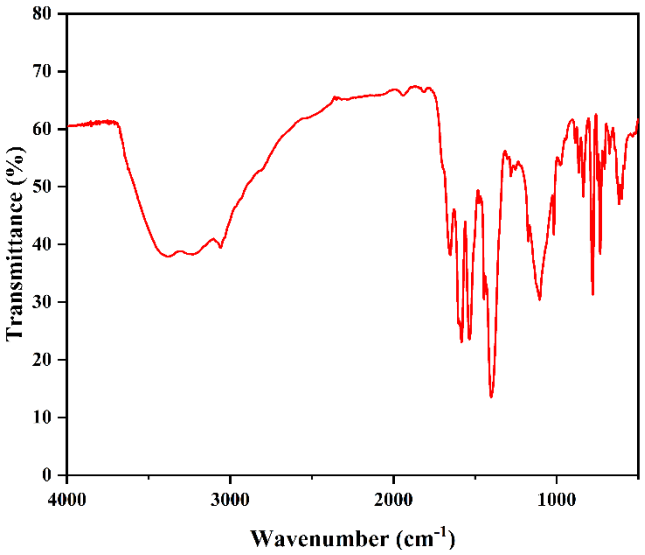

Fig. S5 The IR spectrum of **1**.

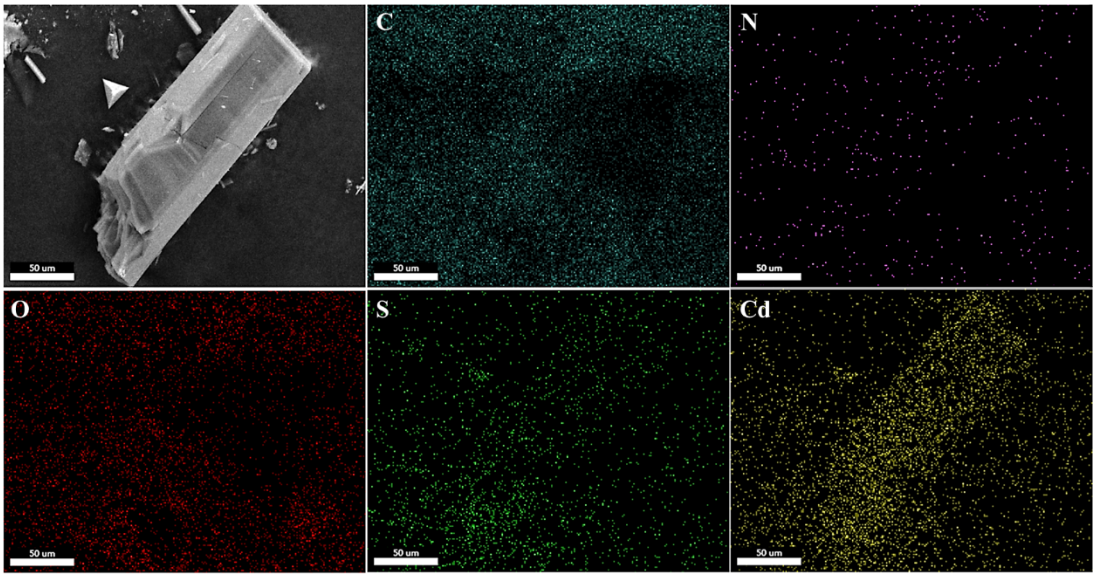

Fig. S6 The Elemental mapping for **1**.

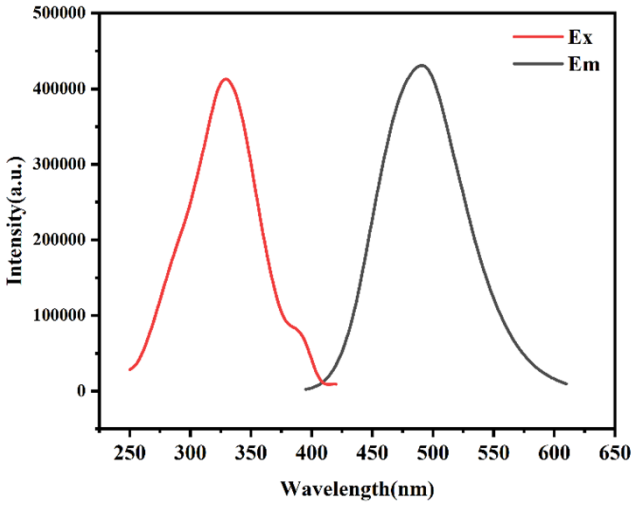

Fig. S7 Excitation and emission spectra of **1**.

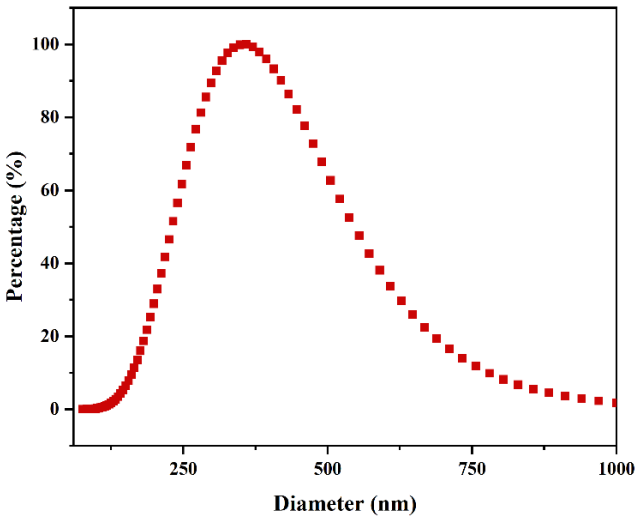

Fig. S8 The particle size distributions of **1** dispersed in H_2O after 48h.