Supporting Information

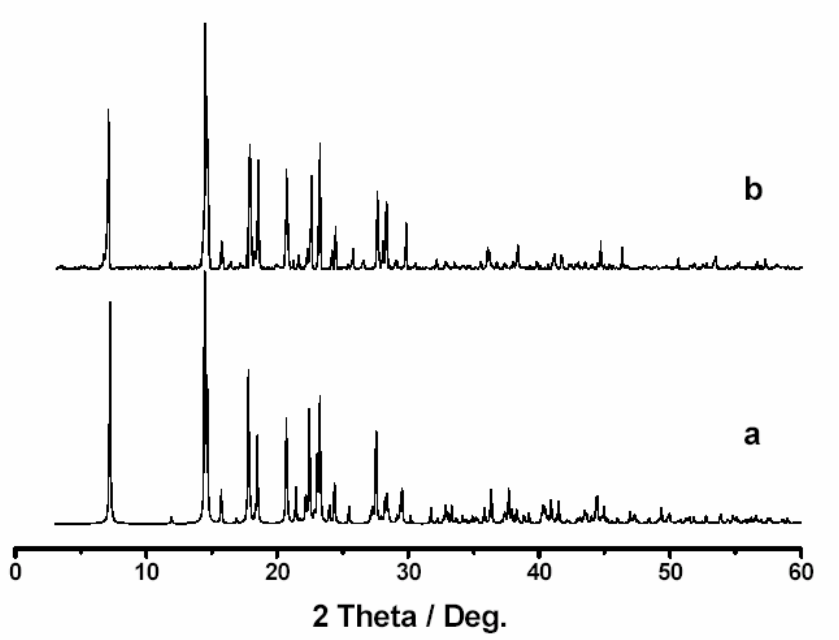
Highly-thermostable metal-organic frameworks (MOFs) of zinc and cadmium 4,4'-(hexafluoroisopropylidene)diphthalates with a unique fluorite topology

Ru-Qiang Zou,[a,b] Rui-Qin Zhong,[a,b] Miao Du,[a] Tetsu Kiyobayashi [a] and Qiang Xu*,[a,b]

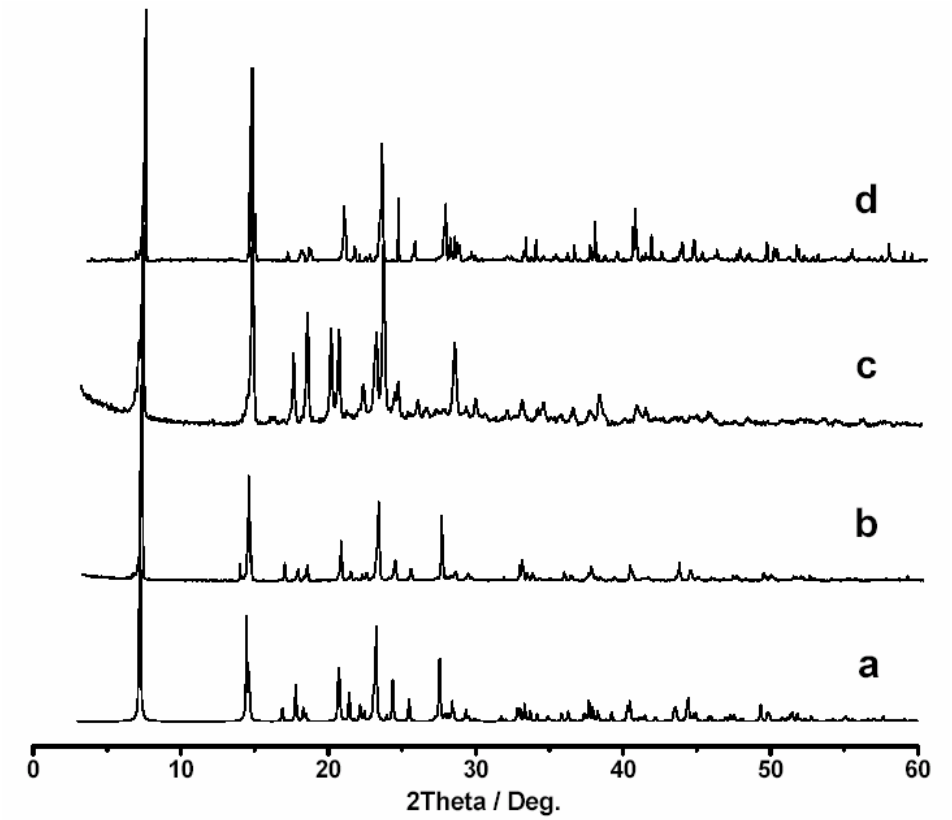
[a] National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, and [b] Graduate School of Science and Technology, Kobe University, Nada Ku, Kobe, Hyogo 657-8501, Japan; E-mail: q.xu@aist.go.jp

Experimental section

Materials and general methods. All the solvents and reagents for synthesis and analysis were commercially available and used as received. IR spectra were recorded on a Bruker ISS/v6 apparatus at a spectral resolution of 2 cm^{-1} accumulating 80 scans. The dry sample powder was mixed by Al_2O_3 and treated directly in the purpose-made diffuse-reflectance IR cell. The latter was connected to a vacuum-adsorption apparatus with a residual pressure below 10^{-3} Pa. The cell allowed the IR measurements to be performed at ambient temperature. Elemental analyses were performed on a Perkin-Elmer 2400 Series II analyzer. Thermogravimetric analysis (TGA) was carried out on a Shimadzu DTG-50 thermal analyzer from room temperature to 600 °C at a ramp rate of 5 °C/min in a helium atmosphere. Powder X-ray diffraction (PXRD) patterns were recorded on a Rigaku X-ray diffractometer at 40 kV, 100 mA for Cu Kα radiation (λ = 1.5406 Å). Solid-state emission spectra were taken on a Perkin Elmer LS50B luminescence spectrophotometer.



SI-1 PXRD patterns of **1**: (a) the simulated one from single crystal data and (b) the original one at room temperature.

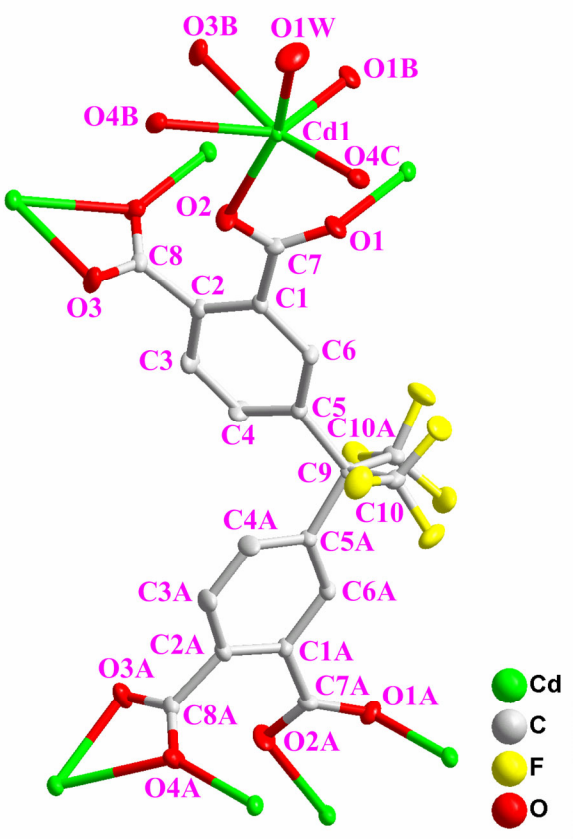


SI-2 PXRD patterns of **2**: (a) the simulated one from single crystal data, (b) the original one at room temperature, (c) the dehydrated one *via* heating to 270 ºC, and (d) the re-hydrated one.

SI-3. Selected bond distances (Å) and angles (°) for complex **1**.

Zn(1)-O(2)	1.941(4)	Zn(1)-O(3)#1	1.927(4)
Zn(1)-O(4)#2	1.962(4)	Zn(1)-O(1)#3	1.992(4)
O(2)-Zn(1)-O(3)#1	110.2(2)	O(2)-Zn(1)-O(4)#2	119.87(19)
O(3)#1-Zn(1)-O(4)#2	118.5(2)	O(2)-Zn(1)-O(1)#3	110.22(19)
O(3)#1-Zn(1)-O(1)#3	98.96(18)	O(4)#2-Zn(1)-O(1)#3	95.26(17)

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

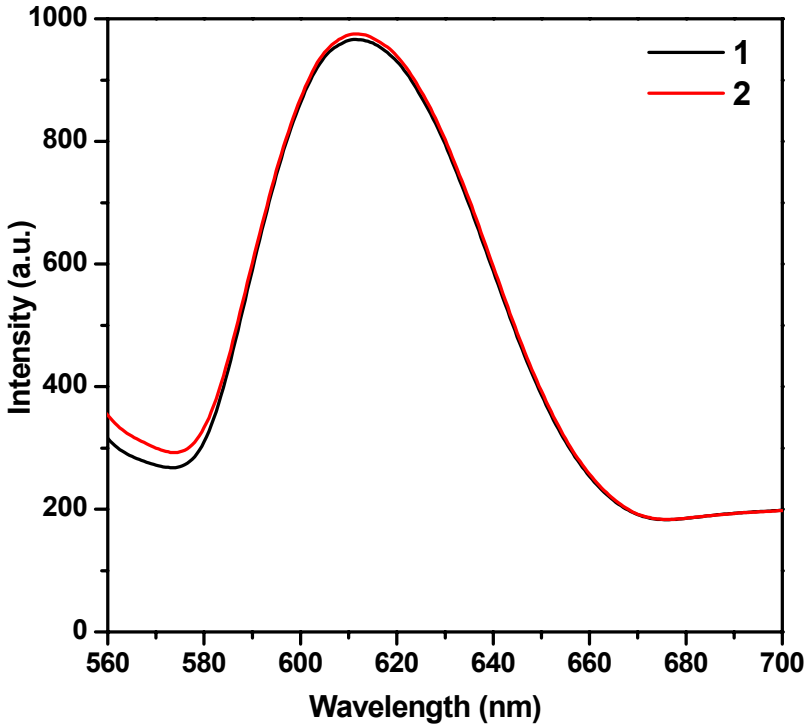


SI-4 A view showing the coordination environment of Cd(II) and the binding mode of **L** ligand. Symmetry codes: A $-x + 1, y, -z + 1/2$; B $-x - 1/2, -y - 1/2, -z + 1$; C $x, -y, z + 1/2$.

SI-5 Selected bond distances (Å) and angles (°) for complex **2**.

Cd(1)-O(4)#1	2.2533(19)	Cd(1)-O(1)#2	2.268(2)
Cd(1)-O(2)	2.284(2)	Cd(1)-O(3)#3	2.293(2)
Cd(1)-O(1W)	2.338(2)	Cd(1)-O(4)#3	2.5579(19)
O(4)#1-Cd(1)-O(1)#2	96.35(9)	O(4)#1-Cd(1)-O(2)	107.81(8)
O(1)#2-Cd(1)-O(2)	108.24(8)	O(4)#1-Cd(1)-O(3)#3	155.56(8)
O(1)#2-Cd(1)-O(3)#3	86.42(7)	O(2)-Cd(1)-O(3)#3	94.19(8)
O(4)#1-Cd(1)-O(1W)	74.11(8)	O(1)#2-Cd(1)-O(1W)	95.43(9)
O(2)-Cd(1)-O(1W)	155.68(10)	O(3)#3-Cd(1)-O(1W)	81.46(9)
O(4)#1-Cd(1)-O(4)#3	119.26(3)	O(1)#2-Cd(1)-O(4)#3	139.70(8)
O(2)-Cd(1)-O(4)#3	79.83(7)	O(3)#3-Cd(1)-O(4)#3	53.32(7)
O(1W)-Cd(1)-O(4)#3	78.43(8)		

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



SI-6 Fluorescent emission spectra of **1** and **2** (λ_{ex} = 456 nm).