

Supporting Information

Tb(III)-functionalized a new layer-like Cd MOF as luminescent probe for highly selectively sensing Cr³⁺

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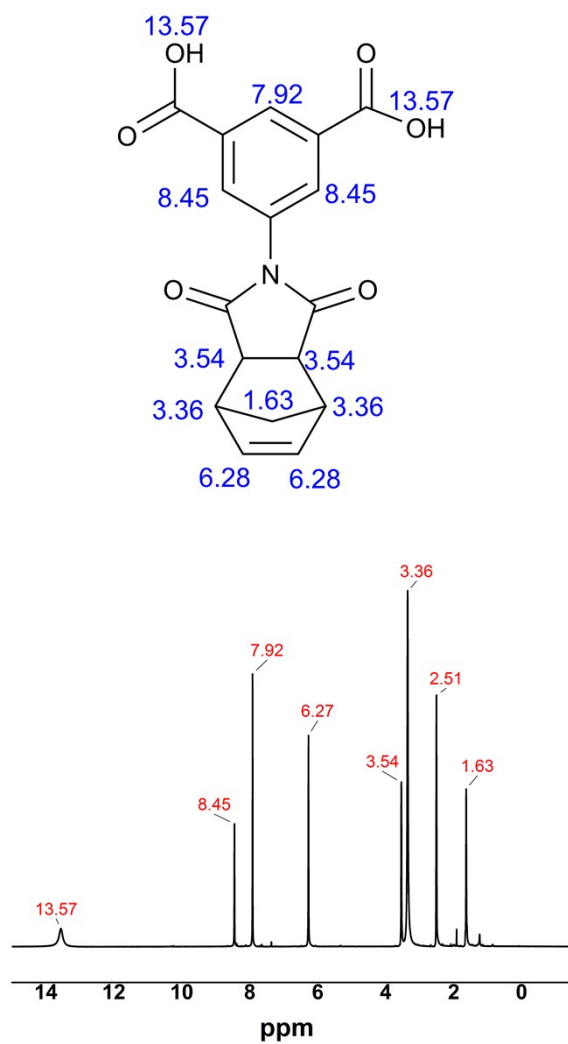


Fig .S1 ¹H-NMR spectrum of organic ligand

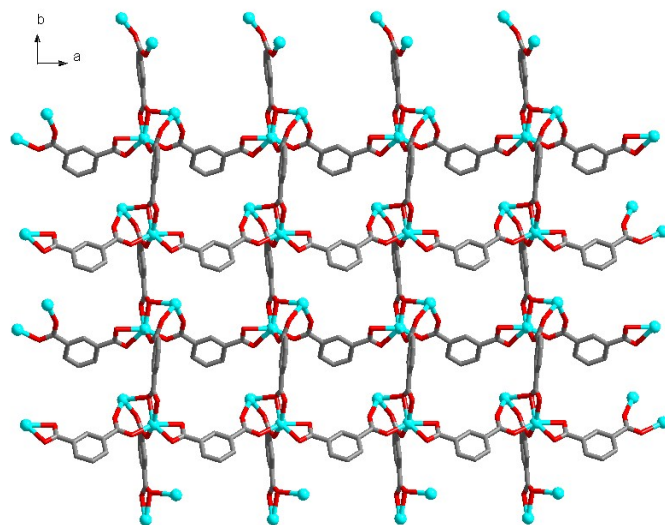


Fig. S2 2D layers of Cd-MOF

Table S1. Crystal data and structure refinement for Cd-MOF.

Identification code	2
Formula weight	2207.31
Crystal system,	Monoclinic
space group	P21

a	10.3650(2) Å
b	15.4064(3) Å
c	28.5396(5)
α	90 deg.
β	94.720(2) deg.
γ	90 deg.
Volume	4541.96(15) Å ³
Z, Calculated density	2, 1.614 Mg/m ³
Absorption coefficient	1.011 mm ⁻¹
F(000)	2228.0
θ range, deg.	2.74 - 27.00
Reflections collected	37227

Refinement method Full-matrix least-squares on F^2

Final R indices [$I > 2\sigma(I)$] $R1 = 0.0457$, $wR2 = 0.0917$

R indices (all data) $R1 = 0.0597$, $wR2 = 0.0994$

Absolute structure parameter $0.41(3)$

Largest diff. peak and hole 0.742 and $-0.575 \text{ e. \AA}^{-3}$

Table S2. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for Cd-MOF.

Cd(1)-O(3)	2.197(5)
Cd(1)-O(7)#1	2.216(5)
Cd(1)-O(2)	2.310(5)
Cd(1)-O(6)	2.335(5)
Cd(1)-O(1)	2.356(4)
Cd(1)-O(5)	2.434(5)
Cd(2)-O(13)	2.236(6)
Cd(2)-O(4)	2.243(5)
Cd(2)-O(8)#1	2.246(5)

Cd(2)-O(14)	2.280(6)
Cd(2)-O(6)	2.324(4)
Cd(2)-O(15)	2.338(4)
O(3)-Cd(1)-O(7)#1	91.3(2)
O(3)-Cd(1)-O(2)	95.71(18)
O(7)#1-Cd(1)-O(2)	105.9(2)
O(3)-Cd(1)-O(6)	110.12(19)
O(7)#1-Cd(1)-O(6)	99.42(17)
O(2)-Cd(1)-O(6)	143.19(17)
O(3)-Cd(1)-O(1)	151.88(19)
O(7)#1-Cd(1)-O(1)	93.7(2)
O(2)-Cd(1)-O(1)	56.34(17)
O(6)-Cd(1)-O(1)	96.34(17)
O(3)-Cd(1)-O(5)	98.2(2)
O(7)#1-Cd(1)-O(5)	154.59(18)
O(2)-Cd(1)-O(5)	96.54(18)
O(6)-Cd(1)-O(5)	55.19(14)
O(1)-Cd(1)-O(5)	89.0(2)
O(13)-Cd(2)-O(4)	91.9(2)
O(13)-Cd(2)-O(8)#1	165.3(2)
O(4)-Cd(2)-O(8)#1	102.3(2)
O(13)-Cd(2)-O(14)	83.9(2)
O(4)-Cd(2)-O(14)	170.8(2)
O(8)#1-Cd(2)-O(14)	82.53(19)

O(13)-Cd(2)-O(6)	90.61(18)
O(4)-Cd(2)-O(6)	91.95(18)
O(8)#1-Cd(2)-O(6)	85.17(17)
O(14)-Cd(2)-O(6)	96.3(2)
O(13)-Cd(2)-O(15)	100.71(19)
O(4)-Cd(2)-O(15)	83.53(19)
O(8)#1-Cd(2)-O(15)	84.86(19)
O(14)-Cd(2)-O(15)	89.1(2)
O(6)-Cd(2)-O(15)	167.91(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+2 #2 -x+1,y-1/2,-z+2
#3 x-1,y,z #4 x+1,y,z #5 -x,y+1/2,-z+1
#6 -x,y-1/2,-z+1

Table S3 The luminescent data of the Cr³⁺ concentration, I and I₀/I-1.

Cr ³⁺ concentration (M)	I	I ₀ /I-1
50*10 ⁻⁶	81980	9.07063
25*10 ⁻⁶	147040	4.61473
10*10 ⁻⁶	356010	1.31901
7.5*10 ⁻⁶	403010	1.04856
5*10 ⁻⁶	431760	0.91215

$2.5 \cdot 10^{-6}$	521580	0.58286
$7.5 \cdot 10^{-7}$	650600	0.26897
$5 \cdot 10^{-7}$	677710	0.21821
$2.5 \cdot 10^{-7}$	700720	0.1782

$I_0=825590$