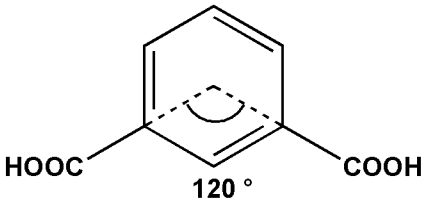
Supporting Information

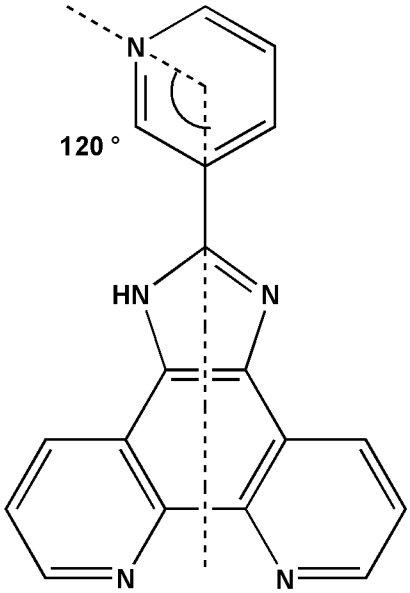
A novel 3D Cd(II) metal-organic framework with an unprecedented (5,6)-connected topology based on isophthalate and 2-(3-pyridyl)imidazo[4,5-*f*]1,10-phenanthroline

Xiuli Wang*, Guocheng Liu, Jinxia Zhang, Yongqiang Chen, Hongyan Lin, Wenyan Zheng

Faculty of Chemistry and Chemical Engineering, Bohai University, Jinzhou 121000, P. R. China



1,3-H_2BDC



PIP

Scheme S1 The ligands used in this paper.

Supporting Information

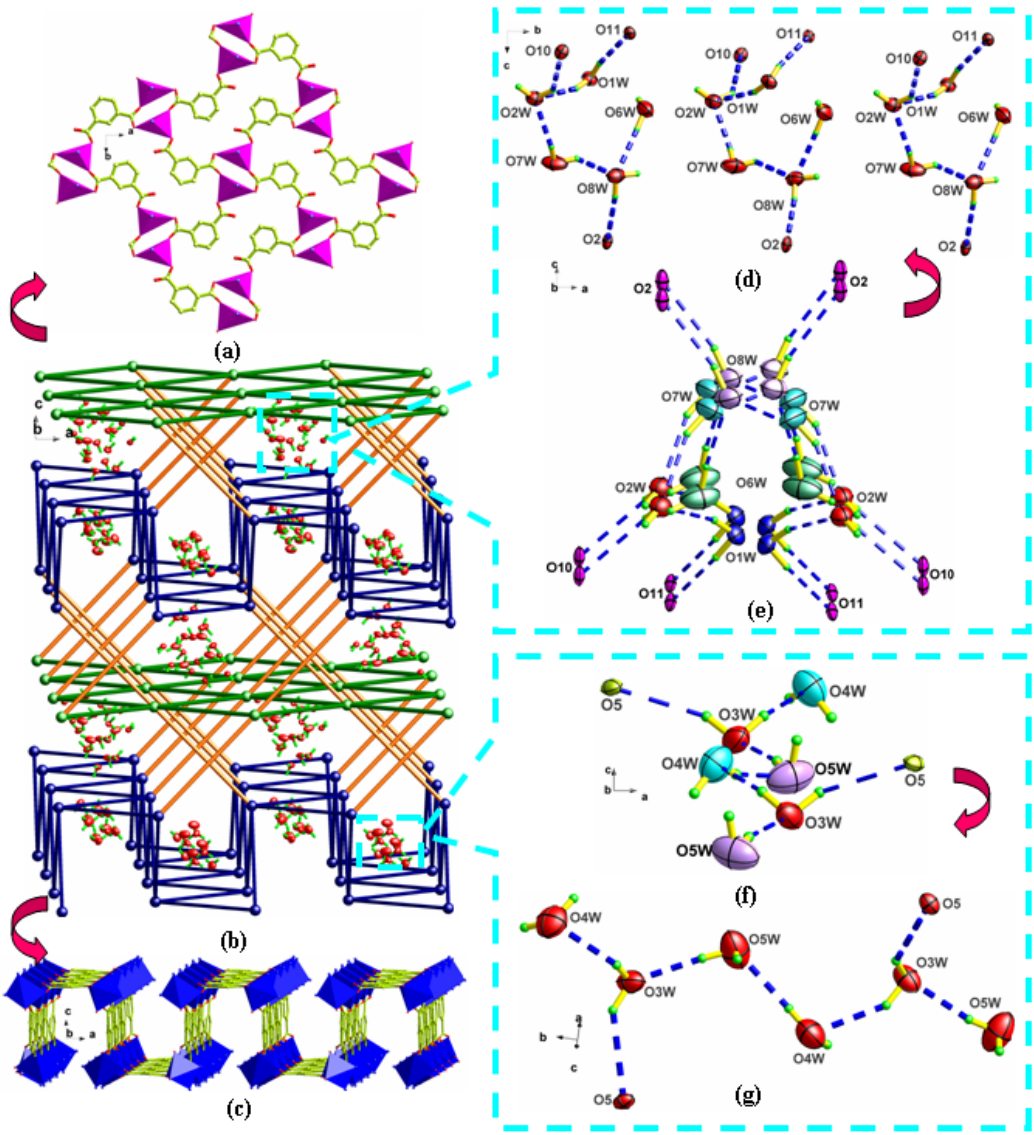


Fig. S1 Schematic view of the 3D framework in **1**. (a) 2D planar SBU based on Cd(II)-1,3-BDC. (b) (5,6)-connected network with two kinds of 1D arrays of water molecules viewed along the *b* axis. (c) 2D flexuous SBU based on Cd(II)-1,3-BDC. (d) 1D supramolecular arrays of incompletely cyclic $(H_2O)_5$ water molecules viewed along the *a* axis, and (e) the *b* axis. (f) 1D zigzag water chain viewed along the *b* axis, and (g) about the *c* axis.

Supporting Information

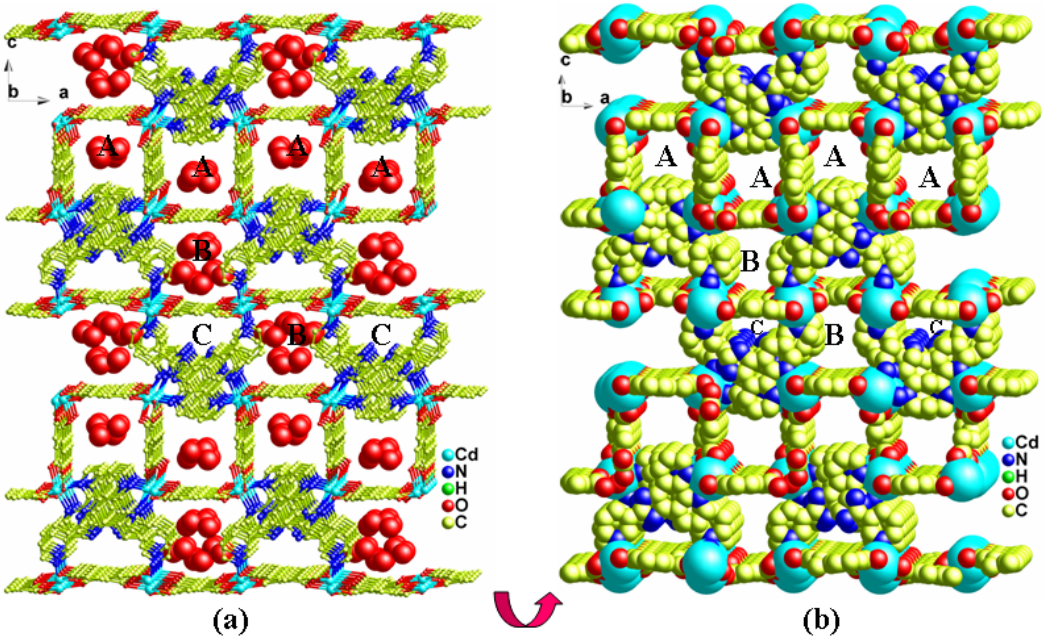


Fig. S2 View of 3-D framework with three kinds of 1-D channels.

Supporting Information

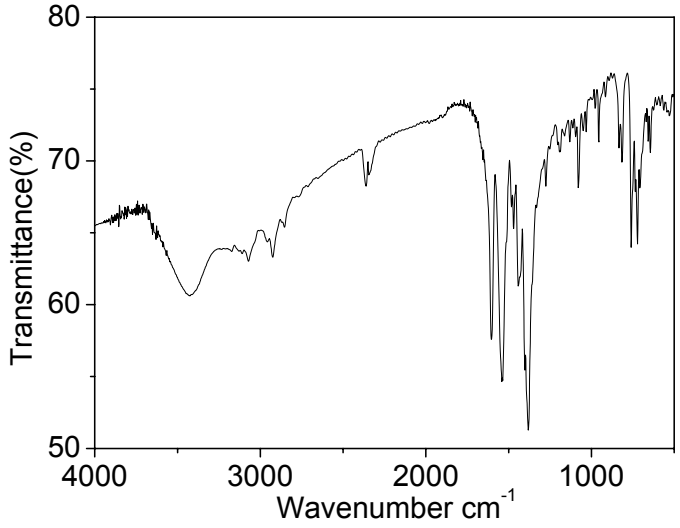


Fig. S3 IR spectrum of **1**. Strong peaks at 1381, 1541 and 1604 cm^{-1} are due to the vibrations of carboxylate groups. The bands in the range of 721–758 cm^{-1} are assigned to the PIP ligands. The strong broad band at around 3423 cm^{-1} was assigned to the vibrations of lattice water molecules in the compound.

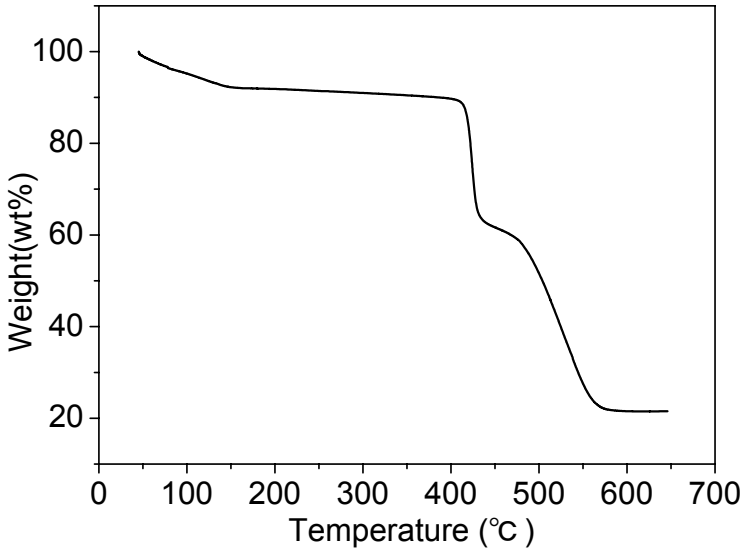


Fig. S4 TG curve of **1**. The TG curve exhibits three weight loss stages in the range of 25—650 °C. The water molecules are eliminated from the framework (calcd. 9.18 %; found 9.21 %) when the temperature is increased from room temperature to about 170 °C. The second and the third weight loss in the range of 400～600 °C was attributed to the decomposition of the framework to form CdO as a final product. (calcd. 21.50 %; found 21.53 %).

Supporting Information

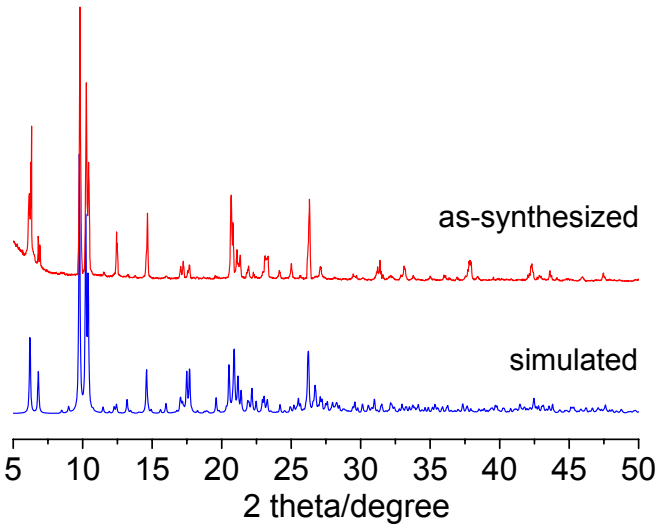


Fig. S5 Power XRD patterns of **1**.

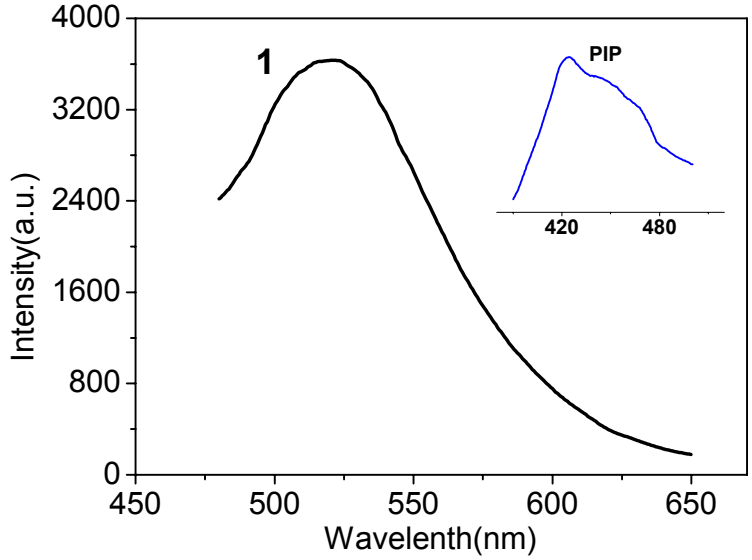


Fig. S6 Luminescence spectra of **1** in solid state.

Supporting Information

Table S1. Selected Bond Distances (Å) and Angles (°) for Complex **1**

Cd(1)–O(7A)	2.225(3)	Cd(1)–O(4)	2.257(3)
Cd(1)–O(6)	2.286(3)	Cd(1)–N(4)	2.311(3)
Cd(1)–N(3)	2.358(3)	Cd(2)–O(2)	2.206(3)
Cd(2)–O(5)	2.230(3)	Cd(2)–N(2)	2.278(3)
Cd(2)–O(3)	2.286(3)	Cd(2)–N(1)	2.320(3)
Cd(3)–O(9B)	2.244(3)	Cd(3)–O(11)	2.280(3)
Cd(3)–N(9)	2.310(3)	Cd(3)–N(10C)	2.315(3)
Cd(3)–O(12C)	2.404(3)		
O(7A)–Cd(1)–O(4)	91.32(12)	O(7A)–Cd(1)–O(6)	87.80(12)
O(4)–Cd(1)–O(6)	91.46(12)	O(7A)–Cd(1)–N(4)	137.81(12)
O(4)–Cd(1)–N(4)	108.47(12)	O(6)–Cd(1)–N(4)	127.04(12)
O(7A)–Cd(1)–N(3)	91.03(12)	O(4)–Cd(1)–N(3)	176.51(13)
O(6)–Cd(1)–N(3)	86.05(11)	N(4)–Cd(1)–N(3)	71.30(11)
O(2)–Cd(2)–O(5)	97.26(12)	O(2)–Cd(2)–N(2)	97.75(12)
O(5)–Cd(2)–N(2)	164.28(12)	O(2)–Cd(2)–O(3)	97.55(12)
O(5)–Cd(2)–O(3)	99.21(12)	N(2)–Cd(2)–O(3)	83.43(11)
O(2)–Cd(2)–N(1)	135.33(12)	O(5)–Cd(2)–N(1)	92.62(12)
N(2)–Cd(2)–N(1)	73.33(12)	O(3)–Cd(2)–N(1)	123.69(12)
O(9B)–Cd(3)–O(11)	141.76(11)	O(9B)–Cd(3)–N(9)	95.41(11)
O(11)–Cd(3)–N(9)	90.12(11)	O(9B)–Cd(3)–N(10C)	89.08(11)
O(11)–Cd(3)–N(10C)	89.41(11)	N(9)–Cd(3)–N(10C)	173.30(13)
O(9B)–Cd(3)–O(12C)	86.70(10)	O(11)–Cd(3)–O(12C)	131.39(10)
N(9)–Cd(3)–O(12C)	87.80(12)	N(10C)–Cd(3)–O(12C)	87.50(11)

Symmetry operations: A) – x + 3, y – 1/2, – z – 1/2; B) x – 1/2, – y – 1/2, – z; C) – x + 4, – y – 1, – z

Supporting Information

Table S2. Hydrogen–Bonding Geometry (Å, °) for complex **1**

D–H···A	D–H	H···A	D···A	<D–H···A
O5W–H5WA···O3W(A)	0.85	1.89	2.730(9)	168
O4W–H4WA···O5W	0.85	1.99	2.820(9)	166
O3W–H3WB···O4W	0.85	2.03	2.772(8)	145
O3W–H3WA···O5	0.85	2.29	2.979(6)	139
O6W–H6WB···O8W(B)	0.85	2.01	2.853(7)	174
O7W–H7WB···O2W(C)	0.85	2.05	2.845(6)	156
O1W–H1WB···O2W(C)	0.85	2.10	2.925(5)	163
O7W–H7WA···O8W	0.85	2.27	2.885(8)	129
O8W–H8WA···O2(D)	0.85	2.18	3.012(6)	166
O2W–H2WA···O10	0.85	2.25	2.904(5)	133
O1W–H1WA···O11	0.85	1.99	2.834(5)	170
N6–H6A···O8(E)	0.88	1.93	2.792(4)	166
N8–H8B–O1(F)	0.88	1.98	2.839(4)	164

Symmetry operations: A) 5/2 – x, 1/2 + y, z; B) 9/2 – x, 1/2 + y, z; C) –1/2 + x, –1/2 – y, –z; D) 1 + x, y, z; E) 1/2 + x, y, –1/2 – z; F) 7/2 – x, –1/2 + y, z.

Supporting Information

The coordinates and point symbols of each vertex

Atom coordinates (Here V1 = $[Cd_2N_4O_6]$ as 5-conntected SBU and V2 = $[Cd_2N_4O_6]$ as 6-conntected SBU)

Name	x	y	z
V1	0.4790	0.4566	0.8269
V2	0.5000	0.0000	0.0000

Connectivity of the selected node with coordinates and distances.
Atom V1 V2 links by bridge ligands and has Common vertex with R (A-A)

Atom V1 composes claster with					R (Å-Å)
V1	0.0210	0.9566	0.8269	(0 0 0)	10.340 Å
V1	0.0210	-0.0434	0.8269	(0-1 0)	10.340 Å
V1	0.5210	-0.0434	0.6731	(1-1 1)	10.509 Å
V1	0.5210	0.9566	0.6731	(1 0 1)	10.509 Å
V2	1.0000	0.5000	1.0000	(0 0 1)	12.632 Å

Atom V2 composes claster with					R (Å-Å)
V2	0.0000	-0.5000	0.0000	(-1-1 0)	10.889 Å
V2	1.0000	0.5000	0.0000	(0 0 0)	10.889 Å
V2	0.0000	0.5000	0.0000	(-1 0 0)	10.889 Å
V2	1.0000	-0.5000	0.0000	(0-1 0)	10.889 Å
V1	-0.0210	0.0434	0.1731	(-1 0 1)	12.632 Å
V1	1.0210	-0.0434	-0.1731	(1-1-1)	12.632 Å

Coordination sequences

V1:	1	2	3	4	5	6	7	8	9	10
Num	5	17	46	99	160	228	316	417	530	659
Cum	6	23	69	168	328	556	872	1289	1819	2478

V2:	1	2	3	4	5	6	7	8	9	10
Num	6	24	56	100	160	234	320	420	536	664
Cum	7	31	87	187	347	581	901	1321	1857	2521

Vertex symbols for selected sublattice
V1 Schläfli symbol: $(4^4.6^6)$
With circuits: $[4.4.4.4.6_3.6_3.6_5.6_5.6_5.6_5]$
V2 Schläfli symbol: $(4^4.6^{10}.8)$
With circuits: $[4.4.4.4.6_2.6_2.6_2.6_2.6_4.6_4.6_8.6_8.6_8.6_8.8_8]$

Supporting Information

The highest symmetry embedding (or Systre key) of this new topology

Highest symmetry group and coordinates in the relaxed cell:

Group: *Cmca*

CELL: 1.48986 4.40042 1.31789 90.0000 90.0000 90.0000

NODE 15 0.00000 0.32555 0.00080

NODE 26 0.00000 0.00000 0.00000 (Explicit edges)

EDGE 0.00000 0.00000 0.00000 0.50000 0.00000 0.50000

EDGE 0.00000 0.32555 0.00080 0.50000 0.32555 -0.50080

EDGE 0.00000 0.00000 0.00000 0.00000 0.17445 -0.49920

EDGE 0.00000 0.32555 0.00080 0.50000 0.17445 -0.00080