Electronic Supplementary Information (ESI) for *CrystEngComm*

Spontaneous chiral resolution of a 3D (3,12)-connected MOF with unprecedented ttt topology consisting of cubic $[Cd_4(\mu_3\text{-}OH)_4]$ cluster and propellerlike ligand

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1. General Information.

All chemicals and solvents used in the syntheses were of analytical grade and used without further purification. IR spectra were recorded on a Nicolet AVATAT FT-IR360 spectrometer as KBr pellets in the frequency range of 4000-400 cm^{-1}. The elemental analyses (C, H, N contents) were determined on a Vario EL III analyzer. Powder X-ray diffraction (PXRD) data were collected on a Philips X'Pert Pro MPD X-ray diffractometer with Cu K_{α} radiation equipped with an X'Celerator detector. Thermogravimetric analyses (TGA) were performed on a Netzsch STA 449C thermal analyzer from room temperature to 800 ° C under nitrogen atmosphere at a heating rate of 10° C/min.

2. Synthesis of [Cd(tipa)(μ_3-OH)·NO_3·EtOH·DMF]$_n$ (1).

A mixture of $Cd(NO_3)_2·4H_2O$ (61.7 mg, 0.2 mmol) and tipa (6.65 mg, 0.015 mmol) were stirred in DMF-EtOH mixed solvent (4 mL, v/v: 1/1). Then aqueous NH_3 solution (25 %) was dropped into the mixture to give a clear solution under ultrasonic treatment. The resultant solution was allowed to evaporate slowly at room temperature for two weeks to give colorless crystals of **1** (yield, 51 %). They were washed with small volumes of cold EtOH and diethyl ether. Anal. for $CdC_{32}H_{35}N_9O_5$: calcd. C 52.07, H 4.78, N 17.08; found C 52.37, H 4.99, N 16.69. IR (KBr): ν (cm^{-1}) = 1661(s), 1521(s), 1384(s), 1305(s), 1117(s), 1062(m), 960 (w), 931 (w), 833 (s), 745 (m), 654 (w).

3. Transformation of 1 to [Cd(tipa)(μ_3-OH)·I_3·DMF]$_n$ (2).

When crystals of **1** were immersed in a solution of DMF-EtOH (*v*:*v* = 1:1) solution of iodine (0.2 mol L^{-1} KI + 0.1 mol L^{-1} I_2) for two weeks, the colour of the crystals changed from colorless to red with no discernible degradation of its macroscopic integrity. They were washed ten times with 20 mL cold EtOH for each time.

4. Crystal structure determination of 1 and 2.

Single crystals of the complexes **1** and **2** with appropriate dimensions were chosen under an optical microscope and quickly coated with high vacuum grease (Dow Corning Corporation) before being mounted on a glass fiber for data collection. Data for them were collected on a Bruker Apex II CCD diffractometer with graphite-monochromated Mo Kα radiation source (λ = 0.71073 Å) at 173K. A preliminary orientation matrix and unit cell parameters were determined from 3 runs of 12 frames each, each frame corresponds to a 0.5^{o} scan in 5 s, followed by spot integration and least-squares refinement. For **1-2**, data were measured using ω scans of 0.5^{o} per frame for 40 s until a complete hemisphere had been collected. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. In all cases, the highest possible space group was chosen. All structures were solved by direct methods using SHELXS-97 and refined on F^2 by full-matrix least-squares procedures with SHELXL-97. Atoms were located from iterative examination of difference *F*-maps following least squares refinements of the earlier models. Hydrogen atoms were placed in calculated positions and included as riding atoms with isotropic displacement parameters 1.2-1.5 times U_{eq} of the attached C atoms. All structures were examined using the Addsym subroutine of PLATON to assure that no additional symmetry could be applied to the models. Pertinent crystallographic data collection and refinement parameters are collated in Table S1. Selected bond lengths and angles are collated in Table S2.

5. Table S1. Crystal Data Collection and Structure Refinement for 1*Δ* and 1*Λ*.

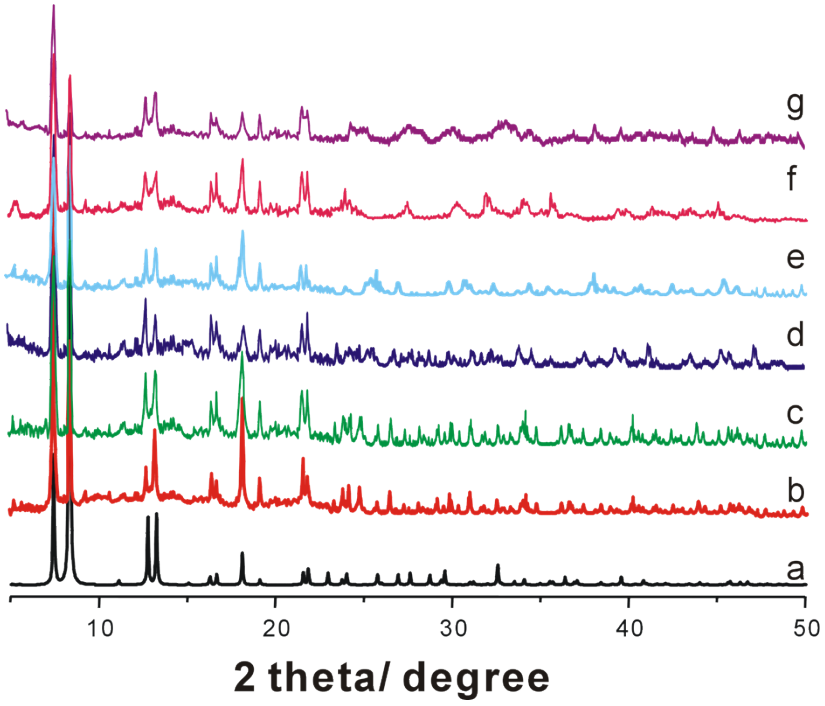
Complex	**1*Δ***	**1*Λ***
Empirical formula	$C_{32}H_{35}CdN_9O_6$	$C_{32}H_{35}CdN_9O_6$
Formula weight	754.09	754.09
Temperature/K	173(2)	173(2)
Crystal system	cubic	cubic
Space group	F23	F23
a/Å	25.3961(9)	25.704(3)
b/Å	25.3961(9)	25.704(3)
c/Å	25.3961(9)	25.704(3)
α/°	90.00	90.00
β/°	90.00	90.00
γ/°	90.00	90.00
Volume/Å^3	16379.5(10)	16983(3)
Z	16	16
ρ_{calc}mg/mm^3	1.223	1.180
μ/mm^{-1}	0.580	0.560
F(000)	6176.0	6176.0
2Θ range for data collection	5.32 to 50°	5.26 to 49.94°
Reflections collected	18992	10189
Independent reflections	2412[R(int) = 0.0810]	2402[R(int) = 0.0826]
Data/restraints/parameters	2412/72/97	2402/0/109
Final R indexes [I>=2σ (I)]	R_1 = 0.0689, wR_2 = 0.1884	R_1 = 0.0529, wR_2 = 0.1259
Final R indexes [all data]	R_1 = 0.0955, wR_2 = 0.2091	R_1 = 0.0811, wR_2 = 0.1337
Largest diff. peak/hole / e Å^{-3}	0.66/-0.29	0.51/-0.32
Flack parameter	-0.08(13)	0.04(8)

6. Table S2. Selected bond lengths (Å) in 1*Δ* and 1*Λ*.

1*Δ*			
Cd1—N1^{i}	2.271 (9)	Cd1—O1	2.450 (7)
Cd1—N1^{ii}	2.271 (9)	Cd1—O1^{iii}	2.450 (7)
Cd1—N1	2.271 (9)	Cd1—O1^{iv}	2.450 (7)
N1^{i}—Cd1—N1^{ii}	87.4 (3)	N1—Cd1—O1^{iii}	93.3 (3)
N1^{i}—Cd1—N1	87.4 (3)	O1—Cd1—O1^{iii}	85.8 (4)
N1^{ii}—Cd1—N1	87.4 (3)	N1^{i}—Cd1—O1^{iv}	93.3 (3)
N1^{i}—Cd1—O1	178.9 (3)	N1^{ii}—Cd1—O1^{iv}	93.5 (3)
N1^{ii}—Cd1—O1	93.3 (3)	N1—Cd1—O1^{iv}	178.9 (3)
N1—Cd1—O1	93.5 (3)	O1—Cd1—O1^{iv}	85.8 (4)
N1^{i}—Cd1—O1^{iii}	93.5 (3)	O1^{iii}—Cd1—O1^{iv}	85.8 (4)
N1^{ii}—Cd1—O1^{iii}	178.9 (3)		
Symmetry codes: (i) −*y*+1/2, −*z*+1/2, *x*; (ii) *z*, −*x*+1/2, −*y*+1/2; (iii) −*x*+1/2, *y*, −*z*+1/2; (iv) −*x*+1/2, −*y*+1/2, *z*.			

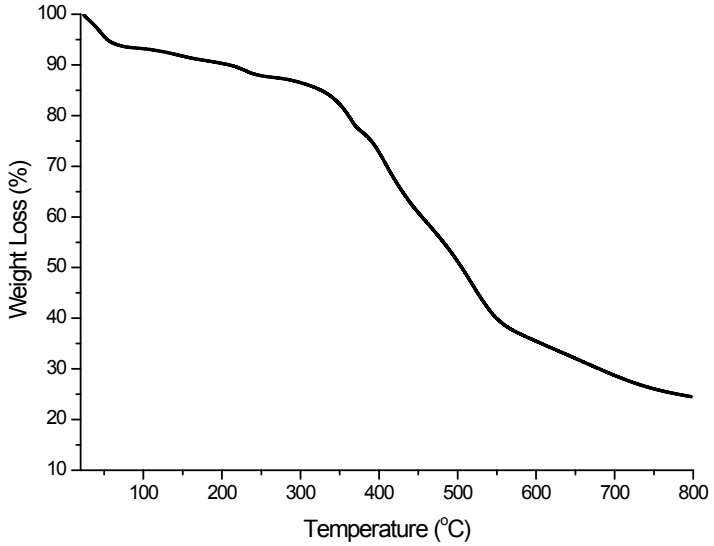
1*Λ*			
Cd1—N1	2.347 (6)	Cd1—O1^{iii}	2.529 (5)
Cd1—N1^{i}	2.347 (6)	Cd1—O1	2.529 (5)
Cd1—N1^{ii}	2.347 (6)	Cd1—O1^{iv}	2.529 (5)
N1—Cd1—N1^{i}	86.6 (2)	N1^{ii}—Cd1—O1	93.1 (2)
N1—Cd1—N1^{ii}	86.6 (2)	O1^{iii}—Cd1—O1	86.8 (3)
N1^{i}—Cd1—N1^{ii}	86.6 (2)	N1—Cd1—O1^{iv}	179.68 (17)
N1—Cd1—O1^{iii}	93.1 (2)	N1^{i}—Cd1—O1^{iv}	93.1 (2)
N1^{i}—Cd1—O1^{iii}	93.5 (2)	N1^{ii}—Cd1—O1^{iv}	93.5 (2)
N1^{ii}—Cd1—O1^{iii}	179.68 (17)	O1^{iii}—Cd1—O1^{iv}	86.8 (3)
N1—Cd1—O1	93.5 (2)	O1—Cd1—O1^{iv}	86.8 (3)
N1^{i}—Cd1—O1	179.68 (17)		
Symmetry codes: (i) −*y*+1, *z*+1/2, −*x*+1/2; (ii) −*z*+1/2, −*x*+1, *y*−1/2; (iii) −*x*+1/2, −*y*+3/2, *z*; (iv) *x*, −*y*+3/2, −*z*+1/2; (v) −*z*+1, *x*+1/2, −*y*+3/2; (vi) *y*−1/2, −*z*+3/2, −*x*+1.			

7. Figure S1. XRD patterns.



a) **1** simulated, b) **1** measured, c) the solid after the anion-exchange with d) $NaClO_4$, e) NH_4PF_6, and f) $NaBF_4$. g) iodine-included **1**.

8. Figure S2. The TGA for 1.



Thermogravimetry indicates complex **1** releases lattice solvent molecules start around the room temperature and the complete loss all solvents (DMF and EtOH) to 330 °C (Cal. 16.1%; Found. 15.3%), then the guest–free framework begins to decompose above 330 °C along with the release of NO_3^-, OH^- and organic ligands. These results are well agreement with crystal structure of **1**.

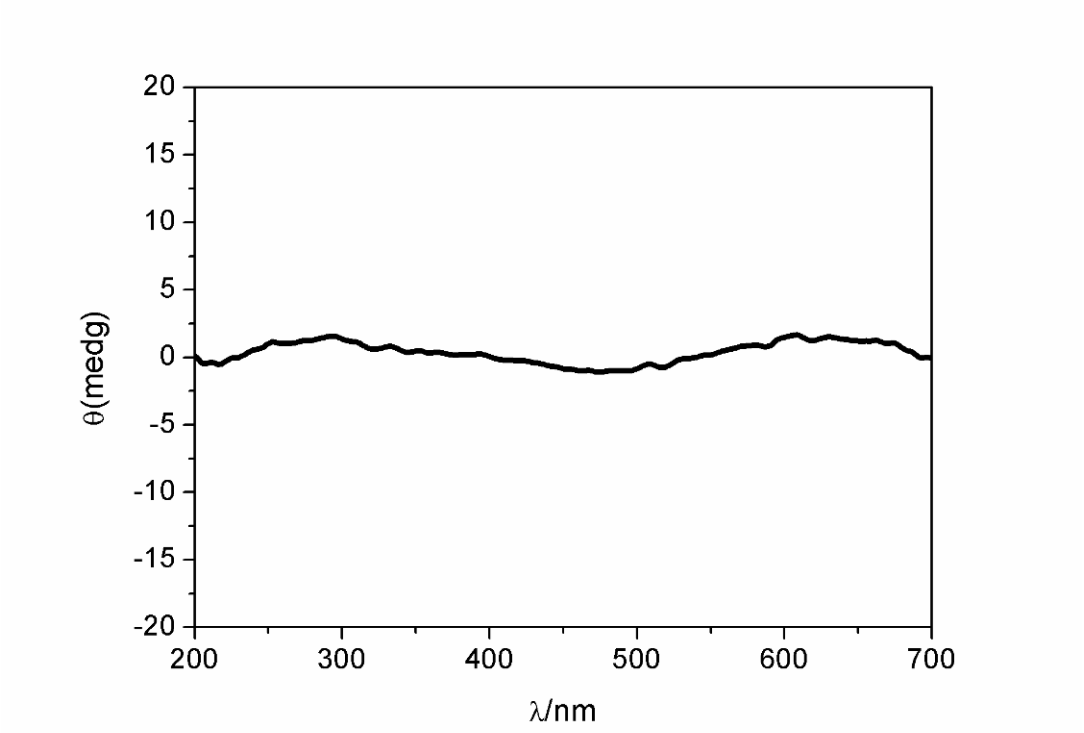
9 Table S3. The comparison between reported (3,12)-connected networks and 1.

Formulae	topology	Schläfli symbol	reference	Cluster-based SBU
$[Na_{0.5}Zn_{4.75}(\mu_3\text{-}OH)_2(BTB)_2(HBTB)(H_2O)_{0.5}]\cdot 5DMF\cdot 1.5EtOH\cdot 10H_2O$ (H_3BTB=Benzene-1,3,5-tribenzoic acid)	N/A	$\{4^{12}\cdot 6^{36}\cdot 8^{18}\}_2\{4^{12}\cdot 6^{24}\cdot 8^{30}\}\{4^3\}_{12}$	*Chem. Commun.*, **2008**, 34, 4019	$[NaZn_6(\mu_3\text{-}OH)_2(COO)_{12}]$ and $[Zn_7(\mu_3\text{-}OH)_4(COO)_8(COO)_8(H_2O)_2]$
$[Co_5(\mu_3\text{-}OH)_2(5\text{-}NH_2\text{-}bdc)_4(H_2O)_2]\cdot 37.5H_2O$ (5-NH_2-bdc=5-aminoisophthalate)	N/A	$\{4^{19}\cdot 6^{27}\cdot 8^{20}\}\{4^3\}_4$	*Cryst. Growth & Des.,* **2009**, 9, 4239	$[Co_5(\mu_3\text{-}OH)_2]$
$[Ln_4(OH)_4(3\text{-}SBA)_4(H_2O)_4]\cdot nH_2O$, [Ln=Eu, n=10; Gd, n=10; Tb, n=8; 3-SBA= 3-sulfobenzoate]	N/A	$\{4^{20}\cdot 6^{28}\cdot 8^{18}\}\{4_3\}_4$	*Inorg. Chem.* **2010**, 49, 1865	$[Ln_4(OH)_4]$
$[Co_8(\mu_3\text{-}OH)_4(SO_4)_2(dcpbpy)_4(H_2O)_4]\cdot 12DMF\cdot 4EtOH\cdot 24H_2O$ (H_2dcpbpy=2,6-di-pcarboxyphenyl-4,4'-bipyridine)	N/A	$\{4^{12}\cdot 6^{34}\cdot 8^{20}\}\{4_3\}_4$	*Chem. Commun.*, **2010**, 46, 6311	$[Co_8(\mu_3\text{-}OH)_4(SO_4)_2]$
$[Zn_8(\mu_3\text{-}OH)_4(oba)_6(bbi)(H_2O)_2]$, ($H_2$oba= 4,4′-oxybis(benzoate), bbi=1,1′-(1,4-butanediyl)bis(imidazole))	N/A	$\{3^2\cdot 4\}^2\{3^8\cdot 4^{2\cdot 2}\cdot 5^{16}\cdot 6^{18}\cdot 7^2\}$	*Cryst. Growth & Des,* **2008**, 8, 3490.	$[Zn_8(\mu_3\text{-}OH)_4]$
$[Ln(TTP)_2]\cdot(CF_3SO_3)_3\cdot C_3H_6O\cdot 5H_2O$ (Ln = Eu,Gd)	N/A	$\{4^{20}\cdot 6^{28}\cdot 8^{18}\}\{4^3\}_4$	*Chem. Commun.,* **2011**, 47, 4234.	Ln_2
$[Cd(tipa)(\mu_3\text{-}OH)\cdot NO_3\cdot EtOH\cdot DMF]_n$ (tipa = tris(4-(1H-imidazol-1-yl)phenyl)amine)	**ttt**	$\{4^{12}\cdot 6^{42}\cdot 8^{12}\}\{4^3\}_4$	This work	$[Cd_4(\mu_3\text{-}OH)_4]$

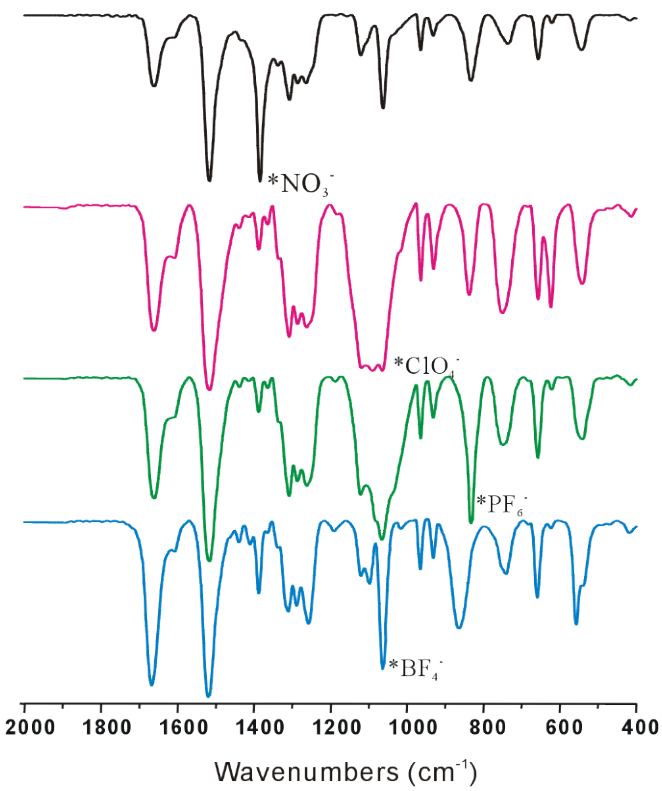
As we know, only limited (3,12)-connected coordinated networks have been documented until now. Hardie et. al., reported the first (3,12)-connected supramolecular network built up by hydrogen bonds between tetrameric clusters of cyclotriveratrylene. Then, Chen group reported the first (3,12)-connected coordination

network based on heptanuclear heterometallic [$NaZn_6(\mu_3\text{-}OH)_2(COO)_{12}$] cluster, following this work, they obtained another octanuclear [$Co_8(\mu_3\text{-}OH)_4(SO_4)_2(COO)_8$] cluster based (3,12)-connected network with a Schläfli symbol of $\{4^{12}\cdot6^{34}\cdot8^{20}\}\{4^3\}_4$. Su et. al., also show us a dinuclear Ln cluster based (3,12)-connected network with a Schläfli symbol of $\{4^{20}\cdot6^{28}\cdot8^{18}\}\{4^3\}_4$.

10. Figure S3. The CD spectrum of all crystals of a single batch for 1.



11. Figure S4. The FT-IR spectra of anion-exchange for 1.

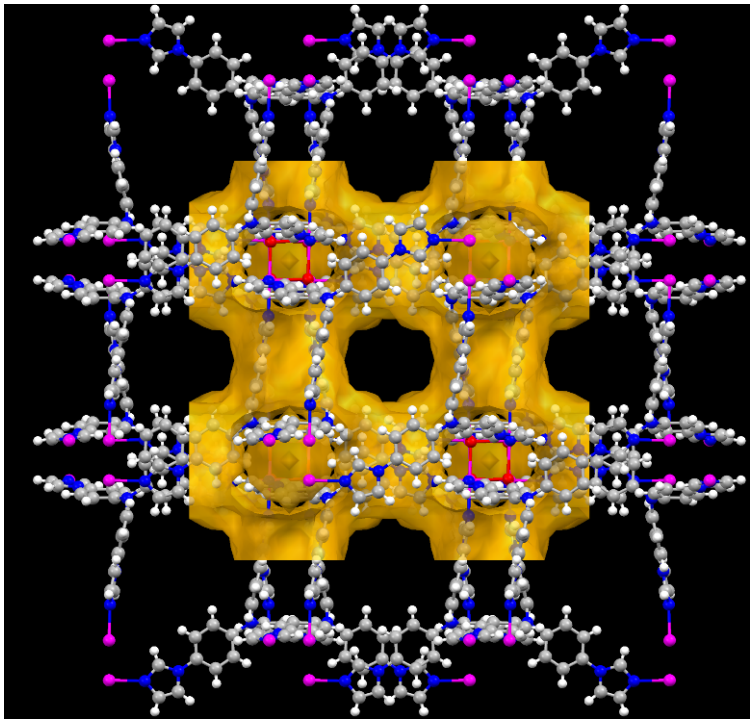


FT-IR spectra of the as-synthesized complex **1** (black), the solid sample treated with saturated DMF solution of $NaClO_4$ (pink), NH_4PF_6 (green), and $NaBF_4$ (cyan).

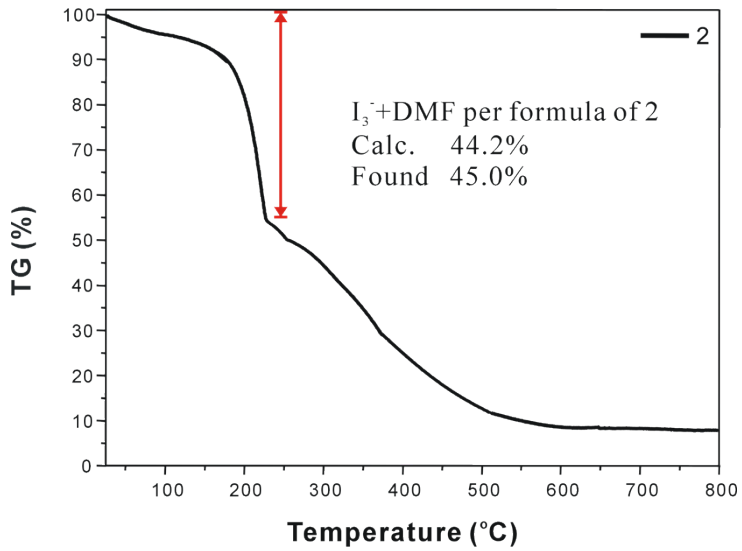
12. Table S4. Crystal Data Collection and Structure Refinement for 2

Empirical formula	$C_{32}H_{35}CdN_9O_6$
Formula weight	754.09
Temperature/K	120(2)
Crystal system	Cubic
Space group	F23
a/Å	25.49(3)
b/Å	25.49(3)
c/Å	25.49(3)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	16556(32)
Z	16
ρ_{calc}mg/mm^3	1.210
m/mm^{-1}	0.574
F(000)	6176.0
Crystal size/mm^3	0.12 × 0.10 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.3 to 49.92°
Index ranges	$-30 \le h \le 28$, $-30 \le k \le 20$, $-22 \le l \le 29$
Reflections collected	14740
Independent reflections	2445 [R_{int} = 0.1424]
Data/restraints/parameters	2445/24/109
Goodness-of-fit on F^2	0.833
Final R indexes [I>=2σ (I)]	R_1 = 0.0594, wR_2 = 0.1264
Final R indexes [all data]	R_1 = 0.1095, wR_2 = 0.1411
Largest diff. peak/hole / e Å^{-3}	0.57/-0.34
Flack parameter	0.17(9)

13. Figure S5. The porous structure of 1⊿.



14. Figure S6. The TGA and Elemental Analysis for 2.



Analysis calculated for $C_{30}H_{29}O_2N_8CdI_3$ (**2**): C 35.09, H 2.85, N 10.91 %; found: C 35.82, H 2.91, N 11.24 %.

15. TOPOS result.

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1:C27 H21 Cd N7 O

##################

Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Ti 1	-0.2500	0.7500	0.2500	(0 1 0)	10.734A	1
Ti 1	0.2500	0.2500	0.2500	(0 0 0)	10.734A	1
Ti 1	0.2500	0.7500	0.7500	(0 1 1)	10.734A	1

Topology for Ti1

Atom Ti1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 1	0.1465	-0.1465	0.1465	(0 0 0)	10.734A	1
Sc 1	-0.1465	0.3535	0.3535	(0 1 0)	10.734A	1
Sc 1	0.3535	0.1465	0.6465	(0 0 0)	10.734A	1
Sc 1	-0.1465	0.1465	0.1465	(0-1 0)	10.734A	1
Sc 1	0.3535	0.3535	-0.1465	(1 0 0)	10.734A	1
Sc 1	0.1465	0.6465	0.3535	(0 0 0)	10.734A	1
Sc 1	0.3535	-0.1465	0.3535	(0 0 1)	10.734A	1
Sc 1	0.6465	0.3535	0.1465	(0 0 0)	10.734A	1
Sc 1	0.1465	0.1465	-0.1465	(0-1-1)	10.734A	1
Sc 1	0.6465	0.1465	0.3535	(1 0 1)	10.734A	1
Sc 1	0.1465	0.3535	0.6465	(0 1 1)	10.734A	1
Sc 1	0.3535	0.6465	0.1465	(1 1 0)	10.734A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with TiSc4

Coordination sequences

Sc1:	1	2	3	4	5	6	7	8	9	10
Num	3	30	22	144	61	336	120	608	199	960
Cum	4	34	56	200	261	597	717	1325	1524	2484

Ti1: 1 2 3 4 5 6 7 8 9 10

Num 12 12 88 42 244 92 480 162 796 252

Cum 13 25 113 155 399 491 971 1133 1929 2181

TD10=2423

Vertex symbols for selected sublattice

Sc1 Point symbol:{4^3}

Extended point symbol:[4.4.4]

Ti1 Point symbol:{4^12.6^42.8^12}

Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(4).6(4).6(4).6(4).6(4).6(4).8(20).8(20).8(20).8(20).8(20).8(20).8(20).8(20).8(20).8(20).8(20).8(20)]

Point symbol for net: {4^12.6^42.8^12}{4^3}4

3,12-c net with stoichiometry (3-c)4(12-c); 2-nodal net

Topological type: ttt; Be5Au (topos&RCSR.ttd) {4^12.6^42.8^12}{4^3}4 - VS [4.4.4] [4.4.4.4.4.4.4.4.4.4.4.4.6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(4).6(4).6(4).6(4).6(4).6(4).8(4).8(4).8(4).8(4).8(4).8(4).8(4).8(4).8(4).8(4).8(4).8(4)] (72849 types in 11 databases)

Non-equivalent circuits

Circuit No 1; Type=4a; Centroid: (0.000,0.500,0.302)

Atom	x	y	z
Sc1	0.1465	0.6465	0.3535
Ti1	0.2500	0.2500	0.2500
Sc1	-0.1465	0.3535	0.3535
Ti1	-0.2500	0.7500	0.2500

Circuit No 2; Type=6a; Centroid: (0.899,0.101,0.351)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465
Ti1	0.7500	-0.2500	0.2500

Sc1	0.6465	0.1465	0.3535
Ti1	0.7500	0.2500	0.7500
Sc1	0.8535	0.3535	0.3535

Circuit No 3; Type=6b; Centroid: (0.899,0.052,0.399)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465
Ti1	0.7500	-0.2500	0.2500
Sc1	0.6465	-0.1465	0.6465
Ti1	0.7500	0.2500	0.7500
Sc1	0.8535	0.3535	0.3535

Circuit No 4; Type=6c; Centroid: (0.351,0.851,0.149)

Atom	x	y	z
Ti1	0.2500	1.2500	0.2500
Sc1	0.1465	0.8535	0.1465
Ti1	0.2500	0.7500	-0.2500
Sc1	0.3535	0.6465	0.1465
Ti1	0.7500	0.7500	0.2500
Sc1	0.3535	0.8535	0.3535

Circuit No 5; Type=6d; Centroid: (0.448,0.052,0.948)

Atom	x	y	z
Ti1	0.2500	0.2500	1.2500
Sc1	0.1465	-0.1465	1.1465
Ti1	0.2500	-0.2500	0.7500
Sc1	0.6465	-0.1465	0.6465
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	0.3535	1.1465

Circuit No 6; Type=8a; Centroid: (0.787,0.213,0.250)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500

Sc1	0.6465	0.3535	0.1465
Ti1	0.2500	0.2500	0.2500
Sc1	0.3535	-0.1465	0.3535
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 7; Type=8b; Centroid: (0.750,0.250,0.250)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500
Sc1	0.3535	0.6465	0.1465
Ti1	0.2500	0.2500	0.2500
Sc1	0.3535	-0.1465	0.3535
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 8; Type=8c; Centroid: (0.823,0.250,0.250)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500
Sc1	0.6465	0.3535	0.1465
Ti1	0.2500	0.2500	0.2500
Sc1	0.6465	0.1465	0.3535
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 9; Type=8d; Centroid: (0.912,0.250,0.338)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500
Sc1	0.8535	0.3535	0.3535
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	0.1465	0.3535
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 10; Type=8e; Centroid: (0.011,0.250,0.438)

Atom	x	y	z
Ti1	0.2500	0.2500	0.2500
Sc1	0.1465	0.6465	0.3535
Ti1	0.2500	0.7500	0.7500
Sc1	0.1465	0.3535	0.6465
Ti1	-0.2500	0.2500	0.7500
Sc1	-0.3535	0.1465	0.3535
Ti1	-0.2500	-0.2500	0.2500
Sc1	0.1465	-0.1465	0.1465

Circuit No 11; Type=8f; Centroid: (0.974,0.287,0.438)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	1.2500	0.7500	0.7500
Sc1	0.8535	0.6465	0.6465
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	0.1465	0.3535
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 12; Type=8g; Centroid: (0.912,0.287,0.375)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500
Sc1	0.8535	0.6465	0.6465
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	0.1465	0.3535
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 13; Type=8h; Centroid: (0.912,0.213,0.375)

Atom	x	y	z

Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500
Sc1	0.8535	0.3535	0.3535
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	-0.1465	0.6465
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 14; Type=8i; Centroid: (0.011,0.213,0.474)

Atom	x	y	z
Ti1	0.2500	0.2500	0.2500
Sc1	0.1465	0.6465	0.3535
Ti1	0.2500	0.7500	0.7500
Sc1	0.1465	0.3535	0.6465
Ti1	-0.2500	0.2500	0.7500
Sc1	-0.3535	-0.1465	0.6465
Ti1	-0.2500	-0.2500	0.2500
Sc1	0.1465	-0.1465	0.1465

Circuit No 15; Type=8j; Centroid: (0.974,0.250,0.474)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	1.2500	0.7500	0.7500
Sc1	0.8535	0.6465	0.6465
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	-0.1465	0.6465
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 16; Type=8k; Centroid: (0.912,0.250,0.412)

Atom	x	y	z
Ti1	1.2500	0.2500	0.2500
Sc1	1.1465	0.6465	0.3535
Ti1	0.7500	0.7500	0.2500
Sc1	0.8535	0.6465	0.6465
Ti1	0.7500	0.2500	0.7500

Sc1	0.6465	-0.1465	0.6465
Ti1	0.7500	-0.2500	0.2500
Sc1	1.1465	-0.1465	0.1465

Circuit No 17; Type=8l; Centroid: (0.375,0.213,0.912)

Atom	x	y	z
Ti1	0.2500	0.2500	1.2500
Sc1	0.3535	0.6465	1.1465
Ti1	0.2500	0.7500	0.7500
Sc1	0.3535	0.3535	0.8535
Ti1	0.7500	0.2500	0.7500
Sc1	0.6465	-0.1465	0.6465
Ti1	0.2500	-0.2500	0.7500
Sc1	0.1465	-0.1465	1.1465

Circuit No 18; Type=8m; Centroid: (0.474,0.213,0.011)

Atom	x	y	z
Ti1	0.2500	0.2500	0.2500
Sc1	0.3535	0.6465	0.1465
Ti1	0.7500	0.7500	0.2500
Sc1	0.6465	0.3535	0.1465
Ti1	0.7500	0.2500	-0.2500
Sc1	0.6465	-0.1465	-0.3535
Ti1	0.2500	-0.2500	-0.2500
Sc1	0.1465	-0.1465	0.1465

Circuit No 19; Type=8n; Centroid: (0.338,0.250,0.912)

Atom	x	y	z
Ti1	0.2500	0.2500	1.2500
Sc1	0.3535	0.6465	1.1465
Ti1	0.2500	0.7500	0.7500
Sc1	0.3535	0.3535	0.8535
Ti1	0.7500	0.2500	0.7500
Sc1	0.3535	0.1465	0.6465
Ti1	0.2500	-0.2500	0.7500
Sc1	0.1465	-0.1465	1.1465

Circuit No 20; Type=8o; Centroid: (0.437,0.250,0.011)

Atom	x	y	z
Ti1	0.2500	0.2500	0.2500
Sc1	0.3535	0.6465	0.1465
Ti1	0.7500	0.7500	0.2500
Sc1	0.6465	0.3535	0.1465
Ti1	0.7500	0.2500	-0.2500
Sc1	0.3535	0.1465	-0.3535
Ti1	0.2500	-0.2500	-0.2500
Sc1	0.1465	-0.1465	0.1465

Circuit No 21; Type=8p; Centroid: (0.437,0.287,0.974)

Atom	x	y	z
Ti1	0.2500	0.2500	1.2500
Sc1	0.3535	0.6465	1.1465
Ti1	0.7500	0.7500	1.2500
Sc1	0.6465	0.6465	0.8535
Ti1	0.7500	0.2500	0.7500
Sc1	0.3535	0.1465	0.6465
Ti1	0.2500	-0.2500	0.7500
Sc1	0.1465	-0.1465	1.1465

Circuit No 22; Type=8q; Centroid: (0.375,0.287,0.912)

Atom	x	y	z
Ti1	0.2500	0.2500	1.2500
Sc1	0.3535	0.6465	1.1465
Ti1	0.2500	0.7500	0.7500
Sc1	0.6465	0.6465	0.8535
Ti1	0.7500	0.2500	0.7500
Sc1	0.3535	0.1465	0.6465
Ti1	0.2500	-0.2500	0.7500
Sc1	0.1465	-0.1465	1.1465

Circuit No 23; Type=8r; Centroid: (0.250,0.250,0.823)

Atom	x	y	z
Ti1	0.2500	0.2500	1.2500
Sc1	0.3535	0.6465	1.1465

Ti1	0.2500	0.7500	0.7500
Sc1	0.1465	0.3535	0.6465
Ti1	0.2500	0.2500	0.2500
Sc1	0.3535	0.1465	0.6465
Ti1	0.2500	-0.2500	0.7500
Sc1	0.1465	-0.1465	1.1465

Elapsed time: 7.84 sec.