Supporting Information for

A serials of Zn(II) and Cd(II) coordination compounds based on 4-(4*H*-1,2,4-triazol-4-yl)benzoic acid: synthesis, structure and photoluminescent properties

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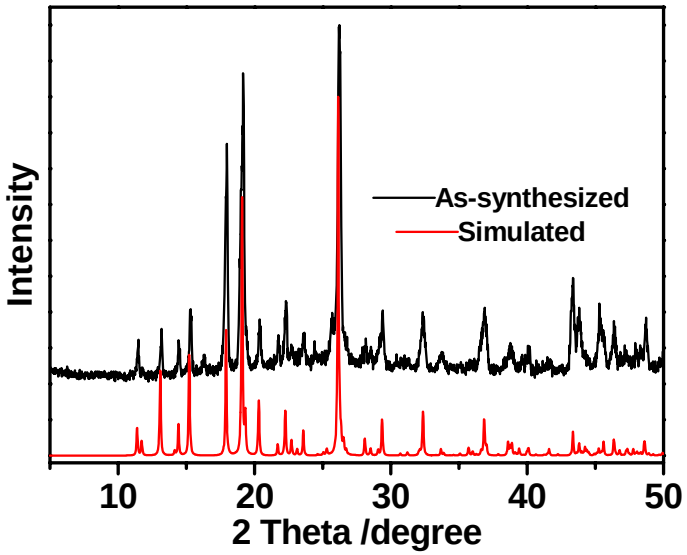

Fig. S1 PXRD of **1**.

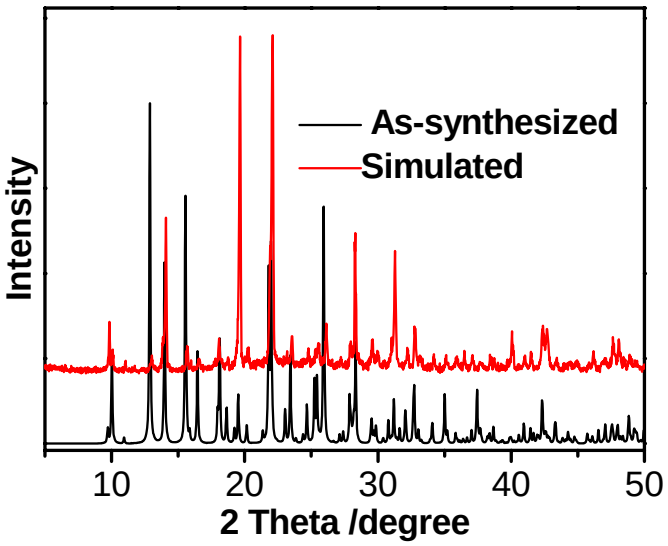

Fig. S2 PXRD of **2**.

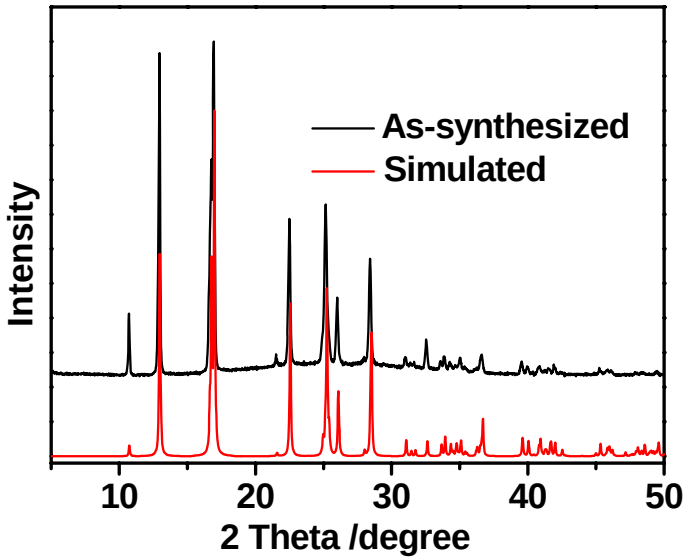

Fig. S3 PXRD of **3**.

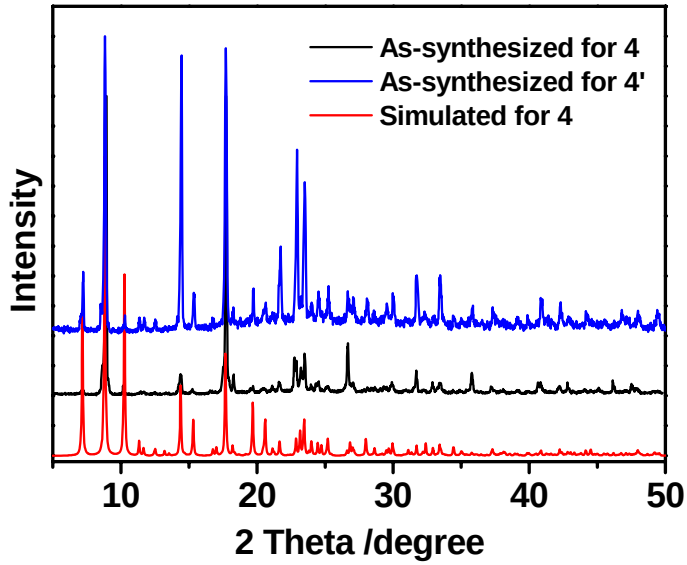

Fig. S4 PXRD of **4**.

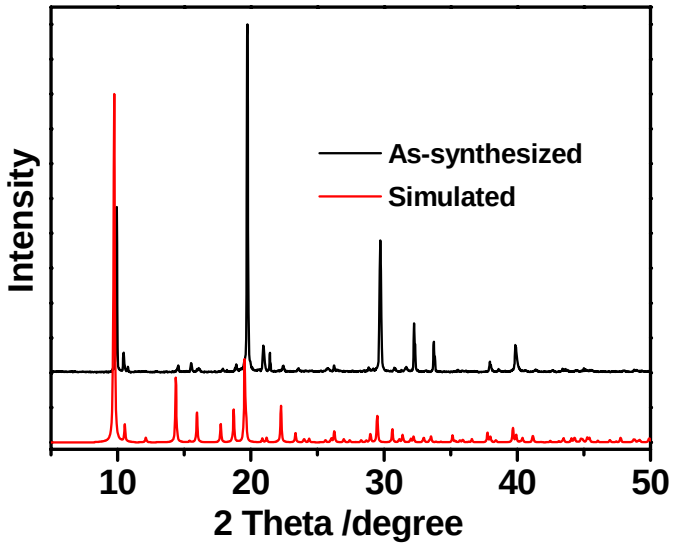

Fig. S5 PXRD of **5**.

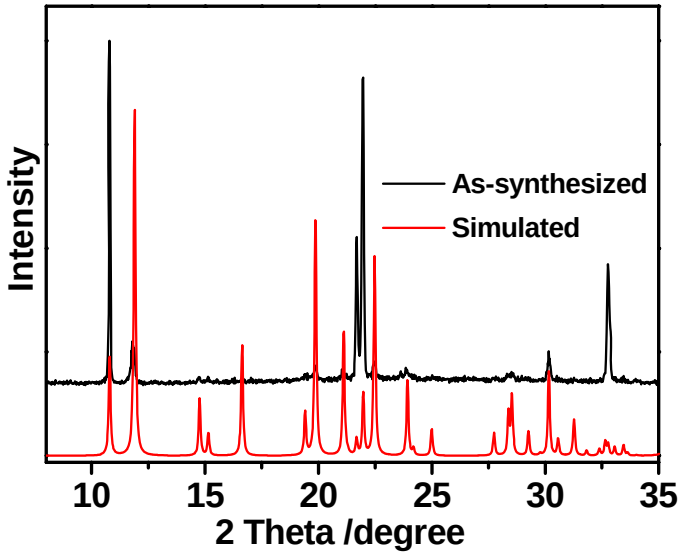

Fig. S6 PXRD of **6**.

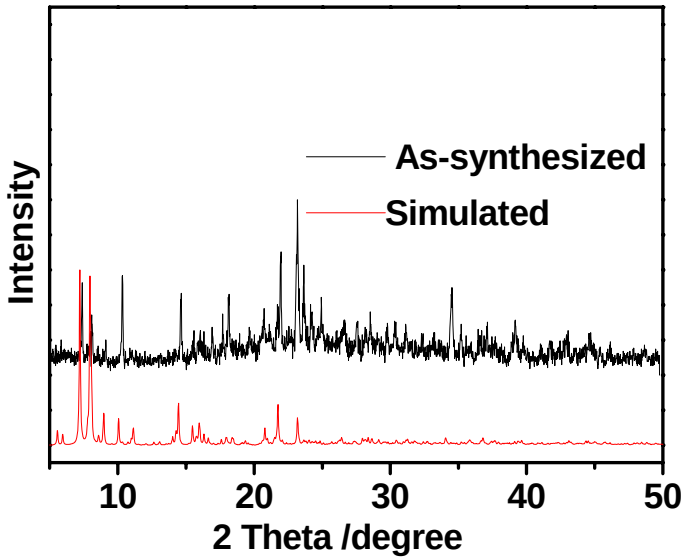

Fig. S7 PXRD of **7**.

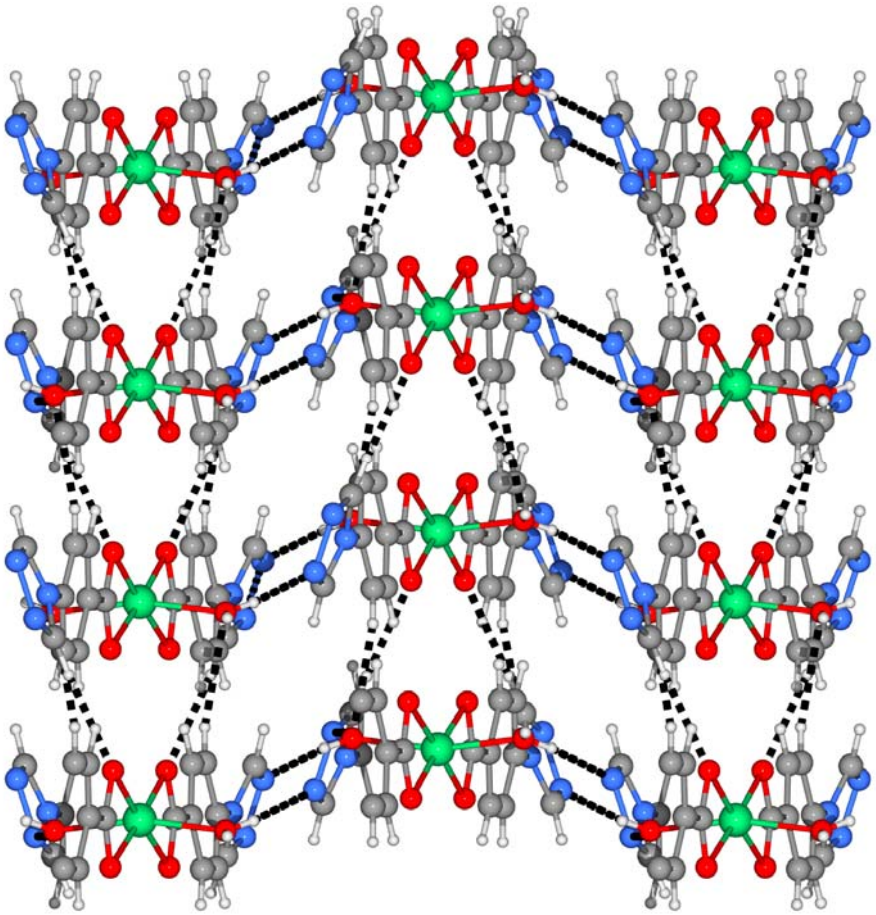

Fig. S8 View of the 3D supramolecular network through the C-H···O weak interactions in **1** along the *a*-axis.

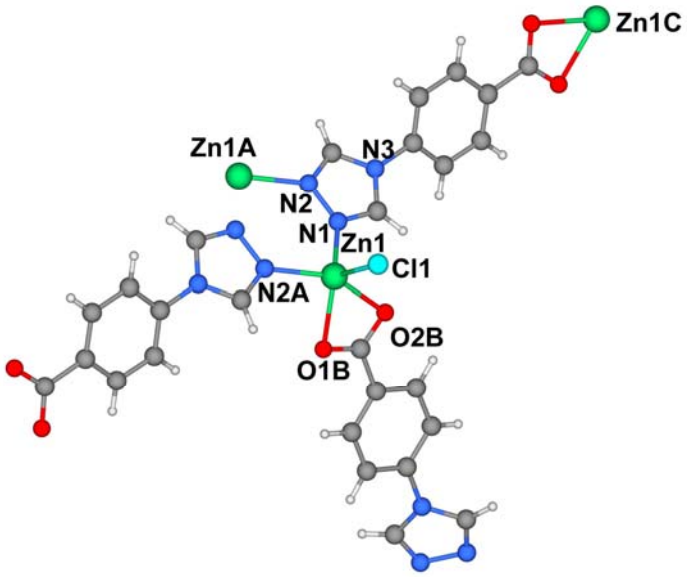

Fig. S9 The coordination environments of the zinc atom and the 4-tba ligand in **2**. Symmetric codes: A: -x, -y, -z; B: x-1, -y+1/2, z-1/2; C: x+1, -y+1/2, z+1/2.

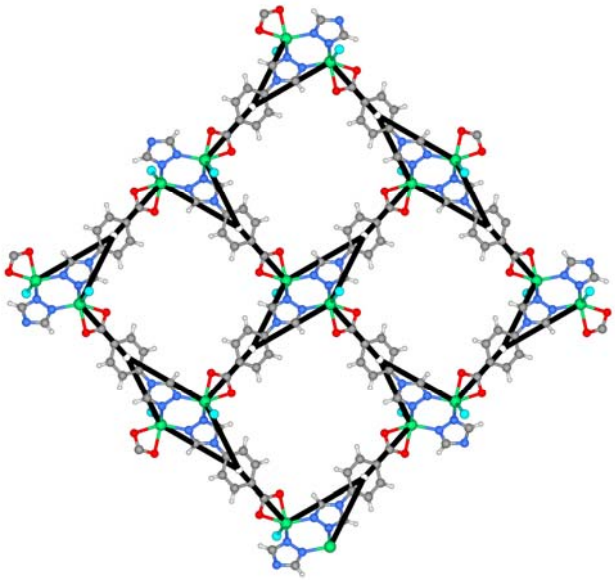

Fig. S10 The 3-connected 4.8^2 topology in **2** when Zn and 4-tba are regarded as two kinds of 3-connected nodes.

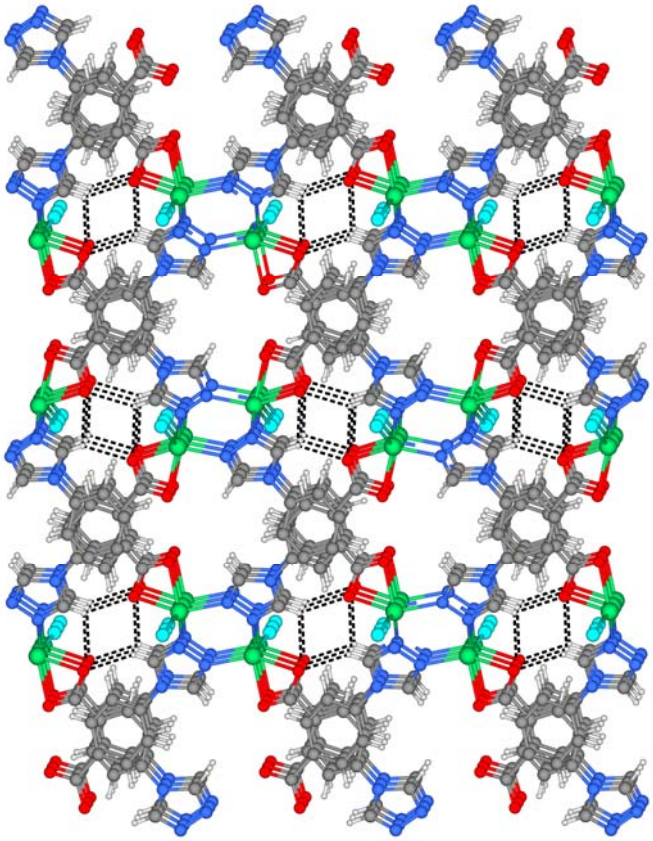

Fig. S11 View of the 3D supramolecular network through the C-H···O weak interactions in **2** along the *c*-axis.

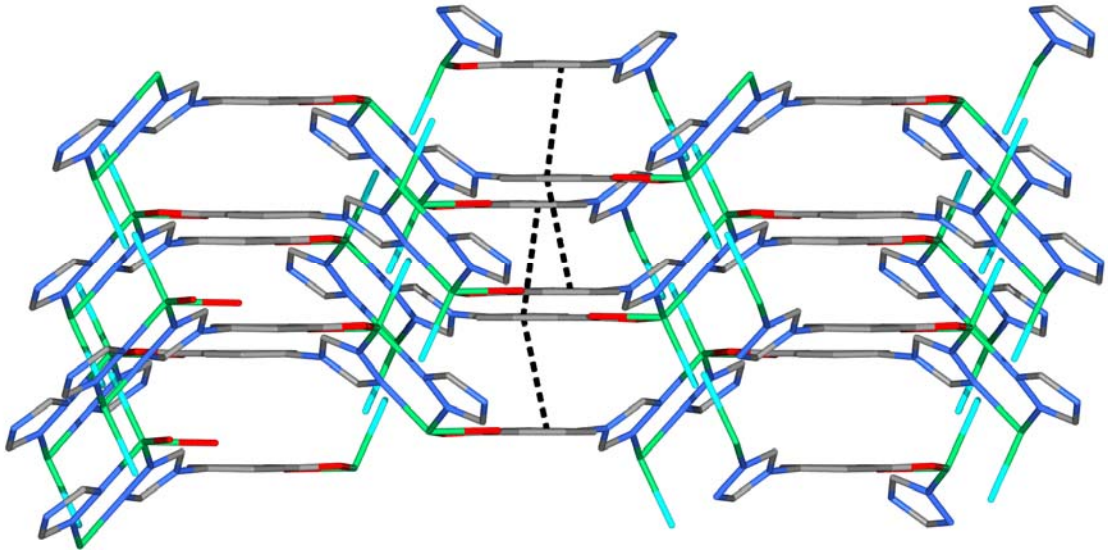

Fig. S12 View of π-π stacking interactions in **2**.

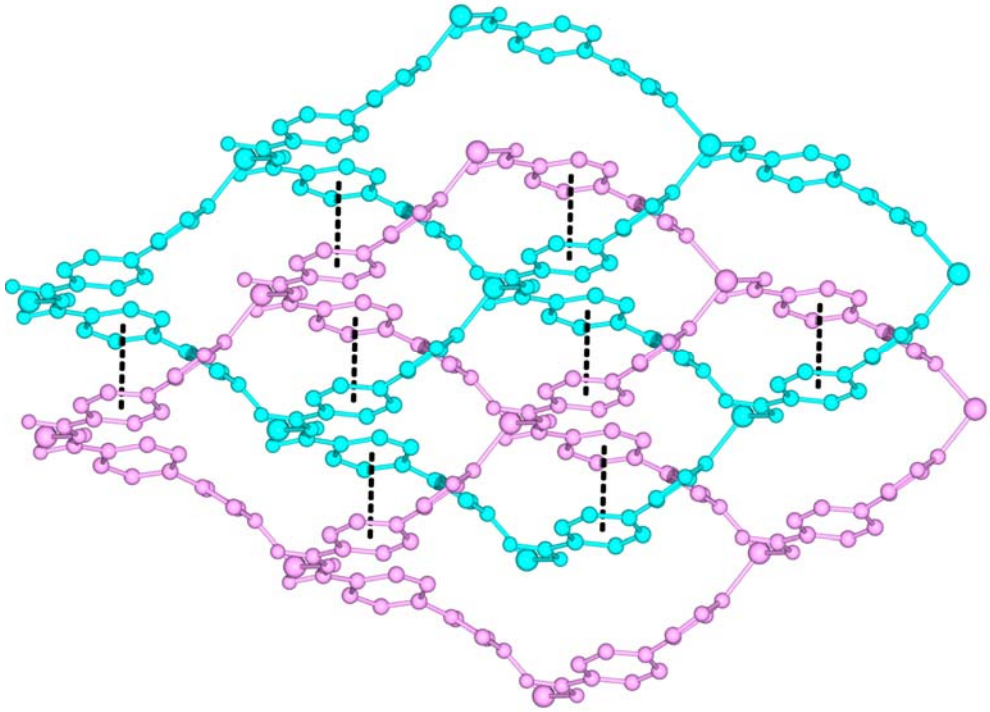

Fig. S13 View of π-π stacking interactions in **3**. The 2-fold interpenetrating 2D layers are shown different color and hydrogen atoms are omitted for clarity.

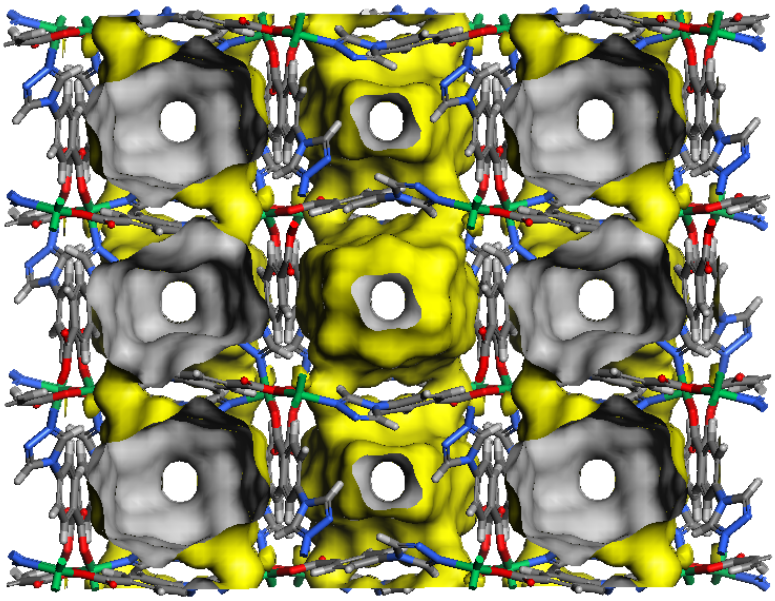

Fig. S14 View of the 3D framework and channel structure of **4** along the *b*-axis.

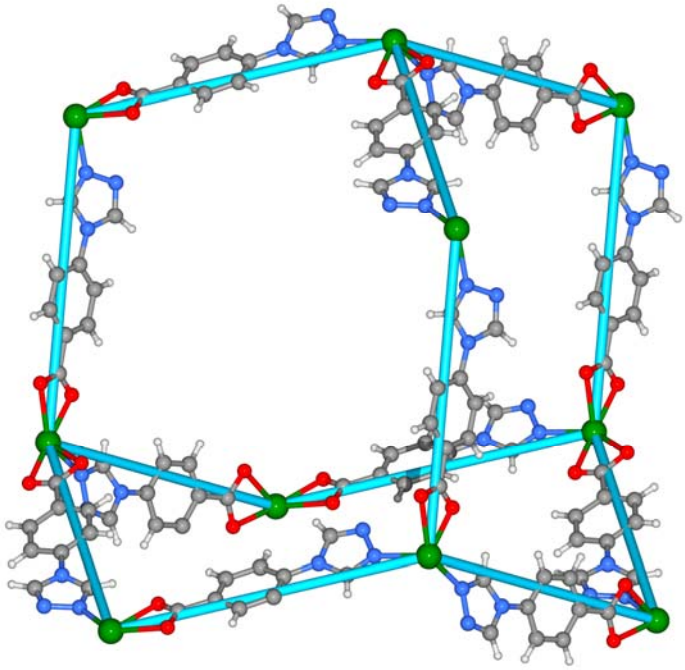

Fig. S15 A single diamond motif in **5**.

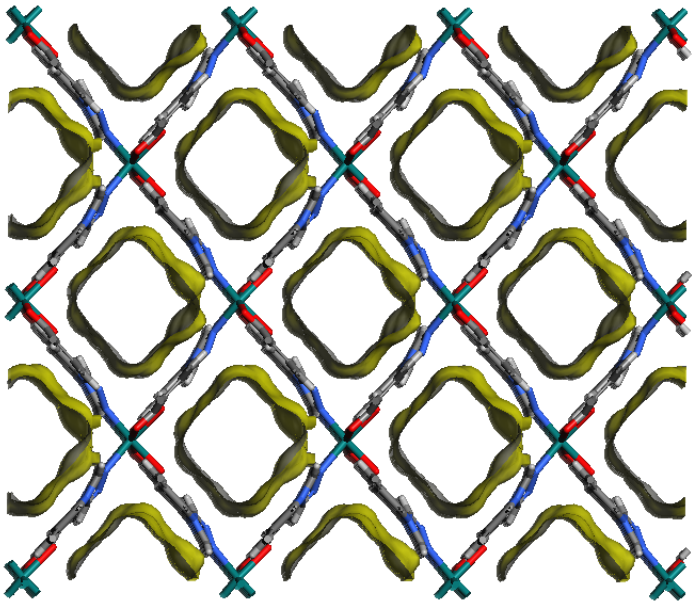

Fig. S16 View of the 3D framework and channel structure of **5** along the *b*-axis.

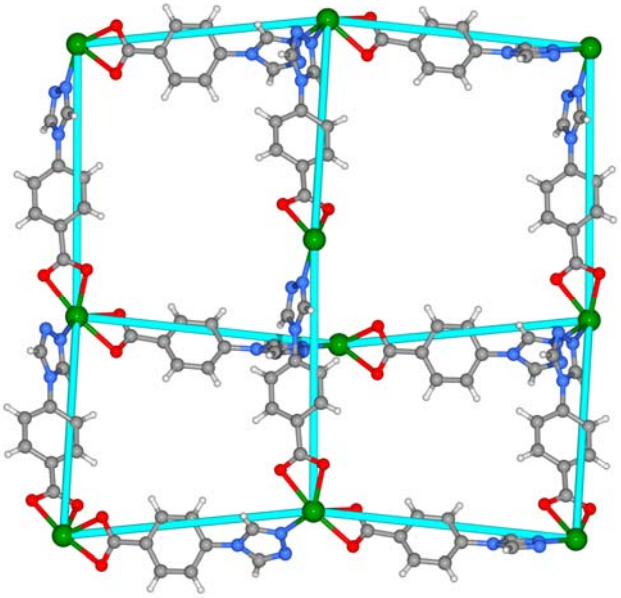

Fig. S17 A single diamond motif in **6**.

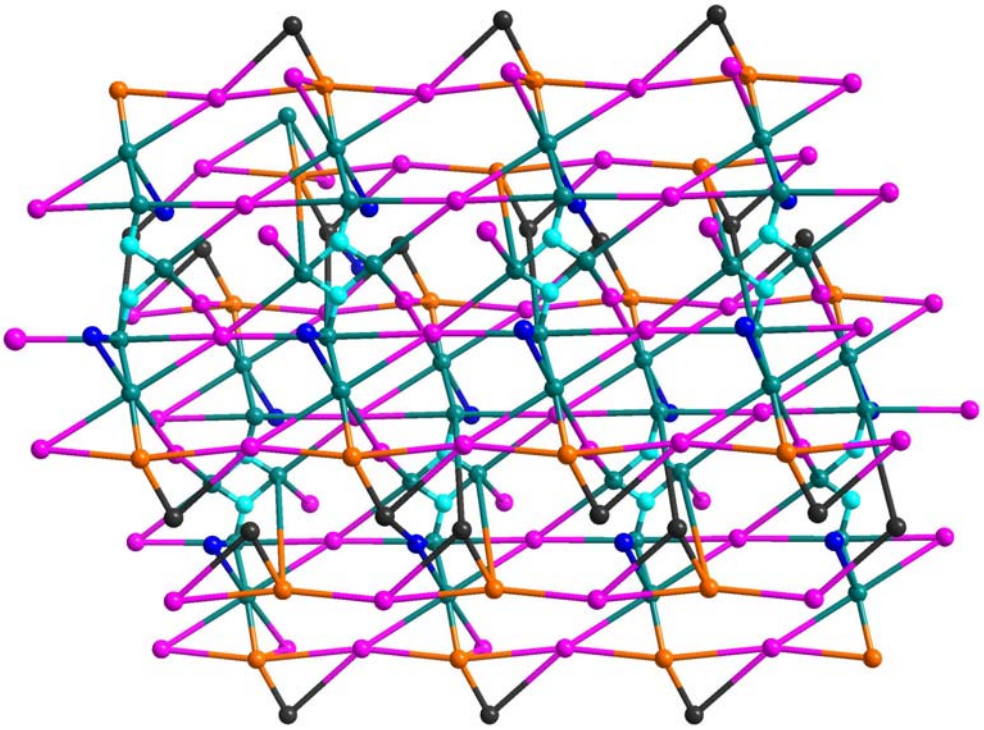

Fig. S18 Topological representation of the10-nodal (3,3,3,4,4,4,5,6,6,6)-connected net of **7**.

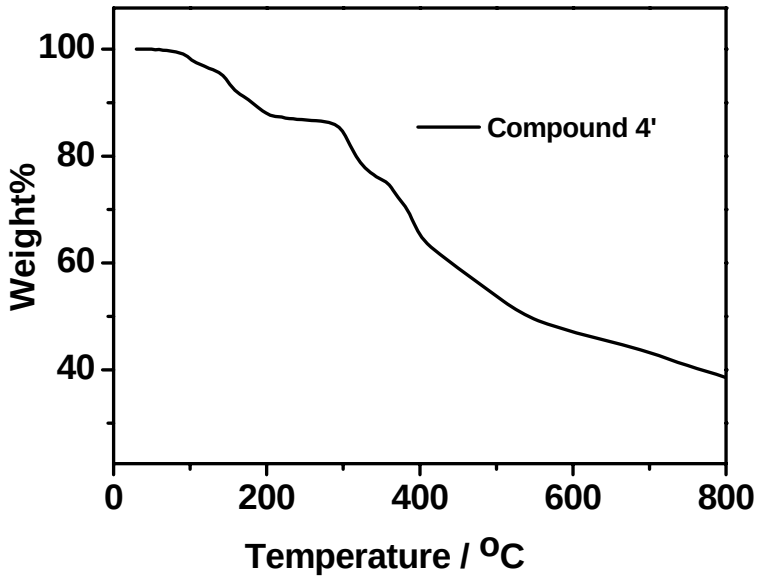

Figure S19. TG curve of compound **4'** synthesized by slow evaporation of the filtrate of 3. The weight loss of 13.35% at temperatures below 238 °C is consistent with the removal of one half of free DMF and two water guest molecules per formula unit (calcd 14.11%).

Table S1 The possible hydrogen bonds for compound**1** and **2**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1				
O(1W')-H(1WA)...N(1a)	0.71	2.06	2.746(17)	164.5
O(1W')-H(1WB)...N(2b)	0.80	2.04	2.790(17)	155.8
C(4)-H(4A)...O(1Wc)	0.93	2.49	3.295(15)	145.3
C(9)-H(9A)...O(1d)	0.93	2.40	3.329(4)	174.3
2				
O(3)-H(3)...O(2e)	0.82	2.01	2.826(6)	173.3
C(6)-H(6A)...O(3b)#5	0.93	2.57	3.496(7)	171.5
C(8)-H(8A)...O(3f)#6	0.93	2.25	3.079(7)	147.4
C(9)-H(9A)...O(1g)#7	0.93	2.48	2.965(6)	112.8
C(9)-H(9A)...O(1e)	0.93	2.47	3.259(7)	142.3

Symmetry code: (a) -x+1, -y+1, -z+1; (b) x-1, y, z; (c) x+1/2, y+1/2, z; (d) x+1/2, y-1/2, z; (e) x, -y+1/2, z-1/2; (f) x-1, -y+1/2, z+1/2; (g) -x+1, y-1/2, -z+1/2.

Table S2 The possible π - π interactions in complexes **1-7** calculated by program PLATON.[S1]

type of π–π interactions	centroid−centroid distance (Å)	closest interplanar distance (Å)	offset angle (°)
1			
benzene ring – triazole ring	3.8662	3.342	13.11
benzene ring – benzene ring	4.1349	3.777	0.00
2			
benzene ring – benzene ring	3.7768	3.363	0.49
3			
benzene ring – benzene ring	3.6562	3.505	0.67
4			
triazole ring – triazole ring	4.2493	3.294	0.04
5			
benzene ring – triazole ring	5.2286	2.642	71.59
6			
benzene ring – benzene ring	4.4961	3.320	16.78
7			
benzene ring – triazole ring	4.2252	3.750	16.29

Topology Analysis of compound 7 by using TOPOS software.[S2]

Topology for Cl1

Atom Cl1 links by bridge ligands and has

Common vertex with					R(A-A)	
Cd 3	0.1675	1.0053	0.4832	(0 1 0)	2.496A	1
Cd 2	0.1763	0.8119	0.4083	(0 0 0)	2.586A	1
Cd 3	-0.1675	0.9947	0.5168	(0 1 1)	2.912A	1

Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Cd 1	0.1746	-0.2232	0.2481	(0-1 0)	5.339A	1

Cd 2	0.1763	-0.1881	0.4083	(0-1 0)	5.457A	1
Cr 1	0.1651	0.5286	0.0038	(0 0 0)	7.238A	1

Topology for Ti1

Atom Ti1 links by bridge ligands and has

Common vertex with					R(A-A)	
Co 1	0.2055	0.7068	0.0765	(0 0 0)	6.293A	1
Cd 1	0.1746	0.7768	0.2481	(0 0 0)	6.402A	1
Cr 1	1.1651	0.5286	0.0038	(1 0 0)	6.502A	1
Co 1	1.2055	0.7068	0.0765	(1 0 0)	6.736A	1

Topology for Ti2

Atom Ti2 links by bridge ligands and has

Common vertex with					R(A-A)	
Cd 3	0.1675	0.0053	0.4832	(0 0 0)	6.274A	1
Co 1	0.2055	0.7068	0.0765	(0 0 0)	6.409A	1
Cd 1	0.1746	0.7768	0.2481	(0 0 0)	6.501A	1

Topology for Ti3

Atom Ti3 links by bridge ligands and has

Common vertex with					R(A-A)	
Cd 3	0.1675	1.0053	0.4832	(0 1 0)	6.407A	1
Cd 2	0.1763	0.8119	0.4083	(0 0 0)	6.449A	1
Cd 1	1.1746	0.7768	0.2481	(1 0 0)	6.528A	1
Cd 2	1.1763	0.8119	0.4083	(1 0 0)	6.541A	1

Topology for Cr1

Atom Cr1 links by bridge ligands and has

Common vertex with					R(A-A)	
Co 1	0.2055	0.7068	0.0765	(0 0 0)	4.136A	1
Ti 1	-0.3267	0.7100	0.1099	(-1 0 0)	6.502A	1
Sc 1	0.1760	0.0991	0.2052	(0 0 0)	7.238A	1
Cd 2	0.1763	0.8119	-0.5917	(0 0-1)	12.394A	1

Topology for Co1

Atom Co1 links by bridge ligands and has

Common vertex with					R(A-A)	
Cr 1	0.1651	0.5286	0.0038	(0 0 0)	4.136A	1
Cd 1	0.1746	0.7768	0.2481	(0 0 0)	4.266A	1
Ti 1	0.6733	0.7100	0.1099	(0 0 0)	6.293A	1
Ti 2	0.1690	0.3811	0.3222	(0 0 0)	6.409A	1
Ti 1	-0.3267	0.7100	0.1099	(-1 0 0)	6.736A	1
Cd 3	0.1675	1.0053	-0.5168	(0 1-1)	12.458A	1

Topology for Cd1

Atom Cd1 links by bridge ligands and has

Common vertex with R(A-A)

Cd 2	0.1763	0.8119	0.4083	(0 0 0)	3.805A	1
Co 1	0.2055	0.7068	0.0765	(0 0 0)	4.266A	1
Sc 1	0.1760	1.0991	0.2052	(0 1 0)	5.339A	1
Ti 1	0.6733	0.7100	0.1099	(0 0 0)	6.402A	1
Ti 2	0.1690	0.3811	0.3222	(0 0 0)	6.501A	1
Ti 3	-0.3323	0.8429	0.3917	(-1 0 0)	6.528A	1

Topology for Cd2

Atom Cd2 links by bridge ligands and has

Common vertex with R(A-A)

Cl 1	0.0554	0.9195	0.4681	(0 0 0)	2.586A	1
Cd 1	0.1746	0.7768	0.2481	(0 0 0)	3.805A	1
Sc 1	0.1760	1.0991	0.2052	(0 1 0)	5.457A	1
Ti 3	0.6677	0.8429	0.3917	(0 0 0)	6.449A	1
Ti 3	-0.3323	0.8429	0.3917	(-1 0 0)	6.541A	1
Cr 1	0.1651	0.5286	1.0038	(0 0 1)	12.394A	1

Topology for Cd3

Atom Cd3 links by bridge ligands and has

Common vertex with R(A-A)

Cl 1	0.0554	-0.0805	0.4681	(0-1 0)	2.496A	1
Cl 1	-0.0554	0.0805	0.5319	(0 1 1)	2.912A	1
Ti 2	0.1690	0.3811	0.3222	(0 0 0)	6.274A	1
Ti 3	0.6677	-0.1571	0.3917	(0-1 0)	6.407A	1
Co 1	0.2055	-0.2932	1.0765	(0-1 1)	12.458A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Cd3CoCrTi3ScCl

Coordination sequences

Cl1:	1	2	3	4	5	6	7	8	9	10
Num	3	11	25	59	105	173	238	317	432	551
Cum	4	15	40	99	204	377	615	932	1364	1915

Sc1:	1	2	3	4	5	6	7	8	9	10
Num	3	10	26	58	99	169	235	331	419	549
Cum	4	14	40	98	197	366	601	932	1351	1900

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

Num 4 13 28 59 105 173 244 335 417 561
Cum 5 18 46 105 210 383 627 962 1379 1940

Ti2: 1 2 3 4 5 6 7 8 9 10
Num 3 11 26 56 105 168 241 330 423 537
Cum 4 15 41 97 202 370 611 941 1364 1901

Ti3: 1 2 3 4 5 6 7 8 9 10
Num 4 15 27 63 112 168 241 341 417 553
Cum 5 20 47 110 222 390 631 972 1389 1942

Cr1: 1 2 3 4 5 6 7 8 9 10
Num 4 13 30 57 111 163 238 327 442 531
Cum 5 18 48 105 216 379 617 944 1386 1917

Co1: 1 2 3 4 5 6 7 8 9 10
Num 6 14 32 66 111 176 248 331 431 563
Cum 7 21 53 119 230 406 654 985 1416 1979

Cd1: 1 2 3 4 5 6 7 8 9 10
Num 6 12 34 62 114 172 261 328 429 545
Cum 7 19 53 115 229 401 662 990 1419 1964

Cd2: 1 2 3 4 5 6 7 8 9 10
Num 6 13 34 65 112 172 242 332 428 554
Cum 7 20 54 119 231 403 645 977 1405 1959

Cd3: 1 2 3 4 5 6 7 8 9 10
Num 5 12 32 63 120 175 243 335 452 536
Cum 6 18 50 113 233 408 651 986 1438 1974

TD10=1939

Vertex symbols for selected sublattice

Cl1 Point symbol:{4^2.6}
Extended point symbol:[4.4.6]

Sc1 Point symbol:{3.7.8}
Extended point symbol:[3.7(2).8(5)]

Ti1 Point symbol:{3^2.6^2.7^2}
Extended point symbol:[3.3.6.6.7(2).7(2)]

Ti2 Point symbol:{3.7.8}
Extended point symbol:[3.7(2).8(5)]

Ti3 Point symbol:{3.4.6^2.7^2}
Extended point symbol:[3.4.6.6.7.7(2)]

Cr1 Point symbol:{3.5.6.7.8^2}
Extended point symbol:[3.8.5(2).8(6).6(3).7(2)]

Co1 Point symbol:{3^3.4.5.6^3.7^6.8}
Extended point symbol:[3.3.3.4.5(2).6.6.6(2).7.7.7.7.7.7(2).8]

Cd1 Point symbol:{3^4.4^2.6^2.7^4.8^2.9}
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Cd2 Point symbol:{3^2.4^2.5^2.6^2.7^4.8^3}
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Cd3 Point symbol:{4^2.5^2.6.7^3.8.9}
Extended point symbol:[4.4.5.5.6.7.7.7.8(2).9]

Point symbol for net:
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3,3,3,4,4,4,5,6,6,6-c net with stoichiometry (3-c)(3-c)(3-c)(4-c)(4-c)(4-c)(5-c)(6-c)(6-c)(6-c); 10-nodal net

References

S1 A. L. Spek, *PLATON*, Utrecht University: Utrecht, The Netherlands, 2003.

S2 The network topology was evaluated by the program TOPOS-4.0; see http://www.topos.ssu.samara.ru.

V. A. Blatov, *IUCr CompComm Newsletter*, 2006, **7**, 4.