Electronic Supporting Information (ESI)

A series of Cd(II) coordination polymers based on flexible bis(triazole) and multicarboxylate ligands: topological diversity, entanglement and properties

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Table S1 Crystallographic data for **1 - 8.**

	1	**2**	**3**	**4**	**5**	**6**	**7**
Formula	$C_{56}H_{56}Cd_5N_{18}$	$C_{14}H_9CdN_3O_4$	$C_{30}H_{18}Cd_3N_6O_{12}$	$C_{20}H_{20}CdN_6O_6$	$C_{21}H_{20}CdN_6O_6$	$C_{40}H_{38}Cd_2N_{12}O_{11}$	$C_{80}H_{78}Cd_4N_1$
Fw	1927.18	395.64	991.70	552.83	564.83	1087.62	2089.14
T/K	293(2)	293(2)	293(2)	293(2)	293(2)	273(2)	223(1)
Crystal	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Orthorhombi
Space group	*C2/c*	*C2/c*	*C2/c*	*P*$\bar{1}$	$P2_1/n$	$P2_1/c$	*Pbca*
a/Å	24.418(7)	17.1401(11)	13.622(3)	9.785(2)	7.641(3)	11.0996(5)	18.4042(5)
b/Å	15.686(4)	6.7651(4)	16.126(3)	10.345(3)	19.081(7)	17.0411(8)	15.8373(3)
c/Å	21.471(6)	22.1684(12)	18.280(4)	11.126(3)	15.210(6)	22.1425(10)	27.9693(7)
α (°)	90	90	90	78.400(9)	90	90	90
β (°)	114.597(5)	94.427(3)	109.949(3)	82.174(12)	91.496(7)	95.1440(10)	90
γ (°)	90	90	90	82.427(11)	90	90	90
V /Å^3	7478(4)	2562.9(3)	3774.5(13)	1086.7(5)	2217.0(14)	4171.4(3)	8152.3(4)
F(000)	3800	1552	1920	556	1136	2184	4200
Z	4	8	4	2	4	4	4
ρ_{calcd} (g cm^{-3})	1.712	2.051	1.745	1.690	1.692	1.732	1.702
μ(mm^{-1})	1.482	1.728	1.738	1.056	1.037	1.097	1.119
Reflections	14392	37678	8322	7926	11719	119670	28280
Unique	6517	2238	3909	3743	3871	10409	7153
Parameter	443	199	231	337	311	604	619
GOF	1.095	1.079	1.076	1.002	1.040	1.038	1.049
R_1 [I > 2σ(I)]	0.0697	0.0229	0.0441	0.0228	0.0769	0.0260	0.0298
wR_2 (all data)	0.1842	0.0565	0.1064	0.0534	0.2475	0.0604	0.0716

GOF = $\{\Sigma w((F_o^2-F_c^2)^2)/(n-p)\}^{1/2}$, $R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2= \{\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2\}^{1/2}$, where n =number of reflections and p = total number of parameters refined.

Table S2 Selected bond lengths [Å] and angles [°] for **1**–**8**.

		1	
Cd(1)-O(1)	2.434(6)	Cd(1)-O(2)	2.415(6)
Cd(1)-O(8A)	2.230(7)	Cd(1)-O(9)	2.414(8)
Cd(1)-N(1)	2.329(8)	Cd(1)-N(5B)	2.328(8)
Cd(2)-O(1)	2.366(6)	Cd(2)-O(3)	2.354(6)
Cd(2)-O(5)	2.546(7)	Cd(2)-O(6)	2.360(6)
Cd(2)-O(10)	2.306(8)	Cd(2)-N(2)	2.388(7)
Cd(2)-N(4B)	2.342(8)	Cd(3)-O(11C)	2.284(7)
Cd(3)-O(11)	2.284(7)	Cd(3)-O(12)	2.312(10)
Cd(3)-O(12C)	2.312(10)	Cd(3)-N(7C)	2.274(10)
Cd(3)-N(7)	2.274(10)	O(2)-Cd(1)-O(1)	54.4(2)
O(8A)-Cd(1)-O(1)	125.7(2)	O(8A)-Cd(1)-O(2)	91.5(2)
O(8A)-Cd(1)-O(9)	75.2(3)	O(8A)-Cd(1)-N(1)	118.6(3)
O(8A)-Cd(1)-N(5B)	136.5(3)	O(9)-Cd(1)-O(1)	156.9(2)
O(9)-Cd(1)-O(2)	143.2(3)	N(1)-Cd(1)-O(1)	75.4(2)
N(1)-Cd(1)-O(2)	129.7(2)	N(1)-Cd(1)-O(9)	86.0(3)
N(5B)-Cd(1)-O(1)	88.1(2)	N(5B)-Cd(1)-O(2)	87.9(3)
N(5B)-Cd(1)-O(9)	79.5(3)	N(5B)-Cd(1)-N(1)	93.9(3)
O(1)-Cd(2)-O(5)	149.3(2)	O(1)-Cd(2)-N(2)	74.0(2)
O(3)-Cd(2)-O(1)	73.1(2)	O(3)-Cd(2)-O(5)	137.4(2)
O(3)-Cd(2)-O(6)	85.0(2)	O(3)-Cd(2)-N(2)	146.2(2)
O(6)-Cd(2)-O(1)	157.3(2)	O(6)-Cd(2)-O(5)	53.0(2)
O(6)-Cd(2)-N(2)	126.3(2)	O(10)-Cd(2)-O(1)	94.6(3)
O(10)-Cd(2)-O(3)	90.8(3)	O(10)-Cd(2)-O(5)	84.0(3)
O(10)-Cd(2)-O(6)	91.6(3)	O(10)-Cd(2)-N(2)	99.5(3)
O(10)-Cd(2)-N(4B)	172.9(3)	N(2)-Cd(2)-O(5)	76.0(2)
N(4B)-Cd(2)-O(1)	88.0(2)	N(4B)-Cd(2)-O(3)	83.7(2)
N(4B)-Cd(2)-O(5)	97.0(3)	N(4B)-Cd(2)-O(6)	83.5(2)
N(4B)-Cd(2)-N(2)	87.5(3)	O(11C)-Cd(3)-O(11)	180.0
O(11C)-Cd(3)-O(12)	85.8(3)	O(11)-Cd(3)-O(12C)	85.8(3)
O(11C)-Cd(3)-O(12C)	94.2(3)	O(11)-Cd(3)-O(12)	94.2(3)
O(12C)-Cd(3)-O(12)	180.0	N(7)-Cd(3)-O(11C)	94.7(3)
N(7C)-Cd(3)-O(11)	94.7(3)	N(7)-Cd(3)-O(11)	85.3(3)
N(7C)-Cd(3)-O(11C)	85.3(3)	N(7C)-Cd(3)-O(12C)	86.3(4)
N(7C)-Cd(3)-O(12)	93.7(4)	N(7)-Cd(3)-O(12C)	93.7(4)
N(7)-Cd(3)-O(12)	86.3(4)	N(7C)-Cd(3)-N(7)	180.0
		2	
Cd(1)-O(1A)	2.325(2)	Cd(1)-O(1)	2.429(2)
Cd(1)-O(2A)	2.521(2)	Cd(1)-O(3B)	2.331(2)
Cd(1)-O(3)	2.370(2)	Cd(1)-N(1)	2.298(3)
Cd(1)-N(2A)	2.448(2)	O(1A)-Cd(1)-O(1)	148.29(6)
O(1A)-Cd(1)-O(2A)	53.65(7)	O(1)-Cd(1)-O(2A)	146.79(8)

O(1A)-Cd(1)-O(3)	79.21(7)	O(1A)-Cd(1)-O(3B)	118.21(7)
O(1)-Cd(1)-N(2A)	83.97(8)	O(1A)-Cd(1)-N(2A)	73.08(8)
O(3)-Cd(1)-O(1)	76.75(7)	O(3B)-Cd(1)-O(1)	77.90(7)
O(3)-Cd(1)-O(2A)	91.91(8)	O(3B)-Cd(1)-O(2A)	116.63(8)
O(3B)-Cd(1)-O(3)	151.40(4)	O(3)-Cd(1)-N(2A)	83.76(8)
O(3B)-Cd(1)-N(2A)	80.61(8)	N(1)-Cd(1)-O(1)	75.26(8)
N(1)-Cd(1)-O(1A)	130.24(8)	N(1)-Cd(1)-O(2A)	76.70(8)
N(1)-Cd(1)-O(3)	101.60(8)	N(1)-Cd(1)-O(3B)	84.45(8)
N(1)-Cd(1)-N(2A)	156.55(8)	N(2A)-Cd(1)-O(2A)	126.29(8)
		3	
Cd(1)-O(1)	2.330(3)	Cd(1)-O(1A)	2.330(3)
Cd(1)-O(6B)	2.203(4)	Cd(1)-O(6C)	2.203(4)
Cd(1)-N(1)	2.428(4)	Cd(1)-N(1A)	2.428(4)
Cd(2)-O(1)	2.386(3)	Cd(2)-O(2)	2.314(4)
Cd(2)-O(3D)	2.308(3)	Cd(2)-O(4D)	2.340(4)
Cd(2)-O(5C)	2.255(3)	Cd(2)-N(2)	2.263(5)
O(1A)-Cd(1)-O(1)	87.55(17)	O(1)-Cd(1)-N(1)	80.57(13)
O(1A)-Cd(1)-N(1)	91.70(13)	O(1)-Cd(1)-N(1A)	91.71(13)
O(1A)-Cd(1)-N(1A)	80.57(13)	O(6B)-Cd(1)-O(1A)	162.33(14)
O(6C)-Cd(1)-O(1)	162.33(14)	O(6C)-Cd(1)-O(1A)	90.86(15)
O(6B)-Cd(1)-O(1)	90.86(15)	O(6B)-Cd(1)-O(6C)	95.8(2)
O(6C)-Cd(1)-N(1A)	105.39(14)	O(6B)-Cd(1)-N(1)	105.39(14)
O(6B)-Cd(1)-N(1A)	81.89(15)	O(6C)-Cd(1)-N(1)	81.89(15)
N(1)-Cd(1)-N(1A)	169.3(2)	O(2)-Cd(2)-O(1)	55.50(11)
O(2)-Cd(2)-O(4D)	88.39(16)	O(3D)-Cd(2)-O(1)	150.53(14)
O(3D)-Cd(2)-O(2)	99.77(15)	O(3D)-Cd(2)-O(4D)	56.00(14)
O(4D)-Cd(2)-O(1)	129.58(14)	O(5B)-Cd(2)-O(1)	86.26(12)
O(5B)-Cd(2)-O(2)	119.80(14)	O(5B)-Cd(2)-O(3D)	122.43(15)
O(5B)-Cd(2)-O(4D)	83.39(15)	O(5B)-Cd(2)-N(2)	83.48(15)
N(2)-Cd(2)-O(1)	84.29(13)	N(2)-Cd(2)-O(2)	128.39(15)
N(2)-Cd(2)-O(3D)	104.07(16)	N(2)-Cd(2)-O(4D)	142.47(17)
		4	
Cd(1)-O(1)	2.2102(17)	Cd(1)-O(3A)	2.3848(18)
Cd(1)-O(4A)	2.4853(17)	Cd(1)-O(5)	2.357(2)
Cd(1)-N(1)	2.3051(19)	Cd(1)-N(4)	2.310(2)
O(1)-Cd(1)-O(3A)	142.74(6)	O(1)-Cd(1)-O(4A)	89.15(6)
O(1)-Cd(1)-O(5)	87.87(7)	O(1)-Cd(1)-N(1)	121.58(7)
O(2)-Cd(1)-N(4)	97.83(8)	O(3A) -Cd(1)-O(4)	53.72(5)
O(5)-Cd(1)-O(3A)	85.07(6)	O(5)-Cd(1)-O(4A)	83.44(6)
N(1)-Cd(1)-O(3A)	95.13(6)	N(1)-Cd(1)-O(4A)	148.63(6)
N(1)-Cd(1)-O(5)	91.03(7)	N(1)-Cd(1)-N(4)	95.29(8)
N(4)-Cd(1)-O(3A)	83.74(8)	N(4)-Cd(1)-O(4A)	85.62(7)
N(4)-Cd(1)-O(5)	167.59(7)		
		5	

Cd(1)-O(1)	2.268(8)	Cd(1)-O(2)	2.393(9)
Cd(1)-O(3A)	2.231(8)	Cd(1)-N(1)	2.291(10)
Cd(1)-N(4)	2.292(10)		
O(1)-Cd(1)-O(2)	56.2(3)	O(1)-Cd(1)-N(1)	125.8(3)
O(1)-Cd(1)-N(4)	98.5(3)	O(3A)-Cd(1)-O(1)	136.1(3)
O(3A)-Cd(1)-O(2)	103.9(3)	O(3A)-Cd(1)-N(1)	92.8(4)
O(3A)-Cd(1)-N(4)	100.7(4)	N(1)-Cd(1)-O(2)	97.4(3)
N(1)-Cd(1)-N(4)	91.4(3)	N(4)-Cd(1)-O(2)	153.4(3)
		6	
Cd(1)-O(1)	2.3819(14)	Cd(1)-O(3)	2.2600(14)
Cd(1)-O(5A)	2.2665(15)	Cd(1)-N(1)	2.2729(16)
Cd(1)-N(8)	2.3221(16)	Cd(1)-N(11B)	2.3498(16)
Cd(2)-O(1)	2.4808(14)	Cd(2)-O(2)	2.4163(15)
Cd(2)-O(7)	2.5209(15)	Cd(2)-O(8)	2.3219(15)
Cd(2)-N(4)	2.2968(17)	Cd(2)-N(7)	2.3183(17)
Cd(2)-N(12B)	2.3899(16)		
O(3)-Cd(1)-O(1)	74.93(5)	O(3)-Cd(1)-O(5A)	109.40(5)
O(3)-Cd(1)-N(1)	94.53(6)	O(3)-Cd(1)-N(8)	84.86(6)
O(3)-Cd(1)-N(11B)	149.96(5)	O(5A)-Cd(1)-O(1)	171.53(5)
O(5A)-Cd(1)-N(1)	86.37(6)	O(5A)-Cd(1)-N(8)	84.79(6)
O(5A)-Cd(1)-N(11B)	100.31(6)	N(1)-Cd(1)-O(1)	100.70(6)
N(1)-Cd(1)-N(8)	170.38(6)	N(1)-Cd(1)-N(11B)	91.54(6)
N(8)-Cd(1)-O(1)	88.43(5)	N(8)-Cd(1)-N(11B)	93.77(6)
N(11B)-Cd(1)-O(1)	75.03(5)	O(1)-Cd(2)-O(7)	147.18(4)
O(2)-Cd(2)-O(1)	53.36(4)	O(2)-Cd(2)-O(7)	96.45(5)
O(8)-Cd(2)-O(1)	157.72(5)	O(8)-Cd(2)-O(2)	148.66(5)
O(8)-Cd(2)-O(7)	54.27(5)	O(8)-Cd(2)-N(12B)	83.33(5)
N(4)-Cd(2)-O(1)	92.49(5)	N(4)-Cd(2)-O(2)	85.09(6)
N(4)-Cd(2)-O(7)	97.81(6)	N(4)-Cd(2)-O(8)	88.06(6)
N(4)-Cd(2)-N(7)	168.22(6)	N(4)-Cd(2)-N(12B)	99.18(6)
N(7)-Cd(2)-O(1)	84.96(5)	N(7)-Cd(2)-O(2)	84.16(6)
N(7)-Cd(2)-O(7)	78.65(5)	N(7)-Cd(2)-O(8)	98.65(6)
N(7)-Cd(2)-N(12B)	91.24(6)	N(12B)-Cd(2)-O(1)	74.59(5)
N(12B)-Cd(2)-O(2)	127.95(5)	N(12B)-Cd(2)-O(7)	133.41(5)
		7	
Cd(1)-O(1)	2.3159(19)	Cd(1)-O(3)	2.287(2)
Cd(1)-O(5A)	2.528(2)	Cd(1)-O(6A)	2.253(2)
Cd(1)-N(1)	2.457(2)	Cd(1)-N(4B)	2.278(3)
Cd(2)-O(2C)	2.267(2)	Cd(2)-O(4)	2.289(2)
Cd(2)-O(7)	2.521(2)	Cd(2)-O(8)	2.269(2)
Cd(2)-N(2)	2.259(2)	Cd(2)-O(1C)	2.6564(19)
Cd(2)-O(3)	2.654(2)		
O(1)-Cd(1)-O(5A)	77.86(7)	O(1)-Cd(1)-N(1)	156.41(8)
O(3)-Cd(1)-O(1)	101.22(7)	O(3)-Cd(1)-O(5A)	91.17(7)

O(3)-Cd(1)-N(1)	82.88(8)	O(6A)-Cd(1)-O(1)	86.18(7)
O(6A)-Cd(1)-O(3)	142.91(8)	O(6A)-Cd(1)-O(5A)	54.54(7)
O(6A)-Cd(1)-N(1)	77.32(7)	O(6A)-Cd(1)-N(4B)	124.81(8)
N(1)-Cd(1)-O(5A)	78.84(8)	N(4B)-Cd(1)-O(1)	110.72(9)
N(4B)-Cd(1)-O(3)	86.78(8)	N(4B)-Cd(1)-O(5A)	171.40(9)
N(4B)-Cd(1)-N(1)	92.61(9)	O(2C)-Cd(2)-O(1C)	52.56(7)
O(2C)-Cd(2)-O(3)	84.51(7)	O(2C)-Cd(2)-O(4)	115.71(8)
O(2C)-Cd(2)-O(7)	141.99(7)	O(2C)-Cd(2)-O(8)	102.20(8)
O(3)-Cd(2)-O(1C)	130.40(6)	O(4)-Cd(2)-O(1C)	161.81(8)
O(4)-Cd(2)-O(3)	52.12(7)	O(4)-Cd(2)-O(7)	94.74(7)
O(7)-Cd(2)-O(1C)	91.80(6)	O(7)-Cd(2)-O(3)	133.44(7)
O(8)-Cd(2)-O(1C)	82.22(7)	O(8)-Cd(2)-O(3)	136.57(6)
O(8)-Cd(2)-O(4)	87.81(7)	O(8)-Cd(2)-O(7)	54.45(7)
N(2)-Cd(2)-O(1C)	83.33(8)	N(2)-Cd(2)-O(3)	82.85(7)
N(2)-Cd(2)-O(2C)	101.92(9)	N(2)-Cd(2)-O(4)	114.19(8)
N(2)-Cd(2)-O(7)	84.01(8)	N(2)-Cd(2)-O(8)	135.23(8)
		8	
Cd(1)-O(1)	2.2892(17)	Cd(1)-O(1A)	2.2892(17)
Cd(1)-O(2B)	2.3357(17)	Cd(1)-O(2C)	2.3357(17)
Cd(1)-N(6B)	2.1691(15)	Cd(1)-N(6C)	2.1691(15)
Cd(1)-N(1A)	2.313(2)	Cd(1)-N(1)	2.313(2)
O(1)-Cd(1)-O(1A)	96.03(8)	O(1)-Cd(1)-O(2B)	177.49(6)
O(1)-Cd(1)-O(2C)	86.45(7)	O(1A)-Cd(1)-O(2B)	86.45(7)
O(1A)-Cd(1)-O(2C)	177.49(6)	O(1)-Cd(1)-N(1)	88.96(8)
O(1)-Cd(1)-N(1A)	97.00(7)	O(2B)-Cd(1)-O(2C)	91.08(9)
N(1)-Cd(1)-O(2B)	90.35(8)	N(1)-Cd(1)-O(2C)	83.41(8)
N(1A)-Cd(1)-O(2C)	90.35(8)	N(1A)-Cd(1)-O(2B)	83.41(8)
N(1)-Cd(1)-N(1A)	171.09(11)		

Symmetry transformations used to generate equivalent atoms: A 3/2-x, 1/2+y, 3/2-z; B 3/2-x, 1/2-y, 2-z; C 1-x, -y, 1-z for **1**; A 1/2-x, -1/2+y, 3/2-z; B 1/2-x, 1/2+y, 3/2-z for **2**; A 1-x, y, 3/2-z; B -1/2+x, 1/2+y, z; C 3/2-x, 1/2+y, 3/2-z; D x, -y, -1/2+z for **3**; A x, -1+y, z for **4**; A -1/2+x, 1/2-y, 1/2+z for **5**; A x, 1/2-y, -1/2+z; B -x, 1/2+y, 1/2-z for **6**; A 3/2-x, 1/2+y, z; B x, 3/2-y, 1/2+z; C 3/2-x, -1/2+y, z for **7**; A 1-x, y, 3/2-z; B x, 1-y, 1/2+z; C 1-x, 1-y, 1-z for **8**.

Table S3 Hydrogen bonds for **1**, **4**, **5**, **6** and **7** (Å and °).

D-H···A	d(D-H)	d(H···A)	D(D···A)	<(DHA)
		1		
O(9)-H(9A)···O(11)^{i}	0.91(2)	2.64(11)	2.901(11)	97(7)
O(9)-H(9A)···O(12)^{ii}	0.91(2)	2.40(3)	3.305(13)	169(10)
O(10)-H(10B)···N(8)	0.90(2)	2.04(2)	2.918(16)	165(3)
O(11)-H(11A)···O(3)^{iii}	0.91(2)	2.58(4)	3.171(9)	124(8)
O(11)-H(11A)···O(4)^{iii}	0.91(2)	1.73(4)	2.633(9)	178(7)

O(11)-H(11B)···O(6)^{iii}	0.92(2)	1.85(2)	2.714(9)	156(4)
O(12)-H(12A)···O(4)^{iii}	0.89(2)	2.24(12)	2.951(13)	137(15)
O(12)-H(12B)···O(8)	0.91(2)	1.95(8)	2.799(13)	156(17)
		4		
O(5)-H(5A)···N(2)^{i}	0.832(19)	2.11(2)	2.910(3)	163(4)
O(5)-H(5B)···O(3)^{ii}	0.851(18)	1.84(2)	2.671(2)	164(4)
O(6)-H(6A)···O(5)^{ii}	0.841(19)	2.10(2)	2.930(3)	171(4)
O(6)-H(6B)···O(2)	0.842(18)	2.02(3)	2.839(12)	165(4)
		5		
O(6)-H(6A)···O(1)	0.90(2)	2.00(2)	2.868(14)	160(8)
O(6)-H(6B)···N(5)^{i}	0.90(2)	2.50(2)	3.349(15)	156(7)
		6		
O(9)-H(9A)···O(3)^{i}	0.944(17)	1.91(2)	2.736(3)	144(3)
O(9)-H(9B)···N(5)^{ii}	0.939(18)	2.05(2)	2.911(3)	152(3)
O(10)-H(10A)···O(4)^{i}	0.881(16)	1830(17)	2.691(2)	165(3)
O(10)-H(10B)···O(6)	0.873(16)	1.974(16)	2.846(2)	177(2)
O(11)-H(11A)···O(10)	0.896(16)	1.913(18)	2.796(2)	168(3)
O(11)-H(11B)···O(2)	0.879(16)	1.962(17)	2.835(2)	171(3)
		7		
O(9)-H(9A)···O(4)	0.845(19)	2.28(3)	3.082(4)	159(5)
O(9)-H(9B)···O(5)^{i}	0.859(2)	1.92(2)	2.773(4)	174(5)
O(10)-H(10C)···O(9)	0.893(19)	1.88(2)	2.766(4)	171(5)
O(10)-H(10D)···O(7)	0.850(19)	2.21(4)	2.866(4)	134(5)
O(11)-H(11A)···O(14)	0.85	2.03	2.841(5)	159.9
O(11)-H(11B)···O(10)^{ii}	0.85	1.97	2.796(5)	163.3

Symmetry transformations used to generate equivalent atoms: i 1/2+x, 1/2-y, 1/2+z; ii 3/2-x, 1/2+y, 3/2-z; iii 1-x, -y, 1-z for **1**; i 1-x, -y, 2-z; ii 1-x, 1-y, 2-z for **4**; i 1/2+x, 1/2-y, -1/2+z for **5**; i x, 1/2-y, 1/2+z; ii 1-x, 1-y, 1-z for **6**; i 3/2-x, 1/2+y, z; ii 1-x, -1/2-y, 1/2-z for **7**.

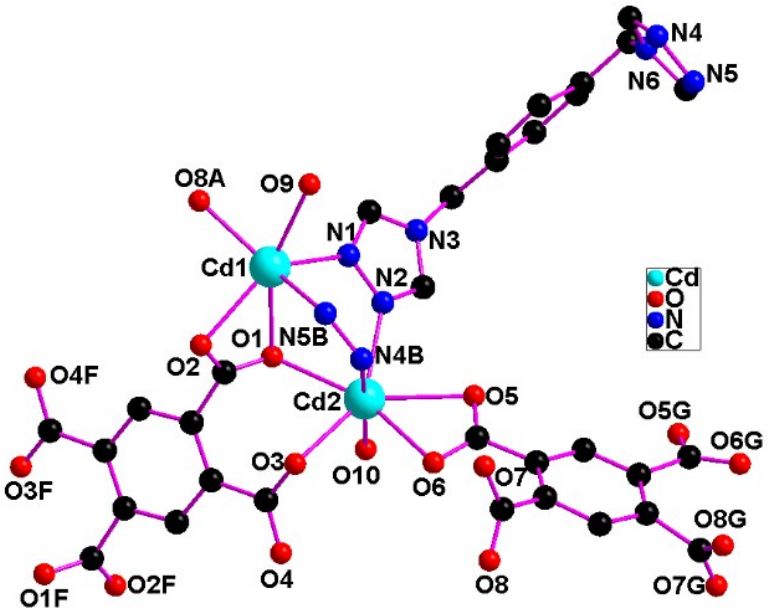

Fig. S1 The coordination environment of the Cd(II) atoms of the 3D motif in **1**. Symmetry transformations used to generate equivalent atoms in **1**: A -x+1/2, y-1/2, -z+1/2; B -x+1/2, -y+1/2, -z+1; F -x+1/2, -y+1/2, -z; G -x, y, -z+1/2; H x-1/2, y+1/2, z.

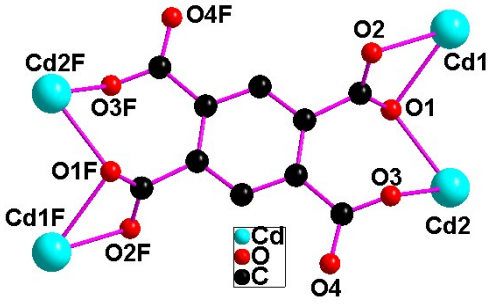

Fig. S2 One kind of btec ligand (O1-O4) in **1**.

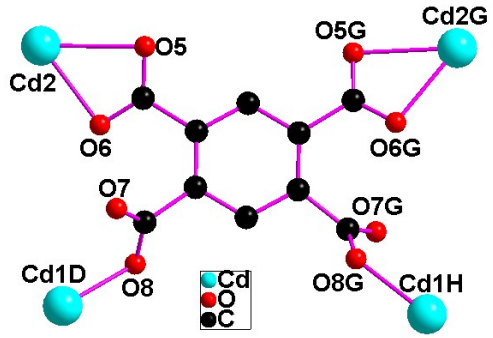

Fig. S3 The other kind of btec ligand (O5-O8) in **1**.

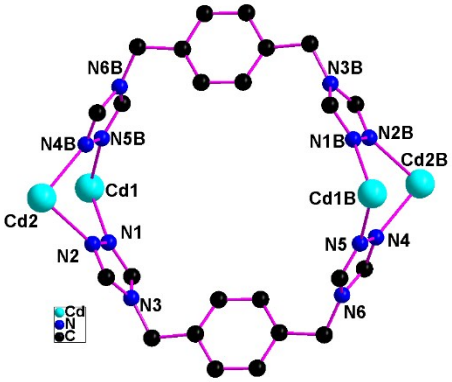

Fig. S4 The $[Cd_4(btrb)_2]$ ring is formed by two btrb ligands and four Cd(II) atoms in **1**.

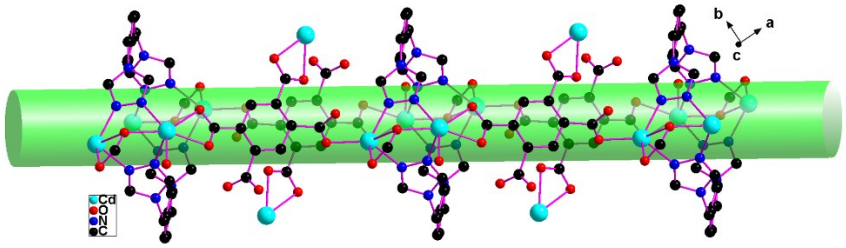

Fig. S5 Side viewing the nano-tunnel in the 3D motif of **1**.

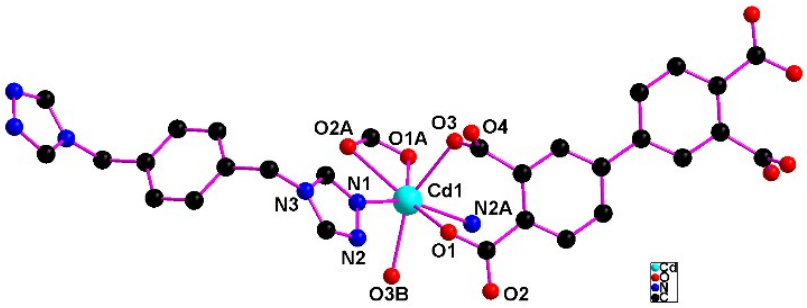

Fig. S6 The coordination environment of the Cd(II) atom in **2**. Symmetry transformations used to generate equivalent atoms in **2**: A 1/2-x, -1/2+y, 3/2-z; B 1/2-x, 1/2+y, 3/2-z.

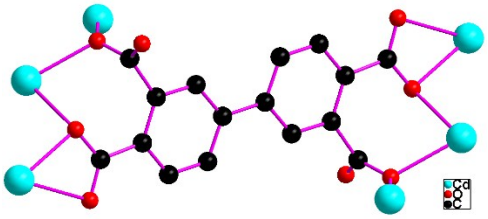

Fig. S7 The coordination mode of bptc ligand in **2**.

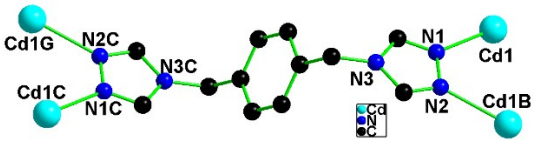

Fig. S8 The btrb ligand coordinates four Cd(II) atoms in **2**.

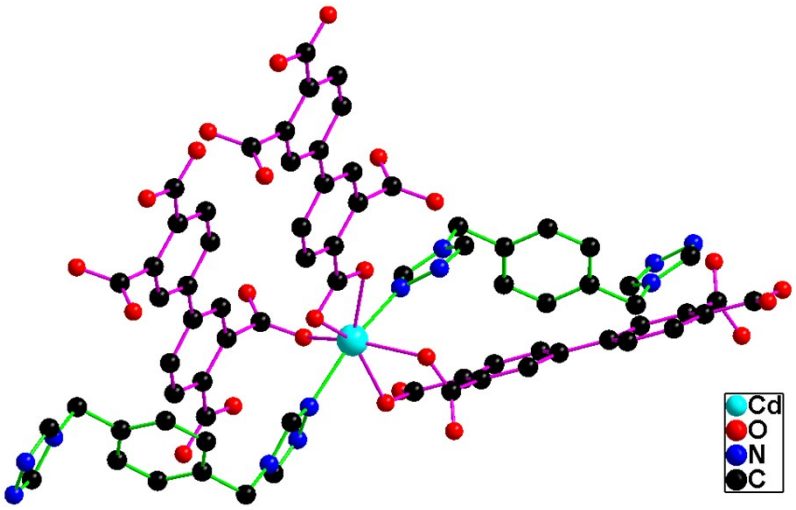

Fig. S9 The 5-connected Cd(II) atom in **2**.

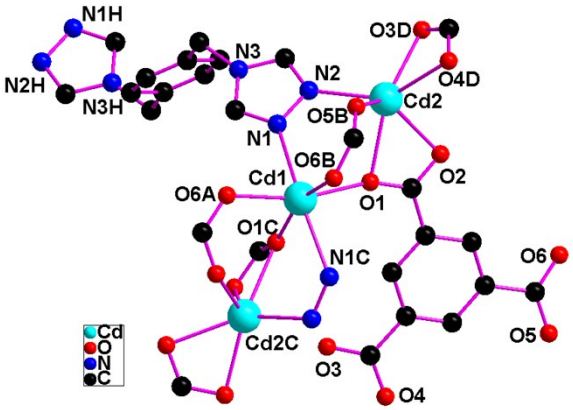

Fig. S10 The coordination environment of the Cd(II) atoms in **3**. Symmetry transformations used to generate equivalent atoms in **3**: A x-1/2, y+1/2, z; B -x+3/2, y+1/2, -z+3/2; C -x+1, y, -z+3/2; D x, -y, z-1/2; H -x, -y, -z+1.

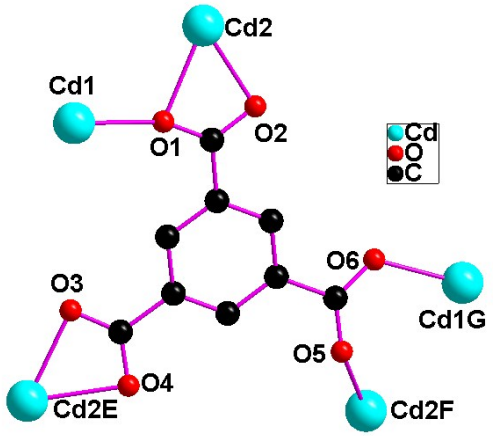

Fig. S11 The coordination mode of the btc ligand in **3**.

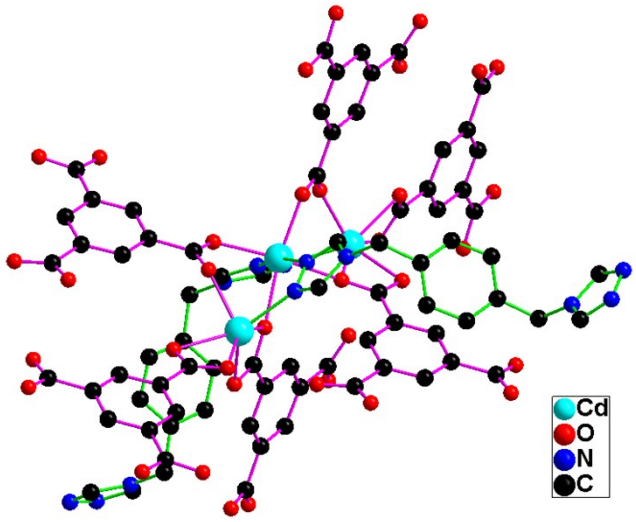

Fig. S12 The 5-connected trimer Cd(II) cluster $[Cd_3(COO)_2]$ in **3**.

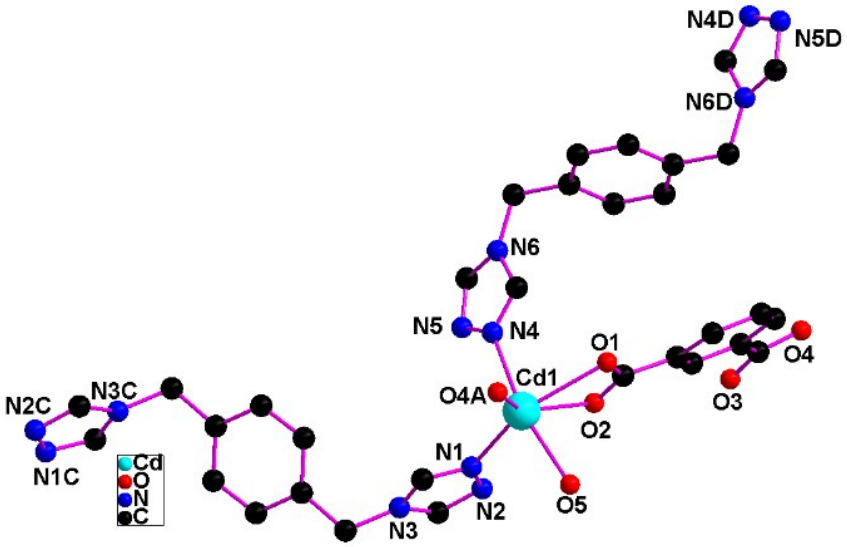

Fig. S13 The coordination environment of Cd(II) atom in **4**. Symmetry transformations used to generate equivalent atoms in **4:** A x, -1+y, z; C 2-x, 1-y, 1-z; D -x, -y, 1-z.

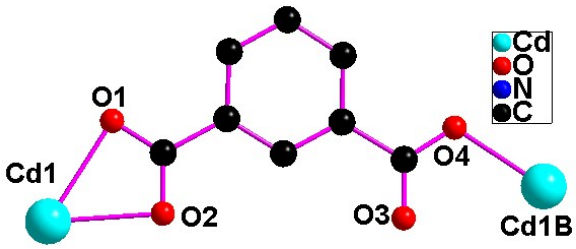

Fig. S14 The coordination mode of the ip ligand in **4**.

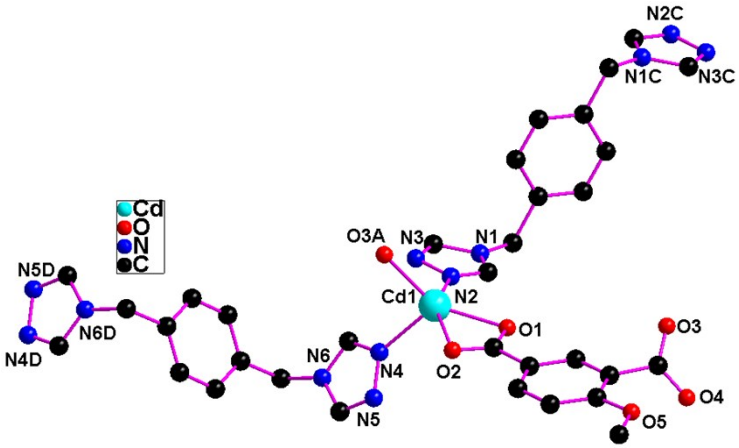

Fig. S15 The coordination environment of the Cd(II) atom in **5**. Symmetry transformations used to generate equivalent atoms in **5**: A x-1/2, -y+1/2, z+1/2; C -x, -y+1, -z; D -x, -y, -z+1.

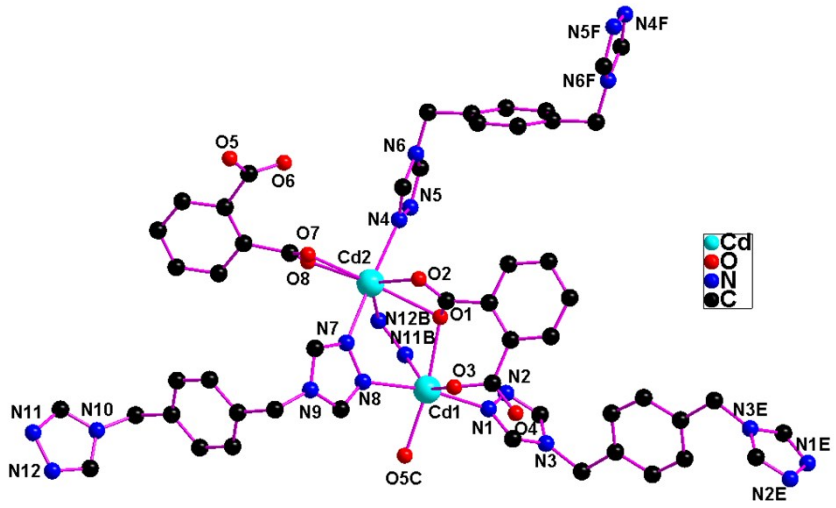

Fig. S16 The coordination environment of the Cd(II) atoms in **6**. Symmetry transformations used to generate equivalent atoms in **6**: B -x, 1/2+y, 1/2-z; C x, 1/2-y, 1/2+z; E 2-x, 1-y, -z; F 2-x, 1-y, 1-z.

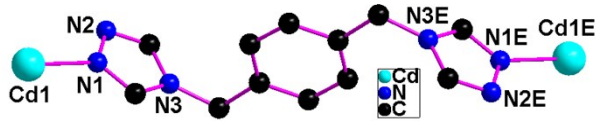

Fig. S17 The coordination mode of two kind of btrb ligands (N1-N3/N4-N5) in **6**.

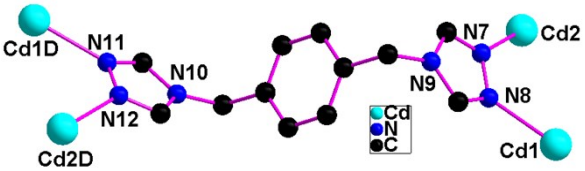

Fig. S18 The coordination mode of the third kind of btrb ligands (N7-N12) in **6**.

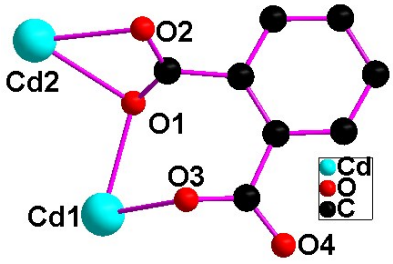

Fig. S19 The coordination mode of one kind of 1,2-bdc ligands (O1-O4) in **6**.

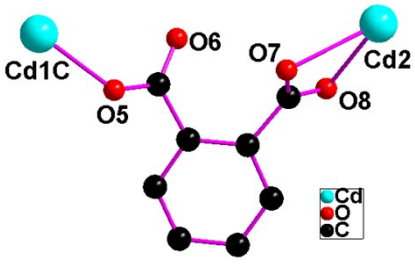

Fig. S20 The other kind of 1,2-bdc ligands (O5-O8) in **6**.

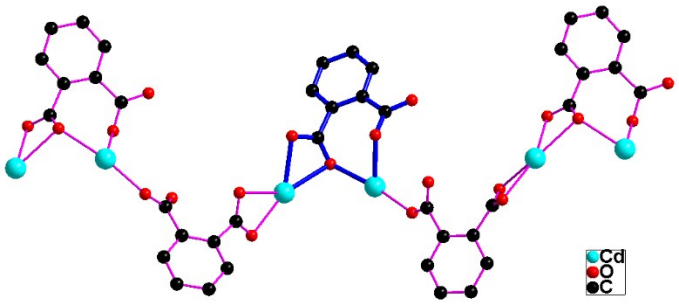

Fig. S21 The $[Cd_2(1,2\text{-bdc})_2]_n$ 1D chain in **6**.

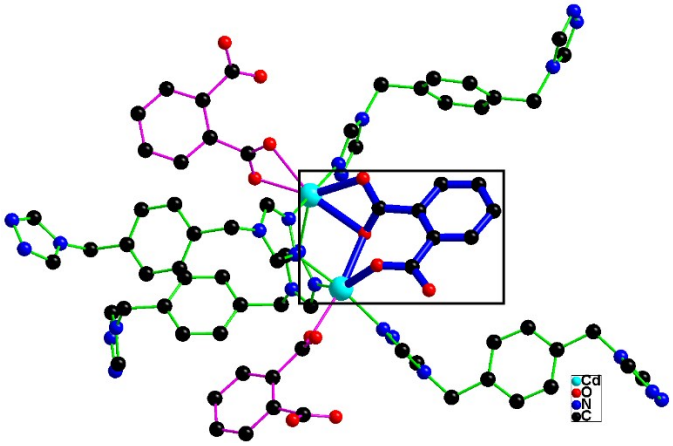

Fig. S22 The 6-connected $[Cd_2(1,2\text{-bdc})]$ dimer in **6**.

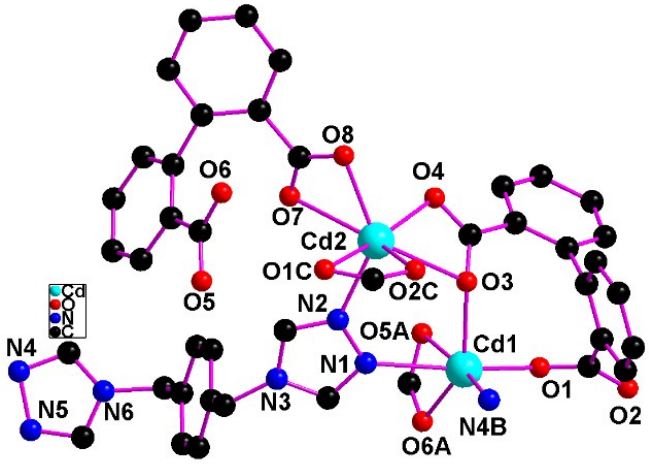

Fig. S23 The coordination environment of **7**. Symmetry transformations used to generate equivalent atoms in **7**: A 1/2-x, 1/2+y, z; B x, 1/2-y, -1/2+z; C 1/2-x, -1/2+y, z.

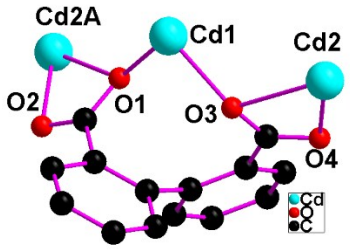

Fig. S24 The coordination mode of first kind of bpdc ligands (O1-O4) in **7**.

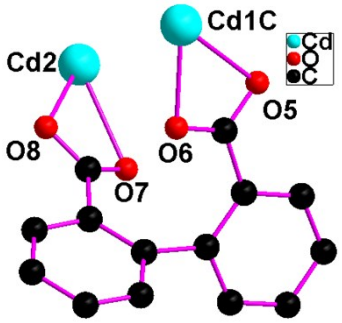

Fig. S25 The coordination mode of other kind of bpdc ligands (O5-O8) in **7**.

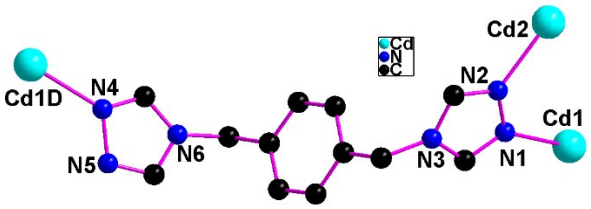

Fig. S26 The coordination mode of the btrb ligand in **7**.

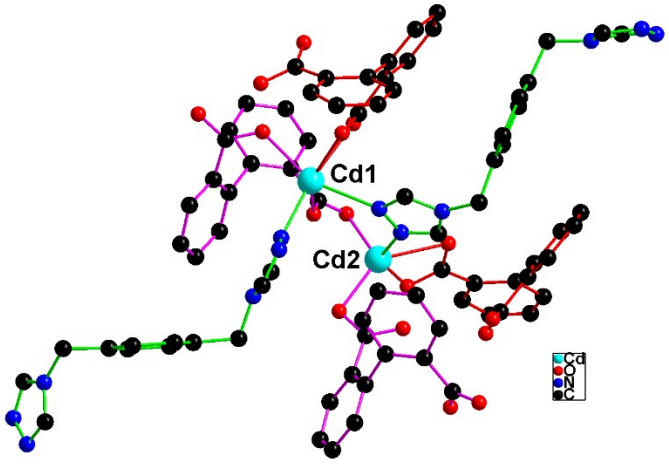

Fig. S27 The 4-connected Cd1 and Cd2 atoms in **7**.

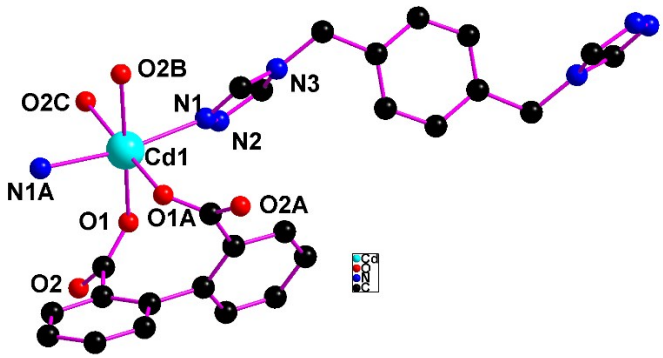

Fig. S28 The coordination environment of the Cd(II) atom in **8**. Symmetry transformations used to generate equivalent atoms in **8**: A 1-x, y, 3/2-z; B x, 1-y, 1/2+z; C 1-x, 1-y, 1-z.

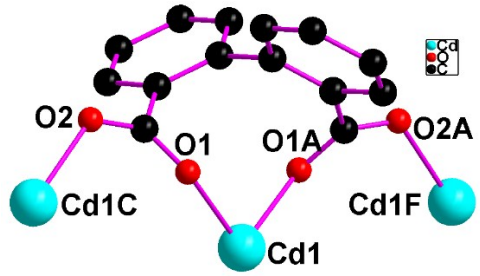

Fig. S29 The coordination mode of bpdc ligand in **8**.

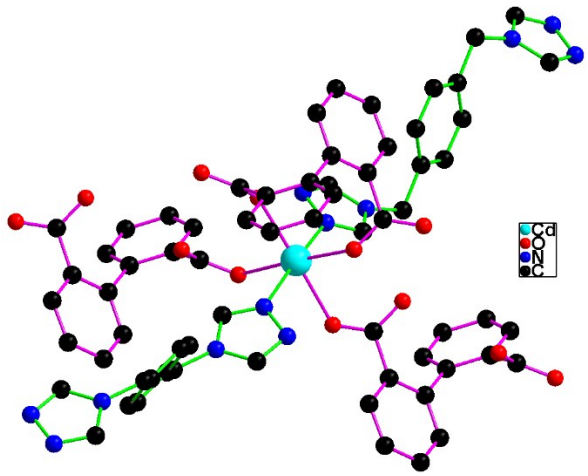

Fig. S30 The 5-connected Cd(II) atom in **8**.

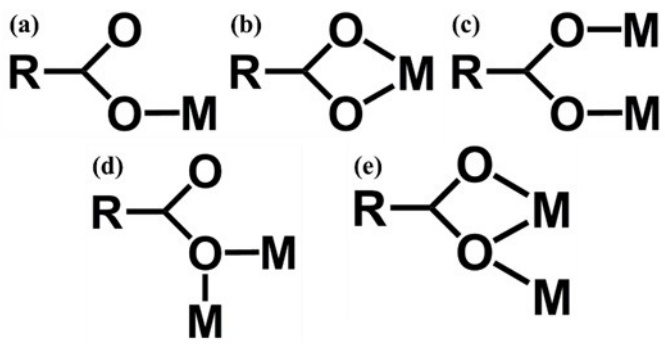

Fig. S31 Five kinds of coordination modes of carboxyl in **1**-**8**.

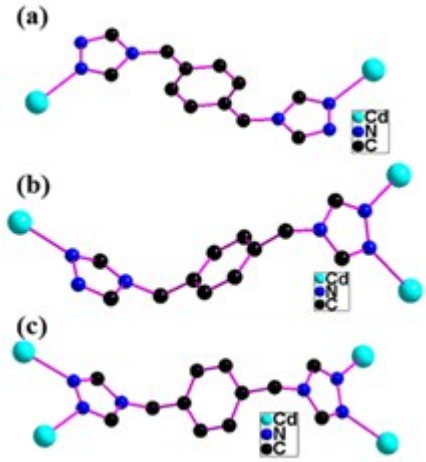

Fig. S32 Three kinds of coordination modes of btrb ligand in **1**-**8**.

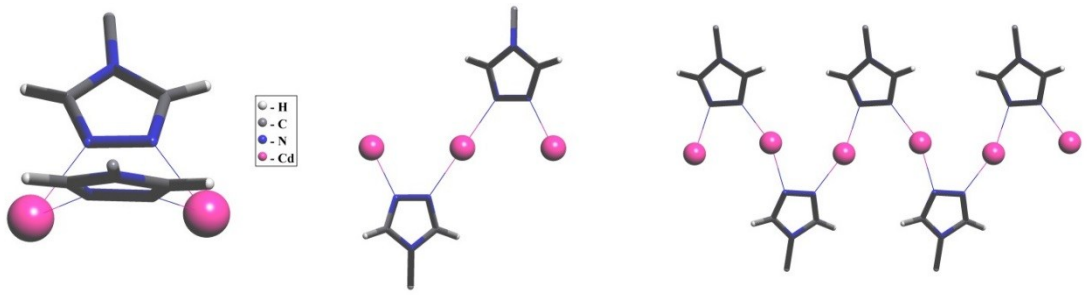

Fig. S33. The methods of connection of Cd atoms by btrb ligands: dimer (in **1** and **6**), trimer (in **3**) and chain (in **2**). Only one of the triazolyl rings of each ligand is shown.

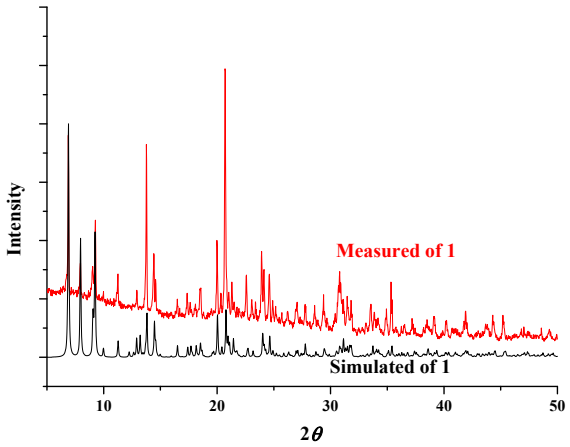

Fig. S34 The measured and simulated PXRD patterns of **1**.

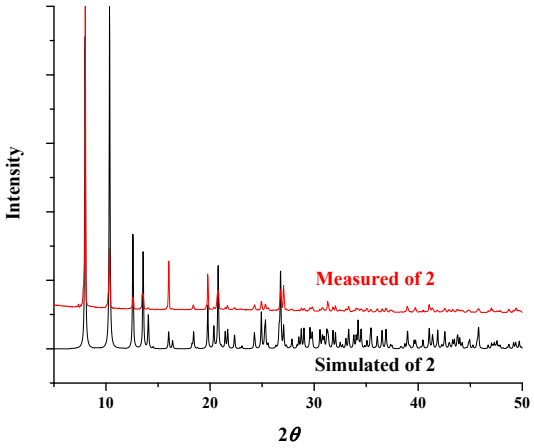

Fig. S35 The measured and simulated PXRD patterns of **2**.

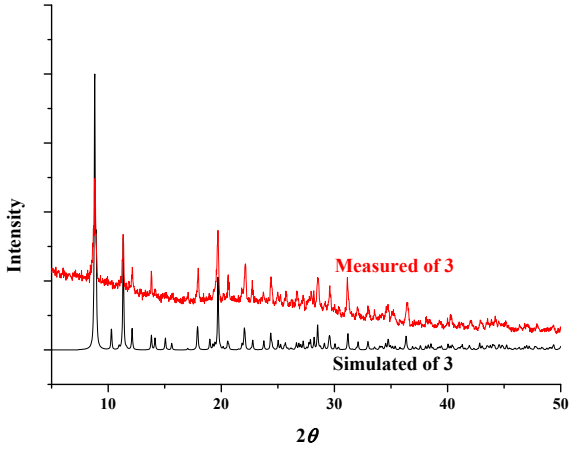

Fig. S36 The measured and simulated PXRD patterns of **3**.

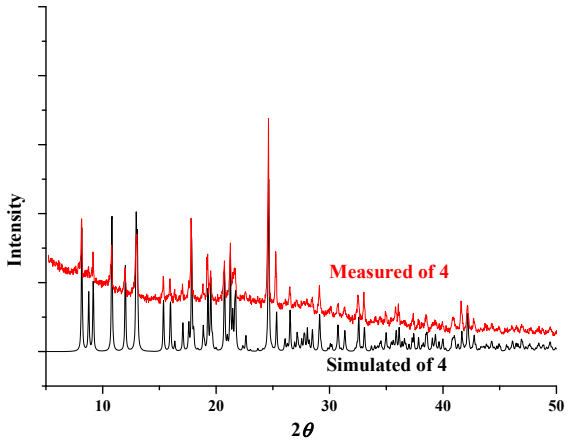

Fig. S37 The measured and simulated PXRD patterns of **4**.

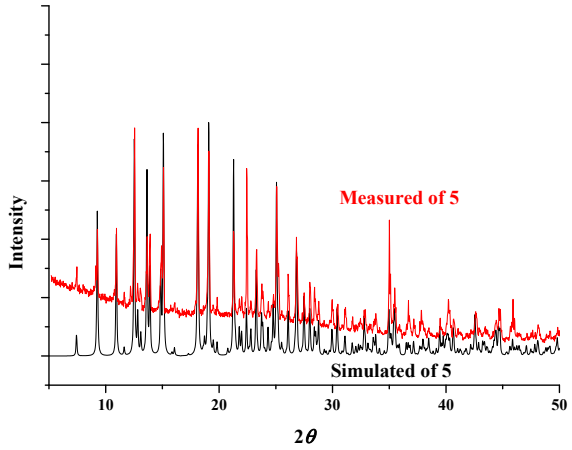

Fig. S38 The measured and simulated PXRD patterns of **5**.

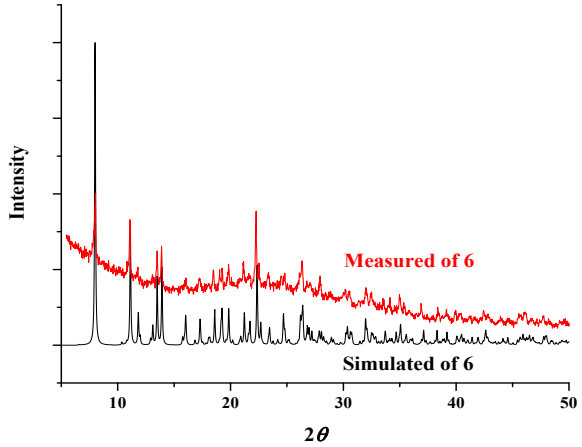

Fig. S39 The measured and simulated PXRD patterns of **6**.

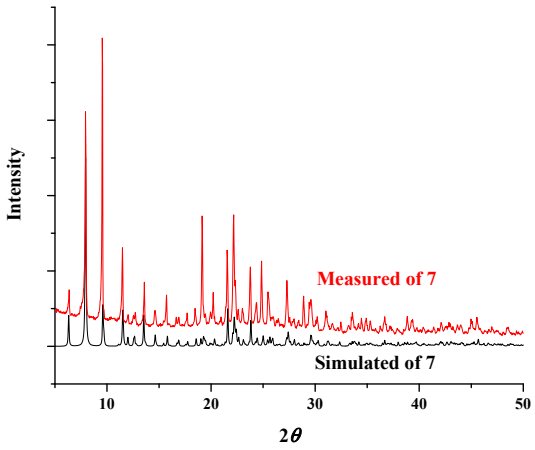

Fig. S40 The measured and simulated PXRD patterns of **7**.

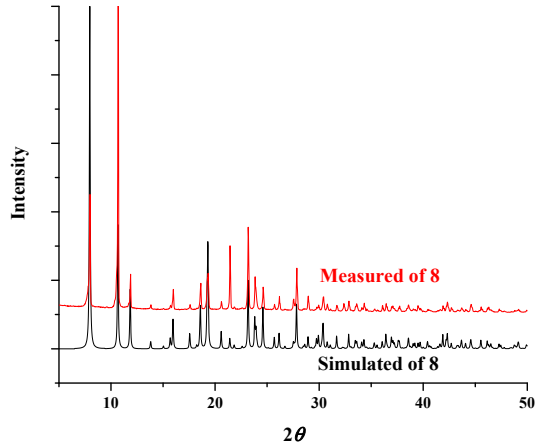

Fig. S41 The measured and simulated PXRD patterns of **8**.

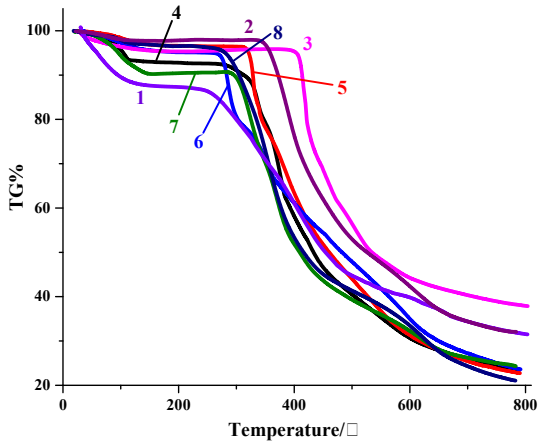

Fig. S42 The TG curves of **1**-**8**.

$$5nCd^{2+}+3nbtrb+2nbtec^{4-}+13nH_2O+2nOH^- \xrightarrow[(2)\ rt.,\ 30d]{(1)\ 110℃,\ 3d} \{[Cd(btrb)(H_2O)_4][Cd_2(btrb)(btec)(H_2O)_2]_2(OH)_2•5H_2O\}n\ (\mathbf{1}•(OH)_2•5H_2O)$$

$$nCd^{2+}+0.5nbtrb+0.5nbptc^{4-}+nH_2O \xrightarrow[3d]{90℃} \{[Cd(btrb)_{0.5}(bptc)_{0.5}]•H_2O\}n\ (\mathbf{2}•H_2O)$$

$$3nCd^{2+}+nbtrb+2nbtc^{3-}+3nH_2O \xrightarrow[3d]{90℃} \{[Cd_3(btrb)(btc)_2]•3H_2O\}n\ (\mathbf{3}•3H_2O)$$

$$nCd^{2+}+nbtrb+nip^{2-}+nH_2O \xrightarrow[3d]{90℃} \{[Cd(btrb)(ip)(H_2O)]•H_2O\}n\ (\mathbf{4})$$

$$nCd^{2+}+nbtrb+nMeOip^{2-}+nH_2O \xrightarrow[3d]{90℃} \{[Cd(btrb)(MeOip)]•H_2O\}n\ (\mathbf{5})$$

$$2nCd^{2+}+2nbtrb+2n1,2\text{-}bdc^{2-}+3nH_2O \xrightarrow[3d]{90℃} \{[Cd_2(btrb)_2(1,2\text{-}bdc)_2]•3H_2O\}n\ (\mathbf{6})$$

$$4nCd^{2+}+2nbtrb+4nbpdc^{2-}+11nH_2O \xrightarrow[3d]{90℃} \{[Cd_2(btrb)(bpdc)_2]_2•11H_2O\}n\ (\mathbf{7})$$

$$nCd^{2+}+nbtrb+nbpdc^{2-}+nH_2O \xrightarrow[3d]{90℃} \{[Cd(btrb)(bpdc)]•H_2O\}n\ (\mathbf{8})$$

Fig. S43 The balanced chemical reaction equations of **1**-**8**.