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Design and syntheses of 1D and 2D coordination polymers resulting from flexible building blocks

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Abstract

Two new mixed-ligand coordination polymers, [Cd(bpp)(cpg)$_2$ (H$_2$O)$_2$] (**1**), [Zn(bpp)(cpg)]·H$_2$O (**2**), have been synthesized. The central cadmium and zinc ions are hexa-coordinate and tetra-coordinate, respectively. X-ray analyses show that different coordination propensity of cadmium and zinc ions leads to different structures, 1D bilayer ladder (**1**) and 2D rectangle grid network (**2**), in which cpg and bpp ligand exist as their stable conformation, respectively (TT-form and TG-form).

Keywords: Hydrothermal reaction; Flexible ligand; Conformation

1. Introduction

The design and construction of inorganic–organic hybrid materials by flexible ligands have received great attention [1–6]. The reason of such structures attracting us is that the flexibility and conformation freedoms of flexible building blocks offer the possibility for obtaining unprecedented frameworks with tailored properties and functions. The fascinating structures of these complexes, coupled with their specific functionality, have made them highly promising in various applications, particularly absorption, catalysis, and molecular magnetization [7–10]. In order for such complex to be potentially useful, it is essential that their structures can be rationally and predictably tuned via variation their constituent building blocks. However, the rational design of these structures is in challenge for two reasons. The first is that different conformations of such flexible building blocks can be incorporated into several different 'supramolecular isomers' where structure prediction becomes difficult [11]. The second is that the design is often complicated by the uncertain coordination propensity of metal ions [12]. Thus, understanding how these considerations affect the formation of the structures is at the heart of the controlling synthesis of complexes resulting from flexible building blocks.

In order to achieve predictability of structures resulting from flexible building units, we have synthesized a series of complexes from the flexible organic ligand with –C$_2$-spacer (4-pyridylacetic acid) in previous works, which are 2D networks with helical chains or rhombic grids, respectively [13]. For further study, we employ mixed flexible ligand of 3-(4-chlorophenyl) glutaric acid (cpg) and 1,3-di(4-bipy)-propane (bpp) in this paper. Both cpg and bpp are flexible ligands with similar –C$_3$-spacer, and the difference between them is the terminal groups (carboxylate groups for cpg and pyridine rings for bpp). We choose cpg and bpp as mixed ligand for 3-fold motives: (1) comparing with 4-pyridylacetic acid, cpg and bpp are more flexible for longer alkyl spacer (–C$_3$- vs –C$_2$-). (2) As shown in Scheme 1, cpg and bpp can exist at least four different conformations, such as TT, TG, GG, and GG$'$ (where T: *trans* and G: *gauche*) [14], which offer interesting possibility for the application in the recognition/separation of molecules. (3) Different terminal groups of cpg and bpp may show different effects on the conformation of alkyl chains. In this paper, we report, our recent results in the design and syntheses of two complexes [Cd(bpp)(cpg)$_2$ (H$_2$O)$_2$] (1), [Zn(bpp)(cpg)].H$_2$O (2), which possess 1D 'bi-layer ladder' and 2D rectangular grid network, respectively.

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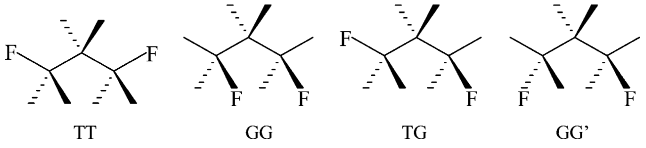

Scheme 1. The possible conformations of cpg and bpp (F: functional group, carboxylate groups for cpg and pyridine rings for bpp).

2. Experimental

2.1. General

$Cd(NO_3)_2 \cdot 4H_2O$, $Zn(NO_3)_2 \cdot 6H_2O$, H_2cpg and bpp were purchased commercially and used without further purification. C, H and N analyses were determined on a Perkin-Elmer 240C analyzer. IR spectra were recorded on a Magna 750 FT-IR spectrophotometer as KBr pallets. Thermogravimetric experiments were performed using a TGA/SDTA851 instrument (heating rate of 10 °C/min, argon stream).

2.2. Synthesis of $[Cd_2(bpp)(cpg)_2(H_2O)_2]$ (**1**)

A mixture of H_2cpg (0.0242 g, 0.1 mmol), bpp (0.0198 g, 0.1 mmol) and $Cd(NO_3)_2 \cdot 4H_2O$ (0.0308 g, 0.1 mmol) in 15 ml distilled water was sealed in a Teflon-lined Stainless autoclave and heated at 165 °C for 3 days under autogenous pressure and then cooled to room temperature during 2 days. Colorless prism-like crystals of **1** suitable for X-ray analysis were obtained in 67%. Anal Calc. for $C_{35}H_{36}Cd_2Cl_2N_2O_{10}$ (940.41): C, 44.70; H, 3.86; N, 2.98. Found: C, 44.74; H, 3.82; N, 3.02. IR data (KBr pellet ν/cm^{-1}): 3215m, 2926m, 1613s, 1557vs, 1491s, 1423vs, 1332s,1296m, 1227w, 1087m, 1014m, 988w, 928w, 827s, 723w, 661m, 619m.

2.3. Synthesis of $[Zn(bpp)(cpg)] \cdot H_2O$ (**2**)

The procedure was similar to that for **1**, except that $Cd(NO_3)_2$ was replaced by $Zn(NO_3)_2$. Light-yellow prism-like crystals of **2** suitable for X-ray analysis were obtained in 40%. Anal Calc. for $C_{24}H_{25}ZnClN_2O_5$ (522.31): C, 55.19; H, 4.82; N, 5.36. Found: C, 55.23; H, 4.78; N, 5.34. IR data (KBr pellet ν/cm^{-1}): 3493m, 3393m, 2933w, 1601vs, 1579s, 1489m, 1429s, 1392s, 1333w, 830m.

2.4. X-ray crystallography

The intensity data of **1** and **2** were collected on a Rigaku CCD diffractometer with graphite-monochromatized Mo Kα ($\lambda = 0.71073$ Å) radiation at 173(2) K. All absorption corrections were performed using the CrystalClear program [15]. The structures were solved by direct methods [16] and refined on F^2 by full-matrix least-squares using the SHELXTL−97 program package [17]. All non-hydrogen atoms were refined anisotropically. The organic hydrogen atoms were generated geometrically (C–H 0.96 Å).

Table 1
Crystal data and refinement parameters of complexes **1** and **2**

	1	**2**
Empirical formula	$C_{35}H_{36}Cd_2Cl_2N_2O_{10}$	$C_{24}H_{25}ClN_2O_5Zn$
Molecular weight	940.36	522.28
Temperature (K)	273	273
Crystal system	Triclinic	Monoclinic
Space group	P-1	*P2(1)/n*
a (Å)	10.232(3)	13.6106(10)
b (Å)	10.255(3)	12.0260(8)
c (Å)	20.201(6)	14.7801(11)
α (°)	96.298(14)	90
β (°)	101.419(11)	97.606(3)
γ (°)	111.508(9)	90
V (A^3)	1894.1	2397.9
Z	2	4
D_{calcd} (g cm^{-3})	1.649	1.447
μ (mm^{-1})	1.320	1.173
Reflection collected/ unique	14,641/8520	14,871/4233
R_{int}	0.0264	0.0497
Goodness-of-fit on F^2	1.037	1.105
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0496$, $wR_2 = 0.0888$	$R_1 = 0.0379$, $wR_2 = 0.0826$
R indices (all data)	$R_1 = 0.0695$, $wR_2 = 0.1010$	$R_1 = 0.0455$, $wR_2 = 0.0866$
Max, min $\Delta\rho$ (e $Å^{-3}$)	1.275, −0.709	0.284, −0.228

The crystallographic data for complexes **1** and **2** are listed in Table 1 and selected bonds and angles in Table 2.

3. Results and discussion

3.1. Syntheses

Our aim is to achieve predictability of structures resulting from flexible building units, so we try to exclude the interfering of different conformations of flexible building units and attempt to clear the uncertainty of coordination propensity of metal ions. As mentioned above,

Table 2
Selected bond lengths (Å) and angles (°) for complexes **1** and **2**

*Complex **1***			
Cd(1)–O(2)	2.378(3)	Cd(2)–O(1)	2.315(4)
Cd(1)–O(3)	2.271(3)	Cd(2)–O(4)	2.291(3)
Cd(1)–O(5)$^{\#1}$	2.383(3)	Cd(2)–O(7)	2.326(3)
Cd(1)–O(6)$^{\#1}$	2.320(3)	Cd(2)–O(8)	2.428(3)
Cd(1)–O(9)$^{\#1}$	2.293(3)	Cd(2)–O(10)$^{\#1}$	2.272(4)
Cd(1)–N(1)	2.403(4)	Cd(2)–N(2)$^{\#2}$	2.359(4)
O(2)–Cd(1)–N(1)	171.56(14)	O(1)–Cd(2)–N(2)$^{\#2}$	165.86(15)
*Complex **2***			
Zn(1)–O(1)	1.9593(18)	Zn(1)–N(1)	2.029(2)
Zn(1)–O(4)$^{\#3}$	1.9736(17)	Zn(1)–N(2)$^{\#4}$	2.075(2)
O(1)–Zn(1)–O(4)$^{\#3}$	112.77(7)	O(1)–Zn(1)–N(2)$^{\#4}$	103.81(8)
O(1)–Zn(1)–N(1)	129.96(8)	O(4)$^{\#3}$–Zn(1)–N(2)$^{\#4}$	96.57(7)
O(4)$^{\#3}$–Zn(1)–N(1)	100.76(7)	N(1)–Zn(1)–N(2)$^{\#4}$	108.14(8)

Symmetry codes: $^{\#1}$ $x+1, y, z$; $^{\#2}$ $-x+1, -y+2, -z+1$; $^{\#3}$ $x+1/2, -y+1/2, z+1/\alpha$; $^{\#4}$ $x, y+1, z$.

both cpg and bpp exist as mixture of different conformations at room temperature. Thus, we introduce hydrothermal reaction method convenient to adjust the reaction temperature, hoping to isolate complex with single conformation of ligand at higher temperature. In this paper, we choose metal ions favoring tetra- (Zn) and hexa-coordination mode (Cd) to examine the effects of metal ions on the formation of structures by using flexible ligands. We first determined the hydrothermal reaction of H_2cpg, bpp and $Cd(NO_3)_2$ at 1:1:1 and obtain complex **1**. Out of our anticipation, the ratio of cpg, bpp and $Cd(NO_3)_2$ in complex **1** is 2:1:2, which prompts us to investigate the reaction of cpg, bpp and $Cd(NO_3)_2$ with different ratios, such as 1:2:1 and 1:3:1. However, the X-ray diffraction shows the structures of products obtained from different ratios are the same as complex **1**. Interested in the effect of coordination propensity of metal centers on the structure, we replaced $Cd(NO_3)_2$ with $Zn(NO_3)_2$, and complex **2** was isolated in 40%. In complex **2**, the ratio of cpg, bpp and $Zn(NO_3)_2$ is 1: 1:1.

*3.2. Crystal structure of complex **1***

Single-crystal X-ray analysis reveals that **1** is a 1D bilayer ladder structure. As shown in Fig. 1, the coordination environments of two Cd centers are similar with four oxygen atoms from one chelating and two bridging-bidentate carboxylate groups, one oxygen atom from coordinated water and one nitrogen atom from bpp. The Cd–O distances range from 2.271 to 2.428 Å, and the Cd–N distances are 2.359 and 2.403 Å, respectively. Through two carboxylate groups, the cpg ligand bridges the cadmium centers forming a $Cd_n(cpg)_n$ chain, and the carboxylate group adopting bridging–bidentate mode bridges two adjacent $Cd_n(cpg)_n$ chains into double chains. As rungs of ladders, the bpp ligands link two double chains forming bilayer ladders. Different from 1D monolayer ladder structure and other 2D bilayer structures [18], the 1D bilayer ladder of complex **1** is seldom reported (Fig. 2). In complex **1**, a cuboidal box forms the fundamental building unit (Fig. 3). This cuboidal structural motif contains eight cadmium (II) ions at the corners, which are connected by four short carboxylate bridges, four long cpg and bpp linkers, making up 12 edges of cuboidal unit. Such cuboidal unit is clearly different from the tetrahedral building blocks used to form other bilayer structures [19,20]. As shown in Fig. 3, two chlorophenyl groups of cpg ligand in each unit orients at different directions occupying the void of the channel. The steric hindrance of two chlorophenyl groups may be the reason that no small molecules locate in the channel. In complex **1**, all dicarboxylate ligands (cpg) are observed as TT-form, and all dipyridine ligand (bpp) exist as TG-form, although they have similar –C_3- spacer (Fig. 4).

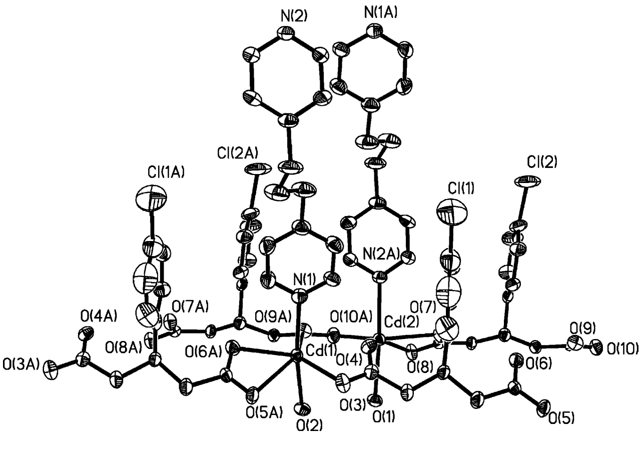

Fig. 1. Coordination environment of complex **1**. Thermal ellipsoids are shown at 30% probability. The related coordination atoms are labeled out. For clarity, all hydrogen atoms were omitted.

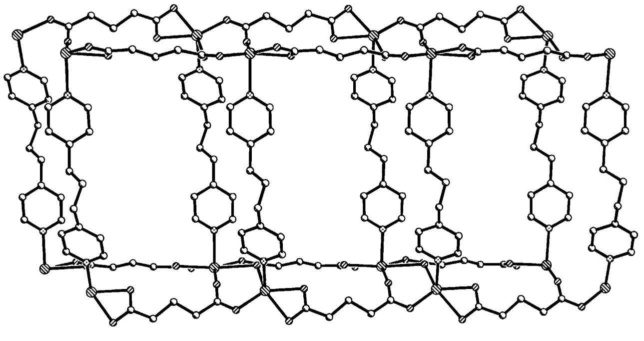

Fig. 2. The 1D bilayer ladder of **1**.

There are two kinds of hydrogen bonds in complex **1**. One kind is hydrogen bonds between coordinated water and carboxylate groups of adjacent ladders (O–O: 2.668–2.759 Å). The other kind exists between two coordinated water molecules of the same ladder (O–O: 2.867 Å). The hydrogen bonds link adjacent ladders into a 3D architecture.

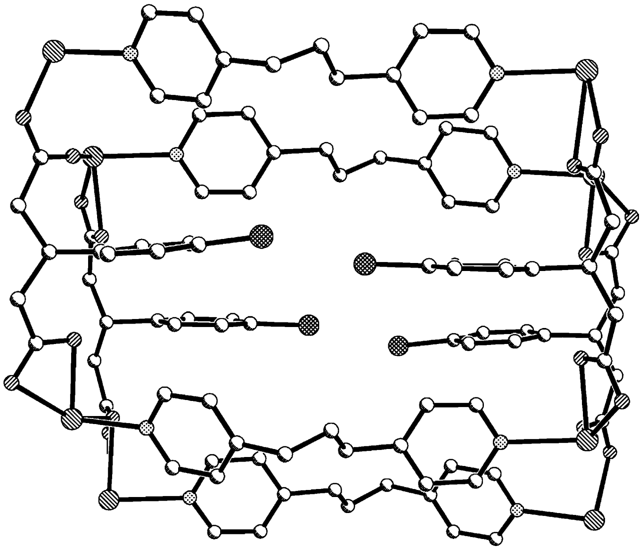

Fig. 3. View of the cuboidal structural motif in **1**.

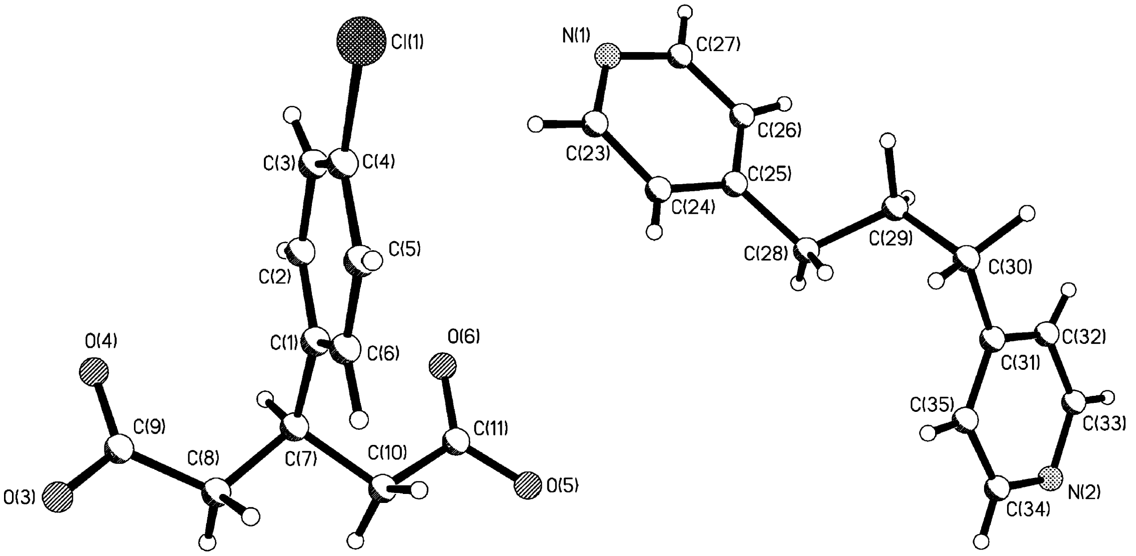

Fig. 4. The TT-form of cpg and TG form of bpp in **1**.

3.3. Crystal structure of complex **2**

Single-crystal X-ray analysis shows that **2** is a two-dimensional network. As shown in Fig. 5, both carboxylate groups of cpg are monodentate, so each Zn center is four-coordinated with two oxygen atoms from two carboxylate groups and two nitrogen atoms from two bpp molecules. The Zn–O distances are 1.974 and 1.959 Å, and the Zn–N distances are 2.075 and 2.029 Å, respectively. Two cpg and two bpp link four Zn atoms forming a Zn_4 grid with the dimension of 12.026 Å × 9.405 Å, which is the basic building unit for the whole 2D network of **2** (Fig. 6). In such unit, the chlorophenyl groups of two cpg ligands orients at the same direction, so only one chlorophenyl group occupies the void of each grid, which leaves space for one free water molecule. The Zn_4 grids are connected to form the ultimate 2D network. In this network, two pyridine rings of one dpp molecule are almost perpendicular (dihedral angle of 74.1°), and at the same time, two pyridine rings coordinated to the same Zn atom are also perpendicular (dihedral angle of 74.2°), which makes the whole network wave-like. Similar to that in complex **1**, all cpg ligands exist as TT-form and bpp are observed as TG-form in complex **2**.

The free water molecules locate at the grids fixed by hydrogen bonds between free water and carboxylate groups (O–O: 2.815, 2.878 Å). The hydrogen bonds between free water and carboxylate groups in adjacent layer link all 2D layers into 3D supramolecular architecture.

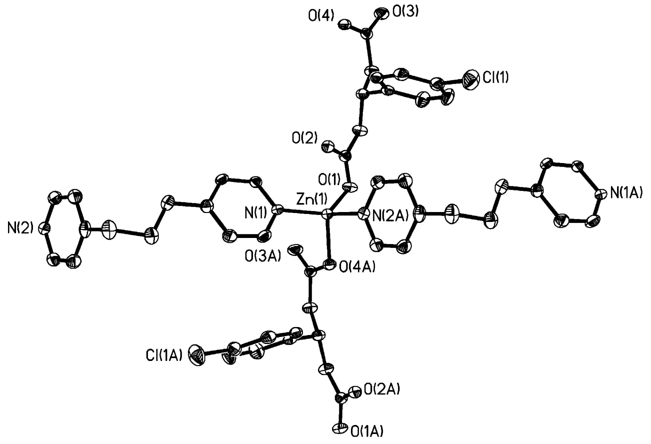

Fig. 5. Coordination environment of complex **2**. Thermal ellipsoids are shown at 30% probability. The related coordination atoms are labeled out. For clarity, all hydrogen atoms were omitted.

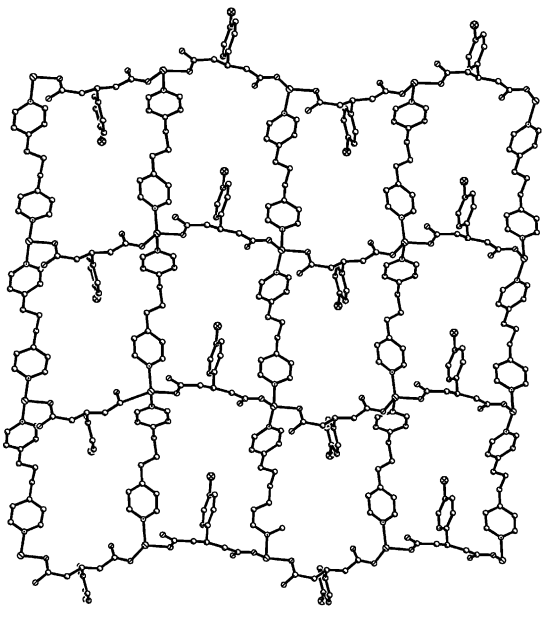

Fig. 6. View of the 2D network in **2** with grids.

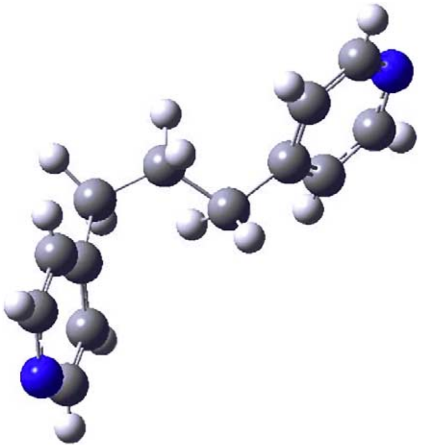

Fig. 7. The TG conformation of the final optimized structure.

3.4. Theoretical calculation

To predict the equilibrium structure of bpp ligand in the ground state, geometry optimization was performed at the Hartree-Fock (HF) level of theory. The basis set 6-31+G* was specified for atoms of C, H and N. The initial geometric parameters were taken from the X-ray experimental data. The convergence criterion of the SCF energy of 10^{-8} a.u. was set. All calculations were accomplished using the GAUSSIAN 03 program package [21]. The final optimized structure was found to be TG conformation (Fig. 7), (the total energy is −609.3582 hartrees and the total dipole moment is 2.9368 Debye). This result showed that the TG-form was the stable configuration for bpp liand, but it is reported that the most stable conformation of aliphatic dicarboxylate is TT-form [4b]. This difference proved that different terminal groups of aliphatic dicarboxylate and aliphatic dipyridine have different effects on the conformation of alkyl chains.

3.5. Vibrational spectra, thermal properties and X-ray powder diffraction

The IR spectrum of **1** shows typical chelating carboxylate asymmetric and symmetric stretching bands at 1557 and 1423 cm^{-1}[22,23]. In the spectra of 2, the bands at 1579 and 1392 cm^{-1} are assigned to the $\nu_{\text{asym}}(\text{CO}_2)$ and $\nu_{\text{sym}}(\text{CO}_2)$ stretching vibrations of monodentate carboxylate of cpg ligand [24]. The difference of IR spectra between **1** and **2** reveals different coordination mode of carboxylate groups in cpg, which is consistent with their crystal structures.

The thermal stability of complexes **1** and **2** has been determined on polycrystalline samples in a nitrogen atmosphere by thermogravimetric analysis (TGA). There was no chemical decomposition up to 285 °C in **1**. For **2**, the total weight loss of 3.47% from 148 to 276 °C corresponds to the loss of one free water molecule per formula unit (ca. 3.45%), indicating the presence of hydrogen bonding interaction between water molecule and carboxyl group of cpg. This complex starts decomposition after 312 °C.

The original samples and dehydrated samples of **1** and **2** were characterized by X-ray Powder diffraction (XRPD) at room temperature. The pattern calculated from the single crystal X-ray data of **1** and **2** were in good agreement with the observed one. Compared to the original samples, the dehydrated solids obtained by heating crystals of **1** and **2** up to 280 °C show almost identical XRPD patterns. These results illustrate that the framework of **1** is retained before 280 °C and the main framework of **2** remains after removal of all the water molecules.

4. Conclusion

Two coordination polymers have been prepared and characterized from the mixed flexible carboxylate and pyridine ligand of cpg and bpp. In complex **1**, the cadmium centers are hexa-coordinated, leading to a 1D bilayer ladder structure, and in complex **2**, the zinc centers adopt tetra-coordination, which results a 2D grid network. Adopting hydrothermal reaction method, we isolate complexes **1** and **2** successfully, in which cpg and bpp ligand exist as their stable conformation, respectively (TT-form and TG-form). The successful synthesis of 1D (**1**) and 2D (**2**) architectures provide useful materials for the rationalizing design of complexes constructing from flexible building units.

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Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.molstruc.2005.07.031. Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Center, CCDC 272765and 272766 (for 1 and 2). These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the cambridge Crystallographic Data Center, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (inernat.)+44 1223/336 033; email: deposit@ccdc.acm.ac.uk].

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