

Synthesis, Structure and Characterization of a Helical Seven-Coordinated Pyridine-2,6-dicarboxylate-Bridged Cadmium(II) Complex

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Abstract

[Cd(C₇H₃NO₄)(H₂O)_{1.5}]_n or [Cd(2,6-pydc)(H₂O)_{1.5}]_n, (**1**) (2,6-pydc = pyridine-2,6-dicarboxylate) was obtained from the reaction of pyridine-2,6-dicarboxylic acid and 4-hydroxypyridine-2,6-dicarboxylic acid with cadmium(II) nitrate tetrahydrate in the presence of piperazine and characterized by elemental analysis, IR spectra and X-ray single crystal diffraction. Complex (**1**) is a novel carboxylate-bridged one-dimensional pincer-shaped helical chain of cadmium(II) polymer. Each Cd atom is seven-coordinate and exhibits an approximately pentagonal-bipyramidal CdNO₆ coordination geometry. The metal fragments are linked *via* the central four-membered Cd₂O₂ ring and the structural analysis showed that 4-hydroxypyridine-2,6-dicarboxylic acid and piperazine do not appear in the structure.

Keywords: Chelating ligands, Cadmium(II) complex, Pyridine-2,6-dicarboxylic acid, Helical chain.

1. Introduction

The design and construction of transition metal coordination polymers and supramolecular architectures, especially helical chains have attracted attention. Such studies mainly focus on the construction of metal-organic frameworks having novel topology and on the crystal engineering of the molecular complexes. One of the strategies for constructing of coordination polymers is to bridge metal ions by carboxylate ligands.^{1–3}

The multi-carboxylate ligands are known as the good spacers for formation of 1D, 2D or 3D frameworks owing to their rich coordination modes. Recent investigations have focused on the usage of this series molecules such as 2,3-pydcH₂ (pydc = pyridine-dicarboxylate), 2,5-pydcH₂, 2,6-pydcH₂, 3,5-pydcH₂, 2,4-pydcH₂.^{4–6} Pyridine-2,6-dicarboxylic acid (2,6-pydcH₂) is an attractive ligand. It can bind metal ions as a tridentate chelating agent in neutral (pydcH₂), monoanionic (pydcH)[–] or dianionic (pydc)^{2–} form. The coordination chemistry in the dianionic form (pydc)^{2–}, which itself has a planar geometry, has been extensively investigated.^{7–13} For complexes having two planar (pydc)^{2–} molecules, coordination to metal ions in two independent perpendicular planes generates a six-coordinate octahedral geometry.¹⁴ The mixed ligand metal complexes containing one (pydc)^{2–} and an auxiliary

ligand like a H₂O or N-based heterocycle, usually form a four- or five-fold coordination geometry.¹⁵

However, in the complex [Cd(2,6-pydc)(H₂O)_{1.5}]_n, dianionic (pydc)^{2–} acts as a bridging ligand to form a seven-coordinate carboxylate-bridged coordination polymer. We here report the syntheses, and structural characterization of a helical one-dimensional cadmium(II) coordination polymer [Cd(2,6-pydc)(H₂O)_{1.5}]_n which has clearly different structure from other reported metal complexes containing Pyridine-2,6-dicarboxylate ligand.^{7–13}

2. Experimental

2.1. Materials and Instrumentations

Pyridine-2,6-dicarboxylic acid, 4-hydroxypyridine-2,6-dicarboxylic acid, cadmium(II) nitrate tetrahydrate and piperazine, were purchased from Merck and used without further purification. IR spectra were recorded on a Bruker FT-IR Tensor 27 spectrometer (KBr pellets, Nujol mulls, 4000–400 cm^{–1}). Elemental analyses were performed using a Costech ECS 4010 CHNS analyzer. X-ray structure analysis of suitable single crystals was carried out on a Bruker APEX-DUO CCD area detector (Mo K α radiation, graphite monochromator, $\lambda = 0.71073$ Å at 150 K).

2. 2. Synthesis of Complex (1)

Pyridine-2,6-dicarboxylic acid (167 mg, 1 mmol) was dissolved in 20 ml deionized water containing 183 mg (1 mmol) of 4-hydroxypyridine-2,6-dicarboxylic acid and 172 mg (2 mmol) of piperazine and stirred at 60 °C for 1 hour. An aqueous solution of 308 mg (1 mmol) of $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ was added to the above solution. Reaction mixture was stirred at 60 °C for 4 hours. Colorless needle crystals of $[\text{Cd}(\text{2,6-pydc})(\text{H}_2\text{O})_{1.5}]_n$ were obtained after allowing the mixture to stand for 3 weeks at room temperature. The structure showed 4-hydroxypyridine-2,6-dicarboxylic acid and piperazine were not bonded in the product. IR (KBr) (cm^{-1}): 3495 (m), 3449 (m), 3394 (s), 3148 (m), 2684 (w), 1725 (s), 1695 (s), 1635 (s), 1506 (s), 1460 (s), 1435 (s), 1377 (s), 1278 (s), 1151 (m), 1079 (m), 1018 (m), 984 (m), 910 (m), 822 (m), 780 (m), 766 (m), 730 (m), 698 (m), 667 (m) cm^{-1} . (Found: C, 26.19; H, 1.73; N, 4.28%. Calc. for $\text{C}_{14}\text{H}_{12}\text{Cd}_2\text{N}_2\text{O}_{11}$ (609.06): C, 27.58; H, 1.98; N, 4.59%).

2. 3. Crystallography

The data for (1) were collected on a Bruker Kappa APEX-DUO diffractometer using monochromated $\text{MoK}\alpha$ radiation and were measured using a combination of scans and scans. The data were processed using APEX2 and SAINT.¹⁶ Absorption corrections were carried out using SADABS.¹⁶ The structure was solved and refined using SHELXTL¹⁷ for full-matrix least-squares refinement that was based on F^2 . H atoms bonded to C atoms were included in calculated positions and allowed to refine in riding-motion approximation with U_{iso} derived from the car-

rier atom. H atoms bonded to O atoms were refined independently with isotropic displacement parameters.

3. Results and Discussion

3. 1. IR Spectra

The IR spectrum of the compound shows broad strong bands at the region 3148–3495 cm^{-1} , which is due to the coordinated water molecules. The two bands at 1635 and 1695 cm^{-1} caused by water molecules overlap the absorption band of COO^- . The stretching vibrations of COO^- illustrate the corresponding bands at 1377 and 1635 cm^{-1} . In the region of 1435–1506 cm^{-1} , sharp and relatively strong peaks are attributed to aromatic $\text{C}=\text{C}$ of (pydc)²⁻ ring.¹⁸

3. 2. Crystal Structure

The molecular structure of $[\text{Cd}(\text{2,6-pydc})(\text{H}_2\text{O})_{1.5}]_n$, (1) with atom numbering, coordination polyhedra around central atoms and a view of the crystal packing are presented in Figures 1–3. The crystallographic data, selected bond lengths, bond angles and torsion angles are listed in Tables 1 and 2, respectively. Complex (1) crystallizes in the monoclinic space group $P2_1/c$ (Table 1). $[\text{Cd}(\text{2,6-pydc})(\text{H}_2\text{O})_{1.5}]_n$ consists of CdO_6N polyhedra and pyridine-2,6-dicarboxylate (pydc) organic groups (see Figure 1). There are two symmetry independent Cd atoms in the structure; both were connected to four oxygen and one nitrogen atoms in the equatorial positions and two oxygen atoms in the axial positions. Thus, a seven-coordinate pentagonal

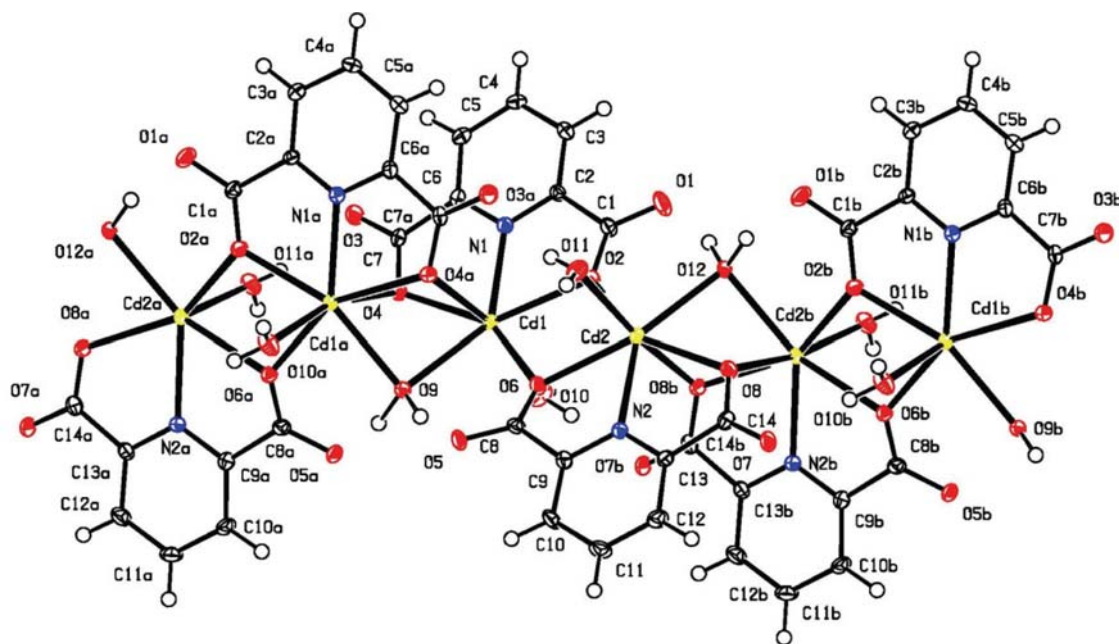


Figure 1. The molecular structure of $[\text{Cd}(\text{2,6-pydc})(\text{H}_2\text{O})_{1.5}]_n$, showing the atom-numbering scheme (The letters *a* and *b* refer to the symmetry operations $a = -x, y, 1/2-z$ and $b = 1-x, y, 1/2-z$).

bipyramidal geometry is observed around the Cd^{II} atom. The five equatorial ligands consist of N atom of the pyridine, three oxygen atoms from the carboxylates and one oxygen atom from the water, and each of the axial oxygen ligands is from the water and the carboxylate group (see Figure 2).

The polymer builds from dimeric units of [Cd₂(2,6-pydc)₂(H₂O)₃]. The Cd1O6N and Cd2O6N groups share their edges through the equatorial oxygen atoms [O2 and O6] of their pydc ligands, respectively and form the edge-sharing Cd2O10N2 dimers. Then the carboxylate groups of the pydc ligands from Cd1O6N and Cd2O6N groups are further coordinated to the other Cd1O6N and Cd2O6N groups, respectively through the axial oxygen atoms and form a 1D helical chain of cadmium(II) polymer that runs parallel to the [100] axis (see Figure 3). As seen in Figure 4, the two CdO6N pentagonal bipyramidal groups with

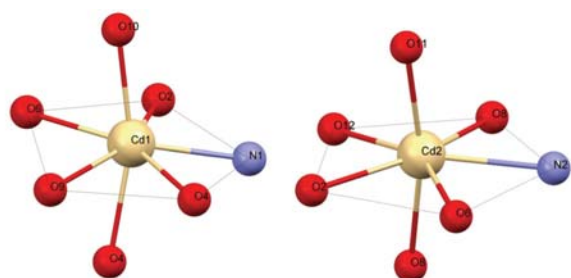


Figure 2. Coordination polyhedra around Cd1 and Cd2 in the complex of (1).

Table 1. Crystal and Structure Refinement Data for Compound 1

<i>Crystal data</i>	
Empirical Formula	C ₁₄ H ₁₂ Cd ₂ N ₂ O ₁₁
Formula weight	609.06
Cell setting, Space group	Monoclinic, <i>P2/c</i>
Unit cell dimensions	<i>a</i> = 13.4751(15) Å <i>b</i> = 9.3657(11) Å <i>c</i> = 13.5363(15) Å <i>β</i> = 93.858(2)°
Unit cell volume	1704.5(3) Å ³
Temperature (K)	150(1)
Absorption coefficient	2.564 mm ⁻¹
Z, Density [g/cm ³]	4, 2.373 /m ³
F(000)	1176
Crystal size (mm)	0.18 × 0.10 × 0.10
<i>R</i> value	0.0259
<i>R_w</i> value	0.0367
<i>θ</i> range (°)	1.51 → 27.60
<i>h</i> range	-17 → 15
<i>k</i> range	-12 → 12
<i>l</i> range	-17 → 17
Reflections collected / unique	3937/3185 [<i>R</i> (int) = 0.0372]
Completeness to <i>θ</i> _{max}	99.1%
Goodness-of-fit on <i>F</i> ²	1.022
Large diff. peak and hole	1.162 and -0.763 e. Å ⁻³

pydc linkers are joined by a bridging water molecule, which makes the shape look like a pair of pincers.

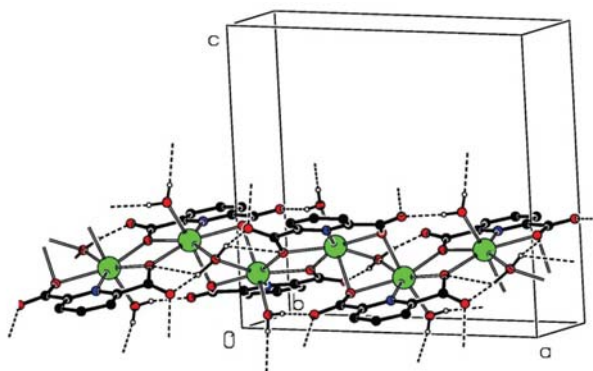


Figure 3. The crystal packing diagram of (1) along the crystallographic *a* axis.

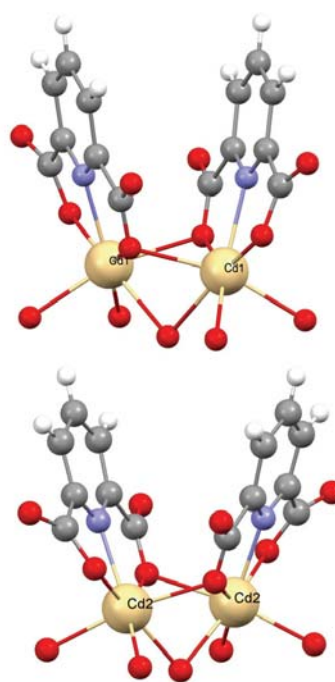
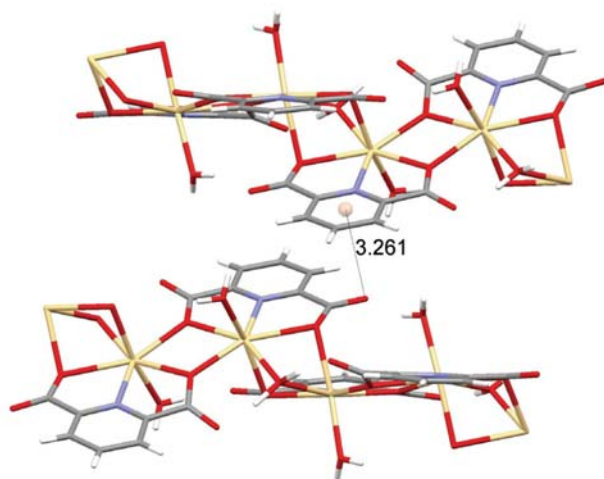


Figure 4. Ball-and-stick model representing a pair of pincer-shaped structure around Cd1 and Cd2 in the complex of (1). The two CdO6N pentagonal bipyramidal groups with pydc linkers are joined by a bridging water molecule (yellow, Cd; blue, N; red, O; gray, C).

The equatorial plane around Cd1 is defined by one nitrogen atom of the pyridine (Cd1–N1, 2.306(3) Å), three oxygen atoms from the carboxylates (Cd1–O2, 2.386(2); Cd1–O4, 2.440(2); Cd1–O6, 2.321(2) Å) and one oxygen atom from the water (Cd1–O9, 2.380(2) Å) and each of the axial oxygen ligands is from the water (Cd1–O10, 2.274(3) Å) and the carboxylate group (Cd1–O4^{*i*}, 2.337(2) Å; *i* = -*x*, *y*, 1/2-*z*). The equatorial plane around Cd2 is built by one N atom (Cd2–N2, 2.3316(3) Å) and four O atoms from the carboxylates (Cd2–O2, 2.306(2);

Table 2. Bond lengths (Å), bond angles and torsion angles (°) for Compound **1**

Distance (Å)			
Cd1–N1	2.306(3)	Cd2–N2	2.331(3)
Cd1–O2	2.386(2)	Cd2–O2	2.306(2)
Cd1–O4	2.440(2)	Cd2–O6	2.421(2)
Cd1–O6	2.321(2)	Cd2–O8	2.480(2)
Cd1–O9	2.380(2)	Cd2–O12	2.365(2)
Cd1–O10	2.274(3)	Cd2–O11	2.259(3)
Cd1–O4 ⁱ	2.337(2)	Cd2–O8 ⁱⁱ	2.304(2)
Angle (°)			
O2–Cd1–N1	68.95(8)	O2–Cd2–N2	139.05(8)
O4–Cd1–N1	68.39(8)	O6–Cd2–N2	68.56(8)
O4 ⁱ –Cd1–N1	90.09(8)	O8–Cd2–N2	66.57(8)
O6–Cd1–N1	139.37(8)	O8 ⁱⁱ –Cd2–N2	92.24(8)
O9–Cd1–N1	135.97(8)	O11–Cd2–N2	98.83(10)
O10–Cd1–N1	106.85(9)	O12–Cd2–N2	136.24(8)
O2–Cd1–O4	137.34(7)	O2–Cd2–O6	70.70(7)
O2–Cd1–O6	71.07(7)	O2–Cd2–O8	152.44(7)
O2–Cd1–O9	151.38(6)	O2–Cd2–O11	82.03(9)
O2–Cd1–O10	88.71(8)	O2–Cd2–O12	82.70(6)
O2–Cd1–O4 ⁱ	99.82(7)	O2–Cd2–O8 ⁱⁱ	87.88(8)
O4–Cd1–O6	150.92(7)	O6–Cd2–O8	134.63(6)
O4–Cd1–O9	69.33(6)	O6–Cd2–O11	85.87(9)
O4–Cd1–O10	103.61(8)	O6–Cd2–O12	151.74(5)
O4–Cd1–O4 ⁱ	80.13(7)	O6–Cd2–O8 ⁱⁱ	95.78(7)
O6–Cd1–O9	81.60(6)	O8–Cd2–O11	107.11(8)
O6–Cd1–O10	78.96(8)	O8–Cd2–O12	70.23(6)
O6–Cd1–O4 ⁱ	89.76(7)	O8–Cd2–O8 ⁱⁱ	79.71(7)
O9–Cd1–O10	94.37(8)	O11–Cd2–O12	100.04(8)
O9–Cd1–O4 ⁱ	71.09(6)	O11–Cd2–O8 ⁱⁱ	168.62(9)
O10–Cd1–O4 ⁱ	162.90(8)	O12–Cd2–O8 ⁱⁱ	73.33(6)
Torsion angles (°)			
N1–Cd1–O2–Cd2	168.82(12)	N2–Cd2–O2–Cd1	9.55(17)
N1–Cd1–O6–Cd2	–7.05(17)	N2–Cd2–O6–Cd1	–179.55(11)
O2–Cd1–O4–Cd1 ⁱ	–123.97(9)	O2–Cd2–O8–Cd2 ⁱⁱ	–30.98(18)
O2–Cd1–O9–Cd1 ⁱ	119.46(13)	O2–Cd2–O12–Cd2 ⁱⁱ	–133.83(6)
O6–Cd1–O4–Cd1 ⁱ	41.11(17)	O6–Cd2–O8–Cd2 ⁱⁱ	121.58(9)
O6–Cd1–O9–Cd1 ^a	136.66(5)	O6–Cd2–O12–Cd2 ⁱⁱ	–114.28(13)

 $i = -x, y, 1/2-z$ $ii = 1-x, y, 1/2-z$ 

Cd2–O6, 2.421(2); Cd2–O8, 2.480(2); Cd2–O12, 2.365(2) Å) and each of the axial oxygen ligands is from the water (Cd2–O11, 2.259(3) Å) and the carboxylate group (Cd2–O8ⁱⁱ, 2.304(2) Å; $ii = 1-x, y, 1/2-z$) (Table 2). The $d(\text{Cd1–N1})$ and $d(\text{Cd2–N2})$ are 2.306(3) Å and 2.331(3) Å, respectively. The average Cd1–O distance and Cd2–O distance both are 2.356 Å, which are comparable to those observed in Cd(II) complexes based on polycarboxylates with identical coordination spheres,¹⁹ but it is

Figure 5 A. View of the C–O... π stacking interaction between the carbonyl group of the pyridine-2,6-dicarboxylate groups and the pyridine ring of pydc²⁻ fragments, with an O... π distance of 3.261(3) Å for C7–O3...Cg1 ($-x, -y, -z$) [Cg1 is the centroid for the (N1/C2–C6) ring].

shorter than that of analogous cadmium complexes.^{20–22}

In the crystal structure there are C–O $\cdots\pi$ stacking interactions between the carbonyl groups of the pyridine-2,6-dicarboxylate groups and the pyridine ring of symmetry related, with an O $\cdots\pi$ distance of 3.261(3) Å (measured to the center of the pyridine ring) for C7–O3 \cdots Cg1 (-x, -y, -z) [Cg1 is the centroid for the (N1/C2–C6) ring] (see Figure 5).

As shown in Table 3, various hydrogen bonds of type O–H \cdots O and C–H \cdots O are also responsible for the expansion of the structure. Both weak and strong hydrogen bonds with D \cdots A distances ranging from 2.613(3) to 3.439(4) Å, are observed in the crystal. The presence of carboxylate and coordinated water molecules in the crystal structure causes the hydrogen bonding network of the system to be more extended, as its hydrogen bonds probably have an important linking role between the molecules of the structure. The structure consists of an infinite two-dimensional network of O–H \cdots O and C–H \cdots O hydrogen-bonded in the (010) plane.

Table 3. Hydrogen-bond geometry (Å, °).

D–H \cdots A	D–A	H \cdots A	D \cdots A	D–H \cdots A
O9–H9O \cdots O5 ⁱ	1.12(4)	1.53(5)	2.634(3)	165(4)
O10–H10B \cdots O5 ⁱⁱⁱ	0.78(5)	2.05(5)	2.819(3)	169(4)
O10–H10C \cdots O7 ⁱⁱ	0.84(5)	1.97(5)	2.805(3)	174(5)
O11–H11B \cdots O7 ^{iv}	0.82(5)	1.99(5)	2.786(4)	165(4)
O11–H11C \cdots O3 ⁱ	0.76(5)	2.00(5)	2.722(3)	159(5)
O12–H12O \cdots O1	0.93(4)	1.71(4)	2.613(3)	165(4)
C3–H3A \cdots O7 ^v	0.95	2.53	3.394(3)	152
C4–H4A \cdots O10 ^{vi}	0.95	2.57	3.439(4)	152
C5–H5A \cdots O5 ^{vii}	0.95	2.36	3.090(3)	134
C10–H10A \cdots O3 ^{ix}	0.95	2.42	3.287(3)	151
C12–H12A \cdots O1 ^{ix}	0.95	2.49	3.187(4)	130
C12–H12A \cdots O11 ^{iv}	0.95	2.51	3.200(5)	130

Symmetry Codes: *i* = -x, y, -z+1/2, *ii* = 1+-x, y, 1/2+z, \rightarrow *iii* = x, -1-y, -1/2+z, *iv* = 1-x, -1-y, 1-z, *v* = 1-x, 1+y, 1/2-z, *vi* = x, 1+y, z, *vii* = -x, 1+y, 1/2-z, *ix* = -x, -1+y, 1/2-z, *ix* = 1-x, -1+y, 1/2-z

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5. Appendix A. Supplementary data

Crystallographic data for the structure reported in this paper has been deposited at the Cambridge Crystallo-

graphic Center, CCDC No. 895784. Copies of the data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033; email: deposit@ccdc.cam.ac.uk]. Structure factor table is available from the authors.

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Povzetek

$[\text{Cd}(\text{C}_7\text{H}_3\text{NO}_4)(\text{H}_2\text{O})_{1.5}]_n$ ali $[\text{Cd}(2,6\text{-pydc})(\text{H}_2\text{O})_{1.5}]_n$, (**1**) (2,6-pydc = piridin-2,6-dikarboksilat) smo pripravili z reakcijo piridin-2,6-dikarboksilne kisline in 4-hidroksipiridin-2,6-dikarboksilne kisline s kadmijevim(II) nitratom tetrahidratom v prisotnosti piperazina. Dobljeno koordinacijsko spojino **1** smo okarakterizirali z elementno analizo, IR spektroskopijo in rentgensko strukturno analizo na monokristalu. Spojina **1** je kadmijev(II) polimer - enodimenzionalna spiralna veriga s karboksilatnimi mostovi, ki ima obliko klešč. Vsak kadmijev atom ima koordinacijsko število sedem, geometrija koordinacijskega poliedra pa je približna pentagonalna bipiramida CdNO_6 . Kovinski fragmenti so povezani preko centralnega štiričlenskega obroča Cd_2O_2 , strukturna analiza pa je pokazala, da molekule 4-hidroksipiridin-2,6-dikarboksilne kisline in piperazina v strukturi niso prisotne.