

## NOTE

## Ni(II) Coordination Polymer with 3D Supramolecular Structure

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One pyridinecarboxylato-bridged coordination polymers  $[\text{Ni}(\text{pbc})_2(\text{H}_2\text{O})_2]_n$  (Hpsc=3-pyrid-3-ylbenzoic acid) has been synthesized by the hydrothermal method and characterized by X-ray single crystal diffraction. The compound  $[\text{Ni}(\text{pbc})_2(\text{H}_2\text{O})_2]_n$  exhibit a 1D chain structure.

**Key Words:** Nickel(II), Coordination polymer, Hydrothermal synthesis, Crystal structure.

The current interest in polymeric coordination networks is rapidly expanding not only for their potential applications in catalysis, molecular adsorption, magnetism, nonlinear optics and molecular sensing, but also for their intriguing variety of topologies<sup>1-5</sup>. The suitable linker must have the quality to afford a wide variety of linking sites. One of the common strategy to construct these polymeric transition metal complexes is to select suitable multidentate ligands to integrate the metal ions to a desired framework. So the multidentate ligands with suitable spacers between the linking groups are good choices to get the infinite architectures. Besides covalent bonds, hydrogen bonds are frequently used as a powerful crystal engineering tool to form frame works<sup>6-8</sup>. Accordingly, the pyridine-carboxylic ligands have been used in many synthetic systems, resulting in great variety of new complexes.

Elemental analysis was carried out on a Carlo Erba 1106 full-automatic trace organic elemental analyzer. FT-IR spectra were recorded with a Bruker Equinox 55 FT-IR spectrometer in dry KBr pullet in the range of 4000~400  $\text{cm}^{-1}$ .

**Synthesis of  $[\text{Ni}(\text{pbc})_2(\text{H}_2\text{O})_2]_n$  (2):** A mixture of 3-pyrid-3-ylbenzoic acid (0.199 g, 1 mmol),  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$  (0.119 g, 0.5 mmol), NaOH (1 mmol, 0.04 g) and distilled water (18 mL) was heated in a 25 mL stainless-steel reactor with a Teflon liner 160 °C for 120 h, followed by slow cooling to room temperature. Green block crystals were obtained in 85 % yield (based on Ni). Anal. calcd. (%) for  $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_6\text{Ni}$ : C, 58.69; H, 4.10; N, 5.70. Found (%): C, 59.20; H, 3.96; N, 5.62. IR (KBr,  $\nu_{\text{max}}$ ,  $\text{cm}^{-1}$ ): 3415 br, 1612 s, 1424 s, 649 m, 402 m.

**X-Crystallography:** Suitable single crystals were selected under a polarizing microscope and fixed with epoxy cement on fine glass fibers which were mounted on a Bruker Smart

1000 CCD diffractometer with a  $\text{MoK}_\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293(2) K. The hydrogen atoms bound to carbon were located by geometrically calculations. All non-hydrogen atoms were refined by full-matrix least-squares techniques. All calculations were performed by the SHELXTL 97 program<sup>9</sup>. Crystal data, intensity collection and structure refinement details are summarized in Table-1. Selected interatomic distances and bond angles are given in Table-2. CCDC: 706295.

TABLE-1  
CRYSTALLOGRAPHIC DATA AND STRUCTURE  
REFINEMENT SUMMARY FOR Ni(II) COMPLEX

Empirical formula	$\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_6\text{Ni}$	Z, Calculated density ( $\text{mg}/\text{m}^3$ )	2, 1.571
Formula weight	491.13	F(000)	508
Crystal system space group	Monoclinic, $P2_1/c$	Limiting indices	$-10 \leq h \leq 12$ $-11 \leq k \leq 12$ $-15 \leq l \leq 14$
Unit cell dimensions	$a = 9.519(5) \text{ \AA}$ $b = 9.417(5) \text{ \AA}$ $c = 11.701(5) \text{ \AA}$	Largest diff. peak and hole ( $e/\text{\AA}^3$ )	0.384 and -0.387
Volume ( $\text{\AA}^3$ )	1038.5(9)	$\theta$ Range for data collection	2.18-28.22
Final R indices [I > 2 $\sigma$ (I)]	$R_1 = 0.0401$ , $wR_2 = 0.0830$	R indices (all data)	$R_1 = 0.0643$ , $wR_2 = 0.0932$

**Structure description  $[\text{Ni}(\text{C}_{12}\text{H}_8\text{NO}_2)_2(\text{H}_2\text{O})_2]_n$ :** The local coordination geometry of polymer  $[\text{Ni}(\text{pbc})_2(\text{H}_2\text{O})_2]_n$  with the atom-numbering scheme is show in Fig. 1. The central Ni(II) ion is surrounded by six coordinate atoms with a

TABLE-2  
SELECTED BOND LENGTHS (Å)  
AND ANGLES (°) FOR COMPLEX

Ni(1)-O(2)*	2.068(2)	Ni(1)-O(2A)**	2.068 (2)
Ni(1)-O(1W)*	2.098(2)	Ni(1)-O(1WA)**	2.098(2)
Ni(1)-N(1)***	2.110(2)	Ni(1)-N(1A)	2.110(2)
O(2)*-Ni(1)-O(2A)**	180.0	O(2)*-Ni(1)-O(1W)*	90.00(8)
O(1W)*-Ni(1)-O(1WA)**	180.0 (1)	O(2)*-Ni(1)-N(1)***	89.70(8)
O(2)*-Ni(1)-N(1A)	90.30(8)	O(1W)*-Ni(1)-N(1)***	88.13(8)
O(1WA)-Ni(1)-N(1)**	91.87(8)	N(1)**-Ni(1)-N(1A)	180.0 (1)

Symmetry code for compounds: \*-1 + x, y, z; \*\*1-x, 2-y, 1-z; \*\*\*-x, 2-y, 1-z.

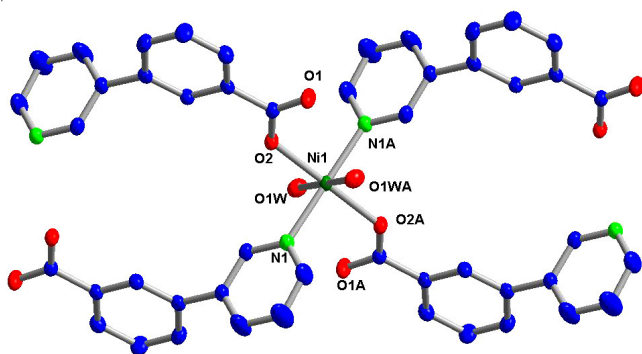


Fig. 1. Coordination environment of Ni(II) ion

octahedron geometry, in which the equatorial positions are occupied by two carboxyl oxygen atoms [Ni(1)-O2=2.068 (17) Å and Ni(1)-O2A=2.068 (17) Å] and two water molecules [Ni(1)-O1W=2.098(2) Å and Ni(1)-O1WA=2.098(2) Å] and the axial positions are occupied by two N<sub>pyridinyl</sub> [Ni(1)-N(1)=2.110(2) Å and Ni(1)-N(1A)=2.110(2) Å] with N-Ni-N angle of 180°.

Crystal packing analysis of complex shows the formation of independent inter-chain [O(3)-H(2)···O(1)] as well as intra-chain [O(3)-H(1)···O(1)] hydrogen bonds (Fig. 2). In the formation of the inter-chain O(3)-H(2)···O(1) hydrogen bond, the O-H group of the coordination water molecule of one chain is linked through the uncoordinated oxygen atoms of the adjacent chain at a D···A distance of 2.832(3) Å and an O-H···O angle of 166(3)° (symmetry code: x, 1/2-y, -1/2 + z). The

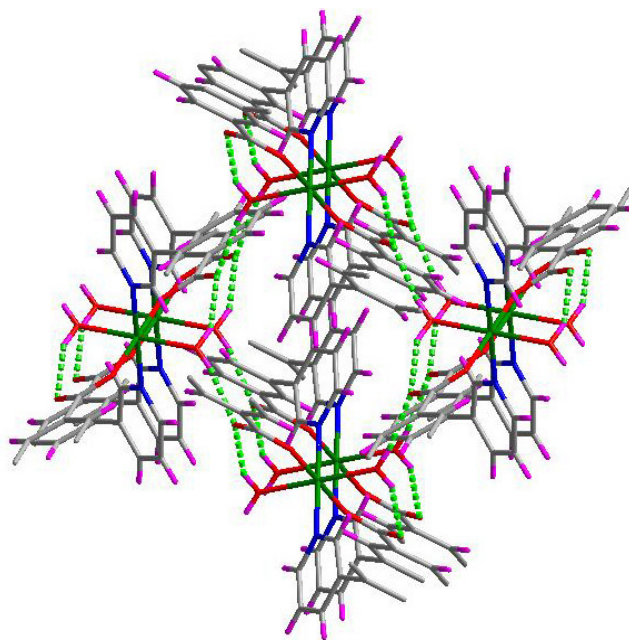


Fig. 2. Supramolecular structure formed by hydrogen bonds indicated by blue dashed lines for compound

intra-chain hydrogen bond is formed between the O-H group of the coordinated water molecule and an uncoordinated carboxylate oxygen at a D···A distance of 2.681(3) Å and an O-H···O angle of 155(2)° (symmetry code: -x, 1-y, -z).

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