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NOTE

Hydrothermal Synthesis and Crystal Structure of a Nickel(II) Coordination Polymer Assembled by 5-(3'-Carboxylphenyl)nicotinic Acid

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A novel nickel(II) coordination polymer with 5-(3'-carboxylphenyl)nicotinic acid [L=5-(3'-carboxylphenyl)nicotinic acid] has been prepared by hydrothermal synthesis and characterized by single-crystal X-ray diffraction X-ray diffraction analysis reveals that the ligand (L) adopt chelating bidentate and monodentate modes. The L ligands bridge Ni(II) ions to give rise to a two-dimensional structure.

Key Words: Coordination polymer, Nickel(II).

In recent years, coordination polymers have attracted much attention, owing to their potential application as functional materials[1-3]. It is well-known that the structural and functional information of such target materials were constructed by the metal-ligand coordination bonds In this case, the design of new types of ligands such as pyridyl and/or carboxylate groups have been proven to the most important strategy, due to their potential multiple coordination mode[4-7].

As a part of our work towards rational design and preparation of functional coordination frameworks, I selected 5-(3'-carboxylphenyl)nicotinic acid as assembly ligand to construct a new compound $\{[Ni(L)(H_2O)]\cdot H_2O\}_n$.

Preparation of compounds $[Ni(L)(H_2O)_2]n$: A mixture of H_2L (1 mmol), $NiCl\cdot 6H_2O$ (1 mmol), NaOH (2 mmol) and distilled water (15 mL) was heated to 160 ºC for 96 h in a 25 mL stainless steel reactor with a Teflon liner, followed by slow cooling to room temperature. Green crystals for compound were obtained in 46 % yield (based on Ni).

X-ray 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 MoK_α radiation (λ = 0.71073 Å) 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[8]. Crystal data, intensity collection and structure refinement details are summarized in Table-1. Selected interatomic distances and bond angles are given in Table-2.

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{13}H_{11}NO_6Ni$	Z, Calculated density (mg/m^3)	4,1.870
Formula weight	335.94	Absorption coefficient(mm^{-1})	1.657
Crystal system space group	Monoclinic, $P2_1/c$	F(000)	688
Unit cell dimensions	a =13.386(4) Å b =11.708(3) Å c = 7.691 (2) Å	Limiting indices	-17 ≤ h ≤ 17 -15 ≤ k ≤ 15 -9 ≤ l ≤ 9
Volume(Å^3)	1192.9(6)	Largest diff. peak and hole (e/Å^3)	2.116 and -1.961
θ Range for data collection	1.54-27.49	Reflections collected/unique	2700/2700
Final R indices [I > 2 σ(I)]	R_1 = 0.0671, wR_2 = 0.1633	R indices (all data)	R_1 = 0.0961, wR_2 = 0.1792

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

Ni(1)-O(4)^i	2.020(5)	Ni(1)-N(1)^{ii}	2.127(5)
Ni(1)-O(6)	2.028(5)	Ni(1)-O(1)	2.152 (5)
Ni(1)-O(5)	2.082(5)	Ni(1)-O2	2.174 (5)
O(4)^i-Ni(1) -O(6)	91.1(2)	O(6)-Ni(1)-N(1)^{ii}	87.0(2)
O(4)^i-Ni(1)-O(5)	90.1(2)	O(5)-Ni(1)-N(1)^{ii}	90.8(2)
O(6)-Ni(1)-O(5)	177.80(19)	O(4)^i-Ni(1)-O(1)	88.07(18)
O(4)^i-Ni(1)-N(1)^{ii}	119.0(2)	O(6)-Ni(1)-O(1)	91.1(2)

Symmetry codes: (i) *x*-1, -*y*+1/2, *z*-1/2; (ii) -*x*+1, -*y*+1, -*z*+1

Description of the crystal structure: The single-crystal X-ray diffraction analysis reveals that the compound crystallizes in the monoclinic, space group P21/c. The local coordination geometry of polymer $[Ni(L)(H_2O)_2]_n$ with atomic numbering scheme is shown in Fig. 1. The central Ni(II) ion is six-coordinated with a distorted octahedron, in which the equatorial plane consists of three carboxyl oxygen atoms and one nitrogen atom, and the axial positions are occupied by two water molecules with the O-Ni-O angel of 177.82º.

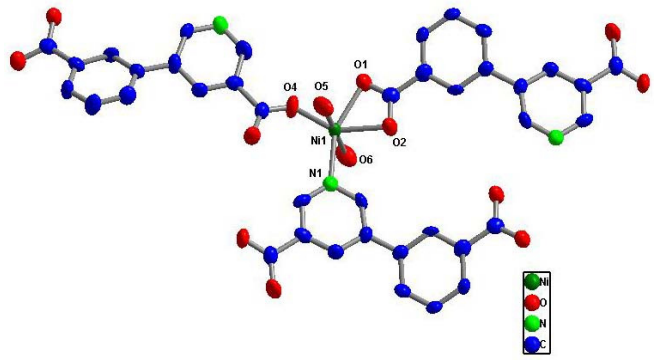

Fig. 1. Coordination environment of Ni(II) ion

Each L anions connects to three nickek(II) atoms and each nickel(II) is link by three L anions. So, the 2D complex framework can be simplified to 3-connected topology. The combination of nodes and connectors provides the 3-connected network of compound with the topological notation of (4.82) (Fig. 2).

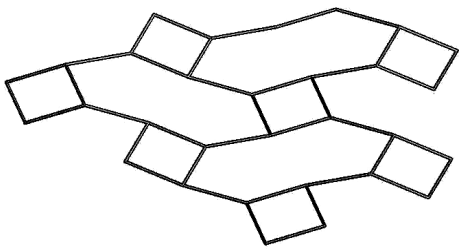

Fig. 2. Schematic description of the 3-connected framework

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