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NOTE

Hydrothermal Synthesis and Crystal Structure of Cd(II) Coordination Polymer

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By hydrothermal method, the compound $[Cd(nia)_2(H_2O)]_n$ (nia = nicotinate) was synthesized and its structure was characterized with elemental analysis and X-ray diffractometer. The crystal is orthorhombic, space group Pbca with a =11.458(s), b = 12.113(2), c = 17.435(3) Å, $\alpha = \beta = \gamma = 90°$, M_r = 374.62, V = 2419.8(7)Å^3, D_c = 2.057 g/cm^3, F(000) = 1472 and Z = 8. The Cd(II) center adopt a distorted octahedron geometry which is surrounded by 6 coordination atoms from nicotinate and water molecule.

Key Words: Hydrothermal, Synthesis, Crystal structure, Cd(II), Coordination polymer.

More attentions have been paid in recent years to supramolecular chemistry reflecting the intense contemporary interest in the rational design of functional materials with extended architectures. The most useful strategy is to employ appropriate multidentate bridging ligands capable to bind metal ions either by strong covalent interactions or supramolecular contacts as hydrogen bonding or staking forces which can be obtained the higher dimensional complex[1-6].

All reagent and solvents employed were commercially available and used as received without further purification. Elemental analysis was carried out on a Carlo Erba 1106 full-automatic trace organic element analyzer.

Synthesis of the Cd(II) coordination polymer compound: A mixture of nicotinate (0.166 g, 1 mmol), NaOH (0.4 g, 1 mmol), $Cd(OAc)_2{\cdot}2H_2O$ (0.5 mmol, 0.133 g) and distilled water (18 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 160 ºC for 96 h, followed by slow cooling to room temperature. Colourless crystals of the complex formed. Yield 70 % (base Cd). Anal. calcd. (%) for C 38.47; H 2.67; N 7.47. Found (%): C 39.01; H 2.62; N 7.39.

X-Ray crystallography: A suitable colourless crystal was mounted on a glass fiber and the data collected on a Bruker Smart 1000 CCD diffractometer with a MoK_α radiation (0.71073 A) at 293(2) K by using an ω scan mode in the range of $3.4° < \theta < 27.5°$. The hydrogen atoms bound to carbon were located by geometrical calculations and their positions and thermal parameters were fixed during the structure

refine. The highest and lowest residual peaks in the final difference Fourier map are 0.35 and -0.25 e/Å^3, respectively. All calculations were performed by the SHELXTL 97 program[7]. The selected bond lengths and bond angles are listed in Table-1. CCDC: 715177.

TABLE-1
SELECTED BOND LENGTHS (Å) AND ANGLES (º) of $[Cd(nia)_2(H_2O)]_n$

Cd1–O3	2.2503 (16)	Cd1–N1^i	2.3504 (17)
Cd1–O2	2.2758 (16)	Cd1–O1W	2.3826 (17)
Cd1–N2	2.3053 (17)		
O3–Cd1–O2	80.57 (6)	N2–Cd1–N1^i	91.99 (6)
O3–Cd1–N2	127.63 (6)	O3–Cd1–O1W	91.55 (7)
O2–Cd1–N2	147.43 (6)	O2–Cd1–O1W	85.98 (6)
O3–Cd1–N1^i	102.85 (6)	N2–Cd1–O1W	78.20 (6)
O2–Cd1–N1^i	97.21 (6)	N1^i–Cd1–O1W	165.57 (6)

Symmetry codes: (i) –x+1, y+1/2, –z+1/2

The local coordination geometry of polymer $[Cd(nia)_2(H_2O)]_n$ with numbering scheme is depicted in Fig. 1. It is shown that Cd(II) is three carboxylate oxygen atoms, two N atoms and one water molecules. O1, O2, O3 and N2 form the equatorial plane (the equation of plane is 0.026x + 6.821y + 14.408z = 5.5051). N1 and O1w occupy the axial sites. The ligands have two coordination mode: μ_2-N,O and μ_2-N,O,O. Through nia ligands, the 3D net is generated shown in Fig. 2.

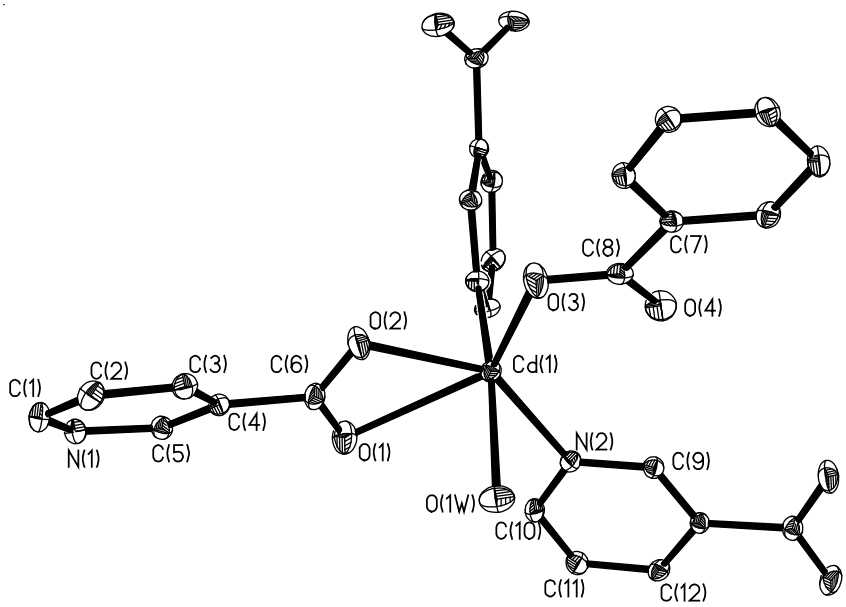

Fig. 1. Local coordination geometry of polymer $[Cd(nia)_2(H_2O)]_n$ with the atom-numbering scheme

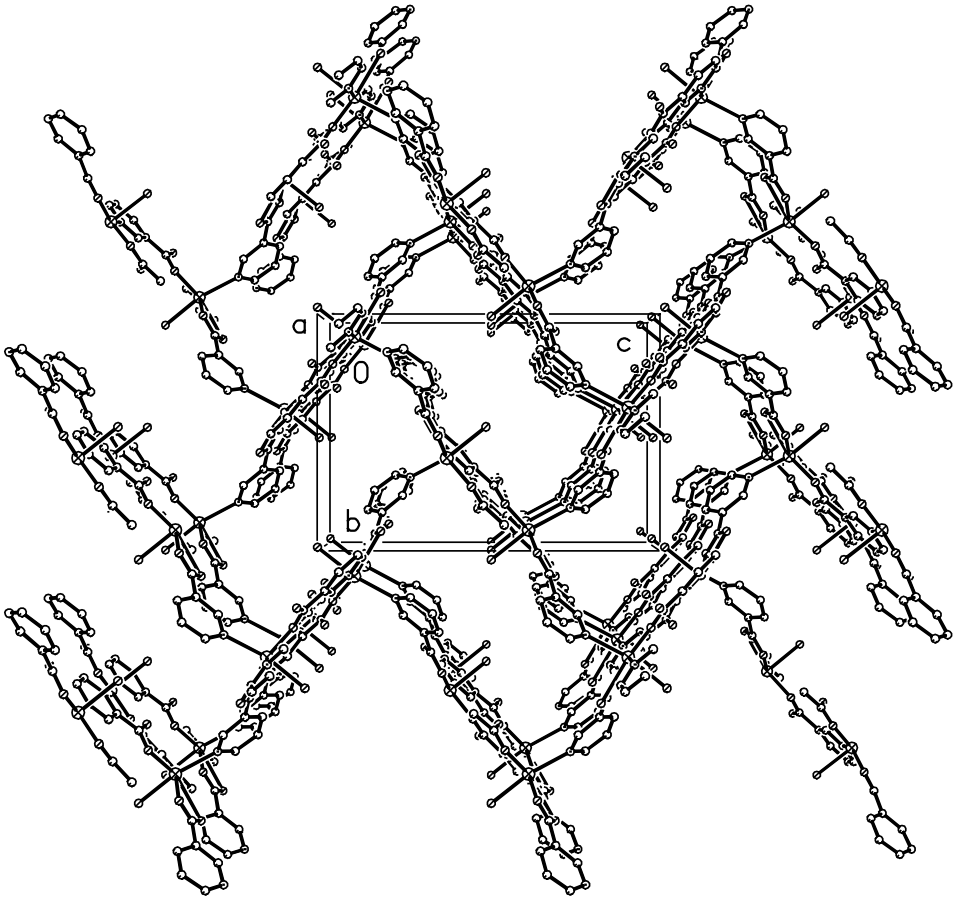

Fig. 2. 3D Structure of $[Cd(nia)_2(H_2O)]_n$ (nia = nicotinate)

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