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SHORT COMMUNICATION

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A Zn(II) COORDINATION POLYMER BASED ON 4,4'-BIPYRIDINE AND ACETATO

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Abstract: A novel Zn(II) coordination polymer, $[Zn(bpy)(acetato)_2]_n$ (bpy = 4,4'-bipyridine), has been synthesized and characterized by elemental analysis and single-crystal X-ray diffraction. The Zn(II) coordination polymer is triclinic, space group *P*-1 with a = 8.046(3) Å, b = 9.161(3) Å, c = 10.663(3) Å, α = 109.769(4)º, β = 99.966(5)º, γ = 101.666(5)º, V= 699.1(4) Å^3, Z = 2, Dc = 1.614 mg·m^{-3}, μ = 1.774 mm^{-1}, F(000) = 348, and final R_1 = 0.0541, ωR_2 = 0.1605. X-ray diffraction analysis reveals that the Zn(II) center is six-coordination with a N_2O_4 distorted octahedral coordination environment. The Zn(II) complex forms 1D chain structure by the bridge of 4,4'-bipyridine and acetato.

Keywords: *Zn(II) coordination polymer, synthesis, structural characterization*

INTRODUCTION

The design and synthesis of Zn(II) coordination polymers have attracted a great deal of interests, not only because of their new structural architectures and topologies, but also because of their potential applications as important functional materials in luminescence, biochemistry, catalysis, gas storage and so on [1 - 5]. Poly-functional ligands, such as carboxylic acid and 4,4'-bipyridine have proven to be good candidates for the construction of new coordination polymers [6 - 8]. Kim and his research group have reported a Zn(II) coordination polymer based on 4,4'-bipyridine and acetato ligands [9], however, the synthetic method and some crystal parameters are different from my research. Taking account of the above, in this paper, a coordination polymer $[Zn(bpy)(acetato)_2]_n$ obtained by the reaction of 4,4'-bipyridine and $Zn(CH_3COO)_2{\cdot}2H_2O$ was reported.

EXPERIMENTAL

Materials and methods

$Zn(CH_3COO)_2{\cdot}2H_2O$, 4,4'-bipyridine and solvents employed were commercially available and used without further purification. Elemental analysis (C, H, N) was carried out on a Elementar Vario III EL elemental analyzer. The crystal data was collected on a Bruker smart-100 CCD Area Detector.

Synthesis of the $[Zn(bpy)(acetato)_2]_n$

A mixture of 4,4'-bipyridine (1.0 mmol, 0.156 g) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (1.0 mmol, 0.219 g) were dissolved in 10 mL CH_3CH_2OH/H_2O (v:v = 1:1). Then the mixture was continuously stirred for 4 h at 70 °C. After cooling to room temperature, filtered, then the filtrate was evaporated at room temperature, the colourless crystals were obtained after 10 days. Elementary analysis: calcd for $C_{14}H_{14}N_2O_4Zn$: C, 49.46; H, 4.12; N, 8.24 %; found: C, 49.18; H, 4.32; N, 7.89 %.

Crystal data and structure refinement

A suitable colourless block crystal with dimensions of 0.30 × 0.26 × 0.24 mm was selected for measurement. Diffraction data of the single crystal were collected by φ~ω scan mode using a graphite-monochromatic Mo $K\alpha$ radiation (λ = 0.71073 Å) at 293 (2) K on a Bruker Smart Apex CCD diffractometer. Empirical formula: $C_{14}H_{14}N_2O_4Zn$; Formula weight: 339.64; Crystal system: triclinic; Space group: P-1; a: 8.046(3) Å; b: 9.161(3) Å; c: 10.663(3) Å; α: 109.769(4)º; β: 99.966(5)º; γ: 101.666(5)º; V: 699.1(4) $Å^3$; Z; 2; Dc: 1.614 $mg{\cdot}m^{-3}$; μ: 1.774 mm^{-1}; F(000): 348; Refl'ns collected: 3628; Independent refl'ns [R(int)]: 2415 [0.0595]; Refl'ns observed (>2δ): 2090; Refinement method: Full-matrix least-squares on F^2; Goodness-of-fit: 1.010; Final R indices [I > 2δ(I)]: 0.0541, 0.1605; R indices (all data): 0.0597, 0.1648; Limiting indices: $-9 \le h \le 9$, $-10 \le k \le 10$, $-12 \le l \le 7$; Min. and max. resd. dens. ($e/Å^3$): 1.453, -0.562; The program packages of SHELXL-97 and SHELXTL-97 were used to refine structure [10, 11].

RESULTS AND DISCUSSION

The crystal structure of the Zn(II) complex is shown in Figure 1. The crystal structure analysis shows that the symmetric unit consists of one Zn(II) atom, two acetatos and one 4,4'-bipyridine ligand. As shown in Figure 1, Zn(II) is six-coordinated three oxygen atoms of coordinated acetato (O1, O2, O3, O4) and two nitrogen atoms of the 4,4'-bipyridine ligand (N1, N2B). The acetato groups adopt monodentate and bidentate coordination mode, respectively. The Zn(II) ion adopts a distorted octahedral coordination environment. In the coordination polyhedral structure of Zn(II) ion, O1, O2, O3, and O4 locate at the equatorial positions, while N1 and N2 locate at the axial positions. The complex molecule forms 1D chain structure by the bridge of 4,4'-bipyridine, and also forms 2D layered structure by the bridge of acetato and the π-π interaction of 4,4'-bipyridine (Figure 2).

Selected bonds: Zn1-O1 2.295(4) Å; Zn1-O2 2.169(4) Å; Zn1-O3 2.008(3) Å; Zn1-O4 2.023(3) Å; Zn1-N1 2.175(4) Å; Zn1-N2B 2.175(4) Å; C13-O3 1.244(6) Å; C11-O2 1.252(6) Å; C11-O1 1.225(6) Å; C1-N1 1.344(6) Å; C5-N1 1.344(6) Å; C9-N2 1.344(6) Å; C8-N2 1.345(6) Å;

Selected angles: O3-Zn1-O4 123.02(16)°; O2-Zn1-O3 147.80(16)°; O2-Zn1-O4 89.00(15)°; O3-Zn1-N1 86.16(14)°; N1-Zn1-O4 87.39(13)°; O2-Zn1-N1 92.67(15)°; O3-Zn1-O1 90.95(15)°; O1-Zn1-O4 145.90(16)°; O1-Zn1-O2 56.93(14)°; O1-Zn1-N1 92.59(15)°; O1-Zn1-N2B 89.89(15)°; N1-Zn1-N2B 176.76(13)°; O2-Zn1-N2B 90.43(15)°; O4-Zn1-N2B 91.72(14)°; O3-Zn1-N2B 91.72(13)°; C8-N2-C9 115.6(4)°; O1-C11-O2 118.7(5)°; O3-C13-O4A 127.1(4)°;

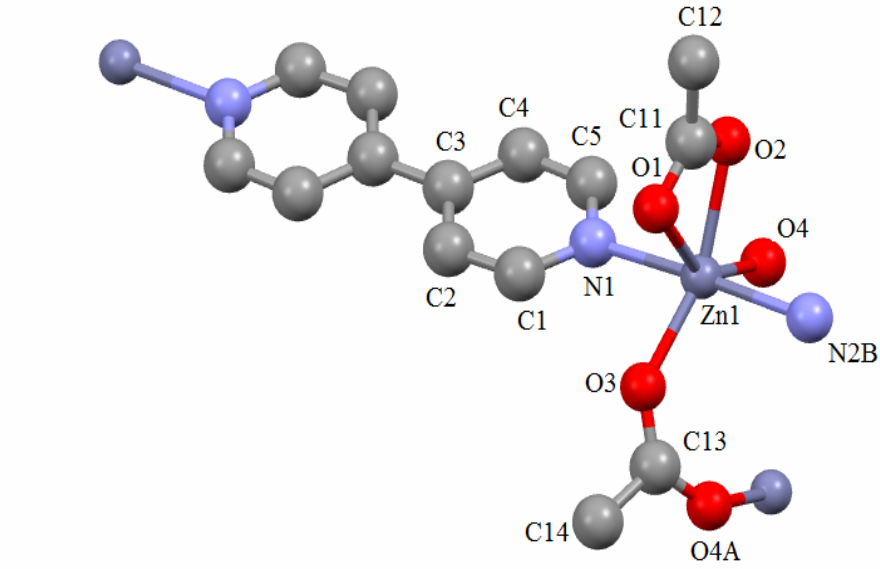

Figure 1. *The symmetrical molecular structure of the Zn(II) complex, Symmetry code: x, y+1, z+1*

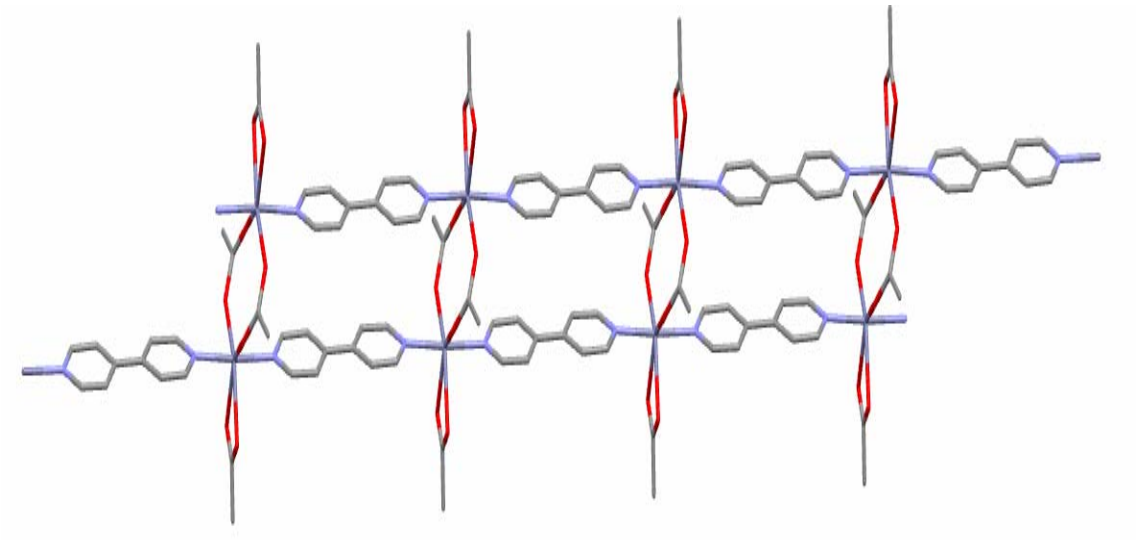

Figure 2. *1D chained structure and 2D layered structure of the Zn(II) coordination polymer*

CONCLUSIONS

A novel Zn(II) coordination polymer, $[Zn(bpy)(acetato)_2]_n$, has been synthesized and characterized by elemental analysis and single-crystal X-ray diffraction. Single crystal X-ray analysis reveals that the Zn(II) center is six-coordination with a N_2O_4 distorted octahedral coordination environment. The complex molecule forms 1D chain structure by the bridge of 4,4'-bipyridine and acetato.

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