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NOTE

Hydrothermal Synthesis and Crystal Structure of 1D Zigzag Chain $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$

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A novel coordination polymer of $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$ (Hbsal = 5-bromosalicylate, 4,4'-bipy = 4,4'-bipyridine) was synthesized by hydrothermal reaction and characterized by elemental analysis and X-ray single crystal diffraction. The crystal is monoclinic, space group C2/c with a = 20.561(4), b = 9.207(2), c = 14.769(3) Å, α = 90°, β = 121.92(3)°, γ = 90°, M_r = 653.58, V = 2373.0(8) Å^3, D_c = 1.829 g/cm^3, F(000) = 1288 and Z = 4. The structure analysis shows that the complex exhibits a 1D zigzag chain structure.

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

Salicylic acid and its substituted derivatives continue to attract attention because of its versatile coordination modes and biological applications[1-5]. Many complexes with salicylic acid and N-donor ligands, such as 2,2'-bipyridine, 1,10-phenanthroline and 4,4'-bipyridine, were found to display diverse structure types[6-9]. Herein, we report the hydrothermal synthesis and crystal structure of a Zn(II) complex, $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$.

All chemicals were of AR grade and used as received from commercial sources. Elemental analyses were conducted on a Perkin-Elmer 2400 CHN elemental analyzer.

Synthesis of $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$: A mixture of $Zn(NO_3)_2 \cdot 6H_2O$ (0.030 g, 0.1 mmol), 4,4'-bipy (0.016 g, 0.1 mmol), 5-bromosalicylic acid (0.043 g, 0.2 mmol) and distilled water (10 mL) was put into a Teflon-lined autoclave (20 mL) and then heated at 433 K for 48 h. Yellow block-like crystals of the complex formed. Yield 30 % (based on Zn). Anal. calcd. (%) for $C_{24}H_{16}N_2O_6Br_2Zn$: C, 44.10; H, 2.47; N, 4.28. Found (%): C, 44.30; H, 2.35; N, 4.35.

X-Ray crystallography: A yellow block-like single crystal with dimension of 0.18 mm × 0.15 mm × 0.14 mm for $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$ was used for X-ray diffraction analysis. Data collection was carried out at 293 K on a Rigaku RAXIS-RAPID Weissengberg IP diffractometer with graphite monochrocmated MoK_α radiation (λ = 0.71073 Å). A total of 9271 reflections were obtained and 2147 unique (R_{int} = 0.0516) were collected in the range of 3.25 < θ < 25.25° by ω scan mode, of which 1408 reflections with I > 2σ(I) were used in the succeeding refinement. The final R = 0.0546, wR = 0.1303 ($w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 9.4277P]$, where $P = (F_o^2 + 2F_c^2)/3$). The highest and lowest residual peaks in the final difference Fourier map are 1.125 and -0.907 e Å^{-3}, respectively. All calculations were performed by the SHELXTL 97 program[10]. The selected bond lengths and bond angles are listed in Table-1. CCDC: 786194.

TABLE-1
SELECTED BOND LENGTHS (Å) AND ANGLES (°) OF $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$

Zn1–O1	2.465 (5)	Zn1–N1	2.0 72(5)
Zn1–O2	2.027 (5)	$O2^a$–Zn1–O1	99.33 (2)
O2–Zn1–$O2^a$	149.2(3)	N1–Zn1–$N1^a$	104.8 (3)
O2–Zn1–N1	94.1(2)	N1–Zn1–O1	150.0(2)
$O2^a$–Zn1–N1	104.7(2)	O1–Zn1–$O1^a$	87.2 (2)
O2–Zn1–O1	56.8 (2)	$N1^a$–Zn1–O1	91.0(2)

Symmetry codes a: –x + 2, y, –z + 3/2.

The local coordination around the Zn(II) atom is shown in Fig. 1. The Zn(II) atom in $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$ is coordinated by four O atoms from two 5-bromosalicylate ligands and two N atoms from two 4,4'-bipy ligand in a distorted octahedral coordination geometry. All carboxylic anions of 5-bromosalicylate ligands are bidentately coordinated with Zn(II). Through 4,4'-bipy ligands, the 1D zigzag chain along the a axis is generated shown in Fig. 2.

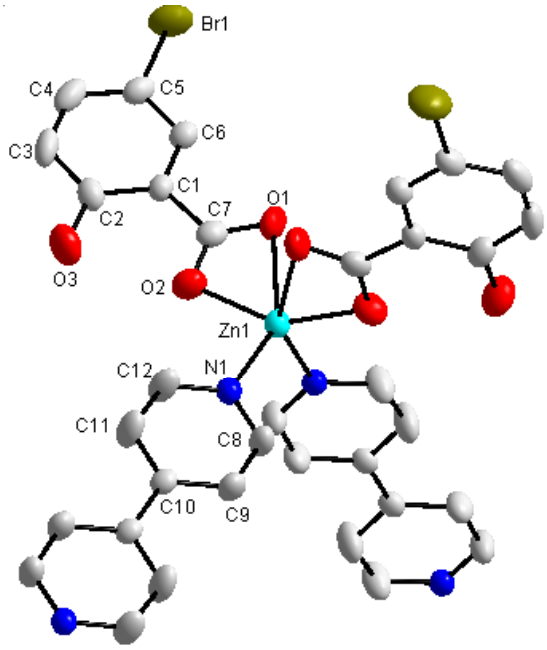

Fig. 1. ORTEP view of coordination environment of $[Zn(Hbsal)_2(4,4'\text{-bipy})]_n$ with 30 % probability ellipsoid

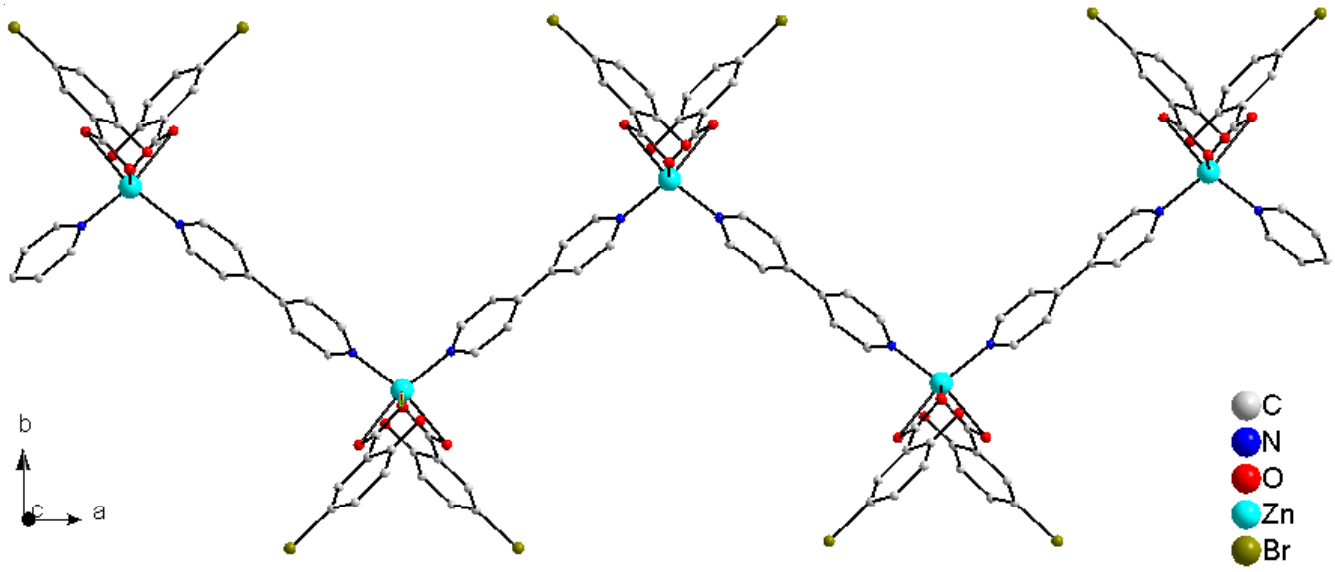

Fig. 2. View of the 1D zigzag chain along the a axis

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