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The crystal structure of *catena-poly* [(m₂-4,4'-bipyridine-κ²N:N)-bis(6-phenylpyridine-2-carboxylato-κ²N,O) zinc(II)], C₃₄H₂₄N₄O₄Zn

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.14 × 0.13 × 0.10 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.91 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ _{max} , completeness:	25.0°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	5980, 2506, 0.027
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2249
<i>N</i> (<i>param</i>) _{refined} :	195
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

A part of the title coordination polymer is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized by one pot method: 6-phenylpyridine-2-carboxylic acid (0.0996 g, 0.5 mmol), Zn(O₂CMe)₂ · 2H₂O (0.0548 g, 0.25 mmol), NaOH (0.020 g, 0.5 mmol), and 4,4'-bipyridine (0.0781 g, 0.5 mmol) were added to water-95% ethanol (20 mL, v:v = 1:1) and stirred to dissolve at room temperature. The mixture was stirred at 70 °C for 4 h and cooled to room temperature. Then the reaction was continued for 3 h at room temperature and filtered. Colorless block crystals of the title compound were received after 20 days. **Anal. Calcd.** for C₃₄H₂₄N₄O₄Zn: C, 66.03; H, 3.88; N, 9.06. Found: C, 65.85; H, 4.18; N, 9.18. **IR:** 1653 cm⁻¹ (C=O), 1602 cm⁻¹ (C–C + C=N), 1436 cm⁻¹ (C–C + C=N), 1403 cm⁻¹ (C–C + C=N), 1369 cm⁻¹ (COO–), 1225 cm⁻¹ (C–H), 1072 cm⁻¹ (C–H).

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Abstract

C₃₄H₂₄N₄O₄Zn, monoclinic, *I*2/*a* (no. 15), *a* = 18.2546(14) Å, *b* = 11.0510(7) Å, *c* = 16.1874(15) Å, β = 119.605(11)°, *V* = 2839.2(5) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0302, *wR*_{ref}(*F*²) = 0.0694, *T* = 200 K.

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Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å). Their *U*_{iso} values were set to 1.2*U*_{eq} of the parent atoms.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
Zn1	0.250000	0.61808 (3)	0.500000	0.01819 (11)
O1	0.37476 (8)	0.62111 (12)	0.57876 (9)	0.0214 (3)
O2	0.49557 (8)	0.72094 (14)	0.63175 (11)	0.0373 (4)
N1	0.29344 (10)	0.79028 (15)	0.44464 (11)	0.0216 (4)
N2	0.25200 (9)	0.48000 (14)	0.40501 (11)	0.0202 (4)
C1	0.16811 (12)	0.8483 (2)	0.29796 (14)	0.0263 (5)
C2	0.10432 (14)	0.9342 (2)	0.25404 (17)	0.0369 (6)
H2	0.111111	1.010632	0.280930	0.044*
C3	0.03147 (15)	0.9070 (3)	0.17135 (19)	0.0454 (7)
H3	-0.010316	0.965367	0.142091	0.055*
C4	0.02049 (15)	0.7946 (3)	0.13225 (19)	0.0519 (7)
H4	-0.028923	0.776384	0.076446	0.062*
C5	0.08244 (14)	0.7074 (2)	0.17516 (17)	0.0429 (6)
H5	0.074527	0.630542	0.148612	0.051*
C6	0.15589 (13)	0.7348 (2)	0.25736 (15)	0.0292 (5)
H6	0.197697	0.676304	0.285838	0.035*
C7	0.24951 (14)	0.87948 (19)	0.38257 (15)	0.0285 (5)
C8	0.28229 (17)	0.9957 (2)	0.39578 (18)	0.0495 (7)
H8	0.250433	1.057140	0.354254	0.059*
C9	0.36150 (18)	1.0207 (2)	0.4698 (2)	0.0589 (8)
H9	0.383379	1.098630	0.479021	0.071*
C10	0.40755 (15)	0.9286 (2)	0.52958 (17)	0.0412 (6)
H10	0.462123	0.942112	0.578787	0.049*
C11	0.37131 (12)	0.81550 (19)	0.51533 (14)	0.0249 (5)
C12	0.41885 (12)	0.71205 (19)	0.58144 (14)	0.0221 (5)
C13	0.32232 (11)	0.44336 (19)	0.40664 (14)	0.0239 (5)
H13	0.372763	0.480487	0.449323	0.029*
C14	0.32460 (12)	0.35377 (19)	0.34881 (14)	0.0246 (5)
H14	0.375693	0.331164	0.353749	0.029*
C15	0.25068 (11)	0.29731 (17)	0.28323 (13)	0.0187 (4)
C16	0.17744 (12)	0.3340 (2)	0.28215 (16)	0.0305 (5)
H16	0.126192	0.297894	0.240549	0.037*
C17	0.18098 (13)	0.4237 (2)	0.34278 (16)	0.0317 (5)
H17	0.130984	0.446749	0.340436	0.038*

Comment

The novel structures and excellent properties of coordination polymers have been highly favored by chemists [5]. For Zn(II) coordination polymers, they show novel structure [6] and potential applications in many ways such as antibacterial activity [7], electrocatalyst [8], fluorescence [9], antitumor activity [10], and so on. According to the literature reports, most of Zn(II) coordination polymers are constructed from ligands containing a carboxy, a carboxylate and an azacyclo-group. In our previous work, some metal complexes with 6-phenylpyridine-2-carboxylate as ligand have been synthesized and structural characterized [11–14]. In this work, we selected 6-phenylpyridine-2-carboxylic acid and 4,4'-bipyridine as starting materials.

We also elaborately used NaOH as modifier to adjust the pH value of the reaction system. With these points in mind, we successfully synthesized a new 1D Zn(II) coordination polymer (1). The structure of **1** was determined by elemental analysis, IR, and X-ray single-crystal diffraction. The results revealed that compound **1** possesses a zig-zag-chain structure. The asymmetrical unit of **1** contains one half of a Zn(II) ion (located on a twofold axis), one 6-phenylpyridine-2-carboxylate ligands and one half of a 4,4'-bipyridine ligand (see the figure). The Zn(II) ion is hexa-coordinated with two nitrogen atoms, two oxygen atoms from two different 6-phenylpyridine-2-carboxylate ligands and two nitrogen atoms from two different 4,4'-bipyridine ligands, forming a distorted ZnN_4O_2 octahedral geometry. The coordination mode of 6-phenylpyridine-2-carboxylate ligands in **1** is consistent with previous work [11–15]. The Zn–O and Zn–N distances are 1.9861(13) Å (Zn1–O1), 2.3991(16) Å (Zn1–N1), and 2.1793(16) Å (Zn1–N2), which is consistent with other Zn(II) complexes. The sum of angles around Zn(II) ion is 365.48° (N2–Zn1–N2a, 91.12(9)°; N1–Zn1–N2, 99.67(6)°; N1–Zn1–N1a, 75.02(8)°; N1a–Zn1–N2a, 99.67(6)°), and the angle of O1–Zn1–O1a is 178.07(8)°, showing that N1, N2, N1a, N2a atoms are at the equatorial plane and O1, O1a atoms are at axial position. The dihedral angle between the phenyl ring and pyridine ring of 6-phenylpyridine-2-carboxylate ligand is 31.7°. Two nitrogen atoms (N1, N1a) of 4,4'-bipyridine ligand coordinated with the two different Zn(II) atoms, respectively. So the molecules form the 1D zig-zag chain coordination polymer by the bridging of the 4,4'-bipyridine ligand.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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