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The crystal structure of phenantroline-κ²N,N′-bis(6-phenylpyridine-2-carboxylato-κ²N,O) copper(II), C₃₆H₂₄N₄O₄Cu

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Abstract
C₃₆H₂₄N₄O₄Cu, monoclinic, I₂/a (no. 15), a = 16.5119(17) Å, b = 11.0747(7) Å, c = 17.6272(17) Å, β = 117.916(13)°, V = 2848.3(5) Å³, Z = 4, Rgt(F) = 0.0335, wRref(F²) = 0.0759, T = 200 K.

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The crystal structure 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.

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Table 1: Data collection and handling.

| Crystal: | Ble block |
| Size: | 0.13 × 0.12 × 0.1 mm |
| Wavelength: | Mo Kα radiation (0.71073 Å) 0.82 mm⁻¹ |
| Diffractometer, scan mode: | SuperNova, ω-scans |
| θmax, completeness: | 25°, >99% |
| n(hkl)measured, N(hkl)unique, Rint: | 5858, 2513, 0.028 |
| Criterion for Iobs, N(hkl)gt: | Iobs > 2σ(Iobs), 2156 |
| N(param)refined: | 204 |
| Programs: | Bruker programs [1], OLEX2 [2], SHELX [3], CrysAlisPRO [4] |

Source of materials

Synthesis of phenantroline-κ²N,N′-bis(6-phenylpyridine-2-carboxylate-κ²N,O)copper(II): a solution of Cu(CH₃COO)₂.H₂O (100 mg, 0.5 mmol) in 5 mL distilled water was added to the solution of 6-phenylpyridine-2-carboxylic
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.

Comment

Pyridine carboxylic acid or 1,10-phenanthroline and their derivatives were widely used to construct metal complexes owing to their abilities to form stable chelates [5]. And their metal complexes exhibited a wide range of potential applications including magnetic properties [6], neurotropic activity [7], fluorescence sensor [8], antimicrobial properties [9], and catalytic activity [10]. We have previously published some metal complexes of Co(II), Cu(II), Zn(II) and Pb(II) with 6-phenylpyridine-2-carboxylic acid as a bidentate primary ligand [11–16]. Continuing to enrich our studies on the synthesis of transition metal complexes using pyridine carboxylic acid derivative ligands, herein we used 6-phenylpyridine-2-carboxylic acid and 1,10-phenanthroline as excellent starting materials to construct a new Cu(II) complex.

The molecular structure is given in Figure 1. The Cu(II) complex contains a Cu(II) ion, two 6-phenylpyridine-2-carboxylate ligands and one neutral 1,10-phenanthroline ligand. The asymmetric unit is one half of a complex located on a twofold axis. The Cu(II) ion forms a distorted octahedral six-coordination geometry by coordinating to two N atoms (N1 and N1a) and two O atoms (O2 and O2a) of two 6-phenylpyridine-2-carboxylate ligands, and two N atoms (N2 and N2a) from one 1,10-phenanthroline ligand. The bond angle of both O2–Cu1–N2 and O2a–Cu1–N2a are 173.26(7)°, showing that O2 and N2 (or O2a and N2a) atoms located on the axial position, and other four atoms (O2a, N1, N2a and N1a, or O2, N1, N2 and N1a) located on the equatorial plane. The Cu–N and Cu–O bond distances are 2.0154(18) Å (Cu1–N2), 2.0155(17) Å (Cu1–N2a), 2.4418(18) Å (Cu1–N1), 2.4418(17) Å (Cu1–N1a), 1.9615(15) Å (Cu1–O2 and Cu1–O2a), respectively, which agrees with the reports [12, 15]. The complex molecules are further interconnected by \( \pi-\pi \) interaction of neighboring aromatic rings to form the 3D network structure.

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References
