Zhao Zeng-Bing, Li Xue-Ping, Yang Shu-Cheng, Yang Bing-Qi, Wang Ze-Tao, Cheng Lan-Xing* and Tai Xi-Shi*

The crystal structure of [(2,2′-bipyridine-6-carboxylato-κ³N,N,O)-(6-phenylpyridine-2-carboxylate-κ²N,O)copper(II)] monohydrate, C₂₃H₁₇N₃O₅Cu

Abstract

C₂₃H₁₇N₃O₅Cu, monoclinic, P₂₁/n (no. 14), a = 11.49510(10) Å, b = 8.69660(10) Å, c = 21.1454(2) Å, β = 105.433(1)°, V = 2037.65(4) Å³, Z = 4, Rgt(F) = 0.0298, wRref(F²) = 0.0862, T = 294 K.

Crystal: Blue block
Size: 0.15 × 0.12 × 0.11 mm
Wavelength: Cu Kα radiation (1.54184 Å)
μ: 1.88 mm⁻¹
Diffractometer, scan mode: XtaLAB Synergy, ω
θmax, completeness: 75.7°, 99%
N(hkl)measured, N(hkl)unique, Rwp: 14,284, 4042, 0.027
Criterion for Iobs, N(hkl)op: Iobs > 2 σ(Iobs), 3836
N(param)refined: 296
Programs: Bruker [1], Olex2 [2], SHELX [3], CrysAlisPro [4]

The molecular 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.

1 Source of materials

The title compound was synthesized by dissolving NaOH (0.040 g, 1.0 mmol), 6-phenylpyridine-2-carboxylic acid (0.9960 g, 0.5 mmol), 2,2′-bipyridine-6-carboxylic acid (0.100 g, 0.5 mmol) in 5 mL aqueous solution with stirring. Then 15 mL of a 95% ethanol solution containing Cu(O₂C-Me)₂·H₂O (0.0999 g, 0.50 mmol) was added. The mixture was stirred at 70 °C for 4.5 h. The filtrate was evaporated at room temperature, and gave a colourless block crystal of the title complex in 15 days. Yield 62%.

Anal. Calcd. for C₂₃H₁₇N₃O₅Cu: C, 57.63; H, 3.55; N, 8.77. Found: C, 57.38; H, 3.82; N, 8.39.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å and O–H = 0.85 Å). Their Uiso values were set to 1.2Ueq or 1.5Ueq of the parent atoms.
Transition metal complexes constructed from carboxylic acid-containing group ligands are an important class of compounds with interesting structures and functional properties. So the study of these compounds has been one of the hot research topics. They can show structural diversity [5], and promising potential applications in many aspects of luminescence property [6], anticancer activity [7], catalytic activities [8, 9], and antibacterial agent [10]. In recent years, we have also synthesized and structurally characterized several transition metal complexes with ligands containing carboxylic acid group [11, 12]. However, no literature reports on the synthesis and structure of copper complex with 2,2′-bipyridine-6-carboxylic acid and 6-phenylpyridine-2-carboxylic acid ligands.

The molecular structure of the title complex is shown in the figure. It consists of one Cu\textsuperscript{II} ion, one 2,2′-bipyridine-6-carboxylato ligand, one 6-phenylpyridine-2-carboxylato ligand and one uncoordinated water molecules. The Cu(II) ion is coordinated to two nitrogen atoms (N1, N2) from one 2,2′-bipyridine-6-carboxylato ligand, one nitrogen atom (N3) from one 6-phenylpyridine-2-carboxylato ligand, one oxygen atom (O2) from one 2,2′-bipyridine-6-carboxylato ligand, and one oxygen atom (O3) from one 6-phenylpyridine-2-carboxylato ligand. The coordination environment around Cu(II) ion is a distorted bi-pyramid with N1, N2, O2 and O3 at the position. The 2,2′-bipyridine-6-carboxylato ligand adopts tridentate coordination mode and the 6-phenylpyridine-2-carboxylato ligand adopts bidentate coordination mode. The dihedral angles of two pyridine rings (N1–C14–C15–C16–C17–C18) and (N2–C19–C20–C21–C22–C23) is 2.33°, showing that the 2,2′-bipyridine-6-carboxylato ligand is coplanar. However, the dihedral angle of pyridine ring (N3–C2–C3–C4–C5–C6) and benzene ring (C7–C8–C9–C10–C11–C12) is 37.83°, showing that the 6-phenylpyridine-2-carboxylato ligand is not coplanar. The Cu–N and Cu–O distances are 1.9163(12)–2.2710(12) Å and 2.0018(11)–1.9176(11) Å. The hydrogen bonds (O–H–O) between the uncoordinated water molecules and O atoms of 2,2′-bipyridine-6-carboxylato and 6-phenylpyridine-2-carboxylato ligands create a 1D structure.

### Author contributions:
All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

References