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The crystal structure of [(2,2'-bipyridine- k^2N,N)-bis(6-phenylpyridine-2-carboxylate- k^2N,O)copper(II)], $C_{34}H_{24}N_4O_4Cu$

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.14 × 0.12 × 0.09 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.85 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	6381, 2368, 0.023
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2201
$N(param)_{refined}$:	195
Programs:	Bruker [1], CrysAlis ^{PRO} [2], Olex2 [3], SHELX [4], Diamond [5]

Source of material

The mixture of 6-phenylpyridine-2-carboxylic acid (0.50 mmol, 0.0996 g), 2,2'-bipyridine (0.25 mmol, 0.039 g), NaOH (0.50 mmol, 0.020 g), and cupric acetate monohydrate (0.25 mmol, 0.0499 g) were dissolved in a 15 mL water (5 mL)-ethanol (10 mL) solution at room temperature. The blue solution gradually became cloudy. The reaction mixture was stirred for 4 h at 75 °C, cooled to room temperature and stirring was continued for 4 h. Then the solution was filtered and the filtrate was left resting for 20 days. The blue crystals of the title complex were obtained from the filtrate.

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

As one of the important research contents of coordination chemistry, the complexes have been widely valued by chemists and material scientists. Because they show a rich variety of structures [6] and many applications such as

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Abstract

$C_{34}H_{24}N_4O_4Cu$, monoclinic, $C2/c$ (no. 15), $a = 17.2931(15)$ Å, $b = 10.3584(5)$ Å, $c = 17.5641(16)$ Å, $\beta = 120.180(12)^\circ$, $V = 2719.8(5)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0282$, $wR_{ref}(F^2) = 0.0681$, $T = 199.99(10)$ K.

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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.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cu1	0.500000	0.57566 (3)	0.750000	0.02216 (11)
O1	0.36127 (10)	0.25220 (13)	0.70883 (11)	0.0391 (4)
O2	0.42283 (9)	0.44497 (12)	0.75858 (9)	0.0275 (3)
N1	0.57369 (10)	0.72313 (14)	0.74800 (10)	0.0222 (3)
N2	0.39380 (10)	0.50940 (15)	0.59600 (10)	0.0238 (3)
C1	0.38453 (12)	0.53909 (19)	0.51727 (13)	0.0266 (4)
C2	0.36522 (15)	0.4455 (2)	0.45335 (14)	0.0373 (5)
H2	0.361309	0.467595	0.400212	0.045*
C3	0.35196 (15)	0.3198 (2)	0.46951 (15)	0.0416 (6)
H3	0.338934	0.256146	0.427421	0.050*
C4	0.35822 (14)	0.2894 (2)	0.54894 (15)	0.0342 (5)
H4	0.347741	0.205658	0.560623	0.041*
C5	0.38041 (12)	0.38610 (18)	0.61069 (13)	0.0251 (4)
C6	0.38899 (13)	0.35681 (18)	0.69949 (13)	0.0267 (4)
C7	0.54308 (13)	0.84129 (17)	0.75096 (12)	0.0226 (4)
C8	0.59072 (14)	0.9520 (2)	0.75708 (13)	0.0317 (5)
H8	0.568612	1.032979	0.759100	0.038*
C9	0.67149 (15)	0.9398 (2)	0.76012 (15)	0.0395 (6)
H9	0.704456	1.012913	0.763969	0.047*
C10	0.70340 (14)	0.8190 (2)	0.75746 (14)	0.0367 (5)
H10	0.757763	0.809301	0.759262	0.044*
C11	0.65292 (13)	0.7129 (2)	0.75208 (13)	0.0294 (5)
H11	0.674625	0.631087	0.751235	0.035*
C12	0.36034 (14)	0.7711 (2)	0.53443 (13)	0.0337 (5)
H12	0.340466	0.747001	0.572719	0.040*
C13	0.39046 (13)	0.67742 (19)	0.49878 (13)	0.0284 (4)
C14	0.42071 (14)	0.7158 (2)	0.44225 (14)	0.0372 (5)
H14	0.440530	0.654206	0.417394	0.045*
C15	0.42138 (16)	0.8446 (2)	0.42301 (16)	0.0471 (6)
H15	0.442714	0.869365	0.386038	0.057*
C16	0.39102 (18)	0.9365 (2)	0.45766 (17)	0.0509 (7)
H16	0.391380	1.023087	0.443921	0.061*
C17	0.35973 (17)	0.9000 (2)	0.51327 (16)	0.0454 (6)
H17	0.338355	0.962065	0.536352	0.054*

antiepileptic drug, fluorescent sensor, photophysical property, anticancer property, and optical property [7–10]. Previous studies from our research group showed that both 6-phenylpyridine-2-carboxylate acid and 2,2'-bipyridine are both excellent ligands. Some ternary metal complexes constructed by Pb(II), Zn(II), and Co(II) with 6-phenylpyridine-2-carboxylate acid ligand have been reported [11–13]. In order to continue our study a new Cu(II) complex [(2,2'-bipyridine-*k*²*N,N*)-bis(6-phenylpyridine-2-carboxylate-*k*²*N,O*)copper(II)] has been synthesized and structural characterized.

The asymmetric unit consists of one half of a Cu(II) ion, one 6-phenylpyridine-2-carboxylate ligands, and one half of a 2,2'-bipyridine ligand (see the figure). The title complex is located on a two fold axis. all ligands adopt the bis-chelating coordination mode. The coordinated environment of Cu(II) center is shown in the Figure (symmetry

code: '1-*x*,+*y*,3/2-*z*'). The Cu(II) ion locates in a distorted octahedral geometry, defined by one O atom (O2) form one 6-phenylpyridine-2-carboxylate ligand and one N atom (N1) from 2,2'-bipyridine ligand at the axial positions (O2–Cu1–N1, 173.37(6)°), one O atom (O2') and two N atoms (N2, N2') form 6-phenylpyridine-2-carboxylate ligand, and one N atom (N1') from the 2,2'-bipyridine ligand in the equatorial plane. The dihedral angle between benzene ring (C12–C13–C14–C15–C16–C17) and pyridine ring (C1–C2–C3–C4–C5–N2) of 6-phenylpyridine-2-carboxylate ligand is 33.4°. The crystal packing is stabilized by the π–π stacking to form a 3D network structure.

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