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Aqua[*N*,*N*′-bis(4-methyl-1,3-benzothiazol-2-yl)-pyridine-2,6-dicarboxamidato(2−)]copper(II)

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.006 Å
R factor = 0.058
wR factor = 0.097
Data-to-parameter ratio = 13.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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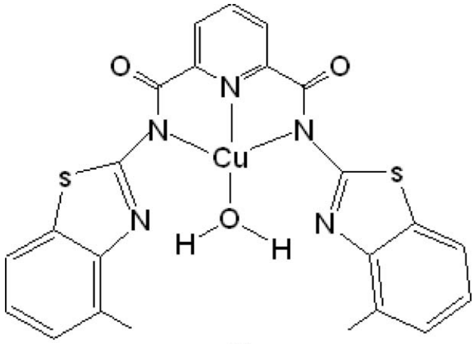
Treatment of deprotonated *N*,*N*′-bis-(4-methyl-2-benzothiazolyl)-2,6-pyridicarboxamide (L^{2-}) with $CuCl_2·2H_2O$ yields the mononuclear title complex, $CuL(H_2O)$ or $[Cu(C_{23}H_{15}N_5O_2S_2)(H_2O)]$. The Cu^{II} atom adopts a distorted square-planar coordination geometry, binding to two deprotonated amide N atoms, the pyridine N atom and the water O atom. In the crystal structure, weak C—H···O and C—H···S hydrogen bonds, and C—H···π and π–π interactions stabilize the crystal structure.

Comment

Investigations of the coordination chemistry of copper(II) continue to be stimulated by interest in developing models for copper proteins and in understanding the factors which give rise to the seemingly infinite variety of distortions from regular stereochemistry observed in copper(II) complexes (Balamurugan *et al.*, 2004). In order to further develop the coordination chemistry of pyridine amide ligands toward copper metal ions, we synthesized the title Cu^{II} complex, (I), based on the *N*,*N*′-bis(4-methyl-2-benzothiazolyl)-2,6-pyridicarboxamidate (L^{2-}) ligand and its structure is reported here (Fig. 1).



(I)

The Cu^{II} cation adopts a distorted square-planar coordination geometry, supported by two strong intramolecular O—H···N hydrogen bonds involving the water molecule and the two thiazole N atoms. Three nitrogen donors are provided by the rigid pyridyl–diamidate chelate with an average Cu—N bond distance of 2.013 (3) Å. The fourth donor site is occupied by the O3 water atom. Atoms N2, N3, N4 and Cu1 are coplanar [r.m.s deviation = 0.044 (3) Å], and O3 lies 0.107 (3) Å from this plane, completing the distorted square-planar coordination. The coordination geometry of the central

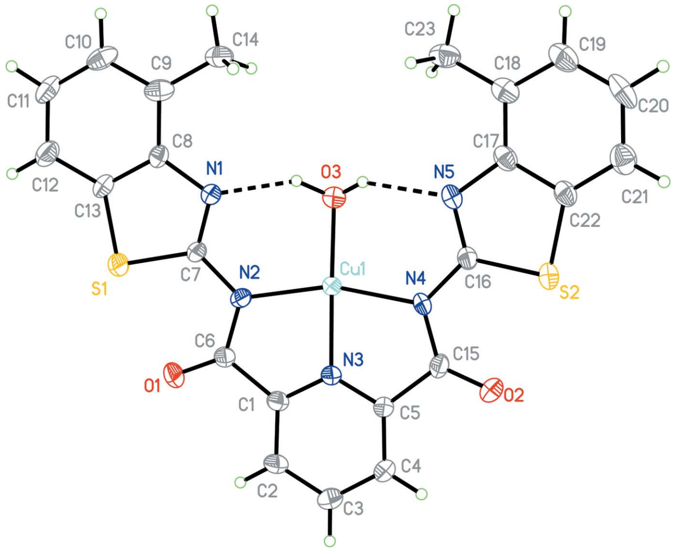


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level and intramolecular hydrogen bonds are shown as dashed lines.

Cu atom is obviously affected by the two-arm structure of the pyridine-2,6-dicarboxamidate ligand (Rowland *et al.*, 2001).

Two adjacent molecules form an inversion related dimer in a head-to-head fashion through weak C12—H12···O1 hydrogen bonds (Table 1). Another weak C23—H23*B*···S2 hydrogen bond links the dimers into a stair-like chain. A C14—H14*B*···π interaction involving the C8–C13 benzene ring [centroid *Cg*1; C14···*Cg*1 = 3.662 (2) Å; symmetry code: $1 - x, 1 - y, 1 - z$] further enhances the interaction between adjacent dimer molecules. A very weak π–π interaction [*Cg*2···*Cg*3 = 4.230 (8) Å; symmetry code: $1 - x, 1 - y, 2 - z$] between the central pyridine ring (centroid *Cg*2) and the six-membered ring of the benzothiazole (centroid *Cg*3) forms a two-dimensional network.

Experimental

The ligand H_2L was synthesized according to a literature method (Liu *et al.*, 2004) using 4-methyl-2-aminobenzothiazole instead of 2-(methylthio)aniline. H_2L (460 mg, 1.0 mmmol) and NaH (48 mg, 2.0 mmol) in DMF (15 ml) were added to a solution of $CuCl_2 \cdot 2H_2O$ (170 mg, 1.0 mmol) in DMF (5 ml). The resulting solution was stirred for 20 min. Exposure of this solution to air for a week gave brown single crystals suitable for structural studies (yield 380 mg, 70.49%). Analysis calculated for $C_{23}H_{17}CuN_5O_3S_2$: C 51.20, H 3.18, N 12.99%; found: C 51.22, H 3.19, N 13.01%.

Crystal data

$[Cu(C_{23}H_{15}N_5O_2S_2)(H_2O)]$
$M_r = 539.11$
Triclinic, $P\overline{1}$
$a = 8.7570$ (11) Å
$b = 11.208$ (2) Å
$c = 11.302$ (2) Å
$\alpha = 89.910$ (3)°
$\beta = 76.450$ (3)°
$\gamma = 89.530$ (3)°
$V = 1078.4$ (3) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.25$ mm^{-1}
$T = 291$ (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Siemens P4 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.70$, $T_{\max} = 0.74$
7899 measured reflections
4243 independent reflections
3302 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.056$
3 standard reflections every 97 reflections intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.097$
$S = 1.05$
4243 reflections
309 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.51$ e Å^{-3}
$\Delta\rho_{\min} = -0.48$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H32···N5	0.74	2.02	2.661 (4)	145
O3—H31···N1	0.94	1.86	2.652 (4)	140
C12—H12···O1$^{\rm i}$	0.93	2.55	3.431 (5)	157
C23—H23*B*···S2$^{\rm ii}$	0.96	2.86	3.734 (5)	151

Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $-x, -y, -z + 1$.

The water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions. All H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.86, C—H = 0.93–0.96 Å and $U_{\rm iso}$(H) = 1.2 or $1.5U_{\rm eq}$(C,N).

Data collection: *XSCANS* (Bruker, 2000); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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m1260 Liu *et al.* • $[Cu(C_{23}H_{15}N_5O_2S_2)(H_2O)]$ *Acta Cryst.* (2007). E**63**, m1259–m1260