metal-organic papers

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Key indicators

Bis(mefenamato-κO)bis(methanol-κO)bis(pyridine-κN)copper(II)

The Cu^{II} centre in the title complex, [Cu(C$_{15}$H$_{14}$NO$_2$)$_2$(C$_5$H$_5$N)$_2$(CH$_3$OH)$_2$], has axially elongated octahedral coordination. It is bonded in a *trans*-square-planar arrangement to the N atoms of two pyridine molecules and one carboxylate O atom from each of the two mefenamate anions. The axial positions are occupied by two methanol molecules coordinated through their O atoms.

Comment

The synthesis and structural characterization of copper(II) complexes with a non-steroidal anti-inflammatory drug, mefenamic acid, have been investigated (Hoang *et al.*, 1992; Melník *et al.*, 2000; Valach *et al.*, 1997); these are similar in structure to the title complex, (I).

(I)
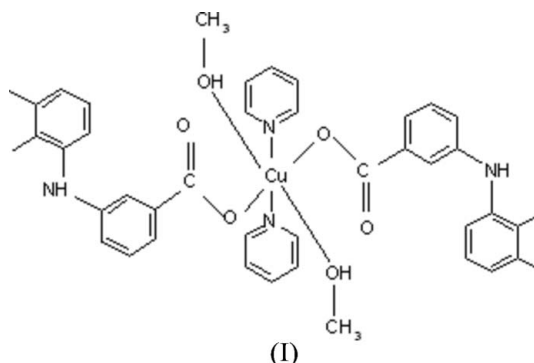
The asymmetric unit of the title complex, (I), consists of a Cu atom located on an inversion centre, one mefenamate anion and one pyridine and one methanol molecule (Fig. 1). Selected bond distances and bond angles are listed in Table 1. The coordination around the central copper(II) atom is axially elongated octahedral. The Cu^{II} atom is coordinated by two carboxylate O atoms from two different mefenamate anions and two N atoms from two different pyridine ligands in a square-planar arrangement. The axial positions are occupied by two methanol molecules [Cu—O3 = 2.449 (2) Å], which complete a distorted square-bipyramidal geometry. The axially elongated octahedral geometry about the Cu^{II} atom is consistent with the Jahn–Teller effect.

Intramolecular O—H···O and N—H···O hydrogen-bonding interactions stabilize the crystal structure of (I) (Table 2).

Experimental

The title complex was prepared by addition of pyridine (0.02 mol) to copper(II) mefenamate (0.01 mol) in hot methanol (20 ml). The

mixture was stirred, filtered and left to cool and stand at room temperature. Blue air-stable crystals of (I) were collected.

Crystal data

[Cu(C$_{15}$H$_{14}$NO$_2$)$_2$(C$_5$H$_5$N)$_2$-(CH$_4$O)$_2$]
$M_r = 766.40$
Triclinic, $P\bar{1}$
$a = 7.544$ (2) Å
$b = 8.448$ (2) Å
$c = 14.865$ (3) Å
$\alpha = 101.09$ (3)°
$\beta = 90.35$ (3)°

$\gamma = 90.55$ (3)°
$V = 929.6$ (4) Å^3
$Z = 1$
$D_x = 1.369$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.64$ mm^{-1}
$T = 100$ (2) K
Prism, blue
$0.30 \times 0.20 \times 0.10$ mm

Data collection

Kuma KM-4 CCD area-detector diffractometer
ω scans
Absorption correction: part of the refinement model (ΔF) (Parkin *et al.*, 1995)
$T_{min} = 0.905$, $T_{max} = 0.937$

6505 measured reflections
4124 independent reflections
3423 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.7°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.092$
$S = 0.97$
4124 reflections
241 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.978 (1)	Cu1—N1	1.991 (2)
Cu1—O3	2.499 (2)		
O1^i—Cu1—O1	180	N1^i—Cu1—N1	180
O1—Cu1—N1^i	90.67 (6)	N1—Cu1—O3	87.43 (6)
O1—Cu1—N1	89.33 (6)		

Symmetry code: (i) $-x, -y, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3—H31$\cdots$O2	0.89	1.81	2.660 (2)	158
N2—H2N$\cdots$O2	0.86	2.02	2.665 (2)	131
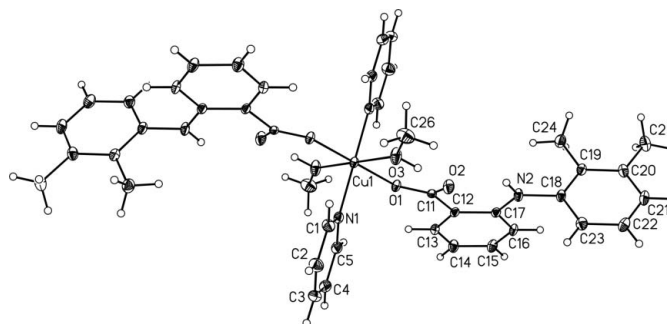
Figure 1
The structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level and H atoms are shown as spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry operation ($-x, -y, -z$).

H atoms were placed in geometrically calculated positions and allowed to ride on their parent atoms, with O—H = 0.89 Å, N—H = 0.86 Å and C—H = 0.93 (aromatic) or 0.96 Å (methyl). The U_{iso}(H) value for all H atoms was fixed at 0.05 Å^2.

Data collection: *KM-4-CCD System Software* (Kuma Diffraction, 1998); cell refinement: *KM-4 CCD System Software*; data reduction: *KM-4 CCD System Software*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1965); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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