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Key indicators

Single-crystal X-ray study
T = 293 K
 Mean σ (C–C) = 0.007 Å
R factor = 0.043
wR factor = 0.062
 Data-to-parameter ratio = 14.8

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

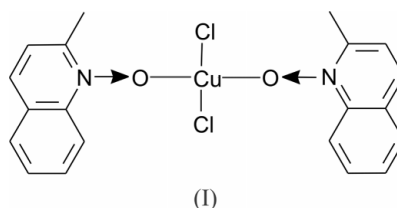
Dichlorobis(2-methylquinoline *N*-oxide- κ O)-copper(II)

The title compound, [CuCl₂(C₁₀H₉NO)₂], has crystallographically imposed twofold symmetry. The Cu atom is surrounded by two Cl atoms and two O atoms in a distorted square-planar configuration.

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Comment

Heteroatomic *N*-oxides and their complexes and salts demonstrate a broad spectrum of biological activity. Some are used as medical remedies (Albini & Pietra, 1991) and plant growth activators (Ponomarenko, 1999). *N*-Oxidation is one of the detoxication pathways of heterocycles in living things (Murray *et al.*, 1997; Hecht, 1996). The necessity of establishing structure–property relationships for this class of compounds led to the crystal structure determination of the title compound, (I).



In the crystal structure of (I), the Cu atom is situated on a twofold axis (see Fig. 1). The coordination polyhedron of the Cu atom is a slightly distorted square, with edge lengths of 3.089 (3) Å (Cl¹··O1) and 2.886 (3) Å (Cl¹··O1ⁱ), and with diagonals of 4.4030 (19) Å (Cl¹··Cl¹) and 3.909 (4) Å (O1··O1ⁱ) [symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, z$]. The term *trans*-square-

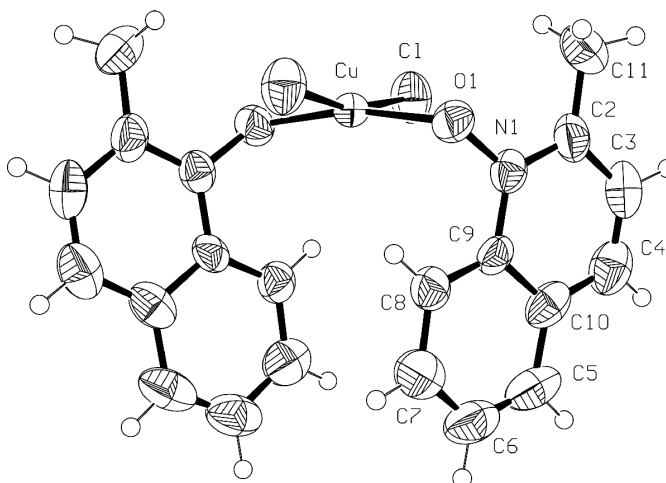


Figure 1
 ORTEP-3 (Farrugia, 1997) view of (I), with 50% probability displacement ellipsoids. H atoms are shown as spheres with arbitrary radii.

planar is used (Johnson & Watson, 1971) because the bond angles are approximately 90°. Selected bond lengths and angles are given in Table 1. The dihedral angle between the methylquinoline and the least-squares Cl/Clⁱ/O1/O1ⁱ plane is 84.56 (5)°. The dihedral angle between the two methylquinoline fragments is 10.88 (8)°. In a similar complex of 2-methylquinoline *N*-oxide with zinc, (II) (Ivashevskaja *et al.*, 2002), the Zn atom is also situated on a twofold axis. The geometries of (I) and (II) are, however, different. The shortest distances between the C atoms of the methyl group, C11ⁱ··C11ⁱ, and between the two methylquinoline moieties, C7ⁱ··C7ⁱ, in (I) are 7.705 (8) and 3.348 (6) Å, respectively, while the same distances, C11ⁱⁱ··C11ⁱⁱ and C7ⁱⁱ··C7ⁱⁱ [symmetry code: (ii) $-x, y, \frac{1}{2} - z$], in (II) are 4.22 (4) and 7.45 (4) Å, respectively. The coordination polyhedron of the Zn atom is a slightly distorted tetrahedron (Ivashevskaja *et al.*, 2002). The main reason for this difference in the Cu and Zn coordination is to be found in the electronic structure of the metal ion. The Cu atom prefers to be in an *sp*²*d*-hybridization state and square-planar coordination, while the Zn atom prefers to be in an *sp*³-hybridization state and tetrahedral coordination. The distortions in the coordination polyhedron are due to the influence of the methylquinoline fragments.

The coordination environment of the Cu atom in (I) is close to that observed in the molecular complexes dichlorobis(4-methylpyridine-1-oxide)copper(II) (Johnson & Watson, 1971), di- μ -(pyridine-1-oxide)bis[dichlorocopper(II)] (Sager *et al.*, 1967) and dichlorobis(2-picoline-1-oxide)copper(II) (Sager & Watson, 1968).

Experimental

2-Methylquinoline *N*-oxide hemihydrate was synthesized according to the procedure described by Ochiai (1953). Compound (I) was prepared by mixing warm saturated 2-methylquinoline hemihydrate and CuCl₂·2H₂O solutions in ethanol in a 2:1 molar ratio. The resulting brown precipitate was washed with ethanol and diethyl ether and then dried in air (yield 60%). The strong N—O band (1244 cm⁻¹) that is present in the IR spectrum of the parent *N*-oxide was absent in the spectrum of (I). On the other hand, in agreement with the literature findings (Garvey *et al.*, 1968), a new strong band at 1187 cm⁻¹, caused by the formation of a donor–acceptor bond between the O atom of quinoline *N*-oxide and a Cu atom, is present. Absorption bands at 353, 335 and 305 cm⁻¹, corresponding to the Cu—Cl bonds, are also present (Whyman *et al.*, 1967).

Crystal data

[CuCl₂(C₂₀H₁₈N₂O₂)]
M_r = 452.80
 Orthorhombic, *Pccn*
a = 7.332 (3) Å
b = 15.185 (5) Å
c = 17.370 (6) Å
V = 1933.8 (12) Å³
Z = 4
D_x = 1.555 Mg m⁻³

Cu *K*α radiation
 Cell parameters from 25 reflections
 θ = 22–25°
 μ = 4.29 mm⁻¹
T = 293 (2) K
 Plate, brown
 0.08 × 0.06 × 0.02 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 Non-profiled $\omega/2\theta$ scans
 1952 measured reflections
 1952 independent reflections
 1046 reflections with $I > 2\sigma(I)$
 θ_{\max} = 74.9°

h = −8 → 0
k = 0 → 19
l = 0 → 21
 1 standard reflection
 frequency: 60 min
 intensity decay: 3%

Refinement

R(*F*²) = 0.043
wR(*F*²) = 0.062
S = 0.88
 1952 reflections
 132 parameters
 Only H-atom *U*'s refined

$w = 1/[\sigma^2(F_o^2) + (0.007P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu—O1	1.968 (3)	C4—C10	1.412 (6)
Cu—Cl	2.2206 (11)	C5—C6	1.348 (6)
O1—N1	1.348 (4)	C5—C10	1.414 (6)
N1—C2	1.322 (5)	C6—C7	1.394 (6)
N1—C9	1.389 (5)	C7—C8	1.384 (6)
C2—C3	1.414 (5)	C8—C9	1.385 (5)
C2—C11	1.473 (5)	C9—C10	1.404 (5)
C3—C4	1.336 (6)		
O1 ⁱ —Cu—O1	166.80 (16)	C3—C4—C10	120.2 (5)
O1—Cu—Cl ⁱ	86.89 (10)	C6—C5—C10	119.9 (6)
O1—Cu—Cl	94.83 (10)	C5—C6—C7	121.3 (6)
Cl ⁱ —Cu—Cl	164.97 (7)	C8—C7—C6	120.5 (5)
N1—O1—Cu	115.5 (2)	C7—C8—C9	118.5 (5)
C2—N1—O1	118.8 (4)	C8—C9—N1	120.5 (4)
C2—N1—C9	124.0 (4)	C8—C9—C10	121.4 (4)
O1—N1—C9	117.1 (3)	N1—C9—C10	118.1 (4)
N1—C2—C3	117.2 (5)	C9—C10—C4	118.2 (5)
N1—C2—C11	118.9 (5)	C9—C10—C5	118.3 (5)
C3—C2—C11	123.9 (5)	C4—C10—C5	123.6 (5)
C4—C3—C2	121.9 (5)		
Cl1—Cu—O1—N1	−44.0 (3)	Cu—O1—N1—C2	106.6 (4)

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, z$.

H atoms were included in calculated positions and refined as riding atoms; C—H bonds lengths are in the range 0.93–0.96 Å and the *U*_{iso}(H) values were allowed to refine.

Data collection: CAD-4 EXPRESS (Enraf–Nonius, 1994); cell refinement: CAD-4 EXPRESS; data reduction: XCAD4 (Harms & Wokadlo, 1995); program(s) used to solve structure: DIRDIF96 (Beurskens *et al.*, 1996); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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