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A copper(II) complex of the fungicide tebuconazole

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In the title copper(II) complex, dichloro[(*RS*)-1-(4-chlorophenyl)-4,4-dimethyl-3-(1*H*-1,2,4-triazol-1-ylmethyl-κN^4)-pentan-3-ol]copper(II) ethanol tetrasolvate, $[CuCl_2(C_{16}H_{22}ClN_3O)_4]\cdot 4C_2H_5OH$, formed with the triazole fungicide tebuconazole, the Cu atom lies on an inversion center and has an elongated octahedral coordination. The molecules are linked to form a network *via* O—H···Cl and O—H···O hydrogen bonds.

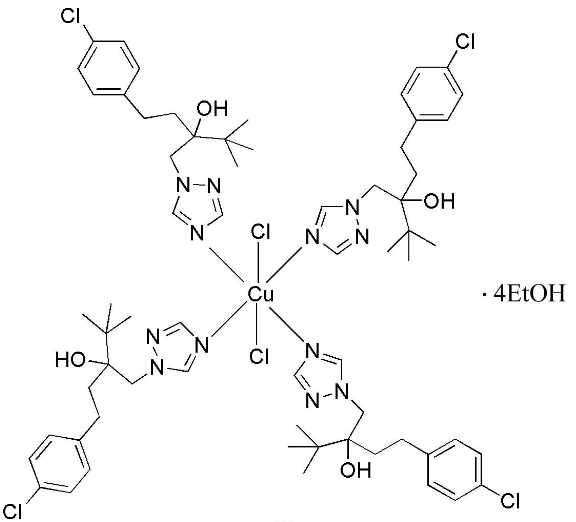
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
Disorder in solvent or counterion
R factor = 0.051
wR factor = 0.118
Data-to-parameter ratio = 15.1

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

Comment

The synthesis of triazole ligands and their interaction with metal ions have attracted a great deal of attention (Arion *et al.*, 2003; Zhang *et al.*, 2003). Many drugs modify their pharmacological and toxicological properties in the form of metallic complexes (El-Bindary & El-Sonbati, 2000). Complexation of pesticides with metals has potential advantages including the enhancement of persistence, longer shelf life, reduction of mammalian toxicity and conversion of non-systemic to systemic pesticides (Kamiya & Kameyama, 2001; Morillo *et al.*, 2002). We report here the preparation and structure of the novel Cu^{II} complex, (I), containing the tebuconazole ligand.



(I)

The Cu atom lies on an inversion center and thus the coordinated N atoms of the triazole ring form a perfect plane including the Cu^{2+} cation. The Cu atom has an elongated octahedral coordination, as shown in Fig. 1. The N atoms of the tebuconazole coordinate to the metal atom in the equatorial plane, whereas the axial positions are occupied by Cl atoms. The Cu—N and Cu—Cl bond distances are 2.006 (2)/

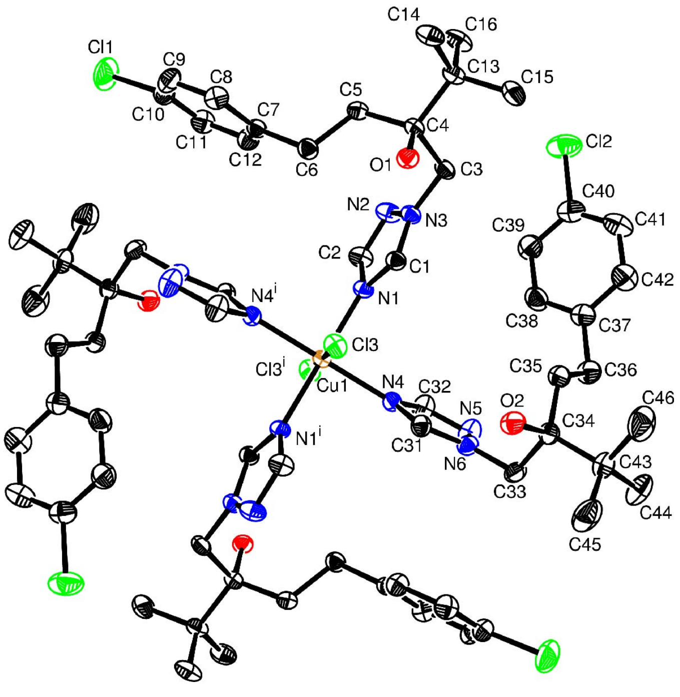


Figure 1
The molecular structure of (I), with ellipsoids at the 30% probability level. H atoms and ethanol solvent molecules have been omitted for clarity. [Symmetry code: (i) 1 − x, 1 − y, 1 − z.]

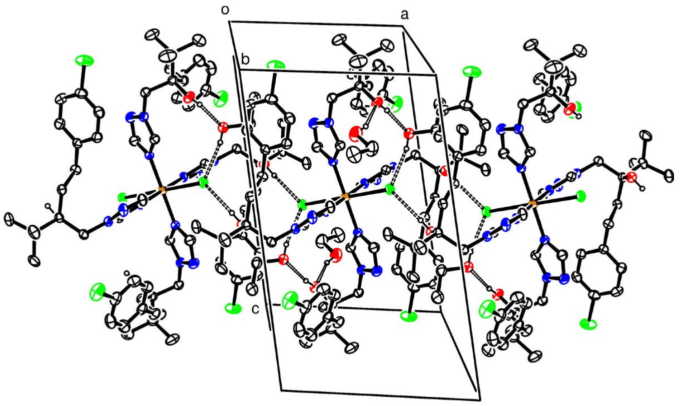


Figure 2
The crystal packing, showing the hydrogen-bonding O—H···O and O—H···Cl interactions (dashed lines), forming a chain parallel to the *a* axis. H atoms not involved in hydrogen bonding have been omitted.

2.021(2) and 2.855 (1) Å, respectively, which are similar to the values found in analogous complexes in which Cl atoms adopt an axial positions in a distorted octahedron around the Cu^{II} atom (Prins *et al.*, 1996). The two triazole rings (N1/C2/N2/N3/C1 and N4/C32/N5/N6/C31) make a dihedral angle of 97.03 (3)°, whereas the dihedral angle between triazole ring N1/C2/N2/N3/C1 and benzene ring C7–C12 is 87.69 (2)°.

Hydrogen-bonding interaction play an important role in the solid-state structure of (I). Indeed, the crystal packing appears to be dominated by O—H···O and O—H···Cl interactions (Table 1). Two of the hydroxy groups, one from the tebuconazole ligand and the other from one ethanol solvent molecule, act as hydrogen-bond donors to atom Cl3. There is also an O—H···O hydrogen bond between an ethanol solvent molecule and the ligand. These hydrogen-bonding interactions lead to the formation of chains parallel to the *a* axis (Fig. 2).

Experimental

To a solution of hydrated copper chloride (0.85 g, 5 mmol) in ethanol (20 ml) was added a solution of tebuconazole (6.0 g, 20 mmol) in ethanol (100 ml). The solution was refluxed for a further 6 h, whereupon a purple–blue product was produced. The solid was filtered off and the filtrate was left to evaporate at room temperature. After a week, single crystals suitable for X-ray analysis were obtained by recrystallization from ethanol.

Crystal data

$[CuCl_2(C_{16}H_{22}ClN_3O)_4]\cdot4C_2H_6O$
$M_r = 1549.98$
Triclinic, $P\overline{1}$
$a = 9.7162$ (1) Å
$b = 14.3502$ (2) Å
$c = 15.8887$ (1) Å
$\alpha = 71.175$ (3)°
$\beta = 79.856$ (3)°
$\gamma = 78.059$ (1)°
$V = 2037.12$ (5) Å^3

$Z = 1$
$D_x = 1.263$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 7526 reflections
$\theta = 2.2$–27.4°
$\mu = 0.52$ mm^{-1}
$T = 273$ (1) K
Chunk, blue
0.26 × 0.23 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.864$, $T_{max} = 0.901$
15280 measured reflections

7023 independent reflections
5140 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 25.4$°
$h = -11 \rightarrow 11$
$k = -17 \rightarrow 17$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.118$
$S = 1.01$
7023 reflections
465 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.9071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H201···O7	0.82	1.91	2.715 (3)	166
O7—H7···Cl3	0.82	2.28	3.083 (2)	167
O1—H101···Cl3^{i}	0.82	2.45	3.247 (2)	166
O6A—H6A1···O2^{ii}	0.82	2.00	2.790 (13)	160

Symmetry codes: (i) −*x*, 1 − *y*, 1 − *z*; (ii) 1 − *x*, 1 − *y*, 1 − *z*.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 (aromatic), 0.96 (CH$_3$) and 0.97 Å (CH$_2$), and O—H distances of 0.82 Å, and with U_{iso}(H) values set at $1.5U_{eq}$(C) (for CH$_3$) or $1.2U_{eq}$(C,O) (for CH$_2$, aromatic CH and O atoms). The two independent ethanol solvent molecules have rather large anistropic displacement parameters. One of these molecules could be modelled as disordered over two positions (site occupancies of 0.50) and refined using the tools available in *SHELXL97* (Sheldrick, 1997).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et* *al.*, 1999); 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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