Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Bis[4-(4-methylphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole]diperchlorato-κ^2O-copper(II)

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Key indicators

Single-crystal X-ray study
T = 571 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.110
Data-to-parameter ratio = 12.2

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

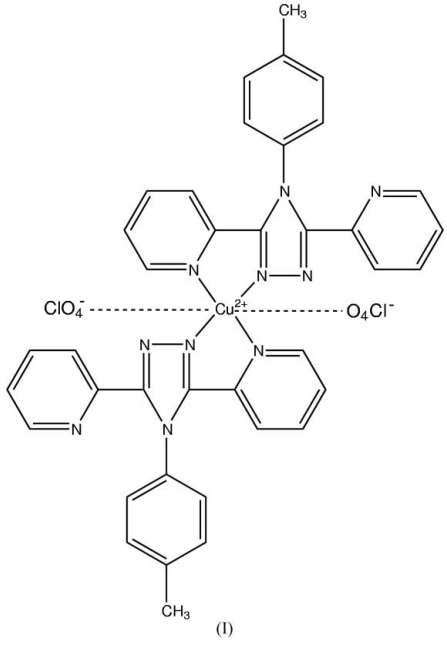
Received 19 January 2005
Accepted 24 January 2005
Online 5 February 2005

In the title centrosymmetric mononuclear copper(II) compound, $[Cu(ClO_4)_2(C_{19}H_{15}N_5)_2]$, the central Cu^{II} atom is coordinated by four N atoms from two 4-(4-methylphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole ligands, and two O atoms from two perchlorate counter-ions. The coordination geometry is slightly distorted octahedral.

Comment

Substituted 1,2,4-triazoles have been actively studied as bridging ligands, coordinating through their N1 and N2 atoms between transition metal(II) ions, since these complexes have interesting structures and magnetic properties (Antolini *et al.*, 1990, 1991; Bencini *et al.*, 1987; Lavrenova *et al.*, 1995).

Recently, we have reported the crystal structure of a nickel(II) complex with the ligand 4-(4-methylphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole (MBPT) (Shao *et al.*, 2004). As an extension of our work, we report here the crystal structure of a new copper(II) complex with the MBPT ligand.



(I)

The title compound, (I), consists of a centrosymmetric mononuclear copper(II) complex cation and two perchlorate counter-ions. In the cation, the central Cu atom lies on a crystallographic inversion centre and is six-coordinated by four N atoms from two inversion-related MBPT ligands, and by the centrosymmetrically related O atoms from two perchlorate counter-ions, forming a slightly distorted octahedral environment (Fig. 1). The MBPT molecule acts as a bidentate ligand. The Cu—N distances of 1.981 (2) and

2.041 (3) Å show normal values. The Cu—$O_{perchlorate\ anion}$ distance of 2.471 (3) Å is shorter than that observed in other copper(II) complexes with perchlorate anions (2.574 Å; Li *et al.*, 1997). The three *trans* angles at the Cu^{II} atom are exactly 180° by virtue of the crystallographic symmetry (Table 1), and the other angles subtended at the Cu^{II} atom are close to 90°, ranging from 80.24 (10) to 99.76 (10)°.

Experimental

Copper(II) perchlorate and two molar equivalents of MBPT were dissolved in methanol with stirring. After allowing the resulting clear purple solution to stand at room temperature in air for 10 d, blue crystals were formed on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using $CaCl_2$. Analysis found: C 51.21, H 3.36, N 15.72%; calculated for $C_{38}H_{30}Cl_2CuN_{10}O_8$: C 51.33, H 3.40, N 15.76%.

Crystal data

$[Cu(ClO_4)_2(C_{19}H_{15}N_5)_2]$	$Z = 1$
$M_r = 889.16$	$D_x = 1.567$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 8.398$ (3) Å	Cell parameters from 3291 reflections
$b = 8.680$ (3) Å	$\theta = 4.5$–$25.1°$
$c = 13.558$ (4) Å	$\mu = 0.79$ mm^{-1}
$\alpha = 93.725$ (5)°	$T = 571$ (2) K
$\beta = 91.749$ (4)°	Block, blue
$\gamma = 106.977$ (4)°	0.43 × 0.37 × 0.29 mm
$V = 942.1$ (5) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3291 independent reflections
	2450 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.018$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -9 \rightarrow 9$
$T_{min} = 0.727$, $T_{max} = 0.803$	$k = -10 \rightarrow 6$
5004 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.6344P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.042$	
$wR(F^2) = 0.110$	
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3291 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
269 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.981 (2)	Cu1—N4	2.042 (3)
N2^i—Cu1—N2	180	N2^i—Cu1—O1	88.83 (11)
N2—Cu1—N4	80.24 (10)	N2—Cu1—O1	91.17 (11)
N2—Cu1—N4^i	99.76 (10)	N4—Cu1—O1	86.28 (10)
N4—Cu1—N4^i	180	N4^i—Cu1—O1	93.72 (10)

Symmetry code: (i) $-x, -y, 2-z$.

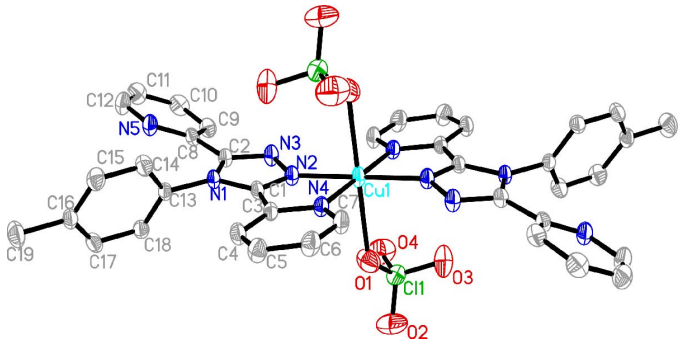


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by $(-x, -y, 2-z)$. H atoms have been omitted for clarity.

The C-bound H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H distances of 0.93 or 0.96 Å, and with U_{iso}(H) values of 1.2 or 1.5 (for methyl) times U_{eq}(carrier atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj300zd.

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