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[1,6-Bis(2-pyridylmethyl)-2,5-diazahexane-κ^4N]chlorocopper(II) perchlorate

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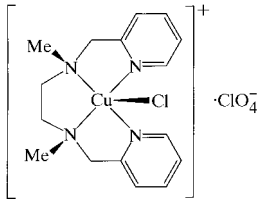
The title mononuclear copper(II) compound, $[CuCl(C_{16}H_{22}N_4)]ClO_4$, shows a slightly tetrahedrally distorted square-pyramidal coordination with the chlorine ligand at the apical position. The directions of the two N—Me bond axes are *syn* to the Cu—Cl bond.

Comment

DNA degradation by the copper(II) complexes with tripodal ligands has been investigated by one (YN) of the authors (Kobayashi *et al.*, 1996, 1998). The structure of



(I)

$[Cu(mep)Cl]ClO_4$, (I), where mep is 1,6-bis(2-pyridylmethyl)-2,5-diazahexane, is reported here.

Experimental

The ligand and its chlorocopper(II) complex were prepared as described previously (Okuno *et al.*, 1997). Crystals of the title compound were grown from a methanol solution.

Table 1
Selected geometric parameters (Å).

Cu1—Cl1	2.421 (1)	Cu1—N3	2.046 (3)
Cu1—N1	2.053 (3)	Cu1—N4	2.031 (3)
Cu1—N2	2.068 (3)		

Crystal data

$[CuCl(C_{16}H_{22}N_4)]ClO_4$	D_x = 1.610 Mg m^{-3}
M_r = 468.83	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
a = 11.044 (2) Å	θ = 10–15°
b = 11.085 (1) Å	μ = 1.436 mm^{-1}
c = 15.858 (1) Å	T = 299 K
β = 95.100 (9)°	Prism, blue
V = 1933.8 (4) Å^3	0.6 × 0.5 × 0.2 mm
Z = 4	

Data collection

Rigaku AFC-5*S* diffractometer	R_{int} = 0.028
θ–2θ scans	θ_{max} = 27.5°
Absorption correction: by integration (Coppens *et al.*, 1965)	$h = 0 \rightarrow 14$
T_{min} = 0.365, T_{max} = 0.764	$k = 0 \rightarrow 14$
4916 measured reflections	$l = -21 \rightarrow 21$
4445 independent reflections	3 standard reflections every 100 reflections
3426 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	H-atom parameters not refined
$R(F)$ = 0.049	$w = 1/[\sigma^2(F_o^2) + \{0.05(F_o^2 + 2F_c^2)/3\}^2]$
$wR(F^2)$ = 0.122	$(\Delta/\sigma)_{max}$ = 0.0006
S = 1.51	$\Delta\rho_{max}$ = 0.98 e Å^{-3}
4445 reflections	$\Delta\rho_{min}$ = −0.68 e Å^{-3}
244 parameters	

Positional parameters of all the H atoms were calculated geometrically and fixed with $U(H) = 1.2U_{eq}$(parent atom). The maximum residual density was located 0.99 Å from the Cu1 atom.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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