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Chloro[*N*′,*N*′-diethyl-*N*,*N*-bis(2-pyridylmethyl)ethylenediamine-κ^4N]-copper(II) perchlorate

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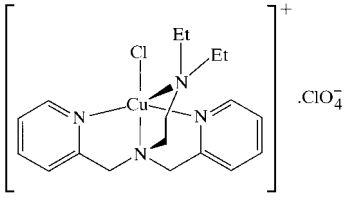
The title mononuclear copper(II) complex, $[CuCl(C_{18}H_{26}N_4)]ClO_4$, shows a square-pyramidal coordination with the diethylamino N atom at the apical position. Large anisotropies in the displacement parameters of the non-H atoms of the ligand seem to be due to rotational disorder of the ClO_4^- anion.

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 $[Cu(Et_2py)Cl]ClO_4$ (where py is pyridine), (I), is reported here.

The U_{eq} values of the perchlorate O1, O2, O3 and O4 atoms are in the range 0.207 (3)–0.349 (6) Å^2, suggesting a rotational disorder of the ClO_4^- anion.



(I)

Experimental

The ligand and its chlorocopper(II) complex were prepared as described previously (Kobayashi *et al.*, 1998). Crystals of the title compound were grown from an aqueous methanol solution.

Crystal data

$[CuCl(C_{18}H_{26}N_4)]ClO_4$	D_x = 1.522 Mg m^{-3}
M_r = 496.88	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
a = 12.513 (2) Å	θ = 10–15°
b = 14.613 (2) Å	μ = 1.285 mm^{-1}
c = 12.569 (2) Å	T = 298 K
β = 109.34 (1)°	Plate, blue
V = 2168.6 (1) Å^3	0.65 × 0.55 × 0.30 mm
Z = 4	

Data collection

Rigaku AFC-5*S* diffractometer	R_{int} = 0.025
θ–2θ scans	θ_{max} = 27.5°
Absorption correction: by integration (Coppens *et al.*, 1965)	$h = 0 \rightarrow 16$
T_{min} = 0.469, T_{max} = 0.701	$k = 0 \rightarrow 19$
5399 measured reflections	$l = -16 \rightarrow 16$
4971 independent reflections	3 standard reflections
2593 reflections with $I > 2\sigma(I)$	every 100 reflections
	intensity decay: none

Refinement

Refinement on F^2	H-atom parameters not refined
$R(F)$ = 0.064	$w = 1/[\sigma^2(F_o^2) + \{0.05(F_o^2 + 2F_c^2)/3\}^2]$
$wR(F^2)$ = 0.161	$(\Delta/\sigma)_{max}$ = 0.003
S = 1.51	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
4971 reflections	$\Delta\rho_{min}$ = −0.43 e Å^{-3}
262 parameters	

Table 1
Selected geometric parameters (Å).

Cu1—Cl1	2.240 (1)	Cu1—N3	2.011 (5)
Cu1—N1	2.008 (5)	Cu1—N4	2.352 (4)
Cu1—N2	2.042 (4)		

Positional parameters of all the H atoms were calculated geometrically and fixed with $U(H) = 1.2U_{eq}$(parent 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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