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μ-Chloro-bis{[benzylbis(2-pyridylmethyl)amine-κ³N]chlorocopper(II)} perchlorate hemihydrate

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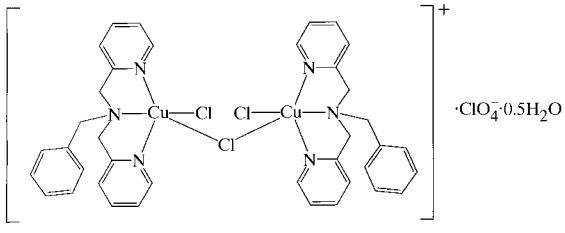
In the title dinuclear Cu^{II} compound, $[Cu_2Cl_3(C_{19}H_{19}N_3)_3]$-$ClO_4{\cdot}0.5H_2O$, the coordination geometry around the Cu atoms is square pyramidal, with the bridging Cl atom at the apical positions. The Cu—Cl—Cu angle is 136.9 (1)° and the Cu···Cu distance is 4.961 (1) Å.

Comment

The abbreviation for the tridentate benzyl(2-pyridylmethyl)-amine ligand in the title compound, (I), is bzpy and that of its 2-hydroxy derivative is phpyH. In the crystals of [Cu(phpyH)Cl]$ClO_4{\cdot}CH_3OH$, which is a model compound for galactose oxidase, a rather long Cu^{II}–phenolic oxygen distance of 2.570 (4) Å was observed (Ito *et al.*, 1998).



(I)

Experimental

The preparation of the bzpy ligand and its chlorocopper(II) complex was carried out by an analagous method to that described previously by Ito *et al.* (1998). Crystals of the title compound, $[Cu_2(bzpy)_2Cl_3]$-$ClO_4{\cdot}0.5H_2O$, were grown from an MeOH/CH_3CN solution.

Crystal data

$[Cu_2Cl_3(C_{19}H_{19}N_3)_2]ClO_4{\cdot}0.5H_2O$	$Z = 2$
$M_r = 920.67$	$D_x = 1.524$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 13.799$ (2) Å	Cell parameters from 25 reflections
$b = 14.488$ (2) Å	$\theta = 10$–15°
$c = 12.608$ (2) Å	$\mu = 1.376$ mm^{-1}
$\alpha = 99.33$ (1)°	$T = 300$ K
$\beta = 111.86$ (1)°	Sphere, blue
$\gamma = 113.14$ (1)°	0.3 mm (radius)
$V = 2005.9$ (6) Å^3	

Data collection

Rigaku AFC-5*S* diffractometer	$R_{int} = 0.012$
θ–2θ scans	$\theta_{max} = 27.5°$
Absorption correction: spherical (*International Tables for Crystallography*, 1992, Vol. C)	$h = 0 \rightarrow 18$
	$k = -19 \rightarrow 19$
$T_{min} = 0.545$, $T_{max} = 0.552$	$l = -16 \rightarrow 16$
9581 measured reflections	3 standard reflections
9196 independent reflections	every 100 reflections
6985 reflections with $I > 2\sigma(I)$	intensity decay: 4.3%

Refinement

Refinement on F^2	H-atom parameters not refined
$R(F) = 0.040$	$w = 1/[\sigma^2(F_o^2) + \{0.1(F_o^2 + 2F_c^2)/3\}^2]$
$wR(F^2) = 0.141$	$(\Delta/\sigma)_{max} = 0.004$
$S = 1.02$	$\Delta\rho_{max} = 0.42$ e Å^{-3}
9196 reflections	$\Delta\rho_{min} = -0.35$ e Å^{-3}
493 parameters	

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.238 (1)	Cu2—Cl2	2.252 (1)
Cu1—Cl3	2.695 (1)	Cu2—Cl3	2.639 (1)
Cu1—N1	2.004 (3)	Cu2—N4	1.988 (3)
Cu1—N2	2.053 (3)	Cu2—N5	2.066 (2)
Cu1—N3	1.999 (3)	Cu2—N6	1.985 (3)
Cl1—Cu1—N2	165.1 (1)	N4—Cu2—N6	164.5 (1)
N1—Cu1—N3	163.3 (1)	Cu1—Cl3—Cu2	136.9 (1)
Cl2—Cu2—N5	153.4 (1)		

The water O atom lies on an inversion centre and the water H atoms were not introduced. Positional parameters of all the other 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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