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# Chlorobis[4,4-bis(hydroxymethyl)-2-(2-pyridyl)-4,5-dihydrooxazole-*N*,*N*′]copper(II) chloride hemihydrate

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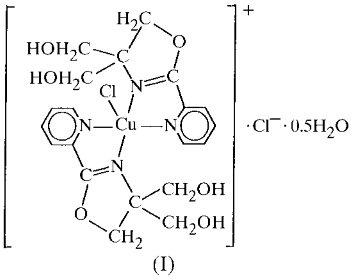
The title compound, $[CuCl(C_{10}H_{12}N_2O_3)_2]Cl\cdot0.5H_2O$, is composed of discrete complex cations, $Cl^-$ anions and water molecules. The O atom of the water molecule lies on a twofold rotation axis. The $[CuN_4Cl]$ coordination polyhedron is intermediate between square pyramidal and trigonal bipyramidal.

## Comment

The 2-oxazoline ring shows an interesting structure and is present in a wide variety of compounds which are of interest in many fields of application (Frump, 1971). The preparation of 2-substituted-2-oxazolines, involving heterocyclic ring-forming processes between nitriles and amino alcohols, is highly desirable (Brunner & Obermann, 1989; Bolm *et al.*, 1991). The formation of some new 2-pyridyl-2-oxazolines and their $Ni^{II}$, $Co^{II}$ and $Cu^{II}$ complexes have already been reported (Segl'a & Jamnický, 1993; Segl'a *et al.*, 1998).



(I)

In the title compound, (I), the $Cu^{II}$ centre is five-coordinated by four N donors from two ligands and by a chloride ligand (Fig. 1). The coordination polyhedron around the $Cu^{II}$ atom is intermediate between square pyramidal and trigonal bipyramidal, and is very similar to that in $[CuBrL_2]Br\cdot0.5H_2O$ (Segl'a *et al.*, 1998). The $\tau$ parameter for both complexes is 0.48 (Addison *et al.*, 1984). The Cu—N bond distances in (I) (see Table 1) are similar to those in the isostructural $[CuBrL_2]Br\cdot0.5H_2O$ complex [Cu—N1 = 2.018 (4), Cu—N2 = 2.093 (4), Cu—N3 = 2.001 (4) and Cu—N4 = 2.201 (5) Å; Segl'a *et al.*, 1998]. The two ligands $L$ in $[CuClL_2]^+$ are almost perpendicular, the dihedral angle between the N1/N2/C5/C6/Cu1 and N3/N4/C15/C16/Cu1 planes being 83.44 (6)°. The OH group (O3—H12) on one oxazoline ring is disordered over two positions with occupation parameters 0.75 for O3—H12 and 0.25 for O3*A*—H12*A* (Fig. 1). The O atom of the water molecule occupies a crystallographic twofold axis. The chloride anion is linked by hydrogen bonds [Cl2···H11 2.30, Cl2···H25$^{i}$ 2.16 and Cl2···H24$^{ii}$ 2.31 Å; symmetry codes: (i) $-x, y, \frac{1}{2} - z$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$]. The O7 atom of the water molecule is hydrogen bonded to H23 (O7···H23 1.97 Å). A similar pattern of hydrogen bonds is seen in $[CuBrL_2]Br\cdot0.5H_2O$ (Segl'a *et al.*, 1998).

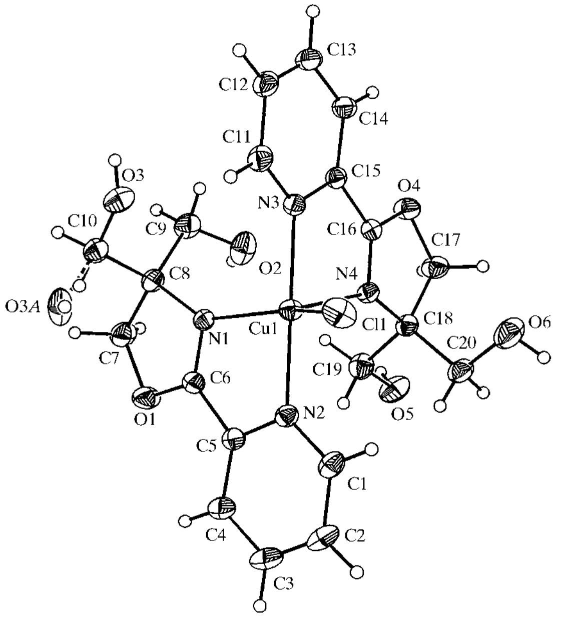


**Figure 1**
A view of the title complex cation with displacement ellipsoids drawn at the 30% probability level and H atoms shown as spheres of arbitrary radii.

## Experimental

The title compound was obtained by an analogous reaction to that described by Segl'a *et al.* (1998). Equimolar quantities of pyridine-2-carbonitrile and 2-amino-2-hydroxymethyl-1,3-propanediol were added to an ethanolic solution of anhydrous copper(II) chloride and the mixture was heated for 30 min at 333 K. After several days, blue–green crystals of (I) appeared.

*Crystal data*

$[CuCl(C_{10}H_{12}N_2O_3)_2]Cl\cdot0.5H_2O$
$M_r = 559.88$
Monoclinic, $C2/c$
$a = 17.995$ (4) Å
$b = 16.601$ (3) Å
$c = 16.879$ (3) Å
$\beta = 114.52$ (3)°
$V = 4587.6$ (15) Å$^3$
$Z = 8$
$D_x = 1.621$ Mg m$^{-3}$
$D_m = 1.62$ Mg m$^{-3}$
$D_m$ measured by flotation in $C_6H_6/CHBr_3$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 4.1$–11.2°
$\mu = 1.233$ mm$^{-1}$
$T = 293$ (2) K
Rectangular prism, green–blue
0.45 × 0.40 × 0.35 mm

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—N1 | 2.0757 (15) | Cu1—N4 | 2.2127 (17) |
| Cu1—N2 | 1.9988 (15) | Cu1—Cl1 | 2.2552 (7) |
| Cu1—N3 | 1.9825 (15) | | |
| N1—Cu1—N2 | 81.03 (6) | N3—Cu1—N4 | 79.56 (6) |
| N1—Cu1—N3 | 96.29 (6) | N1—Cu1—Cl1 | 146.65 (5) |
| N1—Cu1—N4 | 98.96 (6) | N2—Cu1—Cl1 | 92.80 (5) |
| N2—Cu1—N3 | 175.54 (6) | N3—Cu1—Cl1 | 91.38 (5) |
| N2—Cu1—N4 | 97.28 (6) | N4—Cu1—Cl1 | 114.35 (5) |

*Data collection*

Syntex $P2_1$ diffractometer
$\theta$–$2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{\min} = 0.565$, $T_{\max} = 0.650$
5869 measured reflections
5109 independent reflections
3284 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.021$
$\theta_{\max} = 27.57°$
$h = -22 \rightarrow 0$
$k = -21 \rightarrow 21$
$l = -19 \rightarrow 20$
3 standard reflections every 100 reflections intensity decay: 15%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.052$
$S = 0.804$
5109 reflections
323 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0057P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.19$ e Å$^{-3}$

The H atoms on C10 corresponding to the minor disorder component of O3 have not been included. With the exception of H25 (on the water O7 atom) which was located from a $\Delta F$ synthesis and refined as part of a rigid rotating group, H atoms were placed geometrically and refined as part of a riding model.

Data collection: $P2_1$ *Software* (Syntex, 1973); cell refinement: $P2_1$ *Software*; data reduction: *XP*21 (Pavelčík, 1993); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1965); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BM1397). Services for accessing these data are described at the back of the journal.

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*Acta Cryst.* (2000). C**56**, 554–555 Marian Koman *et al.* • $[\mathrm{CuCl}(\mathrm{C_{10}H_{12}N_2O_3})_2]\mathrm{Cl}\cdot 0.5\mathrm{H_2O}$ **555**