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# *catena*-Poly[[[bis(3-aminopyridine-$\kappa N$)copper(II)]-di-$\mu$-chloro] hydrate]

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**Key indicators**

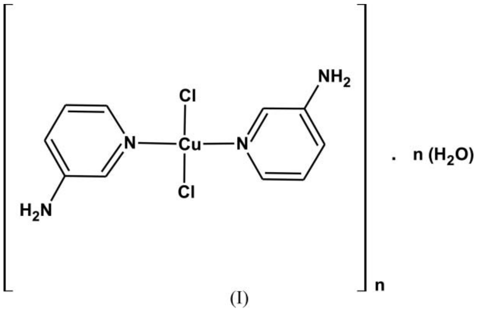
Single-crystal X-ray study
$T$ = 150 K
Mean $\sigma$(C–C) = 0.007 Å
H-atom completeness 86%
Disorder in solvent or counterion
$R$ factor = 0.069
$wR$ factor = 0.222
Data-to-parameter ratio = 23.7

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

The title compound, $\{[CuCl_2(C_5H_6N_2)_2]\cdot H_2O\}_n$, comprises centrosymmetric mononuclear $CuCl_2L_2$ ($L$ = 3-aminopyridine) units, with a *trans* geometry of the ligands, connected into infinite linear chains through bridging chloride ligands. The chains are oriented along the $c$ axis and form channels, which are occupied by disordered water molecules.

## Comment

During the course of systematic investigations on copper–oxalate chemistry with substituted pyridines, the reaction of $CuCl_2\cdot 2H_2O$ with $K_2C_2O_4$ and 3-aminopyridine was performed in methanol solution. Unexpectedly, the title complex, (I), was obtained; the crystal structure of (I) is presented here.



(I)

Complex (I) shows a polymeric chain structure with the basic building block being $CuCl_2L_2$ ($L$ = 3-aminopyridine). The Cu atom lies on an inversion centre and is coordinated by two *trans* 3-aminopyridine ligands and two *trans* chlorides forming a distorted square-planar arrangement (Fig. 1). The

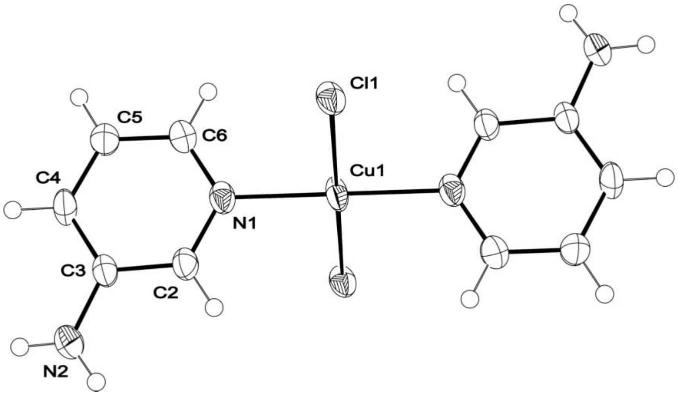


**Figure 1**
The mononuclear building unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by ($1-x$, $y$, $1-z$).

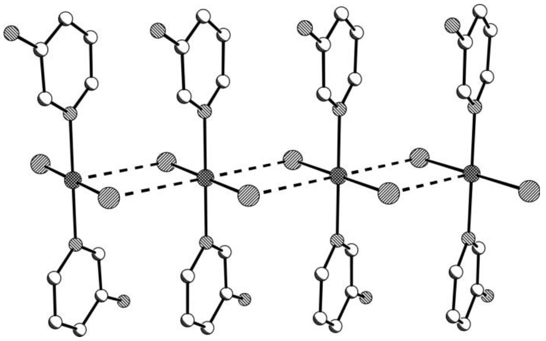


**Figure 2**
The one-dimensional chain structure of (I). H atoms have been omitted.

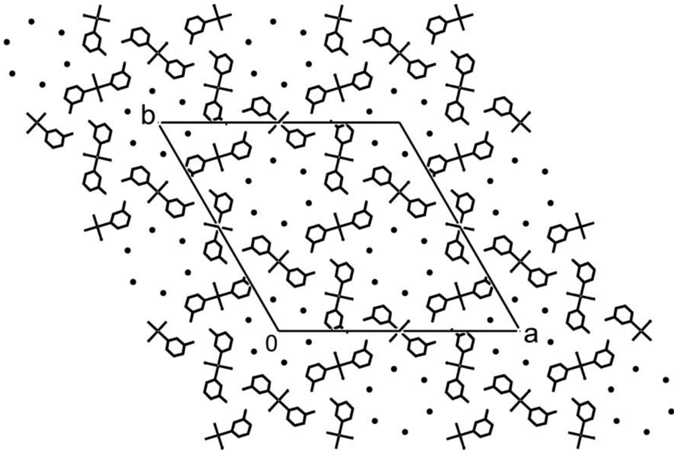


**Figure 3**
A packing diagram of (I), viewed along the *c* axis, showing the channels occupied by water molecules (black circles). H atoms have been omitted.

Cu1—N1 and Cu1—Cl1 distances are 2.006 (3) and 2.2862 (9) Å, respectively; selected geometric parameters are collected in Table 1. The coordination geometry in (I) is similar to those observed in other monomeric complexes with the same stoichiometry and containing substituted pyridines (*e.g.* Stählin & Oswald, 1971; Zhang *et al.*, 2004; Xuan *et al.*, 2003, and references therein). The pyridine ring is twisted with respect to the coordination plane, forming a dihedral angle of 61.1 (1)°. The mononuclear building block is connected into infinite chains (Fig. 2) *via* the coordination of chloride ions of adjacent units to the axial sites at a distance of 3.1926 (12) Å, thus forming the 4 + 2 coordination geometry common to copper halide complexes. The Cu atoms within the chain are separated by 3.9152 (1) Å and the Cu—Cl—Cu$^{i}$ bridging angle is 89.64 (3)° [symmetry code: (i) *x*, *y*, *z* − 1]. Similar chain structures have been observed for complexes containing pyridine (Van Meervelt *et al.*, 2003), 4-methylpyridine (Marsh *et al.*, 1981) and 4-cyanopyridine (Zhang *et al.*, 1997). However, it is noteworthy that the arrangement of the chains in the crystal structure of (I) is different from the aforementioned structures. The chains are oriented along the *c* axis, forming channels that are occupied by (disordered) solvent water molecules, as illustrated in Fig. 3. Adjacent chains are connected *via* N—H···Cl interactions, as detailed in Table 2.

## Experimental

$CuCl_2 \cdot 2H_2O$ (0.10 g) and $K_2C_2O_4$ (0.15 g) were dissolved in methanol (50 ml). 3-Aminopyridine (0.20 g) was added to this solution and the colour changed to brown–green. On standing at room temperature overnight, yellow–green block-shaped crystals were formed. The crystals were extremely unstable when taken from the mother liquor and decomposed rapidly into a blue powder.

*Crystal data*

$[CuCl_2(C_5H_6N_2)_2] \cdot H_2O$
$M_r = 338.68$
Trigonal, $R\overline{3}$
$a = 33.9602$ (7) Å
$c = 3.9152$ (1) Å
$V = 3910.43$ (15) Å$^3$
$Z = 9$
$D_x = 1.294$ Mg m$^{-3}$
Mo *Kα* radiation
Cell parameters from 2142 reflections
$\theta = 1.0$–28.3°
$\mu = 1.56$ mm$^{-1}$
$T = 150$ (2) K
Block, yellow–green
0.15 × 0.10 × 0.10 mm

*Data collection*

Nonius KappaCCD diffractometer
$\omega$ scans at $\kappa = 55°$
Absorption correction: none
3701 measured reflections
1991 independent reflections
1652 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$
$\theta_{\rm max} = 27.5°$
$h = -44 \rightarrow 43$
$k = -36 \rightarrow 37$
$l = -5 \rightarrow 5$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.222$
$S = 1.25$
1991 reflections
84 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1406P)^2 + 3.9571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.002$
$\Delta\rho_{\rm max} = 2.21$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -1.25$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0092 (12)

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

| | | | |
|---|---|---|---|
| Cu1—N1 | 2.006 (3) | C3—C4 | 1.381 (6) |
| Cu1—Cl1 | 2.2862 (9) | C4—C5 | 1.396 (6) |
| Cu1—Cl1$^{i}$ | 3.1926 (12) | C5—C6 | 1.387 (6) |
| Cu1···Cu1$^{i}$ | 3.9152 (1) | N1—C6 | 1.337 (6) |
| N1—C2 | 1.341 (5) | N2—C3 | 1.387 (6) |
| | | | |
| N1—Cu1—Cl1 | 90.10 (10) | C4—C3—C2 | 118.1 (4) |
| N1—Cu1—Cl1$^{i}$ | 91.47 (11) | N2—C3—C2 | 119.6 (4) |
| C6—N1—C2 | 119.6 (4) | C3—C4—C5 | 118.9 (4) |
| N1—C2—C3 | 122.4 (4) | C6—C5—C4 | 119.8 (4) |
| C4—C3—N2 | 122.3 (4) | N1—C6—C5 | 121.2 (4) |

Symmetry code: (i) *x*, *y*, *z* − 1.

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···Cl1$^{ii}$ | 0.86 | 2.61 | 3.394 (4) | 152 |

Symmetry code: (ii) $y + \frac{1}{3}, -x + y + \frac{2}{3}, -z + \frac{5}{3}$.

All H atoms were placed in geometrically calculated positions, and were refined using a riding model (aromatic C—H = 0.93 Å and N—H = 0.86 Å). $U_{\rm iso}$ values were set at $1.2U_{\rm eq}$ of the parent atom. The H atoms of the solvent water molecule were not located. Examination of the structure with *PLATON* (Spek, 2003) showed that it contains solvent-accessible voids. These voids are partially occupied by solvent molecules, but the disorder is so extensive that an atomic model could not be developed; thus, the chemical composition is formulated only on the basis of the modelled water molecule. The highest residual density peak is located at the origin and the deepest hole is 1.85 Å from atom Cl1.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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