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catena-Poly[[chlorocopper(I)]-μ-1,3-di-4-pyridylpropane-κ^2N:N']

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.089
wR factor = 0.200
Data-to-parameter ratio = 13.3

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

The title compound, $[CuCl(C_{13}H_{14}N_2)]_n$, adopts an infinite one-dimensional chain structure. The Cu^I atom, which lies on a crystallographic mirror plane, is coordinated by the N atom from two pyridyl rings [Cu—N = 1.975 (7) Å] and a Cl atom [Cu—Cl = 2.251 (4) Å] in a trigonal-planar geometry. The Cl atom also lies on the mirror plane.

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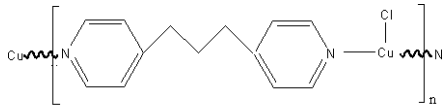
Comment

There are a number of studies on coordination compounds having flexible organic ligands that coordinate to metal centers (Chen *et al.*, 2004; Lu *et al.*, 1999). The 1,3-bis(4-pyridyl)propane heterocycle is an example of such a ligand.



(I)

The present copper(I) chloride adduct, (I) (Fig. 1), which was synthesized hydrothermally with copper(II) chloride as reagent, adopts a linear chain structure. The Cu atom is coordinated by two N atoms from different ligands in a trigonal planar geometry. The Cu and Cl atoms lie on a mirror plane. The bridging mode of the heterocyclic ligand gives rise to the formation of a chain that propagates along the *b* axis of the unit cell (Fig. 2).

Experimental

A mixture of $CuCl_2$ (0.085 g, 0.5 mmol), 1,3-bis(4-pyridyl)propane (0.098 g, 0.5 mmol), KOH (0.028 g, 0.1 mmol) and water (10 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor. The reaction was heated to 433 K for 60 h and then cooled to room temperature over a period of 60 h. Colorless plate-shaped crystals of the title compound were obtained in about 60% yield.

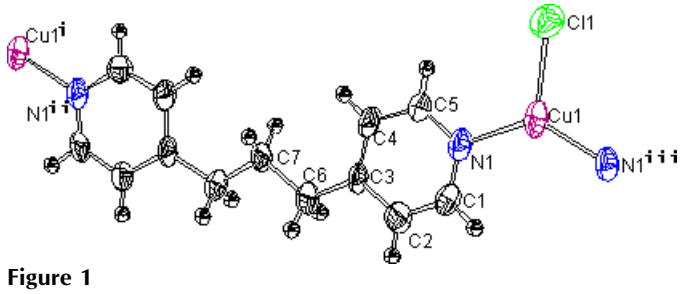


Figure 1
View of a fragment of the title compound, showing 50% probability displacement ellipsoids. [Symmetry codes: (i) $x, y-1, z$; (ii) $x, \frac{1}{2}-y, z$; (iii) $x, \frac{3}{2}-y, z$].

Crystal data

$[CuCl(C_{13}H_{14}N_2)]$
$M_r = 297.25$
Orthorhombic, *Pnma*
$a = 12.699\ (4)$ Å
$b = 13.885\ (4)$ Å
$c = 7.252\ (2)$ Å
$V = 1278.6\ (6)$ Å^3
$Z = 4$
$D_x = 1.544$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 774 reflections
$\theta = 5.2$–$25.1°$
$\mu = 1.89$ mm^{-1}
$T = 293\ (2)$ K
Plate, colorless
$0.34 \times 0.16 \times 0.04$ mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.702$, $T_{max} = 0.927$
2900 measured reflections
1191 independent reflections
774 reflections with $I > 2\sigma(I)$
$R_{int} = 0.088$
$\theta_{max} = 25.1°$
$h = -14 \rightarrow 15$
$k = -11 \rightarrow 16$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.089$
$wR(F^2) = 0.200$
$S = 1.11$
1148 reflections
86 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 10.9684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.976 (7)	Cu1—Cl1	2.251 (5)
N1^{iii}—Cu1—N1	131.5 (5)	N1—Cu1—Cl1	114.2 (2)

Symmetry code: (iii) $x, \frac{3}{2} - y, z$.

H atoms were positioned geometrically and refined using a riding model [aromatic C—H = 0.93 Å and aliphatic C—H = 0.97 Å; U_{iso}(H) = $1.2U_{eq}$(C)].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

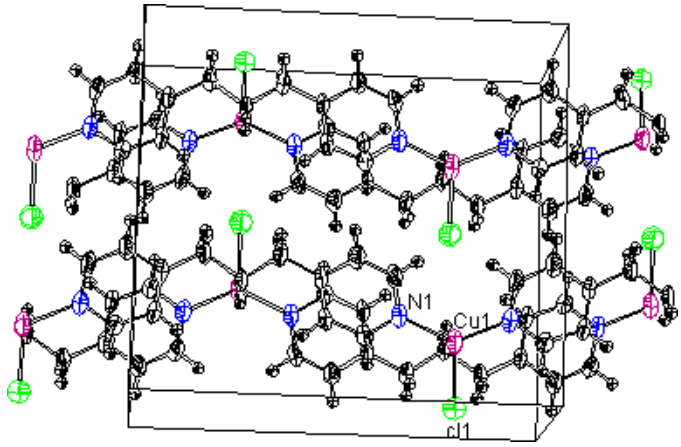


Figure 2
The packing, viewed approximately along the *c* axis.

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