# metal-organic papers

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#### **Key indicators**

Single-crystal X-ray study T = 170 KMean  $\sigma(\text{C-C}) = 0.003 \text{ Å}$  R factor = 0.034 wR factor = 0.089 Data-to-parameter ratio = 23.9

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

# Chlorobis(piperidine-*k*N)copper(I)

In the title compound,  $[CuCl(C_{10}H_{22}N_2)]$ , the Cu atom is connected to two N atoms of two crystallographically independent piperidine ligands and one Cl atom within a distorted trigonal-planar coordination. The complex molecules are stacked in the direction of the crystallographic *b* axis and are connected into chains *via* N-H···Cl hydrogen bonding along the crystallographic *c* axis. Received 14 June 2004 Accepted 22 June 2004 Online 26 June 2004

## Comment

Recently, we have been interested in the synthesis, crystal structures and thermal properties of coordination polymers built up of copper(I) halides and N-donor ligands (Näther & Je $\beta$ , 2002, 2003; Näther, Greve & Je $\beta$ , 2002; Näther, Wriedt & *Je* $\beta$ , 2002). During these investigations, we have synthesized and structurally characterized the ligand-rich title compound, (I). For copper(I) halides and piperidine, only a few structures are known. In the ligand-poorer compound copper(I) iodide–piperidine, Cu<sub>4</sub>I<sub>4</sub> cubes are found, in which each Cu atom is coordinated by three I atoms and one N atom of a piperidine ligand (Schramm, 1978). In the copper(I) halide-rich compounds (CuX)<sub>2</sub>–piperidine–triphenylphosphine (X = Cl, Br, I), (CuX)<sub>2</sub> dimers are found in which each Cu atom is coordinated by one piperidine and one triphenylphosphine ligand (Bowmaker *et al.*, 1994).



In (I), each Cu atom is coordinated by two N atoms of two crystallographically independent piperidine ligands and one Cl atom. The Cu–N bond lengths of 1.9959 (16) and 2.0045 (15) Å and the Cu–Cl bond length of 2.3187 (6) Å are in the range of those found in related structures retrieved from the Cambridge Structural Database (Version 1.6; Allen, 2002). The N–Cu–N and N–Cu–Cl angles are 135.37 (7), 116.68 (5) and 107.92 (5)°, and the Cu atoms show distorted trigonal-planar coordination.

In the crystal structure, discrete copper(I) chloride complexes are stacked in the direction of the crystallographic *b* axis and are connected by  $N-H\cdots$ Cl hydrogen bonding. The Cl atom of one complex is connected to both N atoms of a neighbouring complex; the  $N\cdots$ Cl distances are 3.2807 (17) and 3.31093 (18) Å, the Cl $\cdots$ H distances 2.38 and 2.42 Å and

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### Figure 1

The crystal structure of the title compound, with labelling and displacement ellipsoids drawn at the 50% probability level.

the N-H···Cl angles are 164 and 159°. From this arrangement, infinite chains result, which extend in the direction of the crystallographic c axis.

## **Experimental**

The title compound was prepared by the reaction of 110.8 mg (0.824 mmol) CuCl and 1 ml (10.1 mmol) piperidine in a glass container. After about 7 d, large colourless crystals had grown, which were light-sensitive and had to be stored in the dark.

#### Crystal data

$[CuCl(C_{10}H_{22}N_2)]$	$D_x = 1.390 \text{ Mg m}^{-3}$
$M_r = 269.29$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 7942
a = 20.355(2) Å	reflections
b = 6.5407 (4)  Å	$\theta = 10-23^{\circ}$
c = 9.7669 (11)  Å	$\mu = 1.87 \text{ mm}^{-1}$
$\beta = 98.314 \ (13)^{\circ}$	T = 170 (2)  K
$V = 1286.7 (2) \text{ Å}^3$	Block, colourless
Z = 4	$0.30 \times 0.18 \times 0.07 \ \mathrm{mm}$
Data collection	
Stoe IPDS diffractometer	2373 reflections with $I > 2\sigma(I)$
$\varphi$ scans	$R_{\rm int} = 0.033$
Absorption correction: numerical	$\theta_{\rm max} = 27.9^{\circ}$
(X-SHAPE; Stoe & Cie, 1998)	$h = -26 \rightarrow 26$
$T_{\min} = 0.670, T_{\max} = 0.873$	$k = -8 \rightarrow 8$
7942 measured reflections	$l = -12 \rightarrow 9$
3062 independent reflections	
Refinement	
Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.089$	$(\Delta/\sigma)_{\rm max} = 0.001$
S = 0.97	$\Delta \rho_{\rm max} = 0.63 \ {\rm e} \ {\rm \AA}^{-3}$
3062 reflections	$\Delta \rho_{\rm min} = -0.48 \text{ e} \text{ Å}^{-3}$
128 parameters	Extinction correction: SHELXL97

### Table 1

Selected geometric parameters (Å, °).

H-atom parameters constrained

Cu1-N1 Cu1-N11	1.9959 (16) 2.0045 (15)	Cu1-Cl1	2.3187 (6)
N1-Cu1-N11 N1-Cu1-Cl1	135.37 (7) 116.68 (5)	C1-N1-Cu1 C5-N1-Cu1	112.47 (11) 114.66 (13)
N11-Cu1-Cl1	107.92 (5)		

Extinction coefficient: 0.0148 (17)

H atoms were located in a difference map, but were positioned with idealized geometry (C–H = 0.99 Å and N–H = 0.93 Å) and



#### Figure 2

The crystal structure of the title compound, viewed along the crystallographic *b* axis.  $N-H\cdots$ Cl hydrogen bonding is shown as dashed lines.

refined with fixed isotropic displacement parameters  $[U_{iso}(H) = 1.2U_{eq}(C,N)]$ , using a riding model.

Data collection: *IPDS Program Package* (Stoe & Cie, 1998); cell refinement: *IPDS Program Package*; data reduction: *IPDS Program Package*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997; program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

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