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Chlorotripyridinecopper(I)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.012 Å
R factor = 0.048
wR factor = 0.075
Data-to-parameter ratio = 14.7

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

The Cu atom, the Cl atom and one of the pyridyl rings of the title compound, $[CuCl(C_5H_5N)_3]$, are located on a crystallographic mirror plane. As a result, there is a half molecule in the asymmetric unit. Geometric parameters do not show unusual values.

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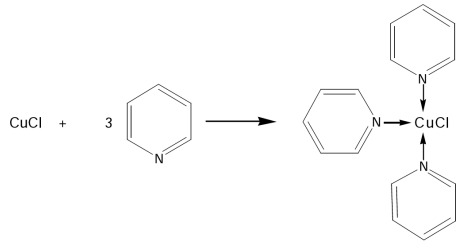
Comment

Clusters containing Cu—P bonds have attracted attention recently due to their structures. We became interested in the reaction of ^{t}Bu$_2$PLi with CuCl. While pure CuCl cannot be dissolved in pentane, addition of pyridine gives a solution from which the title compound, (I), can be isolated.



(I)

The Cu atom, the Cl atom and one of the pyridyl rings of (I) are located on a crystallographic mirror plane. As a result, there is a half molecule in the asymmetric unit.

The Cu—Cl and Cu—N distances are in the same range as in three comparable compounds retrieved from the Cambridge Structural Database (Allen & Kennard, 1993): chlorotris(3-methylpyridine-*N*)copper(I) [CETJUG (Ainscough *et al.*, 1984), CETJUG01 (Dyason *et al.*, 1985)] and chlorotris(3,5-dimethylpyridine-*N*)copper(I) (DUSMUZ; Dyason *et al.*, 1986) (Table 1). The dihedral angles between the aromatic rings are not markedly altered by the different substitution pattern.

Experimental

Pale-yellow crystals of the title compound were obtained from a solution of 0.163 g (1.07 mmol) CuCl and 0.5 ml pyridine in 30 ml pentane (yield 30%).

Crystal data

$[CuCl(C_5H_5N)_3]$
M_r = 336.29
Orthorhombic, $Cmc2_1$
a = 14.349 (2) Å
b = 9.831 (2) Å
c = 11.685 (2) Å
V = 1648.3 (5) Å^3
Z = 4
D_x = 1.355 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4339 reflections
θ = 4.2–25.1°
μ = 1.48 mm^{-1}
T = 173 (2) K
Needle, pale yellow
0.24 × 0.04 × 0.02 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.718, T_{max} = 0.971
6254 measured reflections
1518 independent reflections
1199 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 25.2°
$h = -17 \rightarrow 15$
$k = -11 \rightarrow 11$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.075
S = 0.94
1518 reflections
103 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0115P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Absolute structure: (Flack, 1983)
Flack parameter = 0.05 (4), 738 Friedel pairs

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···Cl1	0.95	2.85	3.519 (6)	128
C16—H16···Cl1	0.95	2.88	3.560 (10)	129
C2—H2···Cl1^{i}	0.95	2.76	3.699 (7)	169

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

Table 2
Comparison of geometric parameters (Å,°).

Structure	Cu—Cl	Cu—N	Angles between aromatic rings
Title compound	2.420 (3)	2.036 (3)	60.3 (2)
		2.058 (8)	59.4 (2)
CETJUG	2.458 (2)	2.021 (5)	62.7
CETJUG01	2.451 (4)	2.029 (10)	63.0
DUSMUZ	2.412 (9)	2.08 (1)	60.0

All H atoms could be located in a difference Fourier synthesis. They were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)], using a riding model (C—H = 0.95 Å).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

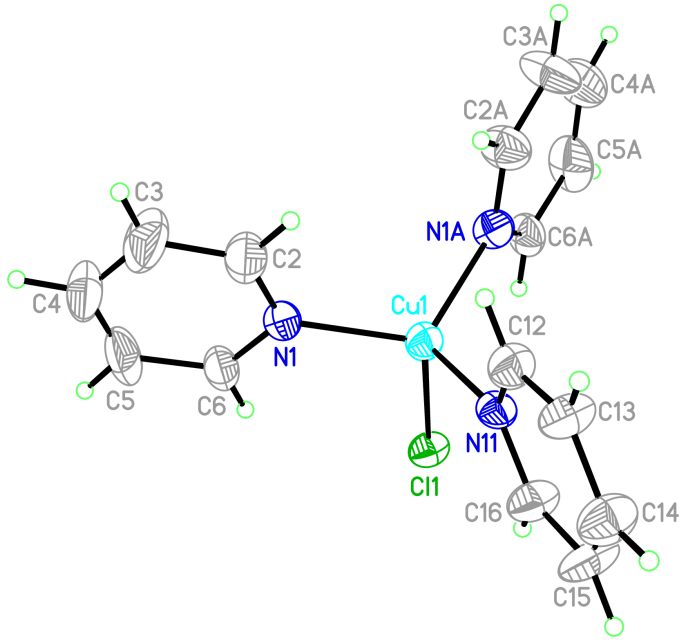


Figure 1
Perspective view of (I) with the atom numbering; displacement ellipsoids are at the 50% probability level.

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