metal-organic papers

{μ-1,4-Bis[2-(2-pyridyl)imidazol-1-yl]butane}-bis[dichlorocopper(II)]

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Key indicators

The title compound, $[Cu_2Cl_4(C_{20}H_{20}N_6)]$, is a dinuclear copper complex. The 1,4-bis[2-(2-pyridyl)imidazol-1-yl]butane ligand bridges two Cu^{II} ions, each in a slightly distorted tetrahedral geometry, consisting of two N atoms from the ligand and two Cl^- anions. The molecule is centrosymmetric.

Comment

In recent years, research into coordination polymers has been expanding rapidly because of the fascinating structural diversity of these compounds and their potential applications as functional materials (Batten & Robson, 1998; Moulton & Zaworotko, 2001). To date, much of the work has been focused on metal complexes with rigid ligands, such as 4,4′-bipyridine, pyrazine and their analogues (Carlucci *et al.*, 1994; Robinson & Zaworotko, 1995). We are interested in utilizing imidazole or substituted 2-(2-pyridyl)imidazole as ligands to prepare new coordination compounds. We report here the structure of the title compound, (I).

(I)
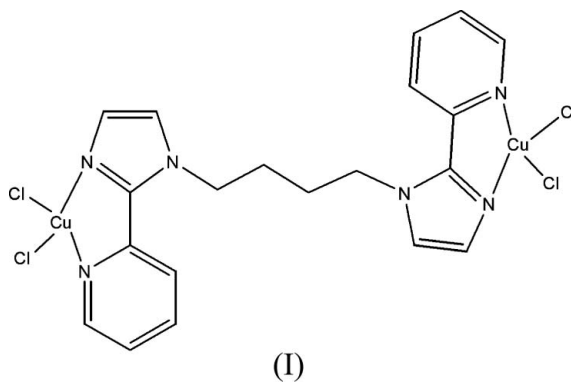
The asymmetric unit of (I) contains one Cu atom, two Cl^- anions and one half of the ligand, the molecule being centrosymmetric. The coordination environment of the Cu^{II} ion is defined by two Cl^- anions and two N atoms from the ligand in a slightly distorted tetrahedral geometry (Fig. 1). Each ligand bridges two Cu^{II} ions through its aromatic N atoms in a bidentate chelating mode. The Cu—N and Cu—Cl distances (Table 1) are similar to the values in other related compounds (Carranza *et al.*, 2003; Ellis *et al.*, 1999).

Experimental

A mixture of $CuCl_2{\cdot}2H_2O$ (0.034 g), 1,4-bis[2-(2-pyridyl)imidazol-1-yl]butane (0.0344 g) and water (10 ml) was stirred for 20 min in air. The mixture was then transferred to a 23 ml Teflon-lined reactor and kept at 438 K for 3 d under autogenous pressure, and then cooled to

room temperature at a rate of $5\,K\,h^{-1}$. Blue crystals of (I) were obtained. These were washed with distilled water and dried at room temperature (yield 60% based on Cu). Analysis, calculated for $C_{20}H_{20}Cl_4Cu_2N_6$: C 39.17, H 3.29, N 13.70%; found: C 39.35, H 3.19, N 13.52%.

Crystal data

$Cu_2Cl_4(C_{20}H_{20}N_6)]$	$Z = 2$
$M_r = 613.30$	$D_x = 1.798\ Mg\ m^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 4.696\ (5)$ Å	$\mu = 2.37\ mm^{-1}$
$b = 16.256\ (5)$ Å	$T = 293\ (2)$ K
$c = 15.000\ (5)$ Å	Block, blue
$\beta = 98.341\ (5)°$	$0.22 \times 0.11 \times 0.10$ mm
$V = 1133.0\ (13)$ Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5593 measured reflections
	2035 independent reflections
φ and ω scans	1619 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan ($SADABS$; Sheldrick, 1996)	$R_{int} = 0.066$
$T_{min} = 0.213$, $T_{max} = 0.298$ (expected range = 0.564–0.789)	$\theta_{max} = 25.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.054$	$\quad + 2.9756P]$
$wR(F^2) = 0.149$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
2035 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
145 parameters	$\Delta\rho_{min} = -0.89$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.973 (5)	Cu1—Cl1	2.212 (2)
Cu1—N1	2.061 (6)	Cu1—Cl2	2.245 (2)
N2—Cu1—N1	80.0 (2)	N2—Cu1—Cl2	91.90 (16)
N2—Cu1—Cl1	165.86 (18)	N1—Cu1—Cl2	168.47 (17)
N1—Cu1—Cl1	94.29 (16)	Cl1—Cu1—Cl2	95.44 (8)

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) and 0.97 Å (CH$_2$), and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: $SMART$ (Bruker, 1997); cell refinement: $SAINT$ (Bruker, 1999); data reduction: $SAINT$; program(s) used to solve
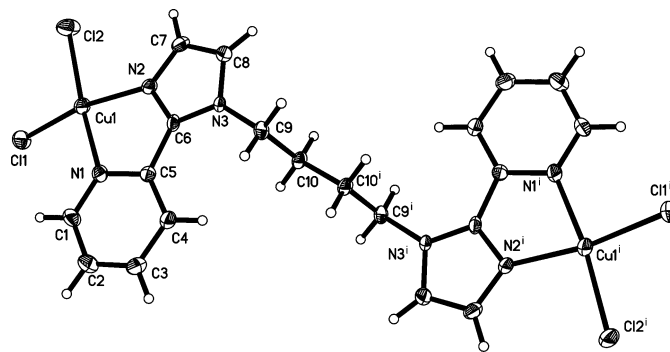

Figure 1
A view of the structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x$, $-y$, $1 - z$.]

structure: $SHELXS97$ (Sheldrick, 1997); program(s) used to refine structure: $SHELXL97$ (Sheldrick, 1997); molecular graphics: $SHELXTL$-$Plus$ (Sheldrick, 1990); software used to prepare material for publication: $SHELXL97$.

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