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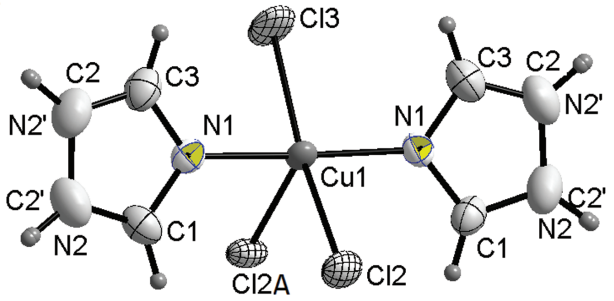
Crystal structure of *catena*-poly[chlorido-(μ_2-chlorido)-bis(imidazole-κ*N*)copper(II)] $C_6H_8Cl_2CuN_4$



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Abstract

$C_6H_8Cl_2CuN_4$, orthorhombic, *Cmc*2$_1$ (no. 26), $a = 12.915(3)$ Å, $b = 10.784(3)$ Å, $c = 6.8037(18)$ Å, $V = 947.6(4)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0368$, $wR_{ref}(F^2) = 0.0905$, $T = 293(2)$ K, Flack parameter: 0.05(4).

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A part of the crystal structure is shown in the figure. Tables 1 and 2 contain details of the crystal structure and measurement conditions and also a list of the atoms including atomic coordinates and displacement parameters.

Source of material

$CuCl_2{\cdot}2H_2O$ (0.0170 g, 0.10 mmol), imidazole (0.0136 g, 0.2 mmol) and water (17 mL) were placed in a 20.0 mL Teflon-lined stainless steel autoclave. It was heated at 383 K for 2 days. After cooling to room temperature, large blue block crystals of the title complex were obtained.

Experimental details

The hydrogen atoms were placed on calculated positions using a riding model (AFIX 43 or AFIX 137 option of the SHELX program [2, 3]).

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.42 × 0.33 × 0.28 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	2.82 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2218, 816, 0.034
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 724
$N(param)_{refined}$:	65
Programs:	Bruker programs [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.12666(8)	0.35629(17)	0.0268(3)
Cl2	0.5000	−0.08247(19)	0.2576(3)	0.0399(6)
Cl3	0.5000	0.34023(17)	0.3815(7)	0.0653(9)
N1	0.3479(3)	0.1274(5)	0.3449(14)	0.0309(10)
N2[a]	0.1869(5)	0.0648(7)	0.3651(14)	0.051(2)
H2[a]	0.1330	0.0204	0.3885	0.061*
C2′[b]	0.1869(5)	0.0648(7)	0.3651(14)	0.051(2)
H2′[b]	0.1286	0.0168	0.3904	0.061*
C1	0.2840(7)	0.0363(6)	0.4036(9)	0.039(2)
H1	0.3054	−0.0370	0.4633	0.046*
C2[a]	0.1898(7)	0.1830(8)	0.2779(11)	0.051(2)
H2A[a]	0.1333	0.2297	0.2365	0.061*
N2′[b]	0.1898(7)	0.1830(8)	0.2779(11)	0.051(2)
H2′A[b]	0.1376	0.2262	0.2396	0.061*
C3	0.2865(7)	0.2141(7)	0.2665(11)	0.0429(19)
H3	0.3103	0.2876	0.2108	0.052*

Occupancies: [a] = 0.44(8), [b] = 0.56(8).

Discussion

The coordination polymers are of current interest owing to their fascinating structures and their potential applications as magnetic, luminescent, catalytic and antibacterial materials [4–8]. Imidazole was studied extensively [9–11]. In addition, the counter ion Cl^- may be incorporated as an essential component leading to high structural complexity and interesting properties in some cases [12]. Therefore, we employed imidazole and copper chloride to construct the title compound.

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The asymmetric unit of the title structure contains one half of a Cu(II) ion, two half chlorine anions, and one neutral imidazole molecule. Each Cu (II) atom is five-coodinated by three chlorine anions and two imidazole N atoms. The Cu—N bond length is 1.966(4) Å, whereas the three different Cu—Cl bond lengths range from 2.310(2) to 2.772(2) Å. The coordination environment is a distorted trigonal bipyramid, since the Cl—Cu—Cl bond angles in the triangular plane are within the range of 92.27–167.68°. The C2 and N2 atoms in a imidazole molecule are disordered. The chlorine anions act as a μ_2-bridge linking the Cu(II) centers into infinite one-dimensional chains.

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