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catena-Poly[[copper(I)-μ-1,4-bis(imidazol-1-ylmethyl)benzene-κ^2N:N'] perchlorate]

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Key indicators

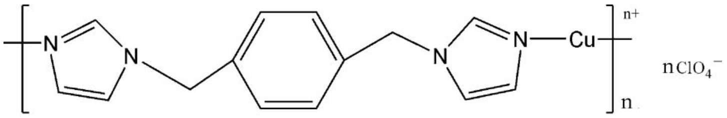
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.054
wR factor = 0.108
Data-to-parameter ratio = 14.2

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

The title compound, $\{[Cu(C_{14}H_{14}N_4)](ClO_4)\}_n$, has been synthesized by the hydrothermal method. The Cu^I atom, lying on a crystallographic twofold rotation axis, is two-coordinate with a linear geometry. The Cl atom also lies on a crystallographic twofold rotation axis. The structure contains one-dimensional chains and a three-dimensional supramolecular network is formed *via* π–π interactions.

Comment

Copper is an important metal ion in biological systems and it plays diverse roles in living organisms (Holm *et al.*, 1996; Kaim & Rall, 1996). The knowledge of the chemistry of well defined coordinatively unsaturated copper(I) complexes is necessary for the understanding of the reactivity of metals in various biological processes. Hydrothermal/solvothermal reactions under pressure have been used as a synthetic strategy to reduce various metal ions, including copper (Lu & Babb, 2002). The simultaneous reduction of Cu^{2+} to Cu^+ and the formation of a stable linear complex of copper(I) at ambient temperature are thus acomplished. Of these compounds, the two-coordinate copper(I) complexes with nitrogen ligands are scarcely represented in the literature and structurally characterized ones are even rarer (Le Clainche *et al.*, 2000; Liang *et al.*, 2002; Sanyal *et al.*, 1993; Sorell & Jameson, 1983).



(I)

Complex (I) consists of chains with alternate Cu^I ions and the bridging ligands. Copper(I) is coordinated by the N atom of each bix ligand unit [bix is 1,4-bis(imidazole-l-ylmethyl)-benzene]. The structure is shown in Fig. 1. The geometry of the cationic portion is a linear bix–Cu^I–bix unit. The Cu—N bond length is quite similar to that previously reported for two-coordinate copper(I) complexes with nitrogen donor ligands (Le Clainche *et al.*, 2000; Liang *et al.*, 2002) The dihedral angle between the two imidazole rings coordinated to Cu^I is 73.7 (3)°. All the bix ligands adopt *trans* conformations to form a one-dimensional chain along the *b* axis, the distance between the Cu ions along the chain being 14.026 (2) Å (Fig. 2). The plane of the imidazole ring is bent relative to the benzene ring, with a dihedral angle between the rings of 80.0 (2)°. It is noteworthy that one imidazole ring interacts with another imidazole ring and a benzene ring belonging to different adjacent chains [symmetry codes: (i) $-x, -y, 1-z$;

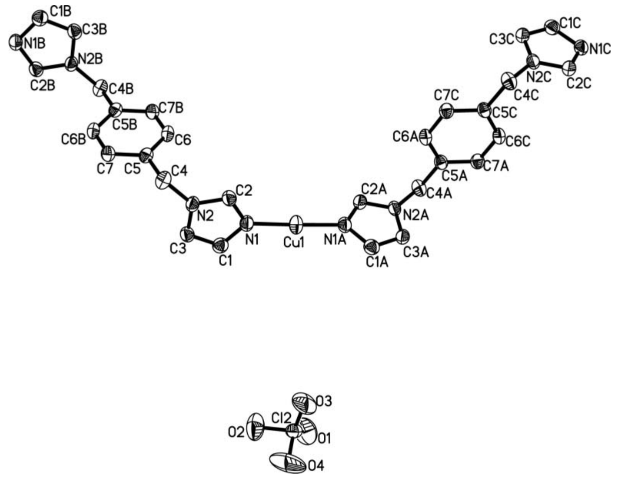


Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) $-x, y, \frac{3}{2} - z$; (B) $\frac{1}{2} - x, -\frac{1}{2} - y, 1 - z$; (C) $\frac{1}{2} + x, -\frac{1}{2} - y, \frac{1}{2} + z$.]

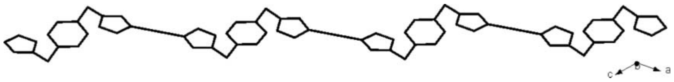


Figure 2
The one-dimensional chain of (I). H atoms have been omitted.

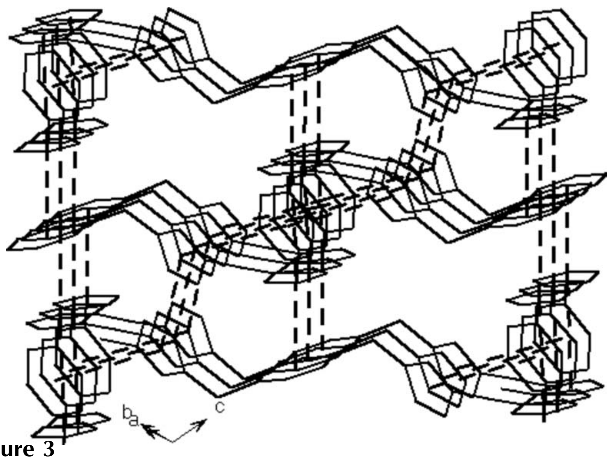


Figure 3
The three-dimensional supramolecular network formed by π–π stacking interactions (dashed lines).

(ii) $x, -y, \frac{1}{2} + z$] [centroid–centroid distances of 3.8408 (10) and 4.0142 (9) Å, respectively], indicating significant π–π interaction (Janiak, 2000). As a result, a three-dimensional supramolecular structure is formed (Fig. 3). Furthermore, packing along the c axis, the cavities form channels occupied by perchlorate anions (Fig. 4).

Experimental

Bix dihydrate was prepared as described by Hoskins *et al.* (1997). Compound (I) was hydrothermally synthesized under autogenous pressure. A mixture of $Cu(ClO_4)_2 \cdot 6H_2O$ (215.2 mg, 0.5 mmol), bix dihydrate (111.2 mg, 0.4 mmol), 2-butynedioic acid (57.1 mg, 0.4 mmol) and H_2O (10 ml) was sealed in a stainless steel reactor with a Teflon liner, which was heated to 433 K for three days. After slow cooling to room temperature, white prismatic crystals of (I) were obtained as a major phase by filtration; these were washed with distilled water and finally dried in air.

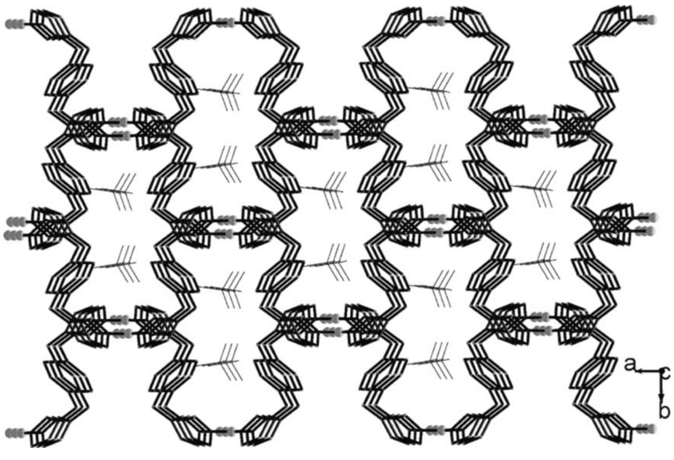


Figure 4
Packing diagram of (I), showing the channels occupied by perchlorate anions.

Crystal data

$[Cu(C_{14}H_{14}N_4)](ClO_4)$
$M_r = 401.28$
Monoclinic, $C2/c$
$a = 15.675$ (3) Å
$b = 11.791$ (3) Å
$c = 11.316$ (4) Å
$\beta = 130.913$ (9)°
$V = 1580.5$ (7) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.58$ mm^{-1}
$T = 173$ (2) K
0.30 × 0.25 × 0.12 mm

Data collection

Rigaku Mercury CCD detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
$T_{\min} = 0.684$, $T_{\max} = 0.827$
5981 measured reflections
1817 independent reflections
1447 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.108$
$S = 1.00$
1817 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.42$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.862 (3)	Cu1—N1$^{\rm i}$	1.862 (3)
N1—Cu1—N1$^{\rm i}$	178.6 (2)	C1—N1—Cu1	128.4 (3)
C2—N1—Cu1	125.8 (3)	N2—C4—C5	112.4 (3)

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

All H atoms bonded to carbon were placed at calculated positions, refined with isotropic displacement parameters, riding on their parent atoms with C—H = 0.95 and 0.99 Å for the aromatic CH and the CH_2 H atoms, respectively; $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$. The O atoms are disordered equally about the crystallographic twofold rotation axis passing through Cl.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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