Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[bis(acetonitrile)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-perchlorato-$\kappa^2O:O'$] perchlorate]

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Received 23 March 2007
Accepted 20 April 2007

Key indicators

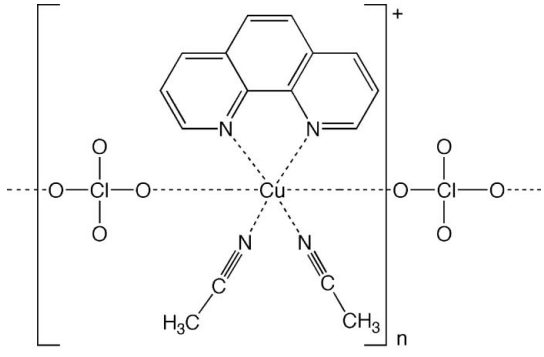
Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.073
Data-to-parameter ratio = 15.6

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

In the title complex $\{[Cu(ClO_4)(C_{12}H_8N_2)(CH_3CN)_2]ClO_4\}_n$, the Cu cations have an N_4O_2 octahedral coordination geometry, being bridged by the perchlorate, chelated by the phenanthroline heterocycles and also coordinated by two acetonitrile ligands. One perchlorate anion acts both as a bridging bis-monodentate ligand between a metal cation and its symmetry equivalents, forming an infinite one-dimensional chain in the *b*-axis direction, and as a counter-ion to balance the charge.

Comment

The perchlorate ion can be strongly bonded to metals in various bonding arrangements: monodentate, bridging or chelating bidentate, simply bridging or simultaneously bridging and chelating tridentate. It is mostly an assembling ligand (Pascal & Favier, 1998). Chelating ligands such as 1,10-phenanthroline have potential antitumour activity which may be increased through chelation to the copper ion (Farrell, 1989). Furthermore, copper(II) complexes of 1,10-phenanthroline and its derivatives have attracted much attention because they exhibit numerous biological activities such as antitumour, anti-Candida, antimycobacterial, and antimicrobial activity *etc* (Sigman & Perrin, 1993; Schaeffer *et al.*,1996; Mahadevan & Palaniandavar, 1998; Zoroddu *et al.*, 1996; Ranford & Sadler, 1993; Geraghty *et al.*, 1999; Saha *et al.*, 2004). In this context, the title complex, (I), of copper(II) with phenanthroline has been prepared and its crystal structure is reported here.



n(ClO_4)$^-$

(I)

Crystals of (I) are pseudo-merohedral twins [twinning by metric merohedry according to Nespolo & Ferraris (2000)] and belong to the non-centrosymmetric space group $P2_1$; the monoclinic angle is 90° within a few standard uncertainties. In

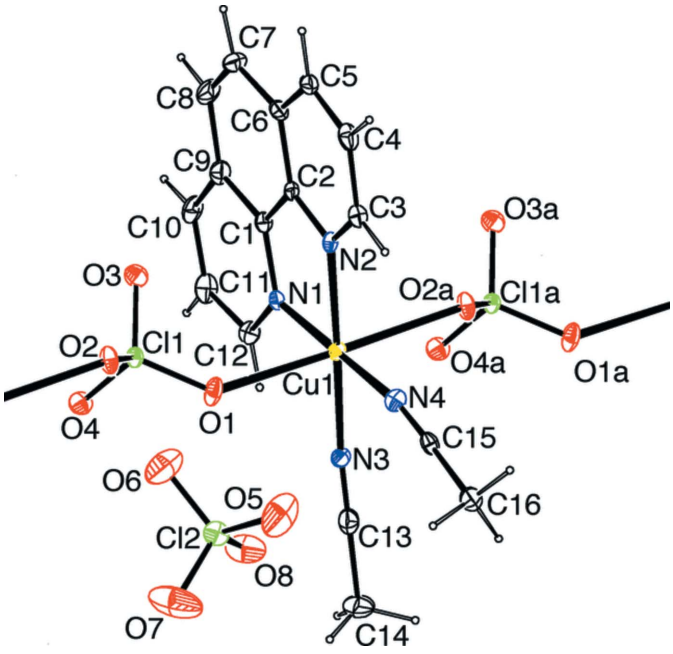


Figure 1
The asymmetric unit of (I), extended to show the complete coordination of Cu. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown with arbitrary radius. [Symmetry code: (a) $x, y-1, z$].

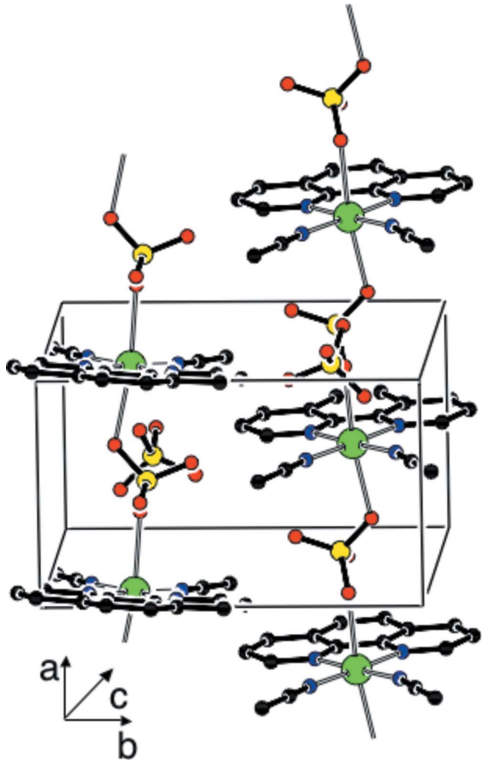


Figure 2
The arrangement of infinite chains in the crystal structure.

addition to pseudo-merohedral twinning, inversion twinning occurs. As no partially overlapped intensities were encountered, the twin refinement gave very satisfactory results and the derived geometrical data have reasonably low standard uncertainties. The metal atom is coordinated in a distorted octahedral fashion, typical for Jahn–Teller systems, by four equatorial N and two axial O atoms. Two of the N atoms belong to the phen ligand, the others to two coordinated acetonitrile molecules. The octahedral coordination is completed by two weakly bonded O atoms from a perchlorate anion and its symmetry equivalent. The bridging perchlorate forms an infinite one-dimensional chain along the *b* axis (Fig. 1). The second perchlorate acts as an uncoordinated counter-ion. Fig. 2 shows the arrangement of infinite chains in the crystal structure. Selected bond lengths and angles are given in Table 1.

Experimental

$Cu(ClO_4)_2\cdot 6H_2O$ (0.371 g, 1 mmol) and 1,10-phenanthroline (0.198 g, 1 mmol) were dissolved in acetonitrile (40 ml) and stirred under reflux to promote formation of the blue title complex. Single crystals suitable for X-ray diffraction were obtained by slow diffusion of benzene into an acetonitrile solution of the complex at room temperature.

Crystal data

$[Cu(ClO_4)(C_{12}H_8N_2)(C_2H_3N)_2]$-$ClO_4$
$M_r = 524.75$
Monoclinic, $P2_1$
$a = 11.578$ (3) Å
$b = 6.943$ (2) Å
$c = 12.542$ (4) Å
$\beta = 90.018$ (3)°
$V = 1008.2$ (5) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.40$ mm^{-1}
$T = 130$ (2) K
0.37 × 0.35 × 0.31 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.625$, $T_{max} = 0.670$
6720 measured reflections
4255 independent reflections
4195 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.073$
$S = 1.01$
4444 reflections
285 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}
Absolute structure: Flack (1983), 1546 Friedel pairs
Flack parameter: 0.39 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.989 (3)	Cl1—O1	1.451 (3)
Cu1—N3	1.983 (3)	Cl1—O2	1.457 (3)
Cu1—N4	1.997 (3)	O2—Cu1^{ii}	2.433 (3)
Cu1—N2	2.010 (3)	Cl2—O5	1.420 (4)
Cu1—O2^{i}	2.433 (3)	Cl2—O8	1.425 (4)
Cl1—O3	1.445 (2)	Cl2—O6	1.435 (3)
Cl1—O4	1.443 (3)	Cl2—O7	1.422 (4)
N1—Cu1—N3	94.89 (11)	N4—Cu1—N2	95.71 (12)
N1—Cu1—N4	178.08 (17)	N1—Cu1—O2^{i}	94.51 (13)
N3—Cu1—N4	86.62 (11)	N3—Cu1—O2^{i}	96.65 (13)
N1—Cu1—N2	82.77 (11)	N4—Cu1—O2^{i}	86.47 (14)
N3—Cu1—N2	177.63 (13)	N2—Cu1—O2^{i}	83.93 (12)

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

H atoms were placed in calculated positions and refined using a riding model, with C—H distances of 0.98 Å and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

MDS gratefully acknowledges financial support from OMNIASIG SA Romania.

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