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(Acetonitrile)bis(1,10-phenanthroline)copper(II) bis(perchlorate)

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Key indicators

Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.049
wR factor = 0.109
Data-to-parameter ratio = 16.1

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

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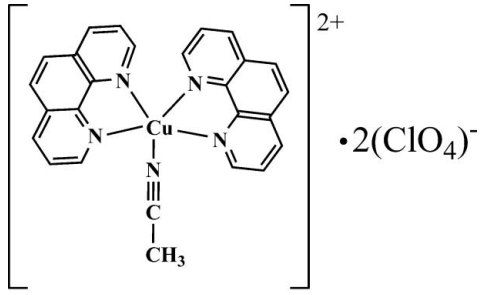
In the title complex, $[Cu(C_{12}H_8N_2)_2(CH_3CN)](ClO_4)_2$, the five-coordinate Cu^{II} ion has a distorted square-pyramidal coordination geometry composed of five N atoms, four from two bidentate chelating phenanthroline ligands and one from acetonitrile. The acetonitrile molecule and the Cu atom are situated on a crystallographic twofold rotation axis.

Comment

Transition metal complexes with potential biological activity are the subject of intensive ongoing research. Copper has been recognized as an essential trace element for living organisms since the late 1930s (Linder, 2001). 1,10-Phenanthroline (phen) is a chelating ligand with high affinity for metal ions (Calatayud *et al.*, 2003; Devereux *et al.*, 1999). Furthermore, Cu^{II} complexes of phen and its derivatives have attracted great attention because they exhibit numerous biological activities such as antitumor, anti-Candida, antimycobacterial and antimicrobial (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 Cu^{II} with phen has been prepared and its crystal structure is reported here.



(I)

The complex crystallizes in the centrosymmetric space group *C*2/*c*. The N atoms of two phen molecules, together with the acetonitrile N atom, form a distorted square-pyramidal geometry. Both the metal atom and the acetonitrile ligand are situated on a crystallographic twofold rotation axis. Selective bond lengths and angles are given in Table 1.

Experimental

$Cu(ClO_4)_2·6H_2O$ (0.371 g, 1 mmol) and phen (0.396 g, 2 mmol) were dissolved in acetonitrile (40 ml) and stirred under reflux to promote the complete formation of the title complex. Single crystals suitable for X-ray diffraction studies were obtained by slow diffusion from a acetonitrile/diisopropylether solution at room temperature.

Crystal data

$[Cu(C_{12}H_8N_2)_2(C_2H_3N)](ClO_4)_2$
$M_r = 663.90$
Monoclinic, $C2/c$
$a = 19.597$ (4) Å
$b = 8.820$ (2) Å
$c = 14.659$ (3) Å
$\beta = 96.618$ (4)°
$V = 2516.9$ (9) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.15$ mm^{-1}
$T = 130$ (2) K
0.32 × 0.16 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.711$, $T_{max} = 0.935$
12454 measured reflections
3125 independent reflections
2663 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.109$
$S = 1.14$
3125 reflections
194 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.9836 (19)	Cu1—N2	2.0984 (19)
Cu1—N3	2.048 (3)		
N1^{i}—Cu1—N1	176.16 (11)	N3—Cu1—N2	124.69 (5)
N1—Cu1—N3	91.92 (5)	N2^{i}—Cu1—N2	110.62 (10)
N1—Cu1—N2	81.55 (7)		

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

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.98 (CH_3) and 0.95 Å (CH), and with U_{iso}(H) = $1.2U_{eq}$(C) or $1.5U_{eq}$(methyl 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*.

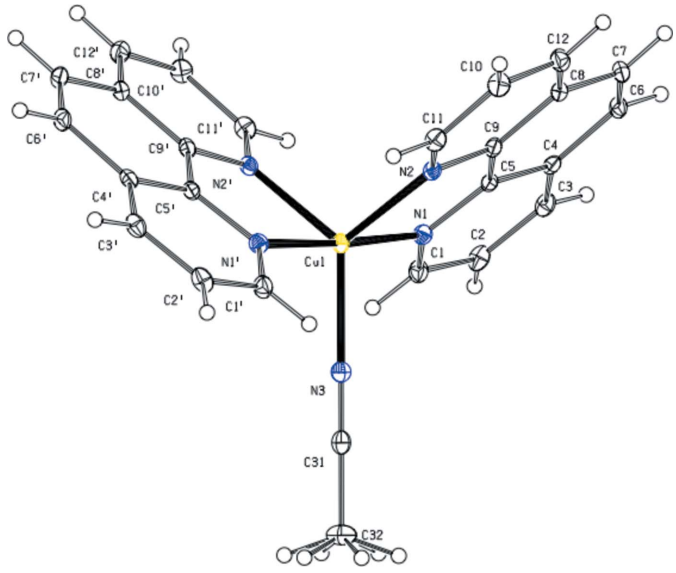


Figure 1
The molecular structure of the title complex, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by spheres of arbitrary radius. Both disorder components are shown.

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