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Chlorobis(1,10-phenanthroline)copper(II) hexafluoroantimonate(V)

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.062
Data-to-parameter ratio = 17.7

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

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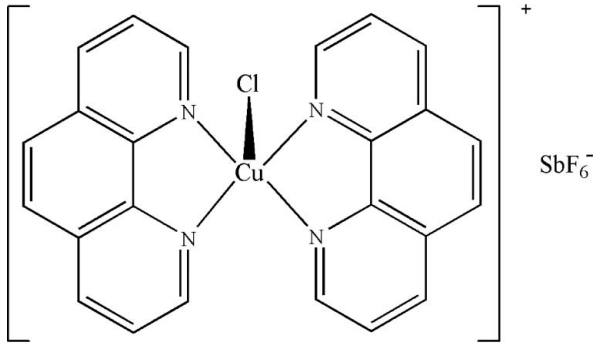
The title compound, $[CuCl(C_{12}H_8N_2)_2][SbF_6]$, was synthesized as green block-shaped crystals by the hydrothermal method. The crystal structure consists of discrete $[CuCl(phen)_2]^+$ (phen is 1,10-phenanthroline) and $[SbF_6]^-$ ions. The Cu atom is coordinated by four N atoms of two 1,10-phenanthroline ligands and by a Cl atom, with a slightly distorted trigonal–bipyramidal stereochemistry.

Comment

Recently, several groups have reported the synthesis of complexes with the $[Cu(phen)_2Cl]^+$ cation (Lu *et al.*, 2004; Zhang *et al.*, 2005). Complexes with the SbF_6^- ligand have attracted much attention, due to their rich structural chemistry, redox chemistry (Ponikvar *et al.*, 2004) and potential applications in doped organic semiconductors (Shen *et al.*, 2003). The hydrothermal synthesis of metal complexes has been developed rapidly in recent years, owing to its effectiveness, simplicity and environmental friendliness (Zhang, 2005), and many metal–organic compounds have been synthesized by this method. In this work, we obtained the title compound, $[CuCl(C_{12}H_8N_2)_2]SbF_6$, (I), by the hydrothermal method for the first time and we report its crystal structure here.



(I)

The crystal structure of (I) is built up of $[Cu(phen)_2Cl]^+$ cations and uncoordinated $[SbF_6]^-$ anions. The asymmetric unit of (I) is illustrated in Fig. 1, and selected geometric parameters are listed in Table 1. No significant differences in geometry were found from similar structures in the literature, *e.g.* Wei & Yang (2004) and Anderson (1975), as representative examples. The Cu atom is five-coordinated by four N atoms from two 1,10-phenanthroline ligands and one Cl^- atom, with a slightly distorted trigonal–bipyramidal stereochemistry. The crystal packing is governed by electrostatic forces.

Experimental

All chemicals were purchased from commercial sources and used without further purification. The title compound was synthesized by the hydrothermal method. Hydrothermal reactions were performed in 30 ml Teflon-lined stainless steel vessels under autogenous pressure with a filling capacity of 60%. A mixture of Sb_2O_3 (0.583 g), $CuCl_2{\cdot}2H_2O$ (0.341 g), 1,10-phenanthroline (0.396 g), H_2MoO_4 (0.396 g), $NaBiO_3{\cdot}2H_2O$ (1.264 g), HF (2 ml) and H_2O (18 ml) in a molar ratio of 1:1:1:1.2:2:57.5:500 was stirred under ambient conditions until it was homogeneous. The mixture was then sealed in a Parr Teflon-lined stainless steel vessel (30 ml) and heated to 453 K for 5 d. After slow cooling to room temperature, the solid product, containing green block-like single crystals, was collected by filtration, washed thoroughly with distilled water and dried at room temperature.

Crystal data

$[CuCl(C_{12}H_8N_2)_2][SbF_6]$	$Z = 4$
$M_r = 695.15$	$D_x = 1.935$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.4442$ (7) Å	$\mu = 2.21$ mm^{-1}
$b = 10.6556$ (5) Å	$T = 273$ (2) K
$c = 17.8305$ (9) Å	Block, green
$\beta = 110.9090$ (10)°	0.36 × 0.28 × 0.18 mm
$V = 2386.1$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	23500 measured reflections
φ and ω scans	5910 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)	5263 reflections with $I > 2\sigma(I)$
$T_{min} = 0.486$, $T_{max} = 0.672$	$R_{int} = 0.017$
	$\theta_{max} = 28.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 1.3196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.062$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.46$ e Å^{-3}
5910 reflections	
334 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.9898 (16)	Cu1—N1	2.1298 (16)
Cu1—N2	1.9981 (16)	Cu1—Cl1	2.3448 (6)
Cu1—N4	2.0726 (16)		
N3—Cu1—N2	177.33 (7)	N4—Cu1—N1	118.36 (6)
N3—Cu1—N4	81.77 (7)	N3—Cu1—Cl1	92.38 (5)
N2—Cu1—N4	97.85 (7)	N2—Cu1—Cl1	89.86 (5)
N3—Cu1—N1	97.12 (7)	N4—Cu1—Cl1	131.23 (5)
N2—Cu1—N1	80.72 (6)	N1—Cu1—Cl1	110.41 (5)

H were placed in idealized position, with Csp^2—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

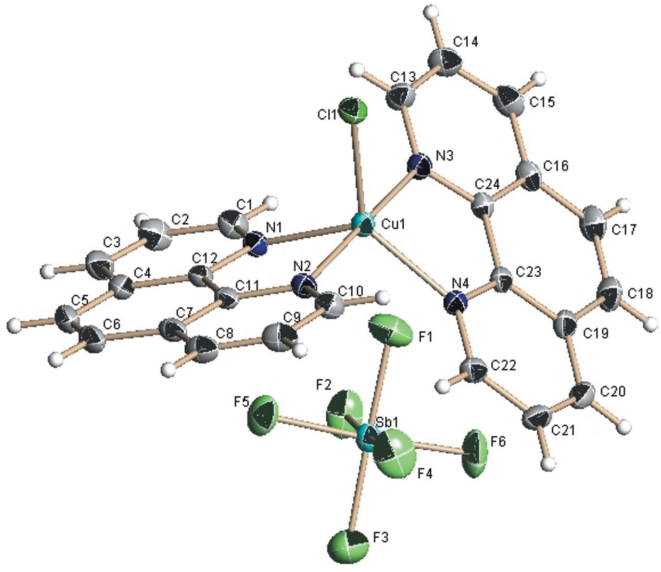


Figure 1
The molecular structure of (I), with the atom-labelling scheme, showing displacement ellipsoids at the 30% probability level.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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