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Formatobis(phenanthroline-κ^2N,N')copper(II) tetrafluoroborate

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Key indicators

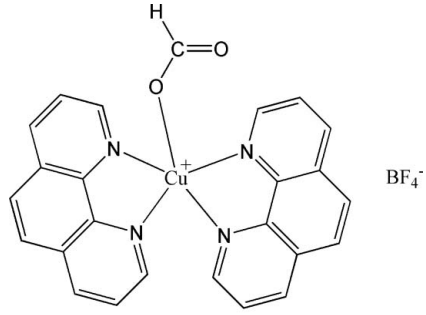
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.102
Data-to-parameter ratio = 13.0

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

The cation and the anion of the title complex, $[Cu(CHO_2)(C_{12}H_8N_2)_2]BF_4$ or $[Cu(phen)_2HCOO]BF_4$ (phen = 1,10-phenanthroline), both lie on crystallographic twofold rotation axes. The Cu^{II} ion is in a distorted square-pyramidal geometry, coordinated by four N atoms from two chelating phen ligands and one O atom from a formate ligand. A crystallographic twofold axis causes the O and H atoms of the formate ligand to be disordered.

Comment

Examples of copper formate complexes appeared in the literature as far back as 1969 and the majority of them contain bipyridyl heterocyclic ligands, *e.g.* 2,2′-bipyridine (Hathaway *et al.*, 1969; Fitzgerald & Hathaway, 1981), 2,4′-bipyridine (Czakis-Sulikowska *et al.*, 2006) and dipyridylamine (Youngme *et al.*, 1999, 2005, 2006). Although the structure of a binuclear copper(II) complex with 1,10-phenanthroline (phen) and formate ligands has been reported (Tokh *et al.*, 1990), the title crystal structure, (I), appears to be the first mononuclear complex of this type.



(I)

The cation and anion both lie on crystallographic twofold rotation axes. The structure of (I) is shown in Fig. 1, and selected bond lengths and angles are given in Table 1. The Cu^{II} ion is in a distorted square-pyramidal geometry, coordinated by four N atoms from two chelating phen ligands and one O atom from a formate ligand. The dihedral angle between the planes of the two phen ligands is 59.4 (4)°. The O and H atoms of the formate ligand are disordered over two sites. The disorder is imposed by a crystallographic twofold axis which runs through atoms Cu1 and C13.

Experimental

The title compound was prepared by adding an acetone solution (5 ml) of phenanthroline (0.198 g, 1 mmol) to an aqueous solution

(5 ml) of copper(II) formate (0.113 g, 0.5 mmol) and KBF_4 (0.063 g, 0.5 mmol). The mixture was stirred at room temperature for half an hour and allowed to stand for several days. Blue crystals suitable for *X* ray diffraction studies were collected and washed with a mixture of acetone and water (1:1).

Crystal data

$[Cu(CHO_2)(C_{12}H_8N_2)_2]BF_4$
M_r = 555.78
Monoclinic, $C2/c$
a = 16.790 (8) Å
b = 11.499 (5) Å
c = 12.524 (6) Å
β = 110.647 (7)°
V = 2262.6 (18) Å^3
Z = 4
D_x = 1.632 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 294 (2) K
Prism, blue
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART 1000 diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.778, T_{max} = 0.852
6279 measured reflections
2314 independent reflections
1655 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.01
2314 reflections
178 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.9129P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.985 (2)	Cu1—N1	2.115 (2)
Cu1—O1	2.041 (5)		
$N2^i$—Cu1—N2	179.25 (13)	$O1^i$—Cu1—$N1^i$	147.40 (17)
N2—Cu1—$O1^i$	90.2 (2)	N2—Cu1—N1	81.40 (9)
N2—Cu1—O1	89.1 (2)	O1—Cu1—N1	97.32 (17)
N2—Cu1—$N1^i$	99.01 (9)	$N1^i$—Cu1—N1	115.05 (12)

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

Atoms O1, O2 and H13*A* are disordered over two sites with equal occupancies. All H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and included in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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: *SHELXTL* (Bruker, 1997).

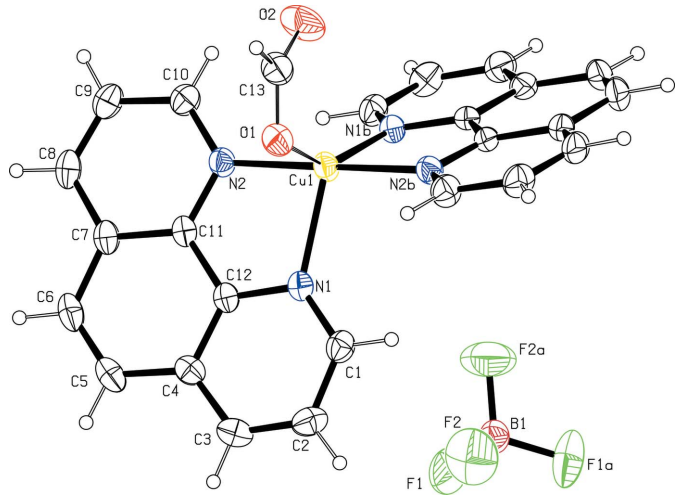


Figure 1
The structure of the cation and anion of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Only one component of the disordered formate ligand is shown. Atoms labeled with suffixes a and b are related by the symmetry codes $(1-x, y, \frac{3}{2}-z)$ and $(1-x, y, \frac{1}{2}-z)$, respectively.

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