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Key indicators

Single-crystal X-ray study
 $T = 299$ K
Mean $\sigma(\text{C}-\text{C}) = 0.009$ Å
Disorder in main residue
 R factor = 0.065
 wR factor = 0.201
Data-to-parameter ratio = 13.2

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

Bis[4-fluoro-*N*-(quinolin-8-yl)benzene-sulfonamidato- $\kappa^2\text{N},\text{N}'$]copper(II) dichloromethane hemisolvate

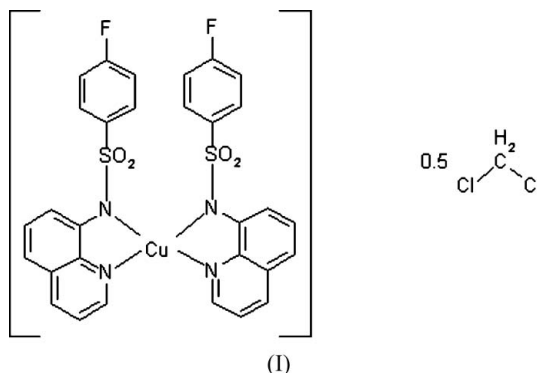
In the title compound, $[\text{Cu}(\text{C}_{30}\text{H}_{20}\text{F}_2\text{N}_4\text{O}_4\text{S}_2)] \cdot 0.5\text{CH}_2\text{Cl}_2$, the Cu^{II} atom is four-coordinated by the N atoms of quinoline and sulfonamide groups in a distorted tetrahedral geometry. The solvent molecule lies on a twofold axis. Intermolecular C—H \cdots O hydrogen bonds link the molecules into a three-dimensional network.

Received 30 May 2006

Accepted 10 June 2006

Comment

Some studies have shown that copper- and zinc-specific chelators have the ability to dissolve amyloid- β plaques, a hallmark of Alzheimer's disease (AD) (Lui *et al.*, 2005). Moreover, there is increasing evidence that interactions between amyloid- β (A β amyloid) and metal ions such as Cu and Zn may play a role in this transformation (Miller *et al.*, 2005; Cardoso *et al.*, 2005). We report here the structure of the title compound, (I), determined as part of our studies to investigate metal chelator probes for neuroprotection in neurodegenerative diseases (da Silva *et al.*, 2006a,b,c,d).



In (I), the Cu^{II} atom has a distorted tetrahedral geometry formed by the N atoms of the quinoline and the sulfonamide (Fig. 1). The dichloromethane molecule occupies a special position on a twofold axis. The Cu—N bonds involving quinoline N atoms are slightly longer than the Cu—N bonds involving the sulfonamide group. Selected bond distances and angles around the central Cu atom are given in Table 1. The quinoline-sulfonamidate ligates through the sulfonamide and the quinoline N atoms, forming a five-membered ring with the Cu atom. In the crystal structure, intermolecular C—H \cdots O hydrogen bonds link the molecules into a three-dimensional network (Fig. 2 and Table 2).

Experimental

The ligand 4-fluoro-*N*-(quinolin-8-yl)benzenesulfonamide was obtained according to the procedure previously described by da Silva

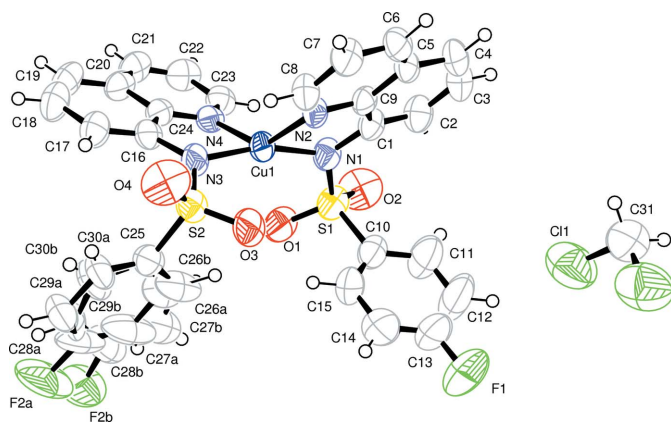


Figure 1

The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. Both disorder components of the benzene ring are shown. The unlabeled Cl atom is related to the corresponding labeled atom by the symmetry operation $(-x, y, \frac{1}{2} - z)$.

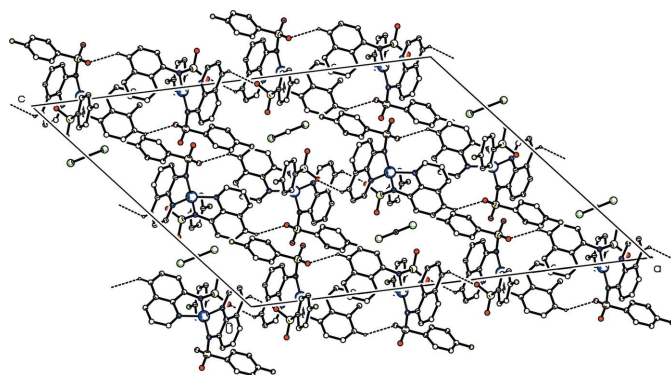


Figure 2

The molecular packing of (I), with hydrogen bonds shown as dashed lines. H atoms not involved in hydrogen bonding and the minor components of the disordered atoms have been omitted for clarity.

et al. (2005). Compound (I) was prepared according to the literature procedure of Macías *et al.* (2002). Single crystals of (I) suitable for X-ray data collection appeared after 2 d from a methanol solution (m.p. 551 K).

Crystal data

[Cu(C₃₀H₂₀F₂N₄O₄S₂)]·0.5CH₂Cl₂
 $M_r = 708.62$
 Monoclinic, $C2/c$
 $a = 32.228$ (3) Å
 $b = 10.405$ (1) Å
 $c = 23.817$ (2) Å
 $\beta = 130.70$ (1)°
 $V = 6054.9$ (13) Å³

$Z = 8$
 $D_x = 1.555$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.00$ mm⁻¹
 $T = 299$ (2) K
 Prism, black
 $0.40 \times 0.30 \times 0.30$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
 ω and φ scans
 Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2004)
 $T_{\min} = 0.690$, $T_{\max} = 0.753$

20303 measured reflections
 6074 independent reflections
 4591 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$
 $\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.065$
 $wR(F^2) = 0.201$
 $S = 1.09$
 6074 reflections
 460 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.1168P)^2 + 6.3418P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.028$$

$$\Delta\rho_{\text{max}} = 1.16 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.73 \text{ e } \text{Å}^{-3}$$

Table 1

Selected geometric parameters (Å, °).

Cu1—N3	1.923 (3)	Cu1—N2	2.005 (3)
Cu1—N1	1.923 (3)	Cu1—N4	2.007 (3)
N3—Cu1—N1	164.82 (15)	N3—Cu1—N4	82.33 (13)
N3—Cu1—N2	104.04 (13)	N1—Cu1—N4	102.70 (13)
N1—Cu1—N2	82.50 (12)	N2—Cu1—N4	135.84 (12)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C19—H19 ⁱ ···O1 ⁱ	0.93	2.58	3.363 (5)	143
C6—H6···O3 ⁱⁱ	0.93	2.51	3.209 (4)	132

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

The unique H atom of dichloromethane was located in a difference map and was refined with restrained geometry [$C-H = 0.98$ (2) Å]. The other H atoms were positioned with idealized geometry and refined using a riding model, with $C-H = 0.93$ Å. All H atoms were refined with isotropic displacement parameters (set at $1.2U_{\text{eq}}$ of the parent atom). Atoms C26–C30 of a benzene ring and F2 are disordered and were refined using a split model. The corresponding site-occupation factors were refined so that their sum was unity [0.69 (3) and 0.31 (3)]. Atoms in each disordered group were restrained to be coplanar and the corresponding bond distances in the disordered groups were restrained to be equal. The highest residual electron density peak is 0.09 Å from Cu1.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank Professor Dr Hartmut Fuess, FG Strukturforschung, FB Material- und Geowissenschaften, Technische Universität Darmstadt, for diffractometer time.

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