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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
Disorder in main residue
R factor = 0.057
wR factor = 0.124
Data-to-parameter ratio = 10.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Aqua(1,10-phenanthroline)[1,1,1-trifluoro-3-(2-thenoyl)acetonato]copper(II) (1,10-phenanthroline)(5-sulfatosalicylato)[1,1,1-trifluoro-3-(2-thenoyl)acetonato]cuprate(II)

The structure of the title complex is built up from a $[\text{Cu}(\text{C}_8\text{H}_4\text{F}_3\text{O}_2\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]^+$ cation and a $[\text{Cu}(\text{C}_8\text{H}_4\text{F}_3\text{O}_2\text{S})(\text{C}_7\text{H}_4\text{O}_6\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)]^-$ anion. Both the cation and anion contain Cu^{II} atoms having a square-pyramidal geometry. Hydrogen bonds between cations and anions generate a one-dimensional chain and stabilize the crystal packing.

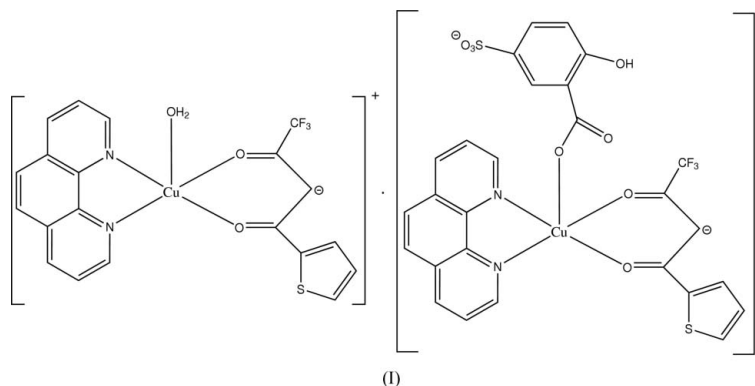
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Comment

The study of cation–anion 5-sulfosalicylate metal complexes has recently been greatly developed in our laboratory. These compounds exhibit interesting assembly topologies (Chen *et al.*, 2005; Fan & Zhu, 2005*a,b*; Fan *et al.*, 2005) in complexes containing 5-sulfosalicylate as the only anionic ligand. Here, we present the results of a combination of 5-sulfosalicylic acid and 2-thenoyltrifluoroacetone, giving the title cation–anion complex containing two different anionic ligands, (I).



In the structure of (I), both cation and anion contain a Cu^{II} atom with a square-pyramidal geometry, in which the basal plane is defined by two N atoms from one 1,10-phenanthroline ligand and two O atoms from one 2-thenoyltrifluoroacetone (ttf) ligand. The apical position in the cation is occupied by the water molecule, whereas in the anion it is occupied by the dianionic 5-sulfosalicylate ligand (Figs. 1 and 2). In both species, the Cu–N bond lengths are close to those of other carboxylate copper complexes containing N donor ligands (Lemoine *et al.*, 2002; Zhu & Kitagawa, 2002), and the Cu–O(ttf) bond lengths are also similar to those of ttf–copper complexes (Yang *et al.*, 2000, 2001).

It is worth noting that the coordinated water molecule in the cation forms hydrogen bonds with the phenolic atom O3 (symmetry code: $x, -1 + y, z$) and the sulfonate atom O6 (symmetry code: $-1 + x, -1 + y, z$) from two adjacent anions, thereby creating a hydrogen-bonded chain (Fig. 3 and Table 1).

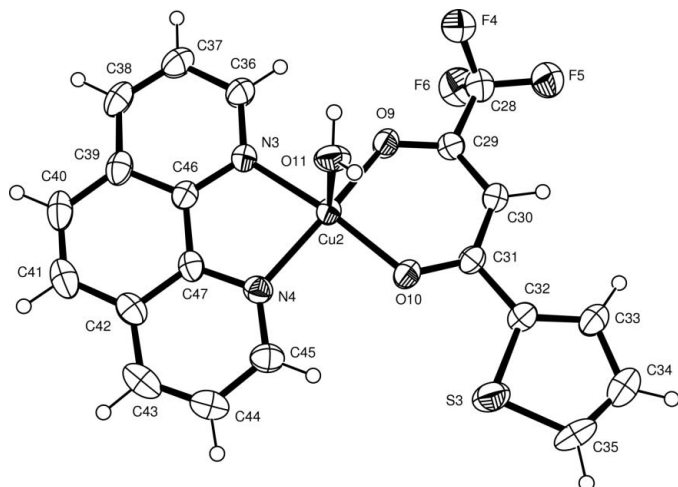


Figure 1
A view of the cation of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. The minor disorder component of the CF₃ group is not shown.

Experimental

A solution of CuSO₄·5H₂O (0.051 g, 0.20 mmol) and 5-sulfosalicylic acid dihydrate (0.051 g, 0.20 mmol) in water (15 ml) was added to a solution of 2-thenyltrifluoroacetone (0.044 g, 0.16 mmol) and 1,10-phenanthroline (0.040 g, 0.20 mmol) in *N,N*-dimethylformamide (10 ml) with stirring. The resulting solution was then set aside and allowed to evaporate. After three weeks, green block-shaped crystals of (I) were obtained and collected by suction filtration.

Crystal data

[Cu(C₈H₄F₃O₂S)(C₁₂H₈N₂)(H₂O)]·
[Cu(C₈H₄F₃O₂S)(C₇H₄O₆S)-
(C₁₂H₈N₂)]
M_r = 1164.01
Monoclinic, *P*2₁/*c*
a = 10.1963 (5) Å
b = 14.0035 (7) Å
c = 32.1357 (17) Å
β = 98.508 (1)°
V = 4538.0 (4) Å³

Z = 4
D_x = 1.704 Mg m⁻³
Mo *Kα* radiation
Cell parameters from 4606
reflections
θ = 2.4–25.5°
μ = 1.17 mm⁻¹
T = 295 (2) K
Block, green
0.17 × 0.10 × 0.08 mm

Data collection

Bruker SMART APEX area-
detector diffractometer
φ and *ω* scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2002)
T_{min} = 0.826, *T_{max}* = 0.912
23617 measured reflections

7984 independent reflections
6409 reflections with *I* > 2σ(*I*)
R_{int} = 0.041
θ_{max} = 25.0°
h = -11 → 12
k = -16 → 16
l = -35 → 38

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.057
wR (*F*²) = 0.124
S = 1.13
7984 reflections
746 parameters
H atoms treated by a mixture of
independent and constrained
refinement

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 1.9253P]$
where $P = (F_o^2 + 2F_c^2)/3$
(Δ/σ)_{max} = 0.003
Δρ_{max} = 0.44 e Å⁻³
Δρ_{min} = -0.34 e Å⁻³

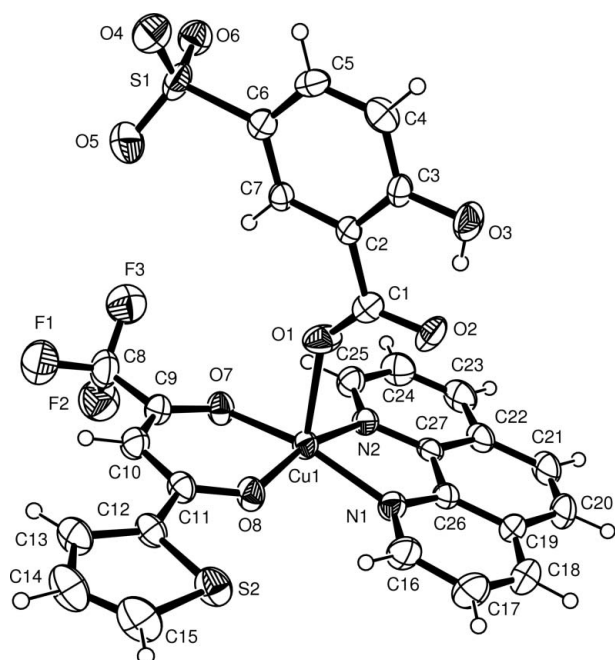


Figure 2
A view of the anion of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. The minor disorder components of the sulfonate and CF₃ groups are not shown.

Table 1

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| O3—H3···O2 | 0.82 | 1.73 | 2.466 (4) | 148 |
| O11—H11A···O3 ⁱ | 0.84 (1) | 2.11 (1) | 2.947 (4) | 172 (4) |
| O11—H11B···O6 ⁱⁱⁱ | 0.85 (1) | 1.87 (2) | 2.695 (16) | 166 (4) |
| O11—H11B···O6 ⁱⁱ | 0.85 (1) | 1.89 (2) | 2.735 (15) | 177 (5) |

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

The H atoms attached to C or O(hydroxyl) atoms were placed in idealized positions and refined as riding on their parent atoms, with C—H = 0.93 Å and O—H = 0.85 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(C,O). Water H atoms were located in difference Fourier maps and were refined with O—H and H···H restraints of 0.85 (1) and 1.39 (2) Å,

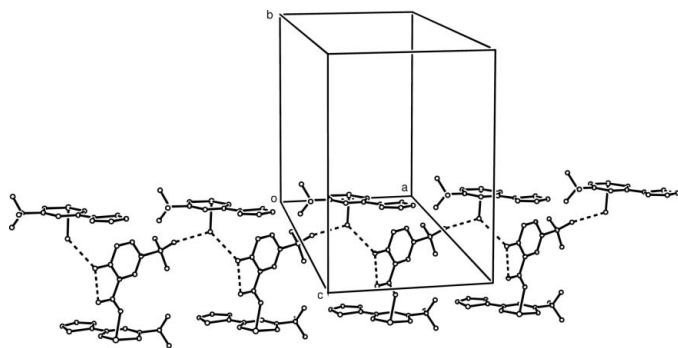


Figure 3
A view of the hydrogen-bonding chain of (I). Hydrogen bonds are drawn as dashed lines. H atoms, 1,10-phenanthroline ligands, and minor disorder components have been omitted for clarity.

respectively, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The sulfonate group and the CF_3 groups are disordered over two positions each and their occupancies are 0.513 (14):0.487 (14) for atoms O4/O5/O6 and O4'/O5'/O6', 0.57 (2):0.43 (2) for atoms F1/F2/F3 and F1'/F2'/F3', and 0.584 (19):0.416 (19) for atoms F4/F5/F6 and F4'/F5'/F6', respectively. The anisotropic displacement parameters for these disordered groups were refined using similarity restraints.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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