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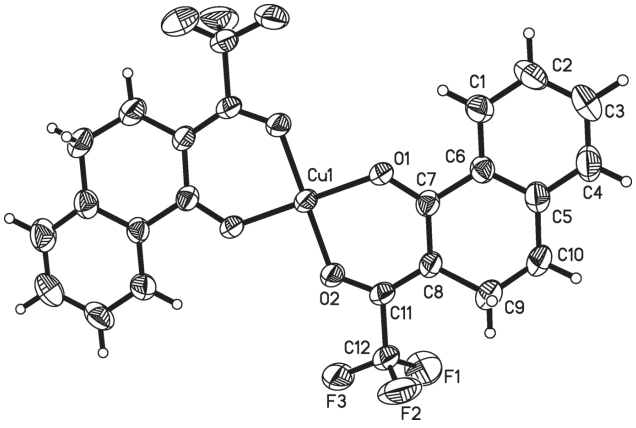
The crystal structure of bis(2-(2,2,2-trifluoroacetyl)-3,4-dihydronaphthalen-1-olato-κ^{2}O,O′)copper(II), $C_{24}H_{16}CuF_6O_4$



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Abstract

$C_{24}H_{16}CuF_6O_4$, triclinic, $P\bar{1}$ (no. 2), $a = 6.5651(7)$ Å, $b = 9.4145(10)$ Å, $c = 9.5014(11)$ Å, $\alpha = 68.668(10)°$, $\beta = 77.063(9)°$, $\gamma = 86.847(9)°$, $V = 532.91(11)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0596$, $wR_{ref}(F^2) = 0.1477$, $T = 293$ K.

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The molecular structure of the title compound is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title complex was synthesized according to the literature [3]. A mixture of 2-(2,2,2-trifluoroacetyl)-3,4-dihydronaphthalen-1(2*H*)-one (0.5 g, 2.06 mmol) and NaOH

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Table 1: Data collection and handling.

Crystal:	Brown block
Size:	0.28 × 0.28 × 0.24 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	11.1 cm^{-1}
Diffractometer, scan mode:	Xcalibur Eos, ω scans
$2\theta_{max}$, completeness:	54.2°, 97.1%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3749, 2280, 0.029
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1853
$N(param)_{refined}$:	160
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.0000	0.5000	0.5000	0.0382(3)
F1	0.9004(6)	1.0404(3)	0.1481(4)	0.0977(12)
F2	0.7123(5)	1.0129(3)	0.3704(5)	0.0925(11)
F3	1.0411(5)	0.9937(3)	0.3385(4)	0.0869(11)
O1	0.7899(4)	0.4722(3)	0.4032(3)	0.0406(6)
O2	0.9917(4)	0.7148(3)	0.4069(3)	0.0426(7)
C1	0.4939(7)	0.3588(5)	0.3087(5)	0.0468(10)
H1	0.5736	0.2916	0.3722	0.056*
C2	0.3482(7)	0.3024(5)	0.2576(5)	0.0563(12)
H2	0.3296	0.1977	0.2857	0.068*
C3	0.2292(7)	0.4031(6)	0.1637(6)	0.0611(13)
H3	0.1284	0.3659	0.1300	0.073*
C4	0.2597(7)	0.5574(6)	0.1204(6)	0.0578(12)
H4	0.1796	0.6236	0.0565	0.069*
C5	0.4066(6)	0.6170(5)	0.1694(5)	0.0441(10)
C6	0.5241(6)	0.5156(4)	0.2668(4)	0.0363(8)
C7	0.6794(5)	0.5728(4)	0.3259(4)	0.0350(8)
C8	0.6950(6)	0.7318(4)	0.2960(5)	0.0431(9)
C9	0.5131(8)	0.8283(5)	0.2372(6)	0.0625(13)
H9A	0.3959	0.8157	0.3240	0.075*
H9B	0.5566	0.9351	0.1923	0.075*
C10	0.4456(7)	0.7846(5)	0.1211(6)	0.0586(12)
H10A	0.5521	0.8185	0.0258	0.070*
H10B	0.3184	0.8370	0.0996	0.070*
C11	0.8542(6)	0.7872(4)	0.3359(5)	0.0388(9)
C12	0.8781(7)	0.9602(5)	0.2964(6)	0.0540(12)

(0.125 g, 2.06 mmol) in a methanol solvent (15 mL) was stirred for 0.5 h. A methanol solution (10 mL) of $CuCl_2{\cdot}2H_2O$ (0.175 g, 1.03 mmol) was added dropwise and allowed to stir for 12 h at room temperature. After removal of a part of the solvent by reduced pressure distillation, the precipitate formed and was filtered off, washed with hexane, and recrystallized. From a mixture of dichloromethane and hexane. Crystals were obtained in about three weeks. Brown crystal, yield: 0.9 g (80%).

Experimental details

All H atoms were placed in idealized positions [C—H = 0.93 (methyl), 0.97 (methylene) and 0.93 Å (aromatic)] and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.5U_{eq}$(methyl C) and $1.2U_{eq}$(methylene and aromatic C).

Comment

Copper complexes have shown great potential for applications in sensors, magnetic materials and catalysts in the past few years [4–6].

The structural analysis reveals that the complex crystallizes in the triclinic space group $P\bar{1}$. The asymmetric unit of the title crystal structure consists of one half of a Cu(II) and one organic ligand (*cf*. the figure). The complex is located on an inversion center. The coordination at the Cu(II) is planar. There are no classic hydrogen bonds found in the title crystal structure. All of the bond distances and bond angles are in normal range [7].

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