

Aqua(furan-2-carboxylato- κO)(furan-2-carboxylato- $\kappa^2 O, O'$)(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II) methanol hemisolvate

Yanfei Li, Junshan Sun,* Shanghua Feng, Ruigang Xue and Jun Wang

Department of Materials and Chemical Engineering, Taishan University, 271021 Taian, Shandong, People's Republic of China
Correspondence e-mail: xiangyz_2008@163.com

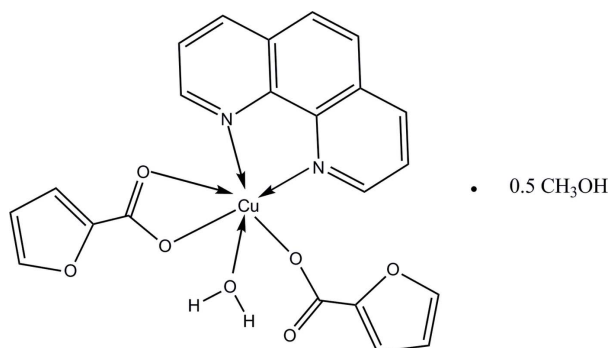
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(C-C) = 0.010$ Å; R factor = 0.055; wR factor = 0.169; data-to-parameter ratio = 12.5.

The asymmetric unit of the title compound, $[Cu(C_5H_3O_3)_2(C_{12}H_8N_2)_2(H_2O)] \cdot 0.5CH_3OH$, contains two Cu^{II} complex molecules and one methanol solvent molecule with the metal centres in strongly distorted octahedral coordination. The coordinated water molecule is involved in intermolecular $O-H \cdots O$ hydrogen bonding, which links the complex molecules into chains propagating along the c axis. Neighbouring chains interact further *via* $\pi-\pi$ interactions between the aromatic rings of 1,10-phenanthroline fragments [centroid-centroid distances = 3.726 (4) and 3.750 (4) Å].

Related literature

For the crystal structures of related carboxylate complexes with 1,10-phenanthroline, see: Ai *et al.* (2007); Li *et al.* (2007); Rodrigues (2004).



Experimental

Crystal data

$[Cu(C_5H_3O_3)_2(C_{12}H_8N_2)_2 \cdot (H_2O)] \cdot 0.5CH_3OH$
 $M_r = 499.93$
Tetragonal, $I4_1/a$
 $a = 34.129$ (17) Å
 $c = 14.450$ (6) Å

$V = 16831$ (14) Å³
 $Z = 32$
Mo $K\alpha$ radiation
 $\mu = 1.09$ mm⁻¹
 $T = 273$ K
 $0.28 \times 0.22 \times 0.17$ mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.750$, $T_{max} = 0.836$

43834 measured reflections
7448 independent reflections
4004 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.100$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.169$
 $S = 0.97$
7448 reflections
595 parameters

792 restraints
H-atom parameters constrained
 $\Delta\rho_{max} = 0.60$ e Å⁻³
 $\Delta\rho_{min} = -0.54$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O14—H14B \cdots O5 ⁱ	0.85	1.76	2.611 (8)	177
O14—H14A \cdots O8	0.85	2.07	2.634 (7)	124
O13—H13B \cdots O11	0.85	1.96	2.749 (7)	154
O13—H13A \cdots O2	0.85	1.87	2.708 (7)	169
O15—H15 \cdots O4	0.82	1.86	2.474 (17)	131

Symmetry code: (i) $x, y, z + 1$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2568).

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supplementary materials

Acta Cryst. (2009). E 65, m858 [doi:10.1107/S1371224109011111] [CODR 2009011111]

(I) $C_{15}H_{11}NO_4$ $M_r = 273.25$ $M_w = 273.25$ $Z = 4$ $a = 10.188(2)$ $b = 10.188(2)$ $c = 10.188(2)$ $\alpha = 90^\circ$ $\beta = 90^\circ$ $\gamma = 90^\circ$ $V = 1060.8(4)$ $D_x = 1.483$ $D_m = 1.483$ $F(000) = 408$ $\mu = 0.71$ $T = 293(2)$ $K = 0.018$ $R = 0.028$ $wR = 0.032$ $S = 1.0$ $h, k, l = 0 \rightarrow 10, 0 \rightarrow 10, 0 \rightarrow 10$

ORTEP diagram of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

Comment

Metal complexes with carboxylates are among the most investigated complexes in the field of coordination chemistry. In recent years, more and more attentions begin to be inclined to complexes with mixed-ligands such as 1,10-phenanthroline ligand (Ai *et al.*, 2007; Li *et al.*, 2007; Rodrigues, 2004). We selected a new carboxylic ligand with the cupric acetate in the presence of 1,10-phenanthroline co-ligand and obtained the title compound, (I).

In (I), the Cu centers exhibit a six-coordinated octahedron geometry with three O atoms from two carboxylic ligands [Cu—O 1.946 (4)–2.255 (4) Å] and one water molecule (Cu—O 1.937 (4) Å) and two N atoms [Cu—N 2.011 (4), 2.023 (4) Å] from 1,10-phenanthroline ligand. The crystal packing exhibits intra- and intermolecular O—H...O hydrogen bonds (Table 1). The latter link the complex molecules into a one-dimensional infinite chain structure.

Experimental

The reaction was carried out in 30 ml methanol solvent. furan-2-carboxylic acid (0.224 g, 2 mmol) and cupric acetate (0.199 g, 1 mmol) and 1,10-phenanthroline (0.180 g, 1 mmol) were mixed in the methanol solvent and stirred for 6 h. The resulting blue solution was filtered. The filtrate was placed for several days yielding blue crystals.

The yield is 76% and elemental analysis: calc. for $C_{15}H_{11}NO_4$: C 54.05, H 3.63, N 5.60; found: C 54.32, H 3.39, N 5.22. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

Refinement

C-bound H atoms were placed in idealized positions, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. O-bound H atoms were located in a difference Fourier map, but placed in idealized positions (O—H 0.82–0.85 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(O)$.

Figures

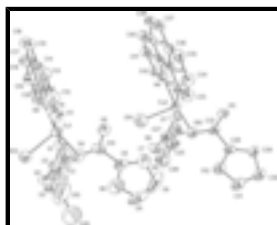


Fig. 1. The content of asymmetric unit of the title compound, with atomic numbering and 30% probability displacement ellipsoids.

