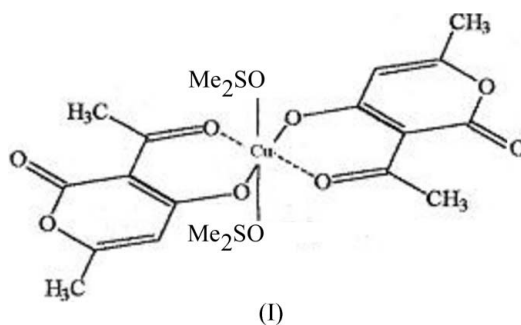


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bouacida_sofiane@yahoo.fr**Key indicators**Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.035
 wR factor = 0.093
Data-to-parameter ratio = 22.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**Bis[3-acetyl-6-methyl-2*H*-pyran-2,4(3*H*)-dionato]bis(dimethyl sulfoxide)copper(II)**

In the structure of the mononuclear title complex, $[\text{Cu}(\text{C}_8\text{H}_7\text{O}_4)_2(\text{C}_2\text{H}_6\text{OS})_2]$, the Cu^{II} atom lies on an inversion centre and has an octahedral coordination geometry of type MO_6 . The bidentate dehydroacetic acid (DHA) ligands occupy the equatorial plane of the complex in a *trans* configuration, and the dimethylsulfoxide (DMSO) ligands are weakly coordinated through their O atoms.

Comment

Mixed *d*-transition metal- β -diketone compounds were used extensively as starting materials in the early days of metallocene chemistry (Smith & Andersen, 1996). Dehydroacetic acid [DHA, 3-acetyl-6-methyl-2*H*-pyran-2,4(3*H*)-dione], a commercially available compound usually obtained through the auto-condensation of ethyl acetoacetate (Arndt *et al.*, 1936), has been shown to possess modest antifungal properties (Rao *et al.*, 1978). The importance of similar pyrones as potential fungicides is reinforced by the existence of several natural fungicides possessing structures analogous to 5,6-dihydrodehydroacetic acid, such as alternaric acid (Bartels-Keith, 1960), the podoblastins (Miyakado *et al.*, 1982) and lachnelluloic acid (Ayer *et al.*, 1988). Also, it has been shown that the complexes of DHA with zinc and with several other transition metal cations are fungistatic (Rao *et al.*, 1978). This has motivated our study of the structural characterization of complexes of dehydroacetic acid. The complex of DHA with Cu was previously reported by Casabò *et al.* (1987), but their characterization of the compound was based only on thermal and elemental analysis, and on IR and NMR spectroscopy. We present here the crystal structure determination of the title complex, $[\text{Cu}(\text{DHA})_2(\text{DMSO})_2]$, (I) (DMSO is dimethylsulfoxide).



The Cu^{II} atom of (I), located on an inversion centre, is surrounded by two DHA ligands occupying the equatorial plane. The two axial positions are occupied by O atoms of two dimethylsulfoxide molecules (Fig. 1). Complexes with related

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structures have been already reported with thiosemicarbazone 2-pyridineformamide (Castiñeiras *et al.*, 2000), and the thiosemicarbazone of acenaphthenequinone (Rodriguez-Argüelles *et al.*, 1997).

(I) is isostructural with the two complexes [Zn(DHA)₂(DMSO)₂] and [Cd(DHA)₂(DMSO)₂] (Zucolotto Chalaça *et al.*, 2002). The O5···Cu bond length for the DMSO in the copper complex, (I) (2.463 Å) is significantly longer than the Zn···O and Cd···O distances of 2.185 and 2.316 Å, respectively, found in the above complexes. This difference is due to the Jahn–Teller distortion for Cu^{II}.

The packing of (I) is stabilized by weak intermolecular C–H···O hydrogen bonds (Table 1) which form a three-dimensional network (Fig. 2).

Experimental

A solution of copper acetate monohydrate was added, with stirring, to a solution of dehydroacetic acid in absolute ethanol in a 1:2 stoichiometric ratio. The title complex precipitated after 1 h. The resulting precipitate of (I) was filtered off and recrystallized by slow evaporation of a dimethylsulfoxide solution.

Crystal data

[Cu(C₈H₇O₄)₂(C₂H₆OS)₂]
M_r = 554.07
 Monoclinic, *P*2₁/*n*
a = 11.580 (5) Å
b = 6.320 (5) Å
c = 16.424 (5) Å
 β = 92.27 (5)°
V = 1201.1 (11) Å³
Z = 2

D_x = 1.532 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 11050 reflections
 θ = 2.1–30.1°
 μ = 1.14 mm⁻¹
T = 294 K
 Prism, blue
 0.1 × 0.1 × 0.1 mm

Data collection

Nonius KappaCCD area-detector diffractometer
 φ scans, and ω scans with κ offsets
 Absorption correction: none
 11050 measured reflections
 3506 independent reflections

2651 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.040
 θ _{max} = 30.1°
h = -13 → 16
k = -6 → 8
l = -22 → 23

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.035
wR (*F*²) = 0.093
S = 1.05
 3506 reflections
 155 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.1877P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.37 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.39 \text{ e \AA}^{-3}$

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>
C2–H2···O5 ⁱ	0.93	2.55	3.475 (3)	170
C9–H9B···O3 ⁱⁱ	0.96	2.55	3.394 (3)	146
C10–H10B···O3 ⁱⁱ	0.96	2.53	3.379 (3)	147
C10–H10C···O1 ⁱ	0.96	2.58	3.486 (3)	158

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

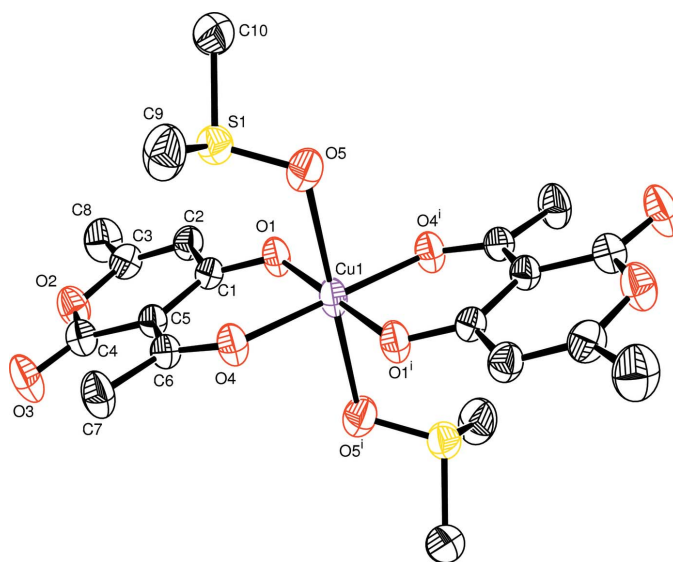


Figure 1
 A view of the title compound, with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $-x, -y, -z$.]

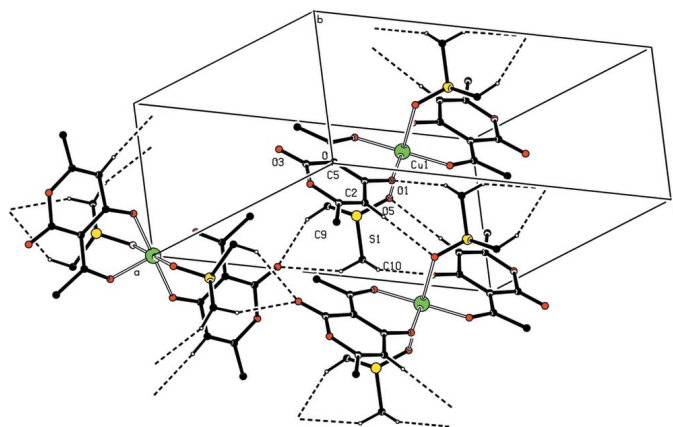


Figure 2
 A packing view, showing the C–H···O hydrogen-bond interactions (dashed lines).

All H atoms were located in difference Fourier maps but introduced in calculated positions and treated as riding on their parent C atoms, with C–H distances of 0.96 Å (CH₃) and 0.93 Å (C_{aromatic}) and with *U*_{iso}(H) = 1.2*U*_{eq}(C_{aromatic}) or 1.5*U*_{eq}(CH₃).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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