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## Key indicators

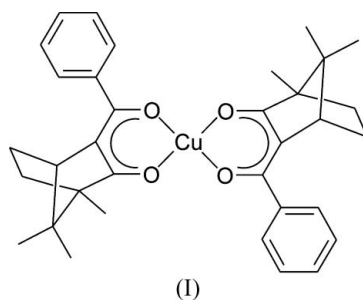
Single-crystal X-ray study  
 $T = 100$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.095  
Data-to-parameter ratio = 19.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*trans*-Bis[(+)-(1*R*,4*R*)-3-benzoylcamphorato- $\kappa^2\text{O},\text{O}'$ ]copper(II)

The title compound,  $[\text{Cu}(\text{C}_{17}\text{H}_{19}\text{O}_2)_2]$ , is the first example of a structurally characterized copper(II) camphorate. The  $\text{Cu}^{\text{II}}$  atom shows an approximately square-planar coordination by four O atoms of the two  $\eta^2$ -bonded benzoylcamphorate groups [average  $\text{Cu}-\text{O} = 1.9196$  (18) Å].

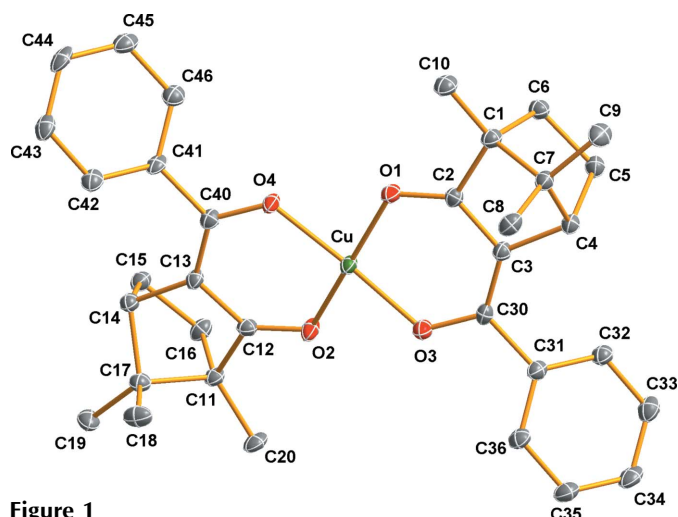
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## Comment

The  $\text{Ce}^{\text{III}}$ -catalysed  $\alpha$ -hydroxylation of  $\beta$ -diketo compounds with molecular oxygen is a mild atom-economic and environmentally friendly method for the synthesis of the biologically important  $\alpha$ -hydroxy- $\beta$ -dicarbonyl group (Christoffers & Werner, 2002; Christoffers *et al.*, 2003, 2004; Rössle *et al.*, 2004). The structure determination of the title compound, (I), was performed as part of a project on the preparation of well defined chiral metal camphorates (Niemeyer & Gan, 2005; Niemeyer *et al.*, 2005) which might be used for enantioselective oxidation reactions.



Crystals of (I) were obtained by the previously described reaction of copper(II) acetate with (1*R*,4*R*)-(+)-3-benzoylcamphor in methanol as the solvent (Pfeiffer *et al.*, 1938). The molecular structure of (I) shows monomeric units (Fig. 1), in which the  $\text{Cu}^{\text{II}}$  atom is bonded to four O atoms of two  $\eta^2$ -chelating camphorate groups. The resulting slightly distorted square planar environment is reflected by the small variation of the  $\text{Cu}-\text{O}$  distances and *cis/trans*-O-Cu-O angles (Table 1). Moreover, a *trans* arrangement of the camphoryl and phenyl substituents, with respect to the central  $\text{CuO}_4$  unit, is observed. The average  $\text{Cu}-\text{O}$  bond length of 1.9196 (18) Å is close to the mean values reported for other  $\text{Cu}^{\text{II}}$ - $\beta$ -diketonates (Gromilov & Baidina, 2004) [*e.g.*  $\text{Cu}(\text{PhCOCHCOCH}_3)_2$ : 1.923 (5) Å (Hon *et al.*, 1966) and  $\text{Cu}(\text{PhCOCHCOC}_4\text{H}_9)_2$ : 1.912 (3) Å (Baidina *et al.*, 1989)]. The six-membered metallacycles *A* (Cu/O1/O3/C2/C3/C30) and *B* (Cu/O2/O4/C12/C13/C40) are not planar. The conformation of rings *A* and *B* is best described as an envelope, with the Cu atom at the flap positions, 0.306 (3) and 0.355 (3) Å,


**Figure 1**

A drawing of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

respectively, from the mean planes through the other five atoms.

Although individual molecules of (I) possess almost non-crystallographic  $C_2$  symmetry, with the twofold axis perpendicular to the central  $\text{CuO}_4$  fragment, there are slightly but significant differences between the two benzoylcamphorato ligands. One concerns the different orientations of the phenyl substituents relative to the  $\text{CuO}_2\text{C}_3$  chelating rings. It is reflected by the torsion angles  $\text{C3—C30—C31—C32}$  [ $-46.1(3)^\circ$ ] and  $\text{C13—C40—C41—C42}$  [ $51.4(3)^\circ$ ].

Finally, the C—C bond-length pattern within the central six-membered  $\text{CuO}_2\text{C}_3$  rings is notable. It indicates a considerable degree of localized bonding and a higher single-bond character for the C—C bonds which are part of the camphorol substituents, thus minimizing ring strain within the bicyclic groups.

## Experimental

The title compound was prepared as described previously by Pfeiffer *et al.* (1938) from (1*R*,4*R*)-(+)-3-benzoylcamphor and  $\text{Cu}(\text{OAc})_2 \cdot (\text{H}_2\text{O})_x$ . Crystals of (I) suitable for X-ray study were grown from a saturated methanol solution (m.p. 513–515 K). Analysis calculated for  $\text{Cu}(\text{O}_2\text{C}_{17}\text{H}_{19}\text{O}_2)_2$ : C 71.12, H 6.67%; found: C 71.10, H 6.62%.

### Crystal data

$[\text{Cu}(\text{C}_{17}\text{H}_{19}\text{O}_2)_2]$	$Z = 2$
$M_r = 574.22$	$D_x = 1.356 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 11.5202(2) \text{ \AA}$	$\mu = 0.81 \text{ mm}^{-1}$
$b = 11.0788(2) \text{ \AA}$	$T = 100(2) \text{ K}$
$c = 12.1686(2) \text{ \AA}$	Plate, olive green
$\beta = 115.1241(9)^\circ$	$0.25 \times 0.20 \times 0.05 \text{ mm}$
$V = 1406.14(4) \text{ \AA}^3$	

### Data collection

Nonius Kappa CCD diffractometer	42111 measured reflections
$\varphi$ and $\omega$ scans	6888 independent reflections
Absorption correction: numerical	6311 reflections with $I > 2\sigma(I)$
( <i>X-SHAPE</i> ; Stoe, 1999)	$R_{\text{int}} = 0.092$
$T_{\text{min}} = 0.854$ , $T_{\text{max}} = 0.952$	$\theta_{\text{max}} = 28.3^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.095$   
 $S = 1.08$   
 6888 reflections  
 361 parameters  
 Only H-atom displacement parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.6865P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983),  
 3226 Friedel pairs  
 Flack parameter:  $-0.006(11)$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cu—O1	1.9269 (18)	C4—C7	1.558 (4)
Cu—O2	1.9305 (18)	C5—C6	1.555 (3)
Cu—O3	1.9102 (18)	C7—C8	1.523 (3)
Cu—O4	1.9106 (18)	C7—C9	1.530 (3)
O1—C2	1.270 (3)	C11—C12	1.518 (3)
O2—C12	1.265 (3)	C11—C16	1.571 (3)
O3—C30	1.299 (3)	C11—C17	1.563 (3)
O4—C40	1.296 (3)	C11—C20	1.511 (3)
C1—C2	1.518 (3)	C12—C13	1.427 (4)
C1—C6	1.570 (3)	C13—C14	1.527 (3)
C1—C7	1.566 (3)	C13—C40	1.378 (4)
C1—C10	1.514 (3)	C14—C15	1.544 (3)
C2—C3	1.410 (4)	C14—C17	1.557 (3)
C3—C4	1.526 (3)	C15—C16	1.551 (3)
C3—C30	1.380 (4)	C17—C18	1.529 (3)
C4—C5	1.555 (3)	C17—C19	1.532 (3)
O1—Cu—O2	172.57 (8)	O2—Cu—O4	93.98 (8)
O3—Cu—O4	174.52 (9)	Cu—O1—C2	121.47 (16)
O1—Cu—O3	94.51 (8)	Cu—O2—C12	121.56 (17)
O1—Cu—O4	85.07 (8)	Cu—O3—C30	125.18 (16)
O2—Cu—O3	87.14 (8)	Cu—O4—C40	125.86 (17)
C3—C30—C31—C32	$-46.1(3)$	C13—C40—C41—C42	$51.4(3)$

The H atoms were positioned geometrically at distances of 1.00 (CH), 0.99 (CH<sub>2</sub>), 0.98 (CH<sub>3</sub>) and 0.95 Å (Aryl-H) and refined in a riding-model approximation, including free rotation for methyl groups. The assigned  $U_{\text{iso}}$  was allowed to refine freely for groups of chemically equivalent atoms. The absolute configuration was assigned on the basis of the known absolute configuration of the starting material (1*R*,4*R*)-(+)-3-benzoylcamphor and confirmed by anomalous scattering effects.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *XDISK* (Siemens, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1998).

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