# metal-organic papers

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#### Key indicators

Single-crystal X-ray study T = 293 K Mean  $\sigma$ (C–C) = 0.005 Å Disorder in main residue R factor = 0.046 wR factor = 0.101 Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

# Tetrakis( $\mu_2$ -4-fluorobenzoato- $\kappa^2 O:O'$ )bis[(ethanol- $\kappa O$ )copper(II)](Cu—Cu)

The title complex,  $[Cu_2(C_7H_4FO_2)_4(C_2H_6O)_2]$ , has a dimeric structure with two  $Cu^{II}$  atoms coordinated by four 4-fluorobenzoate groups and two ethanol molecules. The crystal packing is stabilized by intermolecular  $O-H\cdots O$  hydrogen bonds.

#### Comment

Many dimeric copper(II) carboxylates,  $[Cu(RCOO)_2L]_2$ , have been studied (Kawata *et al.*, 1992; Yang *et al.*, 1997; Del Sesto *et al.*, 2000). We report here the crystal structure of a new dimeric copper(II) complex, *viz.* tetrakis( $\mu_2$ -4-fluorobenzoato- $\kappa^2 O:O'$ )bis[(ethanol- $\kappa O$ )copper(II)], (I) (Fig. 1).



The two Cu<sup>II</sup> atoms in (I) are surrounded by four 4fluorobenzoate groups and two ethanol molecules. The binuclear complex sits on a crystallographic centre of symmetry with a Cu–Cu distance of 2.5843 (8) Å. The O atom from the ethanol ligand has a significantly longer bond with the Cu atom [2.141 (2) Å] than the 4-fluorobenzoate O atoms [average 1.9534 (2) Å], in agreement with other dimeric copper(II) benzoates (Yang *et al.*, 1997). The four O atoms of the bridging 4-fluorobenzoate ligands in the basal plane form an almost perfect square. The octahedral environment about the Cu atom is completed by the other Cu atom of the dimer. The C–O distances in the complex are comparable to those in acetate-bridged dicopper complexes (Koman *et al.*, 1988).

The crystal packing is stabilized by intermolecular  $O-H\cdots O$  hydrogen bonds (Table 1).

### **Experimental**

© 2004 International Union of Crystallography Printed in Great Britain – all rights reserved The title compound was obtained by evaporation of a solution prepared by stirring 4-fluorobenzocopper(II) (1.03 g) in ethanol

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### Figure 1

View of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Only the major component of disordered atom C16 is shown.



#### Figure 2

The crystal packing of (I), showing the  $O-H\cdots O$  hydrogen-bonding interactions as dashed lines.

(10 ml) at 393 K for 12 h. Large blue crystals of (I) crystallized and were collected and washed twice with ethanol, then dried in a vacuum using CaCl<sub>2</sub> (yield: 60.8%). Elemental analysis found: C 49.36, H 3.82, F 9.65%; calculated for  $C_{32}H_{28}Cu_2F_4O_{10}$ : C 49.55, H 3.64, F 9.80%.

#### Crystal data

$Cu_2(C_7H_4FO_2)_4(C_2H_6O)_2$ ]	$D_x = 1.578 \text{ Mg m}^{-3}$
$M_r = 775.62$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3353
$a = 22.489 (4) \text{ Å}_{-}$	reflections
p = 6.6290 (10)  Å	$\theta = 4-27^{\circ}$
z = 22.027 (4)  Å	$\mu = 1.38 \text{ mm}^{-1}$
$\beta = 96.30 \ (3)^{\circ}$	T = 293 (2)  K
$V = 3263.9 (10) \text{ Å}^3$	Plate, blue
Z = 4	$0.20 \times 0.20 \times 0.02 \text{ mm}$

#### Data collection

Bruker SMART CCD area-detector diffractometer $\varphi$ and $\omega$ scans Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996) $T_{\min} = 0.770, T_{\max} = 0.973$ 7200 measured reflections <i>Refinement</i>	3353 independent reflections 2418 reflections with $I > 2\sigma(I)$ $R_{int} = 0.032$ $\theta_{max} = 26.5^{\circ}$ $h = -28 \rightarrow 28$ $k = -8 \rightarrow 4$ $l = -27 \rightarrow 27$
Refinement on $F^2$ $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.101$ S = 1.03 3353 reflections 217 parameters <b>Table 1</b>	H atoms constrained $w = 1/[\sigma^2(F_o^2) + (0.0412P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.002$ $\Delta\rho_{max} = 0.63 \text{ e } \text{Å}^{-3}$ $\Delta\rho_{min} = -0.41 \text{ e } \text{Å}^{-3}$
Hydrogen-bonding geometry (A, °).	

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D - \mathbf{H} \cdots A$
$O5-H1A\cdots O3^{i}$	0.90	2.28	3.089 (3)	149
$O5-H1A\cdots O1^{i}$	0.90	2.38	3.095 (4)	136

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

The methyl C atom of ethanol was found to be disordered and was split into two positions with occupancies of 0.59 (1) and 0.41 (1) and refined isotropically. H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with O–H and C–H distances of 0.90 and 0.96 Å, respectively. They were treated as riding atoms with  $U_{\rm iso}$  values fixed at 0.08 Å<sup>2</sup>.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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