metal-organic papers

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Key indicators

Single-crystal X-ray study T = 263 KMean σ (C–C) = 0.004 Å R factor = 0.033 wR factor = 0.079 Data-to-parameter ratio = 15.4

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

Tetra- μ -methacrylato- $\kappa^{8}O:O'$ -bis[(pyridine- κN)copper(II)]

In the title carboxylate-bridged binuclear copper complex, $[Cu_2\{CH_2C(CH_3)COO\}_4(C_5H_5N)_2]$, the Cu atoms are bridged by four bidentate methacrylate groups. The asymmetric unit consists of two half-molecules, each molecule having inversion symmetry. The Cu···Cu separations are 2.6181 (8) and 2.6442 (10) Å. All bond lengths and angles are normal.

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Comment

Copper complexes with organic acids and other donor ligands exist extensively in living things, playing an important role in a vast range of chemical and biochemical catalytic systems (King, 1994). Numerous papers dealing with copper carboxylate complexes have been published (Du *et al.*, 2004; Hu *et al.*, 2004; Li & Xiao, 2004). We present here a new binuclear copper α -methacrylate complex with pyridine, (I).



The crystal structure of (I) contains two independent binuclear cage complexes, each with inversion symmetry. In each dimer, two Cu atoms are bridged by four μ_2 - $O:O' \alpha$ methacrylate groups, forming a cage structure, and the pyridine ligands are bonded through their N atoms to the Cu atoms in the terminal positions (Fig. 1). All bond lengths and angles in (I) are normal (Table 1). The coordination geometry of each Cu atom is distorted square-based pyramidal. Atom Cu1 is displaced by 0.1960 (19) Å out of the mean plane of atoms O1, O2ⁱ, O3 and O4ⁱ towards the axial pyridine ligand (symmetry codes as in Table 1). Atom Cu2 is displaced by 0.2082 (19) Å out of the mean plane of atoms O5, O6ⁱⁱ, O7 and O8ⁱⁱ towards the axial pyridine ligand. The Cu1...Cu1ⁱ and Cu2...Cu2ⁱⁱ separations are 2.6181 (8) and 2.6442 (10) Å, respectively.

Experimental



Figure 1

View of the title molecule showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. All H atoms have been omitted for clarity. [Symmetry codes are as in Table 1.]

adjusted to 4.0 using 0.5 M NaOH. Pyridine (0.5 M, 2 ml) was added to the mixed solution with stirring. After filtration, the filtrate was allowed to stand at room temperature and single crystals suitable for X-ray work were obtained after one week. Analysis calculated: C 49.91, H 4.83, N 4.48%; found: C 49.69, H 4.74, N 4.51%. IR (KBr, v cm^{-1}): 699, 830, 936, 1036, 1214, 1243, 1369, 1415, 1597, 1650.

Crystal data

$[Cu_2(C_4H_5O_2)_4(C_5H_5N)_2]$	Z = 2
$M_r = 625.60$	$D_x = 1.482 \text{ Mg m}^{-3}$
Triclinic, P1	Mo $K\alpha$ radiation
a = 8.8214 (18) Å	Cell parameters from 7999
b = 9.936 (2) Å	reflections
c = 16.392(3) Å	$\theta = 1.3-27.4^{\circ}$
$\alpha = 100.57 (3)^{\circ}$	$\mu = 1.57 \text{ mm}^{-1}$
$\beta = 92.76 \ (3)^{\circ}$	T = 263 (2) K
$\gamma = 95.88 \ (3)^{\circ}$	Prism, green
V = 1401.6 (5) Å ³	$0.28 \times 0.25 \times 0.24$ mm
Data collection	
Rigaku R-AXIS RAPID	5342 independent reflection
diffractometer	4326 reflections with $I > 2a$
ω scans	$R_{\rm int} = 0.027$
Absorption correction: multi-scan	$\theta_{\rm max} = 25.8^{\circ}$
(ABSCOR: Higashi, 1995)	$h = -10 \rightarrow 10$

 $T_{\min} = 0.651, \ T_{\max} = 0.687$ 11 151 measured reflections

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.079$ S=1.035342 reflections 347 parameters H-atom parameters constrained

tions $2\sigma(I)$ $k = -12 \rightarrow 12$ $l = -20 \rightarrow 20$

 $w = 1/[\sigma^2(F_o^2) + (0.0412P)^2]$ + 0.4712P] where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\rm max} = 0.002$ $\Delta \rho_{\rm max} = 0.47 \ {\rm e} \ {\rm \mathring{A}}^{-3}$ $\Delta \rho_{\rm min} = -0.33 \ {\rm e} \ {\rm \AA}^{-3}$

Table 1		
Selected geometric parameters	(Å,	°).

Cu1-O1	1.9735 (19)	Cu2-O5	1.9757 (19)
Cu1-O2 ⁱ	1.9875 (19)	Cu2-O6 ⁱⁱ	1.9710 (19)
Cu1-O3	1.9672 (18)	Cu2-O7	1.9784 (18)
Cu1-O4 ⁱ	1.9794 (18)	Cu2-O8 ⁱⁱ	1.9717 (19)
Cu1-N1	2.147 (2)	Cu2-N2	2.165 (2)
$\Omega_1 - Cu_1 - \Omega_2^i$	168 63 (8)	$05 - Cu^2 - 07$	89 42 (9)
O1 - Cu1 - O3	87.96 (8)	O5-Cu2-N2	91.80 (8)
$O1-Cu1-O4^{i}$	89.68 (8)	O6 ⁱⁱ -Cu2-O5	167.97 (8)
O1-Cu1-N1	101.92 (8)	O6 ⁱⁱ -Cu2-O7	88.84 (8)
O2 ⁱ -Cu1-N1	89.42 (8)	O6 ⁱⁱ -Cu2-N2	100.23 (8)
$O3-Cu1-O2^i$	91.55 (8)	O7-Cu2-N2	97.60 (8)
$O3-Cu1-O4^{i}$	168.53 (8)	O8 ⁱⁱ -Cu2-O5	89.88 (9)
O3-Cu1-N1	97.32 (8)	O8 ⁱⁱ -Cu2-O6 ⁱⁱ	89.31 (9)
$O4^i - Cu1 - O2^i$	88.55 (8)	$O8^{ii}$ -Cu2-O7	167.79 (7)
$O4^i$ -Cu1-N1	94.15 (8)	O8 ⁱⁱ -Cu2-N2	94.61 (8)

Symmetry codes: (i) 1 - x, 2 - y, 1 - z; (ii) 1 - x, 1 - y, -z.

All H atoms were initially located in a difference Fourier map. All methyl H atoms were then constrained to an ideal geometry, with C-H distances of 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C-C bond. The =CH₂ H atoms and aromatic H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C-H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: RAPID-AUTO (Rigaku, 1998); cell refinement: RAPID-AUTO; data reduction: CrystalStructure (Rigaku/MSC, 2002); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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