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Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.043
 wR factor = 0.114
Data-to-parameter ratio = 18.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Tetrakis(μ -phenylacetato- $\kappa^2\text{O}:\text{O}'$)bis[$(N,N$ -dimethylformamide- κO)copper(II)]

In the crystal structure of the title complex, $[\text{Cu}_2(\text{C}_8\text{H}_7\text{O}_2)_4(\text{C}_3\text{H}_7\text{NO})_2]$, two independent dinuclear Cu^{II} complex molecules, bridged by phenylacetate anions, are located on inversion centres. The $\text{Cu}\cdots\text{Cu}$ separations of 2.6414 (8) and 2.6261 (8) \AA suggest no bonding between the Cu atoms. The Cu^{II} ions exist in a square-pyramidal coordination environment, defined by one N,N -dimethylformamide and four phenylacetate O atoms.

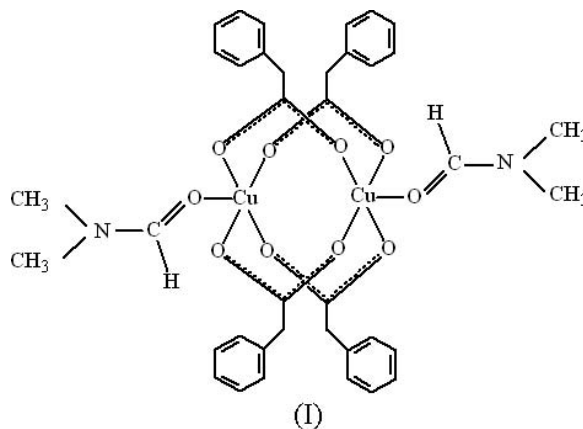
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Comment

The coordination chemistry of centrosymmetric dinuclear Cu^{II} complexes bridged by carboxylates has been widely investigated (Ivanov *et al.*, 1976; Kato & Muto, 1988). In order to explore further the coordination behaviour of the Cu^{II} ion, the title complex, (I), incorporating phenylacetate has been prepared and its crystal structure is reported here.



Two independent molecules of (I) are located on inversion centres. Similar bond distances and angles are observed in these molecules (Table 1). The Cu^{II} ions display approximate square-pyramidal coordination geometry, defined by four carboxylate O atoms of four phenylacetate ligands forming the basal plane and by the O atom of the N,N -dimethylformamide (DMF) molecule occupying the axial position. The $\text{Cu}-\text{O}(\text{DMF})$ bond distances are significantly longer than the $\text{Cu}-\text{O}(\text{carboxylate})$ bond distances (Table 1). Within the dinuclear complex molecules, the $\text{Cu}\cdots\text{Cu}$ separations are 2.6414 (8) and 2.6261 (8) \AA , comparable with the value of 2.641 (1) \AA found in $[\text{Cu}_2(\text{CH}_3\text{CO}_2)_4(\text{pyridine})_2]$ (Uekusa *et al.*, 1989).

Experimental

$\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (2 mmol) was dissolved in a dimethylformamide solution (10 ml) of phenylacetic acid (6 mmol). The mixture was

filtered and allowed to stand at room temperature. Blue prismatic crystals of (I) were obtained after 7 d. Analysis, calculated for $C_{38}H_{42}N_2O_{10}Cu_2$: C 56.08, H 5.20, N 3.44%; found: C 56.11, H 5.21, N 3.56%.

Crystal data

$[Cu_2(C_8H_7O_2)_4(C_3H_7NO)_2]$
 $M_r = 813.84$
 Monoclinic, $P2_1/n$
 $a = 14.291$ (3) Å
 $b = 17.569$ (4) Å
 $c = 15.791$ (3) Å
 $\beta = 107.95$ (3)°
 $V = 3771.7$ (15) Å³
 $Z = 4$

$D_x = 1.433$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 34692 reflections
 $\theta = 3.0$ – 27.5°
 $\mu = 1.19$ mm⁻¹
 $T = 295$ (2) K
 Prism, blue
 $0.42 \times 0.31 \times 0.18$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{min} = 0.636$, $T_{max} = 0.815$
 35794 measured reflections

8596 independent reflections
 6302 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.058$
 $\theta_{max} = 27.5^\circ$
 $h = -17 \rightarrow 18$
 $k = -22 \rightarrow 22$
 $l = -20 \rightarrow 20$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.114$
 $S = 1.05$
 8596 reflections
 473 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.51$ e Å⁻³
 $\Delta\rho_{min} = -0.29$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9611 (19)	Cu2—O5	1.9583 (16)
Cu1—O2 ⁱ	1.9802 (19)	Cu2—O6 ⁱⁱ	1.9719 (16)
Cu1—O3	1.9756 (17)	Cu2—O7	1.9529 (16)
Cu1—O4 ⁱ	1.9546 (17)	Cu2—O8 ⁱⁱ	1.9791 (17)
Cu1—O9	2.1907 (17)	Cu2—O10	2.1609 (17)
Cu1—Cu1 ⁱ	2.6414 (8)	Cu2—Cu2 ⁱⁱ	2.6261 (8)
O4 ⁱ —Cu1—O1	88.65 (8)	O7—Cu2—O5	88.94 (8)
O4 ⁱ —Cu1—O3	167.94 (7)	O7—Cu2—O6 ⁱⁱ	89.56 (8)
O1—Cu1—O3	90.33 (8)	O5—Cu2—O6 ⁱⁱ	168.28 (7)
O4 ⁱ —Cu1—O2 ⁱ	89.64 (8)	O7—Cu2—O8 ⁱⁱ	168.51 (7)
O1—Cu1—O2 ⁱ	168.10 (8)	O5—Cu2—O8 ⁱⁱ	89.94 (9)
O3—Cu1—O2 ⁱ	88.88 (8)	O6 ⁱⁱ —Cu2—O8 ⁱⁱ	89.22 (8)
O4 ⁱ —Cu1—O9	101.21 (7)	O7—Cu2—O10	98.75 (7)
O1—Cu1—O9	101.28 (7)	O5—Cu2—O10	101.03 (7)
O3—Cu1—O9	90.78 (7)	O6 ⁱⁱ —Cu2—O10	90.69 (7)
O2 ⁱ —Cu1—O9	90.60 (7)	O8 ⁱⁱ —Cu2—O10	92.69 (7)

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

The methyl groups were allowed to rotate to fit the electron density [$C-H = 0.96$ Å and $U_{iso}(H) = 1.5U_{eq}(C)$]. The other H atoms were positioned geometrically (aromatic $C-H = 0.93$ Å and aliphatic $C-H = 0.97$ Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$].

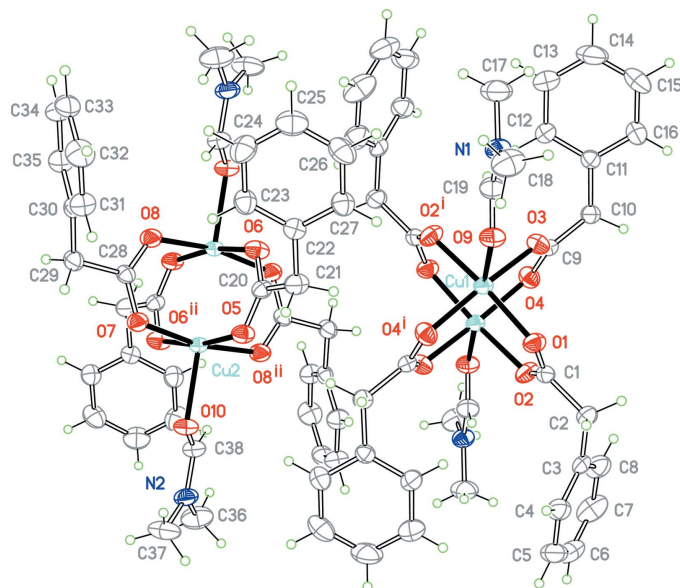


Figure 1

The two independent molecules of (I), with 30% probability displacement ellipsoids. (For symmetry codes, see Table 1).

Data collection: *RAPID AUTO* (Rigaku, 1998); cell refinement: *RAPID AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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