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Tetrakis(μ-2-anilinobenzoato-κ²O:O′)bis-[(*N*,*N*-dimethylformamide-κO)copper(II)]

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Key indicators

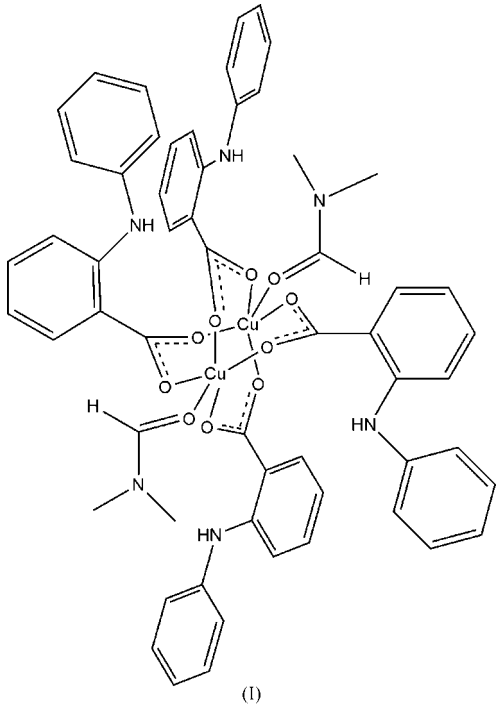
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.108
Data-to-parameter ratio = 14.8

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

The title compound, $[Cu_2(C_{13}H_{10}NO_2)_4(C_3H_7NO)_2]$, is a centrosymmetric paddle-wheel dinuclear complex. The two copper ions are bridged by four caboxylate groups, with a Cu···Cu separation of 2.6168 (7) Å. Additionally, each copper ion is coordinated by one *N*,*N*-dimethylformamide molecule.

Comment

The synthesis of dinuclear and polynuclear complexes for new magnetic materials is still a challenging area of research for inorganic chemists (Kahn *et al.*, 1993; Willet *et al.*, 1985). Among dinuclear species, tetracarboxylate-bridged dimeric copper(II) complexes have been investigated extensively over the past 50 years (Huang *et al.*, 2002; Reyes-Ortega *et al.*, 2005) since the first crystal structure of copper acetate monohydrate was reported by van Niekerk & Schoening (1953). In order to extend the study of this type of dinuclear complex, we report here a new centrosymmetric dinuclear copper complex, (I) (Fig. 1).



(I)

In (I), the two copper(II) cations are bridged by four carboxylate groups of four 2-anilinobenzoates in the *syn–syn* mode, with a Cu···Cu separation of 2.6168 (7) Å. Each copper(II) is also coordinated by an *N*,*N*-dimethylformamide molecule. Thus each copper(II) cation displays an approximate square-pyramidal geometry. The $Cu-O_{carboxylate}$ bond lengths in the basal plane range from 1.961 (2) to 1.969 (2) Å, while the Cu—O bond length in the apical position is

2.148 (2) Å. This dinuclear complex is stabilized by intramolecular hydrogen bonds (Fig. 1 and Table 1). In each anionic ligand, the H atom of the secondary amine participates in hydrogen bonds to the uncoordinated carboxylate O atom in the same ligand. In the crystal packing, each dinuclear subunit interacts with four adjacent dinuclear subunits through offset π–π interactions, with a centroid–centroid distance of 4.3947 (1) Å and a dihedral angle of 24.40 (19)° (Fig. 2).

Experimental

2-Anilinobenzoic acid (2 mmol) and triethylamine (2 mmol) were dissolved in *N*,*N*-dimethylformamide (6 ml). The mixture was heated in a water bath with stirring for 20 min. Copper(II) nitrate (1 mmol) was added to the solution. The mixture was stirred for 10 min at 353 K. The resulting solution was filtered and the filtrate left to stand in air for about 20 h, after which crystals suitable for X-ray analysis were formed. Analysis calculated for $C_{58}H_{54}Cu_2N_6O_{10}$: C 62.08, H 4.85, N 7.49%; found: C 62.05, H 4.89, N 7.51%.

Crystal data

$[Cu_2(C_{13}H_{10}NO_2)_4(C_3H_7NO)_2]$
M_r = 1122.15
Monoclinic, $P2_1/n$
a = 14.1539 (3) Å
b = 11.0440 (2) Å
c = 17.8517 (1) Å
β = 104.2397 (4)°
V = 2704.76 (8) Å^3
Z = 2
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 298 (2) K
Prism, blue
0.20 × 0.15 × 0.12 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.868, T_{max} = 0.903
14382 measured reflections
5115 independent reflections
3784 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 25.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.108
S = 1.11
5115 reflections
345 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 2.0208P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	2.02	2.638 (3)	128
N2—H2···O3	0.86	2.01	2.644 (3)	129

The H atoms of amine groups were located in difference Fourier maps, then positioned geometrically and refined as riding on their parent atoms, U_{iso}(H) = 1.2U_{eq}(N). The methyl H atoms were refined as members of rigid groups, with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(parent atom), allowing for rotation about the C—N bonds. Other H atoms were positioned geometrically, with C—H = 0.93 Å; they were constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C).

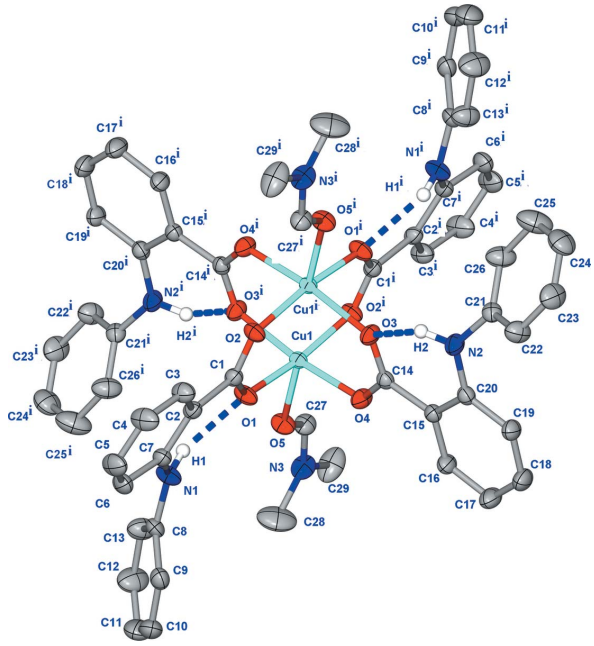


Figure 1
The molecular structure of (I), shown with 30% displacement ellipsoids. Hydrogen bonds are shown as dashed lines. Except for those of amine groups, H atoms have been omitted for clarity. [Symmetry code: (i) $-x$, $1-y$, $-z$.]

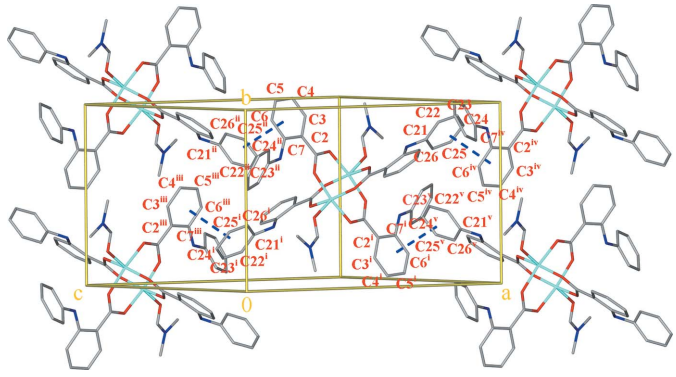


Figure 2
The packing of (I). Offset π–π interactions are shown as blue dashed lines. [Symmetry codes: (i) $-x, 1-y, -z$; (ii) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$; (iii) $-x-\frac{1}{2}, y-\frac{1}{2}, \frac{1}{2}-z$; (iv) $\frac{1}{2}+x, \frac{3}{2}-y, z-\frac{1}{2}$; (v) $\frac{1}{2}-x, y-\frac{1}{2}, -z-\frac{1}{2}$.]

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *XPREP*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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