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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.053
 wR factor = 0.114
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Tetra- μ -phenoxyacetato-bis[(acetonitrile)-
copper(II)]($\text{Cu}-\text{Cu}$)The title centrosymmetric compound, $[\text{Cu}_2(\text{C}_8\text{H}_7\text{O}_3)_4(\text{C}_2\text{H}_3\text{N})_2]$, is a carboxylate-bridged dinuclear Cu^{II} complex with four phenoxyacetate and two acetonitrile molecules as ligands. Each of the four phenoxyacetate anions straddles the pair of Cu atoms, the Cu—Cu distance being 2.6618 (10) Å. A weak $\text{C}-\text{H} \cdots \pi$ interaction connects the dinuclear Cu^{II} units into a one-dimensional chain.

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Comment

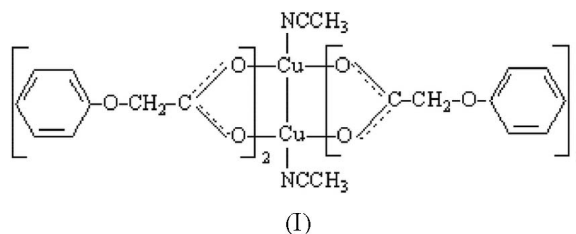
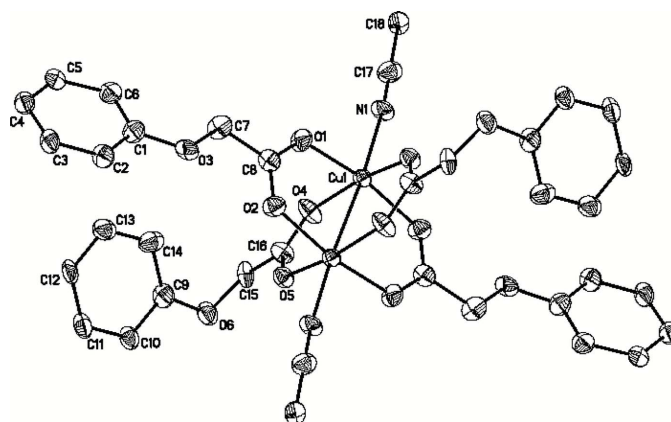
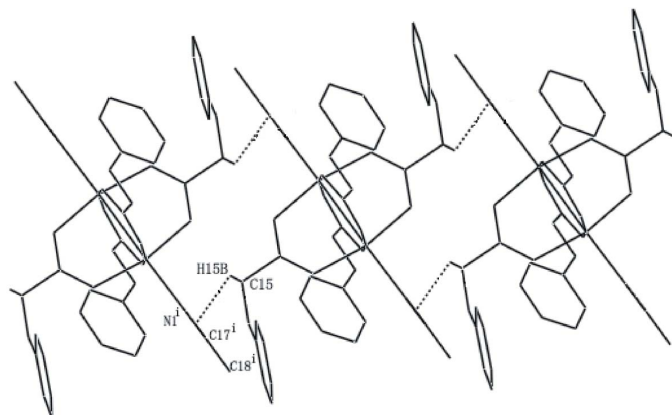
Since the structure of copper(II) acetate monohydrate was reported by van Niekerk & Shoening (1953), interest has focused on understanding Cu—Cu interactions in dinuclear Cu^{II} carboxylates and their magnetic aspects (Hatfield & Whyman, 1969; Herring *et al.*, 1971). A search of the Cambridge Structural Database (Version 5.24; Allen, 2002) for Cu^{II} complexes with phenoxyacetates as ligands yielded five hits. Here, the title compound, (I), a novel dinuclear Cu^{II} complex with acetonitrile as co-ligands, is reported.Complex (I) exists as a centrosymmetric dinuclear unit, with four bidentate phenoxyacetate anions bridging the pair of Cu^{II} atoms (Fig. 1). The Cu—Cu distance is 2.6618 (10) Å. Bond

Figure 1

The structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. (Symmetry code for unlabelled atoms: $\frac{3}{2} - x, \frac{1}{2} - y, -z$.)


Figure 2

A packing diagram for (I), showing chain formation along the *b* axis [symmetry code: (i) $x, -1 + y, z$]. H atoms other than H15*B* have been omitted.

distances and angles involving the Cu^{II} atoms are listed in Table 1. The four O atoms from the two opposing carboxylate anions form a plane, and the Cu—O distances range from 1.946 (3) to 1.965 (3) Å [average 1.957 (3) Å]. In addition, the N atoms from acetonitrile molecules bind to the Cu^{II} atoms nearly in the direction of the Cu—Cu vector in the apical position, to complete a square-pyramidal coordination environment for the Cu^{II} atom. The Cu—N distance is 2.188 (3) Å.

In the crystal structure, a weak C—H... π interaction (Jeffrey, 1997; Ni *et al.*, 2003; Li *et al.*, 2003) plays an important role. The C—H... π interaction between the methylene group of the phenoxyacetate ligand and the cyano group of the acetonitrile ligand (Table 2) connects adjacent Cu^{II} complexes to form a one-dimensional chain along the *b* axis (Fig. 2).

Experimental

[Fe₃O(O₂CCH₂OPh)₆(H₂O)₃](NO₃) was synthesized according to the literature method of Yang *et al.* (2004). [Fe₃O(O₂CCH₂OPh)₆(H₂O)₃](NO₃) (0.241 g, 0.2 mmol) was dissolved in acetonitrile (10 ml) with stirring and then Cu(NO₃)₂·3H₂O (0.047 g, 0.2 mmol) was added. After 30 min, the title complex, (I), formed and was filtered off. Single crystals of (I) suitable for X-ray analysis were grown from the filtrate after one week. The compound obtained was not that expected from the reaction.

Crystal data

[Cu₂(C₈H₇O₃)₄(C₂H₃N)₂]
M_r = 813.73
 Monoclinic, *C*2/*c*
a = 19.064 (4) Å
b = 7.6978 (16) Å
c = 24.864 (5) Å
 β = 98.261 (4)°
V = 3611.0 (13) Å³
Z = 4

D_x = 1.497 Mg m⁻³
 Mo *K* α radiation
 Cell parameters from 935 reflections
 θ = 2.4–25.6°
 μ = 1.24 mm⁻¹
T = 293 (2) K
 Prism, blue
 0.23 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
*T*_{min} = 0.75, *T*_{max} = 0.79
 9410 measured reflections

3544 independent reflections
 2539 reflections with *I* > 2 σ (*I*)
*R*_{int} = 0.048
 θ _{max} = 26.0°
h = -22 → 23
k = -9 → 9
l = -24 → 30

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.053
wR(*F*²) = 0.114
S = 1.05
 3544 reflections
 236 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.55P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.46 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.53 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O5 ⁱ	1.946 (3)	Cu1—O2 ⁱ	1.965 (3)
Cu1—O1	1.956 (3)	Cu1—Cu1 ⁱ	2.6618 (10)
Cu1—O4	1.961 (3)		
O5 ⁱ —Cu1—O1	89.99 (12)	O4—Cu1—N1	94.21 (12)
O5 ⁱ —Cu1—O4	167.49 (10)	O2 ⁱ —Cu1—N1	97.89 (11)
O5 ⁱ —Cu1—O2 ⁱ	87.85 (11)	O5 ⁱ —Cu1—Cu1 ⁱ	82.72 (7)
O1—Cu1—O2 ⁱ	167.03 (11)	O1—Cu1—Cu1 ⁱ	81.34 (8)
O4—Cu1—O2 ⁱ	90.74 (12)	O4—Cu1—Cu1 ⁱ	84.78 (8)
O5 ⁱ —Cu1—N1	98.30 (11)	O2 ⁱ —Cu1—Cu1 ⁱ	85.71 (8)
O1—Cu1—N1	95.07 (11)	N1—Cu1—Cu1 ⁱ	176.28 (9)

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, -z$.

Table 2

Hydrogen-bond geometry (Å, °).

Cg1 is the centre of gravity of the cyano group.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C15—H15 <i>B</i> ...Cg1 ⁱⁱ	0.97	2.87	3.61	134

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

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and *U*_{iso}(H) = 1.2–1.5*U*_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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