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Bis(diacetylacetonato)bis[pyridinecopper(II)]

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Key indicators

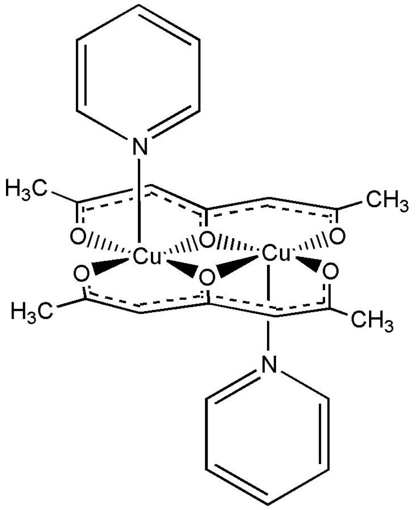
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.080
Data-to-parameter ratio = 33.4

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

In the title compound, $[Cu_2(C_7H_8O_3)_2(C_5H_5N)_2]$, each centrosymmetric molecule contains two square-pyramidally coordinated Cu atoms connected to two O atoms from each of the two diacetylacetonate anions. The Cu atoms and the two diacetylacetonate anions are approximately coplanar, and the pyramidal coordination of Cu is completed by pyridine ligands, which coordinate to the two metals on opposite sides of this plane.

Comment

Polyols have been studied in relation to the fundamental nature of the hydrogen bond (Hibbert & Emsley, 1990). We are interested in diols with adjacent hydrogen bonds, and thus we have probed the coordination ability of of the triketone unit, since the triketone ligand can potentially form polynuclear complexes with constrained geometry. This has led to the synthesis of the title compound, $[Cu_2(C_7H_8O_3)_2(C_5H_5N)_2]$, (I).



(I)

Each Cu atom is coordinated by four O atoms from the two diacetylacetone (diacac) ligands, constituting the basal plane, and the N atom of pyridine acting as the apex of the pyramid. The dimeric molecule is centrosymmetric. The Cu atom lies 0.240 (1) Å above the plane of the four O atoms coordinated to it. The central of the three O atoms of the diacac ligand, O2, has a fundamentally different coordination, as it interacts with both Cu atoms. Thus, O2 exhibits longer Cu—O distances [1.9365 (10) and 1.9628 (10) Å] than O1 and O3 [1.9074 (10) and 1.9095 (10) Å, respectively, for Cu1—O1 and Cu1—O3].

The Cu—N bond distance is 2.2617 (12) Å, significantly longer, as expected, than the basal Cu—O bonds.

The diacac ligands are nominally dianions with the negative charges completely delocalized. However, the distribution of C—O bond lengths within the diacac molecule (Table 1) suggests otherwise [C4—O2 = 1.3136 (16) Å, C6—O3 = 1.2864 (18) Å and C2—O1 = 1.2860 (18) Å]. The shorter the C—O bond, the more double-bond character it has; hence, the longer C4—O2 bond possesses more single-bond character, *i.e.* is slightly more enolate-like than the other C—O bonds. On the other hand, in the heptane backbone of the diacac group, the C3—C4 and C4—C5 bonds are slightly longer [1.411 (2) and 1.410 (2) Å] than the C2—C3 and C5—C6 bonds [1.392 (2) and 1.390 (2) Å], suggesting that the diacac structure results from an even distribution of the three possible resonance forms. If this is the case, the three O atoms should be equally negative, and the differences in the Cu—O bond distances could be ascribed to the different coordination of the O atoms, *i.e.* bridging two Cu atoms (O2) or coordinated to only one Cu atom (O1 and O3).

The diacac ligand is not completely planar; instead there is an r.m.s. deviation of 0.11 Å from the mean plane through the ten constituent atoms. However, on their own the three separate acetyl groups are completely planar, but they become non-coplanar by slight rotations at their connection points, C3 and C5. The Cu centers are 3.0565 (3) Å apart, which suggests that no direct Cu—Cu bonding is present.

Experimental

The crystals were prepared as described by Sagara *et al.* (1968), and crystals suitable for X-ray diffraction were produced by slow evaporation of a solution in pyridine at room temperature.

Crystal data

$[Cu_2(C_7H_8O_3)_2(C_5H_5N)_2]$
$M_r = 565.55$
Triclinic, $P\overline{1}$
$a = 8.4152$ (3) Å
$b = 8.7177$ (3) Å
$c = 9.3451$ (3) Å
$\alpha = 67.769$ (2)°
$\beta = 87.591$ (2)°
$\gamma = 69.878$ (2)°
$V = 592.80$ (4) Å^3
$Z = 1$
$D_x = 1.584$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4210 reflections
$\theta = 2.6$–31.2°
$\mu = 1.84$ mm^{-1}
$T = 100$ (2) K
Block, light green
0.10 × 0.08 × 0.05 mm

Data collection

Bruker SMART APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996).
$T_{min} = 0.776$, $T_{max} = 0.91$
11 199 measured reflections
4448 independent reflections
3703 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 33.1°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.080$
$S = 1.04$
4448 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.063P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

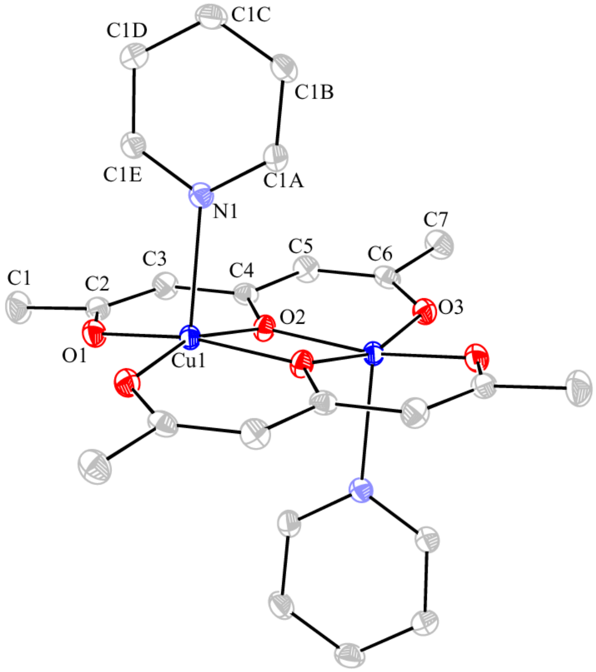


Figure 1
View of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted. Unlabeled atoms are related to labeled atoms by $1 - x$, $1 - y$, $1 - z$.

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9074 (10)	O3—C6	1.2864 (18)
Cu1—O3	1.9095 (10)	C1—C2	1.508 (2)
Cu1—O2	1.9365 (10)	C2—C3	1.392 (2)
Cu1—O2^i	1.9628 (10)	C3—C4^i	1.411 (2)
Cu1—N1	2.2617 (12)	C4—C5	1.410 (2)
O1—C2	1.2860 (18)	C5—C6	1.390 (2)
O2—C4	1.3136 (16)	C6—C7	1.506 (2)
O1—Cu1—O3	93.93 (4)	O2—Cu1—O2^i	76.77 (5)
O1—Cu1—O2	164.19 (5)	O1—Cu1—N1	97.86 (4)
O3—Cu1—O2	93.44 (4)	O3—Cu1—N1	104.37 (4)
O1—Cu1—O2^i	92.32 (4)	O2—Cu1—N1	93.83 (4)
O3—Cu1—O2^i	162.28 (4)	O2^i—Cu1—N1	91.16 (4)

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

H atoms were placed at calculated positions and refined as riding on their parent atom [C—H = 0.95–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$].

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004) and *WinGX* (Farrugia, 1999).

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