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Tetra-μ-benzoato-bis[(6-methylquinoline)copper(II)]

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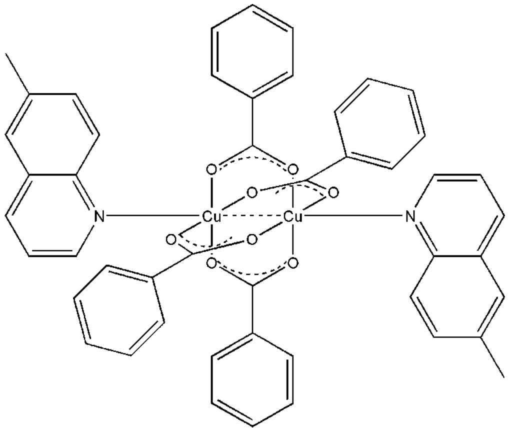
Key indicators: single-crystal X-ray study; T = 288 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.101; data-to-parameter ratio = 14.1.

In the title compound, $[Cu_2(C_7H_5O_2)_4(C_{10}H_9N)_2]$, the paddle-wheel-type dinuclear complex is constructed by four bridging benzoate groups and two terminal 6-methylquinoline ligands. The asymmetric unit contains one-half of the whole molecule, and there is an inversion center at the mid-point of the Cu$\cdots$Cu bond. The octahedral coordination of each Cu atom, with four O atoms in the equatorial plane, is completed by the N atom of the 6-methylquinoline molecule [Cu—N = 2.212 (2) Å] and by another Cu atom [Cu$\cdots$Cu = 2.6939 (13) Å]. The Cu atom lies 0.234 Å out of the plane of the four O atoms. The molecular packing is stabilized by one intramolecular C—H$\cdots$O as well as C—H$\cdots\pi$ and π–π interactions.

Related literature

For related literature, see: Batten & Robson (1998); Chun *et al.* (2005); Cotton & Walton (1993); Janiak (2003); Lee *et al.* (2008); Mines *et al.* (2002); Pichon *et al.* (2007); Yoo *et al.* (2003).



Experimental

Crystal data

$[Cu_2(C_7H_5O_2)_4(C_{10}H_9N)_2]$
M_r = 897.88
Triclinic, $P\bar{1}$
a = 10.420 (7) Å
b = 10.590 (7) Å
c = 10.751 (6) Å
α = 70.399 (11)°
β = 64.234 (10)°
γ = 81.107 (10)°
V = 1006.5 (11) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 288 (2) K
0.10 × 0.08 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*: Bruker, 1997)
T_{min} = 0.898, T_{max} = 0.915
5579 measured reflections
3848 independent reflections
3001 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
S = 1.04
3848 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

*Cg*1 is the centroid of the C22–C27 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$\cdots$O11	0.93	2.50	3.047 (4)	118
C2—H2$\cdots Cg1^{i}$	0.93	2.82	3.734 (3)	168

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

Table 2
π–π interactions (Å, °).

*Cg*2 is the centroid of ring C22–C27. The offset is defined as the distance between *CgI* and the perpendicular projection of *CgJ* on ring *I*.

CgI	*CgJ*	*CgI*$\cdots$*CgJ*	Dihedral angle	Interplanar distance	Offset
*Cg*2	*Cg*2i	3.967 (4)	0	3.39	2.06

Symmetry code: (i) $-x + 2, -y + 2, -z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2146).

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