Tetra-μ-acetato-bis[(9,10-dihydrobenzo-[de]imidazo[2,1-a]isoquinolin-7-one-κN11)-copper(II)]

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The title dinuclear Cu^{II} complex, $[Cu_2(CH_3COO)_4(C_{14}H_{10}N_2O)_2]$, is centrosymmetric. The Cu^{II} ion assumes a distorted square-pyramidal coordination geometry. Four acetate groups bridge two Cu^{II} ions, forming a dinuclear molecule.

Comment

As part of our ongoing studies on transition metal complexes incorporating imidazole and related ligands (Chen *et al.*, 2005; Yang *et al.*, 2004), the title compound, (I), has been prepared and its X-ray crystal structure is presented here.

(I)
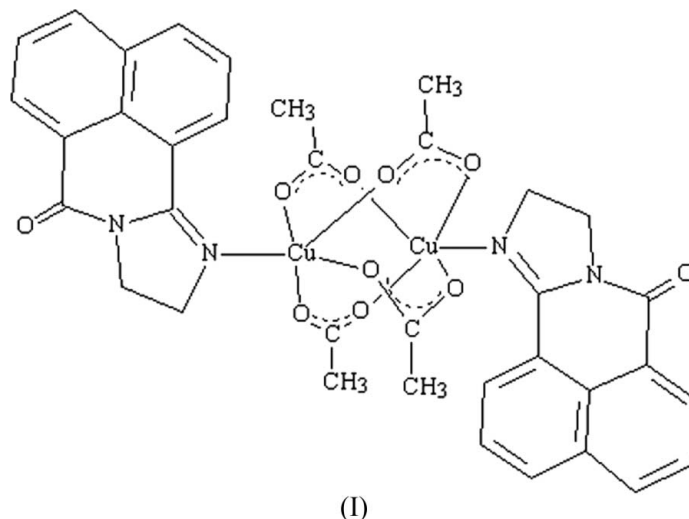
The molecular structure of (I) is shown in Fig. 1. The molecule is centrosymmetric. Each Cu^{II} ion is coordinated by a planar ligand of 9,10-dihydro-benzo[de]imidazo[2,1-a]isoqui-]isoquinolin-7-one (*L*) with a longer Cu—N bond distance (Table 1), indicating the Jahn–Teller distortion. Four acetate groups bridge two Cu^{II} ions, forming the dinuclear molecule. Within the dinuclear molecule, the Cu···Cu separation of 2.6809 (9) Å indicates no bonding between Cu^{II} ions. The coordination geometry around the Cu^{II} ion is therefore distorted square-pyramidal.

Weak C—H···O hydrogen bonding occurs between molecules (Table 2).

Experimental

A methanol solution (10 ml) of *L* (1 mmol) was mixed with an aqueous solution (10 ml) of $Cu(CH_3COO)_2 \cdot H_2O$ (1 mmol). The mixture was stirred for 1 h at room temperature and then filtered. Single crystals of (I) were obtained from the filtrate after 3 d.

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{14}H_{10}N_2O)_2]$
$M_r = 807.76$
Monoclinic, $P2_1/n$
$a = 13.2944\ (12)$ Å
$b = 9.5110\ (8)$ Å
$c = 14.1654\ (12)$ Å
$\beta = 108.393\ (2)°$
$V = 1699.6\ (3)$ Å^3

$Z = 2$
$D_x = 1.578$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.32$ mm^{-1}
$T = 298\ (2)$ K
Prism, blue
$0.17 \times 0.14 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector
  diffractometer
φ and ω scans
Absorption correction: multi-scan
  (*SADABS*; Bruker, 1998)
  $T_{min} = 0.810$, $T_{max} = 0.890$

9815 measured reflections
3698 independent reflections
2465 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.124$
$S = 0.91$
3698 reflections
237 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N1	2.241 (3)	Cu—O4	1.970 (3)
Cu—O2	1.969 (2)	Cu—O5^i	1.968 (3)
Cu—O3^i	1.970 (2)		
O5^i—Cu—O2	88.64 (11)	O4—Cu—O3^i	86.96 (12)
O5^i—Cu—O4	166.57 (11)	O5^i—Cu—N1	99.86 (11)
O2—Cu—O4	91.21 (11)	O2—Cu—N1	100.69 (11)
O5^i—Cu—O3^i	90.11 (11)	O4—Cu—N1	93.36 (11)
O2—Cu—O3^i	166.73 (10)	O3^i—Cu—N1	92.54 (11)

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

Table 2
Hydrogen-bond geometry (Å, °).

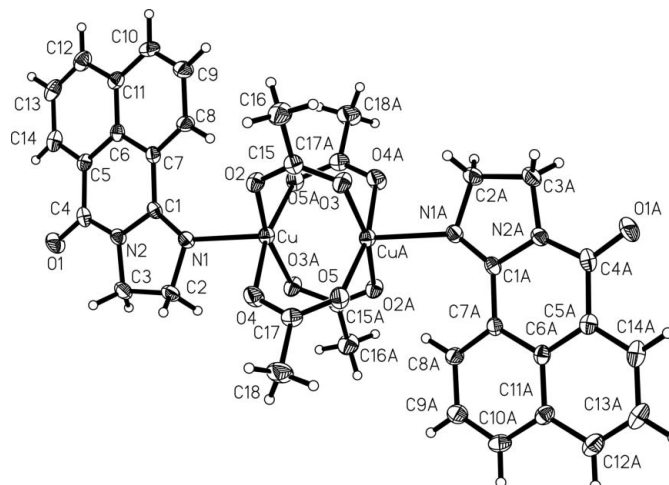| D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$\cdots$O2	0.93	2.34	3.251 (5)	166
C13—H13$\cdots$O3^{ii}	0.93	2.51	3.312 (5)	145

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

Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids [symmetry code: (A) $2 - x, -y, 2 - z$].

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. Other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

References

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