Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetra-μ-benzoato-$\kappa^8O:O'$-bis[(2-benzamidopyridine-κN^1)copper(II)]

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Received 12 March 2006
Accepted 7 May 2006

Key indicators

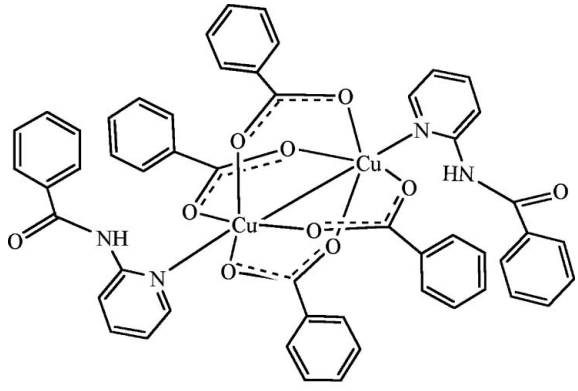
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.054
wR factor = 0.119
Data-to-parameter ratio = 13.4

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

The title complex, $[Cu_2(C_7H_5O_2)_4(C_{12}H_{10}N_2O)_2]$, forms a dimer of the paddle-wheel type located on a crystallographic inversion center. The two Cu^{II} atoms [Cu—Cu = 2.6377 (11) Å] are connected by four benzoate ligands. The apical positions of the square-pyramidal copper coordination polyhedra are occupied by the N atoms of 2-benzamidopyridine ligands. The crystal structure is stabilized by π–π stacking involving the phenyl and pyridine groups.

Comment

Coordination polymers containing symmetric multidentate carboxylate molecules as bridging ligands have attracted increasing attention because of their interesting network structures and potential applications in many fields (Yaghi *et al.*, 1997; Chui *et al.*, 1999). As part of our research interest in 2-benzamidopyridine and benzoic acid bridged polymeric complexes, the title complex, (I), was obtained by the reaction of 2-benzamidopyridine with cuprous chloride and benzoic acid. As shown in Fig. 1, the molecular structure consists of discrete centrosymmetric $[Cu_2(C_7H_5O_2)_4(C_{12}H_{10}N_2O)_2]$ dimers of the paddle-wheel cage type, with an inversion center located at the mid-point of the Cu—Cu vector. These Cu atoms each have a distorted square-pyramidal environment if the Cu—Cu interaction is ignored, with the four basal positions occupied by bridging benzoic acid O atoms. Selected distances and angles are reported in Table 1. Consolidation of the crystal structure is achieved by offset or slipped π–π stacking interactions.



(I)

Experimental

Benzoic acid (2 mmol) and 2-aminopyridine (6 mmol) were dissolved in absolute ethanol (30 ml). The mixture was heated under reflux with

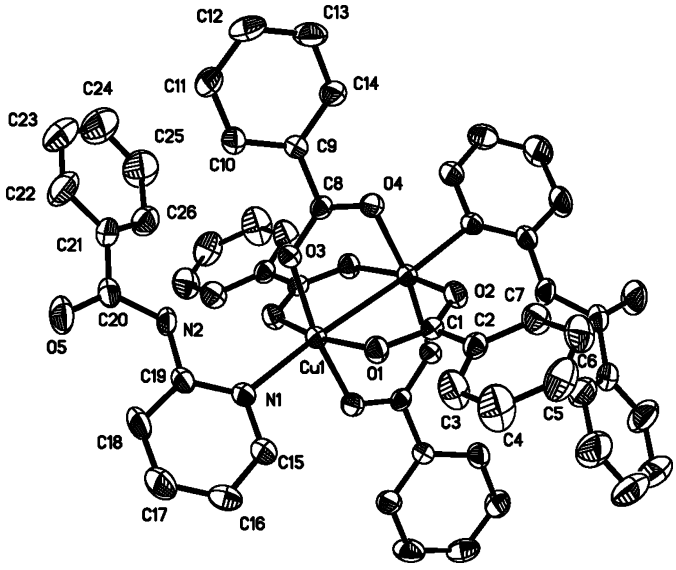


Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted. Unlabeled atoms are related to labeled atoms by the symmetry code $(2 - x, 1 - y, 1 - z)$.

stirring for 1.5 h. Cuprous chloride (2 mmol) was added to the solution. The mixture was stirred for 5 h at room temperature, and half of the solvent was evaporated in a rotary vacuum evaporator. The resulting solution was filtered and the filtrate left in air for about six weeks, after which large green block-shaped crystals suitable for X-ray analysis were formed. Elemental analysis found: C 61.84, H 3.75, N 5.48%; calculated for $C_{52}H_{40}Cu_2N_4O_{10}$: C 61.96, H 3.99, N 5.56%.

Crystal data

$[Cu_2(C_7H_5O_2)_4(C_{12}H_{10}N_2O)_2]$
$M_r = 1007.96$
Triclinic, $P\overline{1}$
$a = 10.209$ (2) Å
$b = 10.730$ (2) Å
$c = 11.075$ (2) Å
$\alpha = 101.661$ (3)°
$\beta = 94.736$ (3)°
$\gamma = 92.709$ (4)°
$V = 1181.5$ (4) Å^3
$Z = 1$
$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.96$ mm^{-1}
$T = 298$ (2) K
Block, green
0.26 × 0.21 × 0.12 mm

Data collection

Siemens SMART 1000 diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.788$, $T_{max} = 0.893$
6272 measured reflections
4112 independent reflections
2543 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.120$
$S = 1.01$
4112 reflections
307 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O4^i	1.950 (3)	Cu1—O1	1.973 (3)
Cu1—O3	1.952 (3)	Cu1—N1	2.208 (3)
Cu1—O2^i	1.961 (3)	Cu1—Cu1^i	2.6377 (11)
O4^i—Cu1—N1	95.03 (13)	O3—Cu1—Cu1^i	83.41 (8)
O3—Cu1—N1	97.21 (13)	O2^i—Cu1—Cu1^i	87.35 (9)
O2^i—Cu1—N1	99.97 (13)	O1—Cu1—Cu1^i	80.95 (9)
O1—Cu1—N1	91.72 (12)	N1—Cu1—Cu1^i	172.67 (10)
O4^i—Cu1—Cu1^i	84.71 (9)		
N1—C19—N2—C20	−178.3 (5)	N2—C20—C21—C22	−152.4 (5)
C19—N2—C20—O5	3.6 (9)	O5—C20—C21—C22	27.5 (8)

Symmetry code: (i) $-x + 2, -y + 1, -z + 1$.

All H atoms were positioned geometrically and treated as riding on their parent atoms, with N—H = 0.86 Å, C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

We acknowledge the Science Foundation of Liao Cheng University, the financial support of the Shandong Province Science Foundation and the State Key Laboratory of Crystal Materials, Shandong University, People's Republic of China.

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