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Tetrakis(μ-2-bromobenzoato-κ^2O,O')-bis[(N,N'-dimethylformamide)copper(II)], a new binuclear complex containing a metal–metal bond

Yu-Liang Zhang,[a] Su-Wen Chen,[a] Wei-Sheng Liu[a]* and Da-Qi Wang[b]

[a]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China, and [b]Department of Chemistry, Liaocheng University, Liaocheng, Shandong 252000, People's Republic of China

Correspondence e-mail:
yuliangzhang@hotmail.com

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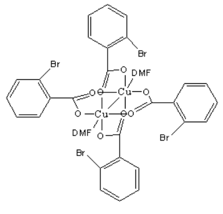
The dimeric neutral title complex, $[Cu_2(C_7H_4BrO_2)_4(C_3H_7NO)_2]$, is centrosymmetric and contains a Cu—Cu bond [2.636 (3) Å].

Comment

It is well known that copper(II) complexes of inactive ligands and active anti-inflammatory drugs are more active than the ligands themselves (Sorenson, 1982), and the most widely used anti-inflammatory drugs are carboxylic acids in which the carboxylate group is available for metal–ligand interaction.



(I)

Recently, the binuclear copper(II) carboxylate compounds $[Cu_2(O_2CR)_4L_2]$ [R = alkyl or phenyl; L = H_2O, DMF, DMSO, pyridine, picoline, diethylamine] were studied (Weder *et al.*, 1999). In the present study, we have isolated the new dimeric complex tetrakis(μ-2-bromobenzoato-κ^2O,O')bis[(N,N'-dimethylformamide)copper(II)], (I) (Fig. 1).

Compound (I) is a centrosymmetric neutral binuclear copper(II) compound with a Cu—Cu^i [symmetry code: (i) $1 - x$, $-y$, $-z$] separation of 2.636 (3) Å. This distance is similar to that found in related Cu–carboxylate dimers (Abuhijhleh, 1994). Each Cu^{II} atom in the complex has a

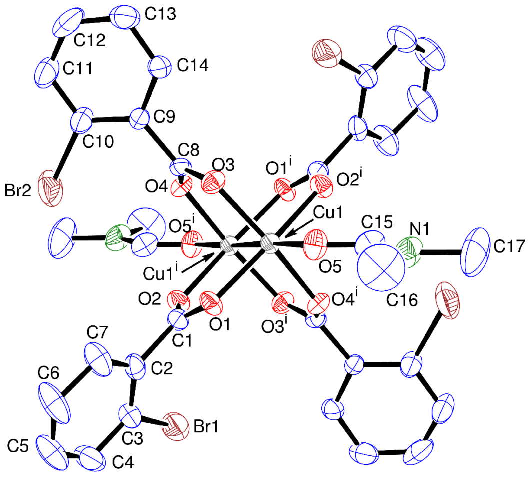


Figure 1
View of the dimeric structure of (I) (50% displacement ellipsoids). H atoms have been omitted for clarity. The symmetry code is as in Table 1.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.049
wR factor = 0.123
Data-to-parameter ratio = 14.5

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

Jahn–Teller-distorted octahedral geometry, with four O atoms from four 2-bromobenzoate groups in the basal plane and one O atom from one dimethylformamide molecule in the axial position. The *trans* angles in the basal plane deviate slightly from 180°, and the four O—Cu—O angles for O5 and the four O atoms in the basal plane are slightly larger than 90° [average 96.0 (2)°], indicating that the coordination geometry around the Cu1 atom in the complex is slightly distorted. The average Cu—O bond length [1.966 (4) Å] in the basal plane is comparable to equivalent bond lengths found in similar complexes.

Experimental

Cupric nitrate was added to sodium 2-bromobenzoate obtained by the reaction of the protonated ligand with sodium hydroxide (wt 10%) in water. The blue residues were collected and dissolved in DMF. Crystals of (I) were isolated by evaporation of the DMF in a vacuum. Spectroscopic analysis, IR (KBr, ν cm^{-1}): 1663, 1616, 1564, 1473, 1409; analysis calculated for $C_{34}H_{30}Br_4Cu_2N_2O_{10}$: C 38.16, H 2.83, N 2.62, Cu 11.88%; found: C 38.30, H 2.61, N 2.75, Cu 11.57%.

Crystal data

$[Cu_2(C_7H_4BrO_2)_4(C_3H_7NO)_2]$
M_r = 1073.32
Monoclinic, $P2_1/n$
a = 10.278 (12) Å
b = 10.885 (13) Å
c = 17.55 (2) Å
β = 92.224 (17)°
V = 1963 (4) Å^3
Z = 2
D_x = 1.816 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1799 reflections
θ = 2.2–20.6°
μ = 5.21 mm^{-1}
T = 293 (2) K
Block, blue
0.37 × 0.33 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.161, T_{max} = 0.391
9841 measured reflections
3407 independent reflections
1731 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.0°
$h = -12 \rightarrow 10$
$k = -12 \rightarrow 8$
$l = -16 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.123
S = 0.86
3407 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cu1^i	2.636 (3)	Cu1—O3	1.968 (4)
Cu1—O1	1.968 (4)	Cu1—O4^i	1.980 (5)
Cu1—O2^i	1.968 (4)	Cu1—O5	2.134 (5)
O1—Cu1—O2^i	167.89 (18)	O1—Cu1—Cu1^i	84.88 (13)
O1—Cu1—O3	89.88 (19)	O2^i—Cu1—Cu1^i	83.03 (13)
O1—Cu1—O4^i	88.47 (19)	O3—Cu1—Cu1^i	87.87 (15)
O1—Cu1—O5	97.60 (19)	O4^i—Cu1—Cu1^i	80.29 (14)
O2^i—Cu1—O3	90.37 (18)	O5—Cu1—Cu1^i	174.05 (14)
O2^i—Cu1—O4^i	88.81 (19)	C1—O1—Cu1	121.7 (4)
O2^i—Cu1—O5	94.37 (18)	C1—O2—Cu1^i	124.3 (4)
O3—Cu1—O4^i	168.14 (17)	C8—O3—Cu1	118.2 (4)
O3—Cu1—O5	97.5 (2)	C8—O4—Cu1^i	126.9 (4)
O4^i—Cu1—O5	94.34 (19)		

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

All the H atoms were placed geometrically and refined as riding (C—H = 0.93 or 0.93 Å; U_{iso} = 1.2 or 1.5U_{eq} of the parent atom).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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