Table 1. *Selected geometric parameters (Å, °)*

Ni7—B3	2.082 (4)	S2—C2	1.665 (5)
Ni7—B8	2.109 (4)	S3—C3	1.676 (4)
Ni7—B11	2.112 (4)	P1—B10	1.906 (5)
Ni7—B2	2.119 (5)	O1—B3	1.480 (5)
Ni7—S3	2.2469 (13)	O2—B8	1.457 (5)
Ni7—S2	2.3405 (13)	O3—B11	1.492 (5)
Ni7—S1	2.3766 (14)	B9—B10	1.823 (6)
S1—C1	1.658 (4)	B10—B11	1.682 (6)
B3—Ni7—B8	50.29 (18)	B8—Ni7—S2	75.25 (13)
B3—Ni7—B11	85.06 (17)	B11—Ni7—S2	117.41 (12)
B8—Ni7—B11	88.79 (17)	B2—Ni7—S2	159.91 (13)
B3—Ni7—B2	49.89 (18)	S3—Ni7—S2	91.97 (5)
B8—Ni7—B2	88.50 (18)	B3—Ni7—S1	82.27 (13)
B11—Ni7—B2	49.25 (17)	B8—Ni7—S1	101.17 (13)
B3—Ni7—S3	146.36 (14)	B11—Ni7—S1	152.86 (12)
B8—Ni7—S3	159.62 (13)	B2—Ni7—S1	105.30 (13)
B11—Ni7—S3	83.04 (12)	S3—Ni7—S1	94.45 (5)
B2—Ni7—S3	100.01 (13)	S2—Ni7—S1	89.63 (5)
B3—Ni7—S2	121.35 (14)		

The cage H atoms were located using Fourier methods and refined isotropically. H atoms on phenyl and CH_3 groups were included at riding positions, with C—H distances and U(H) fixed at 0.93 Å/1.2U_{eq}(C) and 0.96 Å/1.5U_{eq}(C), respectively.

Data collection: *CAD*-4 *Manual* (Enraf–Nonius, 1988). Cell refinement: *CAD*-4 *Manual*. Data reduction: *SDP-Plus* (Frenz, 1985). Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *ZORTEP* (Zsolnai & Huttner, 1994). Software used to prepare material for publication: *SHELXL*97.

The authors acknowledge the support of the Chinese National Science Foundation. JMD acknowledges the support of the Science Foundation of Shandong Province.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1304). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1999). C**55**, 1228–1230

Bis(1-methylimidazole-N^3)bis(salicylato-O,O')copper(II)

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(*Received 23 September 1998; accepted 9 February 1999*)

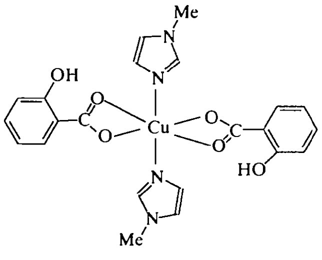
Abstract

The crystal structure of the title complex, $[Cu(C_7H_5O_3)_2(C_4H_6N_2)_2]$, is built of monomeric $[Cu(mim)_2(Sal)_2]$ molecules (mim is N-methylimidazole and Sal is salicylate), which display a distorted octahedral $CuN_2O_2\cdots O'_2$ chromophore. An intramolecular hydrogen bond exists between the hydroxyl group and the carbonyl O atom of the carboxylate group [O···O 2.581 (3) Å].

Comment

The number of reports on monomeric copper(II) complexes containing carboxylate and basic ligands is quite limited. It has been found that by increasing the acidity of the alkylcarboxylate ligands or by increasing the basicity of the basic ligands, the tendency towards formation of monomeric complexes increases (Melnik, 1981; Ahmed & Abuhijleh, 1982; Uruska *et al.*, 1990). Complexes of copper(II) with carboxylate and imidazole ligands have been studied as models for copper proteins containing both functionalities in the side chain (Sigel, 1980; Bernarducci *et al.*, 1983). Some of these copper(II) complexes have been found to possess a variety of pharmacological activities (Tamura *et al.*, 1987; Bhirud & Śrivastava, 1990).

The crystal structure of the title complex, (I), consists of monomeric units in which the copper(II) ion assumes a centrosymmetric distorted octahedral geometry. The coordination of the Cu atom may be described as a $CuN_2O_2\cdots O_2'$ chromophore (Hathaway & Biling, 1970). Two *N*-methylimidazole and two salicylate molecules are coordinated to each Cu atom. The N1 and O1 atoms, together with their respective centrosymmetrically related partners [$N1^i$ and $O1^i$; symmetry code: (i) $-x, -y, -z$], coordinate in a plane around the Cu atom, which lies on a center of symmetry. The Cu—N1 [1.994 (3) Å] and Cu—O1 [1.944 (2) Å] distances are in close agreement with those found for a similar structure (Henriksson, 1977). Both the carbonyl O atoms of the two carboxylate groups (O2 and $O2^i$) interact weakly in axial positions with the Cu^{II} atom, at a distance of 2.785 (2) Å. The tetragonal distortion is clearly indicated by the O1—Cu—O2 angle of 52.25 (8)°. The O2···O3 separation of 2.581 (3) Å indicates an intramolecular hydrogen bond between the hydroxyl group and the carbonyl O atom of the carboxylate group (Rissanen *et al.*, 1987; Hoang *et al.*, 1992).



(I)

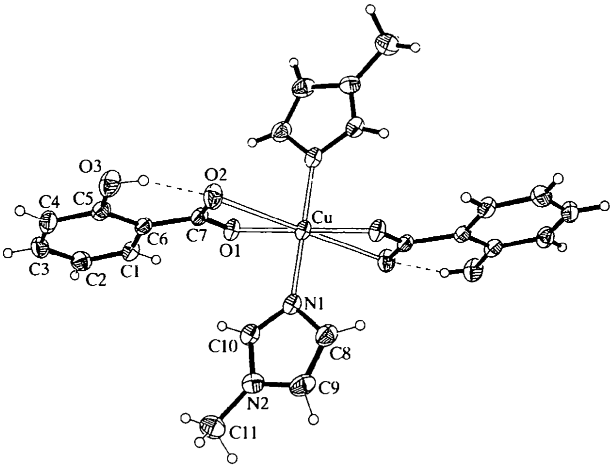


Fig. 1. View of the title compound showing the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level.

Experimental

The title complex was prepared by the reaction of excess *N*-methylimidazole (1 ml) with anhydrous copper(II) disalicylate (1.7 g) in EtOH (50 ml) (Inoue *et al.*, 1964). Single crystals suitable for X-ray analysis were obtained by recrystalization from ethyl acetate solution.

Crystal data

$[Cu(C_7H_5O_3)_2(C_4H_6N_2)_2]$
$M_r = 501.98$
Monoclinic
$P2_1/c$
$a = 7.927\,(3)$ Å
$b = 6.159\,(2)$ Å
$c = 22.47\,(1)$ Å
$\beta = 97.76\,(4)°$
$V = 1087.0\,(7)$ Å^3
$Z = 2$
$D_x = 1.534$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 23 reflections
$\theta = 4$–14°
$\mu = 1.052$ mm^{-1}
$T = 300\,(2)$ K
Parallelepiped
0.30 × 0.20 × 0.15 mm
Blue

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.730$, $T_{max} = 0.853$
2090 measured reflections
2032 independent reflections
1578 reflections with $I > 2\sigma(I)$

$R_{int} = 0.024$
$\theta_{max} = 25.5°$
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 7$
$l = 0 \rightarrow 27$
3 standard reflections every 97 reflections frequency: 60 min intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.107$
$S = 1.054$
2032 reflections
196 parameters
H atoms refined isotropically
$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.530$ e Å^{-3}
$\Delta\rho_{min} = -0.285$ e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.046 (3)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Cu—O1	1.944 (2)	O1—C7	1.278 (3)
Cu—N1	1.994 (3)	O2—C7	1.246 (4)
Cu—O2	2.785 (2)		
O1—Cu—N1	88.75 (10)	$O1^i$—Cu—O2	127.75 (8)
$O1^i$—Cu—N1	91.25 (10)	N1—Cu—O2	90.08 (9)
O1—Cu—O2	52.25 (8)	$N1^i$—Cu—O2	89.92 (9)

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *NRCVAX* (Gabe *et al.*, 1989). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990*a*). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1990*b*). Software used to prepare material for publication: *SHELXL*93.

This work was supported by the NSFC (project 29501001), NSF of Jiangsu Province (project BK950-24401) and IRPA of Malaysia (grant No. 09-02-03-004).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1230). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1999). C**55**, 1230–1234

catena-Poly[[bis(benzimidazole-N^3)copper(II)]-μ-suberato-$O,O':O'',O'''$] and *catena*-poly[[[bis(benzimidazole-N^3)copper(II)]-μ-sebacato-$O,O':O'',O'''$] dihydrate]

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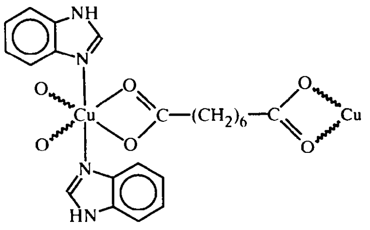
(*Received 10 March 1999; accepted 19 April 1999*)

Abstract

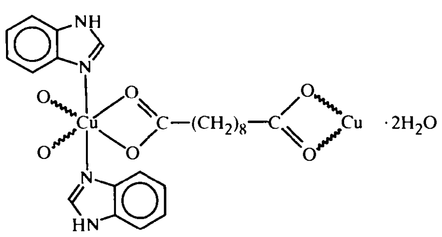
Both title compounds, $[Cu(C_8H_{12}O_4)(C_7H_6N_2)_2]$, (I), and $[Cu(C_{10}H_{16}O_4)(C_7H_6N_2)_2]\cdot 2H_2O$, (II), display inversion symmetry. The Cu centres are bridged by the dicarboxylate ions in a bis-bidentate fashion, forming polymeric chains. In (I) and (II), these chains are differently associated *via* hydrogen bonds. The Cu···Cu intrachain distances are 10.974 (1) Å in (I) and 12.417 (5) Å in (II). In both structures, the base of the elongated octahedron of the Cu^{II} atoms is formed by two short Cu—O and Cu—N bonds [Cu—O 1.973 (1) and 1.974 (2) Å, and Cu—N 1.974 (1) and 1.977 (2) Å in (I) and (II), respectively]. The carboxylate groups form four-membered unsymmetrical chelate rings and complete the Cu^{II} coordination to sixfold by long Cu—O bonds of 2.645 (2) Å in (I) and 2.583 (2) Å in (II). The modes of coordination of the Cu^{II}–dicarboxylic acid ions and benzimidazole molecules are discussed in terms of the computed bond valences and the valences of the Cu and O atoms as the sums of bond valences.

Comment

This work forms part of a continuing study of Cu^{II} complexes with benzimidazole and dicarboxylic acids (Tosik & Bukowska-Strzyżewska, 1992; Tosik *et al.*, 1995*a*,*b*; Sieroń & Bukowska-Strzyżewska, 1998). A dicarboxylate ion is a polydentate ligand and owing to the variable ligation of the carboxylate group, it can form chelate, polynuclear or polymeric complexes. We are interested in the conformation of the aliphatic chains of dicarboxylic acids, the coordination mode of benzimidazole and carboxylate ligands, and the associated types of complexes formed.



(I)



(II)

Sections of the polymeric structures of (I) and (II) are shown in Figs. 1(*a*) and 1(*b*), respectively. In both structures, each Cu atom and dicarboxylate ion is associated with an inversion centre. The Cu atoms are connected by bridging tetradentate dicarboxylate ions to form polymeric chains. The more central C atoms of the $-(CH_2)_n-$ chains adopt fully staggered conformations, with C11—

[†] A holder of the Foundation for Polish Science (FNP) grant.