

Table 2. Selected geometric parameters (Å, °)

Pt—N3	2.023 (6)	Ti—Cl2	2.421 (3)
Pt—N5	2.046 (7)	Ti—Cl3	2.395 (2)
Ti—Cl1	2.440 (2)	Ti—Cl4	2.402 (2)
N3—Pt—N5	92.9 (3)	Cl2—Ti—Cl4	103.7 (1)
Pt—N3—C4	121.8 (5)	Cl2—Ti—Cl3	109.1 (1)
Pt—N3—C2	117.6 (5)	Cl1—Ti—Cl4	107.0 (1)
Pt—N5—C51	119.5 (6)	Cl1—Ti—Cl3	103.9 (1)
Cl3—Ti—Cl4	121.9 (1)	Cl1—Ti—Cl2	111.2 (1)

The highest difference Fourier peak and deepest trough were located near the Pt and Ti atoms, respectively.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CELDIM* (Enraf-Nonius, 1989). Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *MolEN*. Program(s) used to refine structure: *MolEN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BM1076). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-Bis(benzoato-*O,O'*)bis(*N,N*-diethylnicotinamide-*N*¹)copper(II)

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Abstract

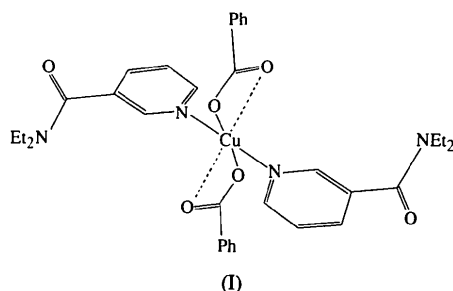
The title molecule, [Cu(C₇H₅O₂)₂(C₁₀H₁₄N₂O)₂], is a crystallographically centrosymmetric mononuclear complex. The two benzoate ions are coordinated to the Cu atom as bidentate ligands. The N and nearest O atoms form a square-planar arrangement around the Cu atom, with the tetragonally distorted octahedral coordination completed by the remaining two carboxylate O atoms.

Comment

N,N-Diethylnicotinamide (DENA) is an important respiratory stimulant (Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1972). The structures of some complexes obtained from the reactions of transition metal(II) ions with DENA have been determined previously; [Cu₂(DENA)₂(C₆H₅COO)₄] (Hökelek, Necefoğlu & Balci, 1995), [Zn₂(C₇H₅O₃)₄(DENA)₂].2H₂O (Hökelek & Necefoğlu, 1996), [Mn(DENA)₂(NCS)₂] (Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1973*a*), [Zn(DENA)₂(NCS)₂(H₂O)₂] (Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1973*b*) and [Cd(DENA)(SCN)₂] (Bigoli *et al.*, 1972). In [Mn(DENA)₂(NCS)₂], DENA is a bidentate ligand, while in [Cu₂(DENA)₂(C₆H₅COO)₄], [Zn₂(C₇H₅O₃)₄(DENA)₂].2H₂O, [Cd(DENA)(SCN)₂] and [Zn(DENA)₂(NCS)₂(H₂O)₂], DENA is a monodentate ligand. In [Cu₂(DENA)₂(C₆H₅COO)₄], the benzoate ion acts as a bidentate ligand, but in [Zn₂(C₇H₅O₃)₄(DENA)₂].2H₂O, two of the benzoate ions act as monodentate ligands, while the other two are bidentate, bridging the two Zn atoms. A series of Cu^{II} alkyl and aryl carboxylates in which the carboxylate is monodentate, cyclic bidentate or bridging, depending on the amount and coordination ability of the solvent molecule, has been reported in the literature (Meln'k, 1981, 1982; Davey & Stephens, 1971*a,b*; Musaev, Movsumov, Mamedov & Amirasanov, 1979; Usabaliev *et al.*, 1980, 1981; Hökelek *et al.*, 1995; Hökelek & Necefoğlu, 1996). The factors influencing the formation of either binuclear or mononuclear carboxylate complexes of Cu^{II} have been investigated, but still no clear understanding exists (Meln'k, 1981). As determined previously, Cu^{II} benzoate forms two types of adduct with DENA, as it

also does with pyridine (Musaev *et al.*, 1979; Usualiev *et al.*, 1980). The differential thermal analysis (DTA) of the adduct in which the Cu:DENA ratio is 1:2 (Nadzhafov & Yasinova, 1990; Necefoğlu, 1995) and the crystal structure of the adduct in which the Cu:DENA ratio is 1:1 both show that dimeric complexes are formed (Hökelek *et al.*, 1995).

The structure determination of the title molecule, (I), a copper complex with two DENA and two benzoate ligands, was undertaken in order to define the ligand properties of the DENA and benzoate ligands, and also to compare the results obtained with those reported previously. The monomeric title complex, $[\text{Cu}(\text{C}_6\text{H}_5\text{COO})_2(\text{DENA})_2]$, has a centre of symmetry and the Cu^{II} atom is surrounded by two DENA and two benzoate ligands.



The two benzoate ions act as bidentate ligands while DENA is a monodentate ligand coordinating through the pyridine N atom, which is more basic than the O atom. A view of the molecule with the atomic numbering scheme is shown in Fig. 1. The Cu—N1 and Cu—O1 bond lengths are 2.004 (3) and 1.995 (2) Å, respectively, and the N1—Cu—O1 bond angle is 89.8 (1)°. The two symmetry-related N atoms of DENA and O atoms of the benzoate groups form a square-planar coordination around the Cu atom. The copper coordination geometry may be considered as square planar or tetragonally distorted octahedral depending on whether or not both O atoms of each benzoate ligand are considered to be bonded to the Cu atom. A weak interaction between the Cu atom and the O atoms of the benzoate ligands is indicated by the Cu...O distance and the large angle between the Cu...O direction and the normal of the Cu, N1, O1, N1', O1' plane. We therefore suggest that an extremely tetragonally distorted octahedron around the Cu atom is completed by the remaining two O atoms of the benzoate ligands at a distance of 2.451 (4) Å. The N1—Cu...O2 and O1—Cu...O2 angles are 90.4 (4) and 58.3 (3)°, respectively. The corresponding angles are 89.6 (1), 89.0 (1) and 55.2 (1)° in $[\text{Cu}(\text{Asp})_2(\text{py})_2]$ (where Asp is acetylsalicylate and py is pyridine) (Greenaway, Pezeshk, Cordes, Noble & Sorenson, 1984). The angle between the directions of Cu...O2 and the normal of the Cu, N1, O1, N1', O1' plane is 31.7 (3)°. The corresponding angles are 36.1, 21.4 and 34.8° in $[\text{Cu}(\text{ClCH}_2\text{COO})_2(2-$

pic)₂] (where 2-pic is 2-picoline) (Davey & Stephens, 1971a), $[\text{Cu}(\text{Cl}_2\text{CHCOO})_2(2-\text{pic})_2]$ (Davey & Stephens, 1971b) and $[\text{Cu}(\text{Asp})_2(\text{py})_2]$ (Greenaway *et al.*, 1984). The Cu atom lies −0.025 (1) Å out of the C1, C2, O1, O2 least-squares plane. The Cu—N1 bond length [2.004 (3) Å] between the Cu atom and N heteroatom of the DENA molecule is shorter than in the dimeric complexes $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{C}_5\text{H}_5\text{N})_2]$ [2.184 (7) Å; Usualiev *et al.*, 1980] and $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{DENA})_2]$ [2.162 (6) Å; Hökelek *et al.*, 1995]. The Cu—O1 bond length [1.995 (2) Å] is in good agreement with the average values reported for other monomeric and dimeric complexes, for example, 1.975 (5) Å in $[\text{Cu}(\text{ClCH}_2\text{COO})_2(2-\text{pic})_2]$ (Davey & Stephens, 1971a), 1.978 (5) Å in $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{C}_5\text{H}_5\text{N})_2]$ (Usualiev *et al.*, 1980) and 1.974 (6) Å in $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{DENA})_2]$ (Hökelek *et al.*, 1995). The bond lengths and angles in the DENA molecule and phenyl ring of the bidentate benzoate anion are in good agreement with the values reported in the literature (Hökelek *et al.*, 1995; Hökelek & Necefoğlu, 1996). The C1—O1 bond length [1.277 (4) Å] is larger than the C1—O2 bond length [1.239 (4) Å] and is in good agreement with the corresponding distances in the monomeric carboxylate pyridine complexes of copper(II) (Davey & Stephens, 1971a,b; Greenaway *et al.*, 1984). The pyridine ring and the O3, C13, N2 plane form a dihedral angle of 102.7 (1)° with one another, which is smaller than in $[\text{Zn}_2(\text{PHB})_4(\text{DENA})_2] \cdot 2\text{H}_2\text{O}$ (where PHB is 4-hydroxybenzoato) (Hökelek & Necefoğlu, 1996). The dihedral angle between the planar carboxyl group (O1, C1, O2) and planar phenyl ring (C2—C7) is 6.7 (9)°. The corresponding angles are 6.08, 7.12 and 5.10, and 1.3°, respectively, in $[\text{Cu}(\text{PBN})_2(\text{py})_2]$ (where PBN is *p*-nitrobenzoato) (Usualiev *et al.*, 1981), $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{py})_2]$ (Usualiev *et al.*, 1980) and $\text{Cu}(\text{PHB})_2 \cdot 8\text{H}_2\text{O}$ (Shnulin, Nadzhafov & Mamedov, 1981).

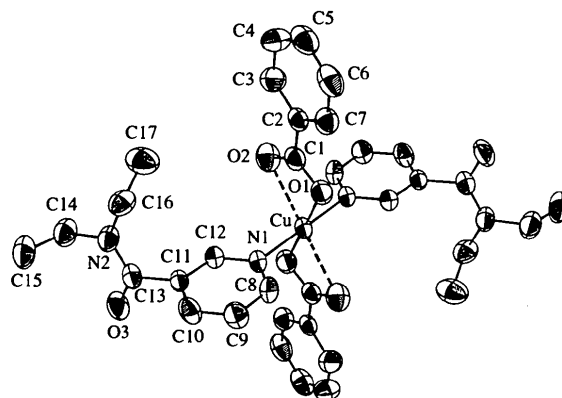


Fig. 1. An ORTEP (Johnson, 1976) drawing of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The Cu atom lies on the centre of symmetry.

Experimental

The title compound was prepared from the reaction of [Cu(C₆H₅COO)₂].3H₂O (0.01 mol) and DENA (0.02 mol) in methanol (100 ml). The mixture was filtered and set aside for crystallization at ambient temperature for a few weeks. Suitable crystals were obtained by recrystallization from ethanol.

Crystal data

[Cu(C₇H₅O₂)₂(C₁₀H₁₄N₂O)₂] Mo K α radiation
M_r = 662.25 λ = 0.71073 Å
 Monoclinic Cell parameters from 25 reflections
*P*₂₁/*n* θ = 10–18°
a = 10.006 (1) Å μ = 0.71 mm⁻¹
b = 14.876 (1) Å *T* = 298 K
c = 11.340 (1) Å Block
 β = 102.93 (1)° 0.56 × 0.16 × 0.14 mm
V = 1645.2 (3) Å³ Deep blue
Z = 2
D_x = 1.34 Mg m⁻³
D_m not measured

Data collection

Enraf–Nonius CAD-4 *R*_{int} = 0.033
 diffractometer θ_{\max} = 26.3°
 $\omega/2\theta$ scans *h* = 0 → 12
 Absorption correction: *k* = 0 → 18
 none *l* = -14 → 13
 3678 measured reflections 3 standard reflections
 3342 independent reflections monitored every 250 reflections
 1920 observed reflections
 [*F* > 2σ(*F*)] intensity decay: 1%

Refinement

Refinement on *F* $(\Delta/\sigma)_{\max}$ = 0.01
R = 0.0427 $\Delta\rho_{\max}$ = 0.12 e Å⁻³
wR = 0.0448 $\Delta\rho_{\min}$ = -0.05 e Å⁻³
S = 1.21 Extinction correction: none
 1920 reflections Atomic scattering factors
 281 parameters from *International Tables*
 All H-atom parameters refined for *X-ray Crystallography*
w = 1/σ²(*F*) (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq}
Cu	0	1/2	0	2.91 (1)
O1	0.1226 (2)	0.5987 (2)	0.0797 (2)	3.91 (6)
O2	0.1622 (3)	0.4776 (2)	0.1944 (2)	4.77 (7)
O3	0.3089 (3)	0.1973 (2)	-0.1743 (3)	5.19 (7)
N1	0.1434 (3)	0.4619 (2)	-0.0879 (2)	2.84 (6)
N2	0.4481 (3)	0.2404 (2)	0.0020 (3)	3.94 (7)
C1	0.1849 (3)	0.5575 (2)	0.1750 (3)	3.47 (8)
C2	0.2894 (3)	0.6101 (2)	0.2635 (3)	3.13 (7)
C3	0.3494 (4)	0.5726 (3)	0.3737 (3)	4.5 (1)
C4	0.4432 (5)	0.6209 (3)	0.4575 (4)	5.7 (1)
C5	0.4769 (4)	0.7062 (3)	0.4317 (4)	5.5 (1)
C6	0.4203 (4)	0.7439 (3)	0.3238 (4)	5.0 (1)
C7	0.3266 (4)	0.6968 (3)	0.2383 (3)	3.88 (9)
C8	0.1826 (4)	0.5152 (2)	-0.1690 (3)	3.67 (8)
C9	0.2790 (4)	0.4894 (3)	-0.2307 (3)	4.11 (8)

C10	0.3380 (4)	0.4062 (3)	-0.2091 (3)	4.01 (8)
C11	0.3019 (3)	0.3510 (2)	-0.1245 (3)	2.82 (7)
C12	0.2033 (3)	0.3816 (2)	-0.0667 (3)	2.98 (7)
C13	0.3550 (4)	0.2559 (2)	-0.1008 (3)	3.52 (8)
C14	0.4904 (5)	0.1466 (3)	0.0318 (4)	5.2 (1)
C15	0.6093 (5)	0.1188 (3)	-0.0184 (5)	6.9 (1)
C16	0.5162 (4)	0.3107 (3)	0.0854 (4)	4.5 (1)
C17	0.4604 (5)	0.3191 (4)	0.1987 (4)	6.5 (1)

Table 2. Selected geometric parameters (Å, °)

Cu—O1	1.995 (2)	N2—C13	1.340 (4)
Cu—N1	2.004 (3)	N2—C14	1.475 (5)
Cu—O2	2.451 (4)	N2—C16	1.471 (5)
O1—C1	1.277 (4)	C1—C2	1.498 (4)
O2—C1	1.239 (4)	C11—C13	1.514 (5)
O3—C13	1.223 (4)	C14—C15	1.488 (7)
N1—C8	1.337 (5)	C16—C17	1.515 (7)
N1—C12	1.334 (4)		
O1—Cu—N1	89.8 (1)	C1—C2—C7	121.7 (3)
Cu—O1—C1	99.5 (2)	N1—C8—C9	122.3 (3)
Cu—N1—C8	121.8 (2)	C10—C11—C12	117.6 (3)
Cu—N1—C12	120.4 (2)	C10—C11—C13	123.1 (3)
C8—N1—C12	117.8 (3)	C12—C11—C13	118.9 (3)
C13—N2—C14	118.0 (3)	N1—C12—C11	123.4 (3)
C13—N2—C16	124.7 (3)	O3—C13—N2	123.6 (3)
C14—N2—C16	117.2 (3)	O3—C13—C11	118.8 (3)
O1—C1—O2	122.4 (3)	N2—C13—C11	117.6 (3)
O1—C1—C2	116.9 (3)	N2—C14—C15	112.8 (4)
O2—C1—C2	120.7 (3)	N2—C16—C17	113.4 (4)
C1—C2—C3	119.6 (3)		

The title structure was solved by direct methods. H-atom positions were obtained from a difference map and refined with isotropic displacement parameters.

Data collection: *MolEN* (Fair, 1990). Cell refinement: *MolEN*. Data reduction: *MolEN*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *MolEN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *MolEN*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: AB1371). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). **C52**, 2473–2475

Polymeric (Aqua-1 κ O)bis[(*R,R*)-tartrato-1 κ^2 O¹,O²:2 κ^2 O³,O⁴]dimanganese(II) Trihydrate

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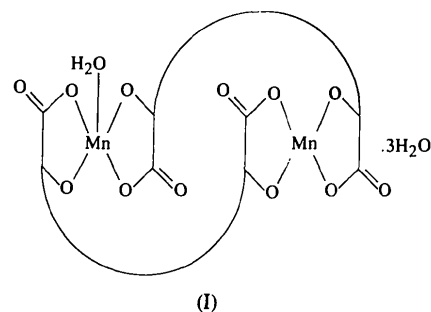
(Received 19 July 1995; accepted 14 May 1996)

Abstract

The structure of the title compound, $\{[\text{Mn}_2(\text{C}_4\text{H}_2\text{O}_6)_2(\text{H}_2\text{O})]\cdot 3\text{H}_2\text{O}\}_n$, is comprised of corrugated polymeric sheets of dimeric $[\text{Mn}_2\{(R,R)\text{-C}_4\text{H}_2\text{O}_6\}_2(\text{H}_2\text{O})]$ units and water molecules (O2W, O3W and O4W). The manganese ions are coordinated by two (*R,R*)-tartrate ligands in a *cis* arrangement. The Mn1...Mn2 intradimeric distance is 5.527 (2) Å.

Comment

This investigation has been motivated by the increasing interest in the coordination of metal atoms with carboxylic acids. The structure of polymeric (aqua-1 κ O)-bis[(*R,R*)-tartrato-1 κ^2 O¹,O²:2 κ^2 O³,O⁴]dimanganese(II) trihydrate, (I), has been determined.



The smallest structural subunit in the title compound, (I), appears to be the dimeric entity $[\text{Mn}_2\{(R,R)\text{-C}_4\text{H}_2\text{O}_6\}_2(\text{H}_2\text{O})]$ (Fig. 1). Each Mn^{2+} ion is coordinated by two halves of two different tartrate dianions *via* chelation through the alcohol and carboxylate groups. The octahedral geometry around the Mn2 ion is completed by a water molecule (O1W) and a non-chelating carboxylate O82 atom of another dimer at $(-x, y - \frac{1}{2}, -z + 1)$. The geometry around Mn1 ion is completed by two non-chelating carboxylate O42 and O52 atoms from two other dimers at $(-x + 1, y + \frac{1}{2}, -z + 1)$ and $(-x, y + \frac{1}{2}, -z)$, respectively.

Bond lengths and angles (Table 2) for each tartrate ligand are usual and do not deviate significantly from

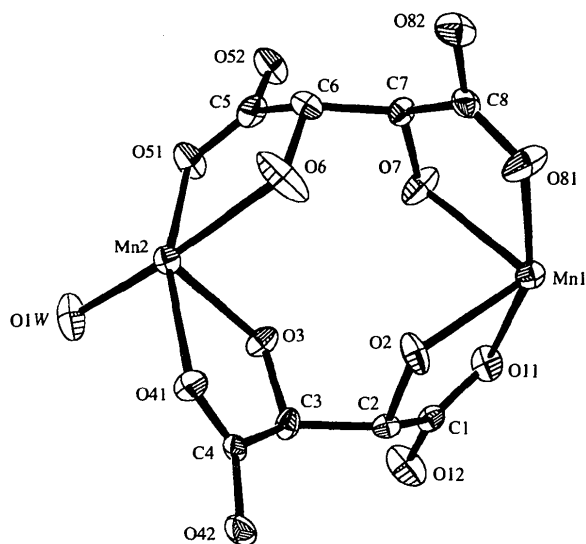


Fig. 1. Perspective drawing of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms and water molecules (O2W, O3W and O4W) have been omitted for clarity.