

Disodium tetrakis(hexanoato-O)-zinc(II)

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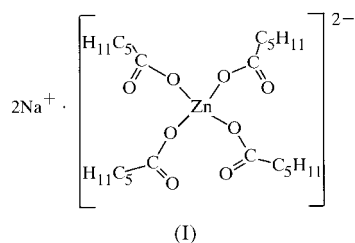
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Received 6 January 2000
Accepted 23 February 2000

The structure of the title compound, $\text{Na}_2[\text{Zn}(\text{C}_6\text{H}_{11}\text{O}_2)_4]$, consists of two-dimensional polymeric sheets. The Zn^{2+} ions are approximately tetrahedrally coordinated by O atoms from different hexanoate anions. Both Na^+ ions are six-coordinated by carboxylate O atoms. One of the hexanoate O atoms is attached to one Zn^{2+} ion and one Na^+ ion, and the remaining O atom is attached to two Na^+ ions.

Comment

During the investigation of the antifungal activity of zinc(II) carboxylates without the presence of other ligating functional groups, an anhydrous zinc(II) hexanoate has recently been prepared (Šegedin *et al.*, 1999). Several crystal structures of different types of anhydrous zinc salts of monocarboxylic acids have been published previously, for example, zinc(II) crotonate (Clegg *et al.*, 1986*a*), two polymorphic forms of acetate (Capilla & Aranda, 1979; Clegg *et al.*, 1986*b*), propionate (Goldschmied *et al.*, 1977; Clegg *et al.*, 1987) and 2-chlorobenzoate (Nakacho *et al.*, 1976; Clegg *et al.*, 1990). Due to the potential use of such complexes as wood preservatives, an attempt was made to increase the water solubility. Therefore, the water soluble title compound, (I), was synthesized.



Clegg *et al.* (1993) published the structure of dilithium zinc crotonate. Despite having the same stoichiometry as (I), the crystal structures of the two compounds differ. The structure of one polymeric sheet in (I) is presented in Fig. 1. All three metal ions lie on special positions; Zn and Na2 are located on a twofold axis, while Na1 resides on a centre of symmetry. Each Zn^{2+} ion is surrounded by four carboxylate O atoms

from different hexanoate groups (Fig. 2). The O—Zn—O angles [92.5 (1)–119.8 (1)°] show large deviations from the regular tetrahedral value of 109.5°. Both Na^+ cations are six-coordinated by O atoms; deformations of the octahedron are larger for the Na^+ ion on the twofold axis (Na1). One of the two remaining hexanoate O atoms is attached to the Zn^{2+} ion and to one Na^+ ion, and the final one is attached to two Na^+ ions.

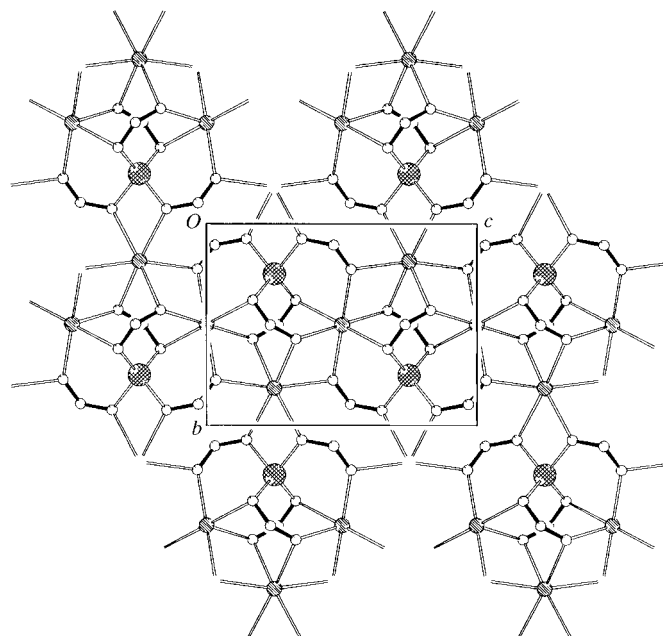


Figure 1
The structure of the framework of one polymeric sheet in (I). Hexanoate chains have been omitted for clarity.

The weak interaction of the hexanoate ligands with the Na^+ ions indicates the monodentate nature of the carboxylate ligand, which was confirmed as an observed difference in the wave numbers of the antisymmetric and symmetric modes of the carboxylate groups in the IR spectra of (I). The difference $\Delta = \nu_{\text{as}}(\text{CO}_2) - \nu_{\text{s}}(\text{CO}_2)$ of 200 cm^{-1} is characteristic for monodentate carboxylate ligands (Deacon & Phillips, 1980), while in the case of zinc hexanoate with *syn-anti* bridging carboxylate ligands, the observed difference is only 136 cm^{-1} (Šegedin *et al.*, 1999).

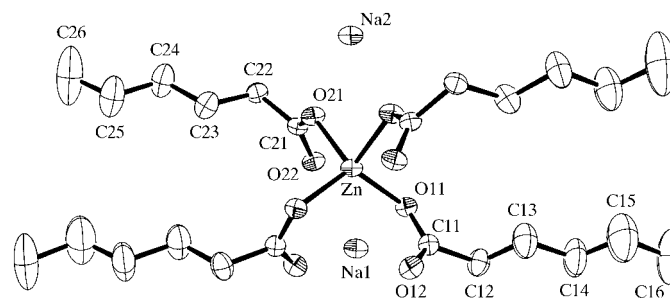


Figure 2
ORTEP (Burnett & Johnson, 1996) view of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

Similar to the structure of dilithium zinc crotonate (Clegg *et al.*, 1993), the structure of (I) is made up of two-dimensional polymeric sheets parallel with the *bc* plane. There is no covalent bonding between the sheets; the hexanoate side chains protrude from the sheets on each side, bringing the hydrophobic parts together. The hydrocarbon chains are in the extended all-*trans* configuration.

Experimental

Complex (I) was obtained by mixing ethanol solutions of sodium hexanoate and zinc hexanoate in a 2:1 molar ratio. Crystals of (I) were deposited at room temperature from the saturated solution.

Crystal data

$\text{Na}_2[\text{Zn}(\text{C}_6\text{H}_{11}\text{O}_2)_4]$	$D_x = 1.255 \text{ Mg m}^{-3}$
$M_r = 571.96$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 75 reflections
$a = 37.605 (7) \text{ \AA}$	$\theta = 8.12\text{--}14.73^\circ$
$b = 7.7797 (6) \text{ \AA}$	$\mu = 0.880 \text{ mm}^{-1}$
$c = 10.347 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 90.82 (2)^\circ$	Plate, colourless
$V = 3026.8 (8) \text{ \AA}^3$	$0.71 \times 0.51 \times 0.10 \text{ mm}$
$Z = 4$	

Data collection

Enraf–Nonius CAD-4 diffractometer	2108 reflections with $I > 2\sigma(I)$
Pure ω scans	$R_{\text{int}} = 0.124$
Absorption correction: by integration (NRCVAX; Gabe <i>et al.</i> , 1989)	$\theta_{\text{max}} = 28^\circ$
$T_{\text{min}} = 0.55$, $T_{\text{max}} = 0.92$	$h = -49 \rightarrow 49$
7288 measured reflections	$k = -10 \rightarrow 0$
3651 independent reflections	$l = -13 \rightarrow 13$
	3 standard reflections every 600 reflections
	intensity decay: 2.1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.1048P]$
$R[F^2 > 2\sigma(F^2)] = 0.055$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.991$	$\Delta\rho_{\text{max}} = 0.68 \text{ e \AA}^{-3}$
3651 reflections	$\Delta\rho_{\text{min}} = -0.81 \text{ e \AA}^{-3}$
164 parameters	Extinction correction: <i>SHELXL97</i> (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.00101 (19)

The space group was deduced from the systematic absences and intensity statistics. H atoms were included at calculated positions using *SHELXL97* (Sheldrick, 1997) and refined using a riding model, with isotropic displacement parameters taken from the attached heavy atoms and multiplied by 1.5 for methyl H atoms and by 1.2 for methylenic H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1994); cell refinement: *PARAM* in *XRAY76* (Stewart *et al.*, 1976); data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn—O11	1.955 (2)	C21—C22	1.502 (4)
Zn—O21	1.964 (2)	C22—C23	1.525 (5)
O12—C11	1.231 (4)	C23—C24	1.498 (5)
O11—C11	1.279 (4)	C24—C25	1.514 (7)
C11—C12	1.511 (4)	C25—C26	1.483 (10)
C12—C13	1.450 (6)	O12—Na1	2.368 (2)
C13—C14	1.532 (7)	Na1—O22 ⁱ	2.3567 (19)
C14—C15	1.418 (9)	Na1—O11 ⁱⁱ	2.460 (2)
C15—C16	1.535 (11)	O21—Na2	2.468 (3)
O21—C21	1.293 (4)	Na2—O22 ⁱⁱⁱ	2.451 (2)
C21—O22	1.235 (4)	Na2—O12 ^{iv}	2.520 (3)
O11 ⁱ —Zn—O11	117.64 (12)	O11—Zn—O21	119.79 (10)
O11 ⁱ —Zn—O21	102.67 (9)	O21—Zn—O21 ⁱ	92.50 (12)

Symmetry codes: (i) $1 - x, y, \frac{3}{2} - z$; (ii) $x, -y, \frac{1}{2} + z$; (iii) $x, 1 - y, \frac{1}{2} + z$; (iv) $x, 1 + y, z$.

structure: *SHELXL97*; molecular graphics: *ORTEP* (Burnett & Johnson, 1996).

The financial support of the Ministry for Science and Technology, Republic of Slovenia, through grants J1-0442 and PS-511, is gratefully acknowledged.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1361). Services for accessing these data are described at the back of the journal.

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