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Anhydrous polymeric zinc(II) octanoate

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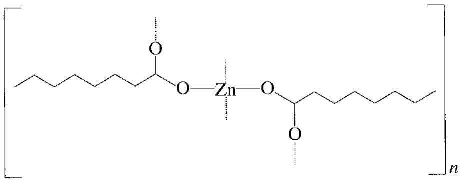
The structure of the title compound, poly[zinc(II)-bis(μ-octanoato-O:O')], $[Zn(C_8H_{15}O_2)_2]_n$, consists of polymeric sheets parallel to (100) in which tetrahedrally coordinated Zn^{2+} cations are connected by carboxylate bridges in a *syn–anti* arrangement.

Comment

The elucidation of the structure of the title compound, (I), follows that already performed for zinc heptanoate, (II) (Peultier *et al.*, 1999). It was undertaken to characterize as well as possible these metal soaps which protect zinc surfaces against corrosion, and to understand the evolution of the structural properties in the $Zn(C_nH_{2n-1}O_2)_2$ series according to n, the number of C atoms in the aliphatic chain.



(I)

Compound (I) clearly shows the structural features of the previously known members of the series, namely, n = 2 (acetate; Clegg *et al.*, 1987; Frada, 1992), n = 3 (propionate; Clegg *et al.*, 1986), n = 4 (butanoate; Blair *et al.*, 1993) and n = 6 (hexanoate; Segedin *et al.*, 1999). The structure is layered, as shown in Fig. 1. Each Zn atom is tetrahedrally coordinated by O atoms belonging to four different octanoate groups (Fig. 2). The Zn tetrahedra are connected by *syn–anti* bridges of the octanoate groups, thus forming layers parallel to (100). The chains constituted by the C2n atoms form an angle of approximately 60°, confirming the tendency of these angles to decrease when n increases (Peultier *et al.*, 1999).

It is mainly the stacking mode of the layers which varies according to n. For example, the addition of a C atom in going from zinc heptanoate to zinc octanoate results in the structure changing from one in which the planes containing the C2n chains of two adjacent layers form an angle of approximately 120° to one in which they are parallel. The structure of (I) (Pc) can be deduced from that of (II) [$Pbc2_1$, a = 4.7651 (6), b = 9.3404 (15) and c = 37.066 (6) Å] by carrying out a rotation of 180° of a layer on two around the c axis, followed by a translation of 4.14 Å along the b axis. This modification in stacking involves the loss of the 2_1 axis parallel with the c axis and of the c glide mirror perpendicular to the b axis, but preserves the b glide mirror perpendicular to the a axis. According to the orientation used to describe the structure of (I), the element of symmetry which is preserved is a c glide mirror perpendicular to the monoclinic b axis, which for (I) leads to a non-centrosymmetric and monoclinic structure (Pc).

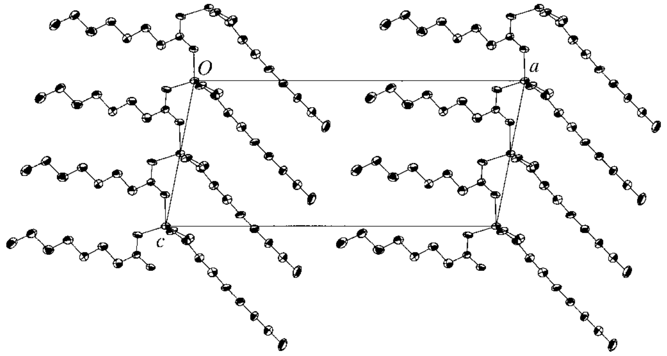


Figure 1
Projection of the structure of (I) along [010] (*ATOMS for Windows*; Dowty, 1995). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

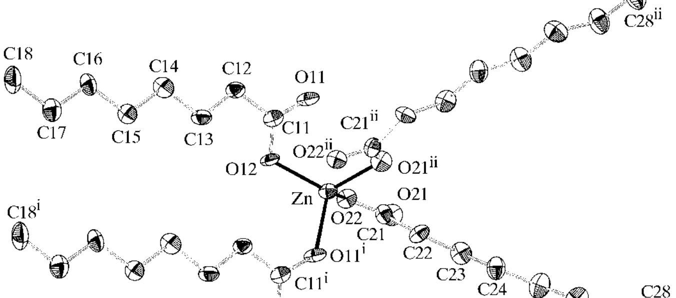


Figure 2
The Zn^{II} tetrahedral environment in (I) showing the orientation of the linear octanoate chains. Displacement ellipsoids are drawn at the 50% probability level (*ATOMS for Windows*; Dowty, 1995). Symmetry codes are as given in Table 1. H atoms have been omitted for clarity.

Experimental

Anhydrous zinc(II) octanoate was synthesized by adding a solution of sodium octanoate in aqueous medium to a weakly acidic solution of zinc nitrate (pH 5.5). The precipitate, (I), was washed with distilled water and dried. Finally, compound (I) was recrystallized from ethanol at room temperature. Colourless crystals appeared as small plates with well developed (100) faces.

Crystal data

$[Zn(C_8H_{15}O_2)_2]$
$M_r = 351.79$
Monoclinic, Pc
$a = 21.093$ (2) Å
$b = 4.6905$ (3) Å
$c = 9.2544$ (9) Å
$\beta = 101.323$ (3)°
$V = 897.78$ (14) Å^3
$Z = 2$
$D_x = 1.301$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 62 153 reflections
$\theta = 0.998$–27.49°
$\mu = 1.380$ mm^{-1}
$T = 150$ (2) K
Plate, colourless
0.30 × 0.20 × 0.02 mm

Data collection

Nonius CCD area detector diffractometer
CCD scans
Absorption correction: empirical, fitted by spherical harmonic functions (*SORTAV*; Blessing, 1995)
$T_{\min} = 0.751$, $T_{\max} = 0.976$
14 913 measured reflections
1574 independent reflections (plus 1410 Friedel-related reflections)
2231 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.095$
$\theta_{\max} = 24.74°$
$h = -24 \rightarrow 24$
$k = -5 \rightarrow 5$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.167$
$S = 1.002$
2984 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0790P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.007$
$\Delta\rho_{\max} = 0.574$ e Å^{-3}
$\Delta\rho_{\min} = -0.662$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.02 (3)

H atoms were placed geometrically but their parameters were not refined. Their individual isotropic displacement parameters were fixed [$U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$].

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS for Windows* (Dowty, 1995); software used to prepare material for publication: *WINWORD* (Version 5.0).

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Table 1
Selected geometric parameters (Å, °).

Zn—O12	1.965 (6)	Zn—O21$^{\rm ii}$	1.988 (6)
Zn—O22	1.966 (5)	O11—C11	1.272 (11)
Zn—O11$^{\rm i}$	1.971 (6)	O12—C11	1.242 (11)
O12—Zn—O22	112.8 (3)	O12—C11—O11	120.4 (8)
O12—Zn—O11$^{\rm i}$	105.1 (3)	O12—C11—C12	118.9 (8)
O22—Zn—O11$^{\rm i}$	102.5 (2)	O11—C11—C12	120.7 (8)
O12—Zn—O21$^{\rm ii}$	115.6 (3)	C21—O21—Zn$^{\rm iv}$	112.0 (6)
O22—Zn—O21$^{\rm ii}$	103.2 (2)	C21—O22—Zn	128.3 (5)
O11$^{\rm i}$—Zn—O21$^{\rm ii}$	117.1 (3)	O21—C21—O22	121.1 (8)
C11—O11—Zn$^{\rm iii}$	133.0 (6)	O21—C21—C22	118.2 (8)
C11—O12—Zn	114.3 (6)	O22—C21—C22	120.7 (7)

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

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1351). Services for accessing these data are described at the back of the journal.

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