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Poly[μ-salicylato-lead(II)]

Qing Yu, Xiu-Qing Zhang, Ji-Hua Deng, He-Dong Bian and Hong Liang*

College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China

Correspondence e-mail: bianhd@mailbox.gxnu.edu.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.030 Å
R factor = 0.076
wR factor = 0.214
Data-to-parameter ratio = 12.0

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

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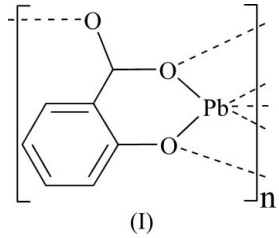
In the title compound, $[Pb(C_7H_4O_3)]_n$, the Pb^{II} atom is coordinated by five O atoms from four salicylic acid ligands with Pb—O distances of 2.318 (16)–2.605 (15) Å. Each ligand acts in a pentadentate mode that leads to the formation of a two-dimensional polymeric network.

Comment

Pb^{II} cations form a range of coordination polymers and polynuclear complexes which display various structural features as a consequence of the large ionic radius, adoption of different coordination modes and the possible occurrence of a stereochemically active lone pair of electrons (Parr, 1997). The absence of crystal field stabilization energy effects also allows the Pb^{II} cations to adopt a range of different coordination geometries not restricted to octahedral, tetrahedral or square-planar (Foreman *et al.*, 2000). We report here the crystal structure of the title compound, (I), a Pb^{II} complex with sa (H_2sa = salicylic acid).



(I)

In (I) (Fig. 1), each sa anion has short contacts with four Pb^{2+} ions through the O atoms. The salicylic anion is tridentate through its carboxy group and bidentate through its phenol O atom. Each Pb^{II} atom is associated with four salicylic anions. The coordination geometry around the Pb^{II} atom may be regarded as midway between square pyramidal and trigonal bipyramidal as described by the τ parameter of 0.69 (Addison *et al.*, 1984). The Pb—O bond distances (Table 1) are reasonable for complexes of this type and agree well with published results (Li *et al.*, 2003).

In the literature, most salicylic acids act as monodentate, bidentate or tridentate ligands (Coyle *et al.*, 2004; Tan *et al.*, 1995; Tan & Tang, 1996). However, in our case, each sa ligand acts in a pentadentate mode that leads to the formation of two-dimensional polymeric layers of two kinds, which differ in the orientations of the benzene rings. These layers are packed alternating along the *b* axis (Fig. 2).

Experimental

Salicylic acid (0.1380 g, 1.0 mmol) was dissolved in ethanol (5 ml), and a solution of $Pb(CH_3COO)_2{\cdot}3H_2O$ (0.3793 g, 1.0 mmol) in water

(5 ml) was added. The mixture was stirred at 333 K for 3 h and then cooled and filtered. The filtrate was allowed to evaporate slowly at room temperature. One month later, an orange block crystal was obtained.

Crystal data

$[Pb(C_7H_4O_3)]$	$Z = 4$
$M_r = 343.29$	$D_x = 3.251$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.8137$ (18) Å	$\mu = 24.00$ mm^{-1}
$b = 18.890$ (5) Å	$T = 298$ (2) K
$c = 6.8843$ (18) Å	Block, orange
$\beta = 111.906$ (3)°	0.36 × 0.12 × 0.10 mm
$V = 701.5$ (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3496 measured reflections
φ and ω scans	1210 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	966 reflections with $I > 2\sigma(I)$
$T_{min} = 0.04$, $T_{max} = 0.09$	$R_{int} = 0.080$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1574P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.076$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.214$	$\Delta\rho_{max} = 6.35$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -6.51$ e Å^{-3}
1210 reflections	Extinction correction: *SHELXL97*
101 parameters	Extinction coefficient: 0.0063 (15)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Pb1—O3^{i}	2.318 (16)	Pb1—O3	2.499 (15)
Pb1—O2	2.437 (15)	Pb1—O1^{iii}	2.605 (15)
Pb1—O2^{ii}	2.465 (14)		
O3^{i}—Pb1—O2	89.5 (5)	O2^{ii}—Pb1—O3	126.6 (5)
O3^{i}—Pb1—O2^{ii}	82.6 (5)	O3^{i}—Pb1—O1^{iii}	80.4 (5)
O2—Pb1—O2^{ii}	64.5 (6)	O2—Pb1—O1^{iii}	168.2 (5)
O3^{i}—Pb1—O3	71.9 (6)	O2^{ii}—Pb1—O1^{iii}	119.7 (5)
O2—Pb1—O3	69.0 (5)	O3—Pb1—O1^{iii}	101.7 (5)

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z$; (iii) $x-1, y, z-1$.

H atoms were positioned geometrically and refined using a riding model, with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron density peak and deepest hole are located 0.98 and 0.97 Å from atom Pb1, respectively.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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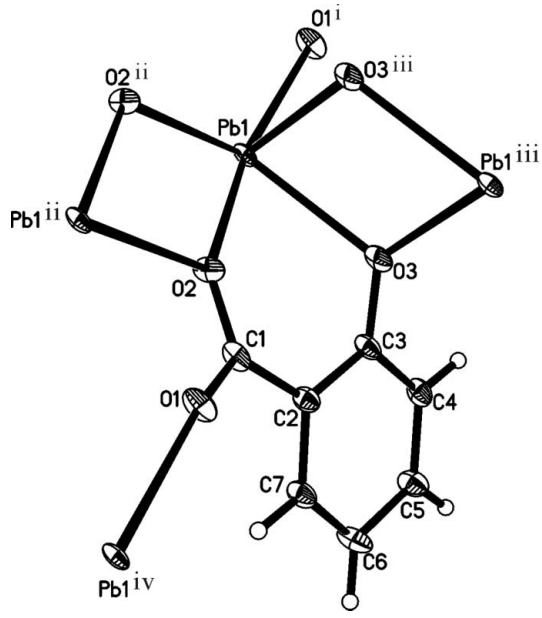

Figure 1
View of a segment of (I) with the atom-labelling scheme and displacement ellipsoids at the 30% probability level [symmetry codes: (i) $-1+x, y, -1+z$; (ii) $1-x, 1-y, -z$; (iii) $-x, 1-y, -z$; (iv) $1+x, y, 1+z$].

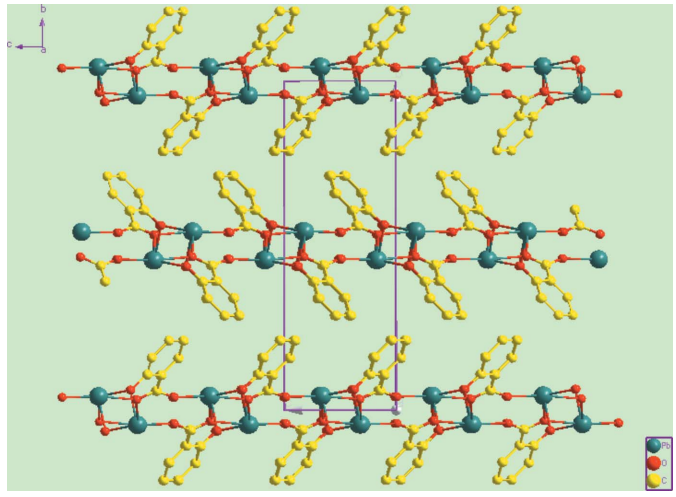

Figure 2
The crystal packing of (I), viewed along the *a* axis and showing alternating two-dimensional polymeric layers. H atoms have been omitted for clarity.

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