

**Ai-Qing Ma, Long-Guan Zhu\*  
 and Guo-Qiang Cai**

Department of Chemistry, Zhejiang University,  
 Hangzhou 310027, People's Republic of China

Correspondence e-mail: chezlq@zju.edu.cn

**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(C-C)$  = 0.009 Å  
 R factor = 0.027  
 wR factor = 0.070  
 Data-to-parameter ratio = 11.7

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

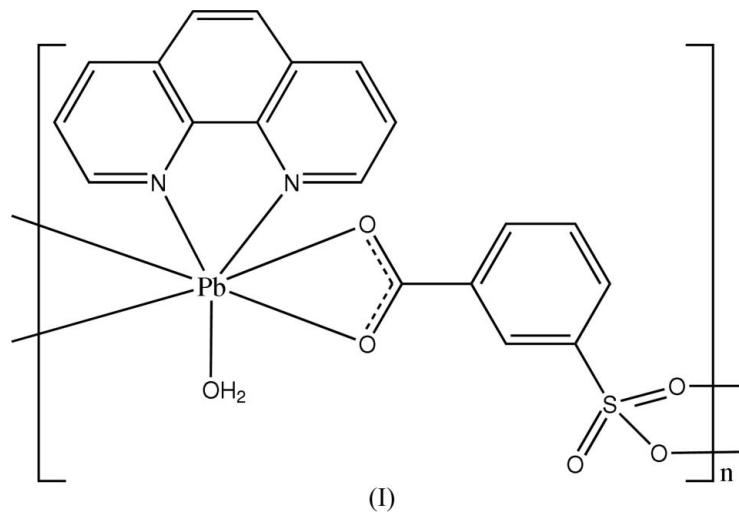
**Poly[[aqua(1,10-phenanthroline)lead(II)]-  
 $\mu_3$ -3-sulfonatobenzoato]**

In the title compound,  $[Pb(C_7H_4O_5S)(C_{12}H_8N_2)(H_2O)]_n$ , each  $Pb^{II}$  atom is coordinated by five O atoms from one water molecule and three 3-sulfonatobenzoate ligands and two N atoms from one 1,10-phenanthroline. The 3-sulfonatobenzoate ligand serves as a  $\mu_3$ -bridge, linking three  $Pb^{II}$  atoms, and extends the structure into a one-dimensional ladder. The O—H...O hydrogen bonds generate a two-dimensional layer and enhance the stability of the structure.

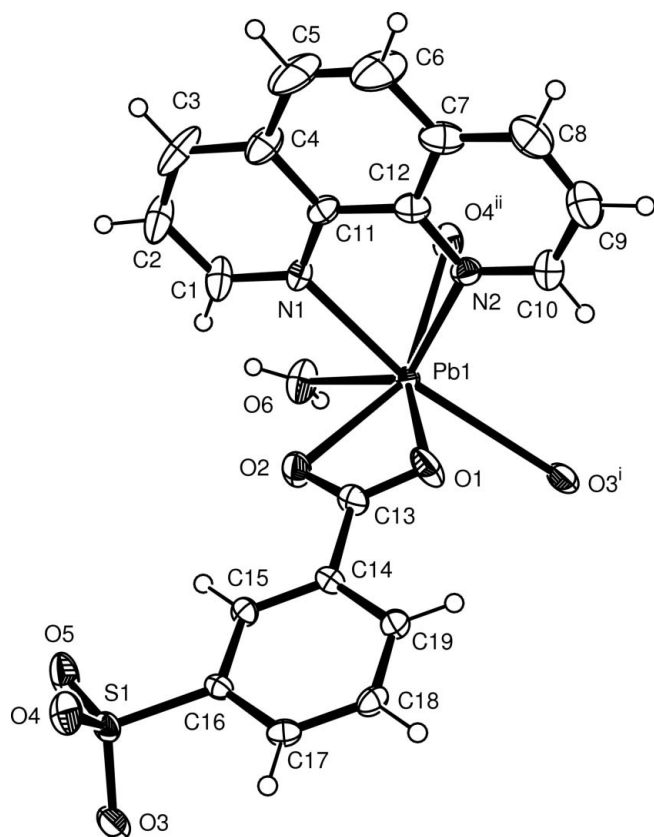
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**Comment**

The structure of the 4-sulfonatobenzoate–lead(II) compound with 1,10-phenanthroline (phen) is a two-dimensional layer (Zhang *et al.*, 2005); however, in the case of 2-sulfonatobenzoate, the structure of the lead(II) compound is a dimer (Li & Yang, 2004). As part of a systematic investigation on sulfobenzoate lead(II) compounds, we present here the 3-sulfonatobenzoate–lead(II) compound, (I).



In (I), the  $Pb^{II}$  atom is coordinated by two N-atom donors from one phen, four O atoms [two from a carboxyl and two from two sulfonate groups of three different 3-sulfonatobenzoato (3-sb) ligands] and one O atom from one water molecule (Fig. 1 and Table 1). A bonding limit to  $<3.10$  Å of Pb—O was applied to search the lead(II) coordination sphere (Soudi *et al.*, 2005); thus, seven-coordinate geometry in the title compound is proposed. The 3-sb chelates a  $Pb^{II}$  atom using its carboxylate group and bridges two other  $Pb^{II}$  atoms in a skew-skew mode using its sulfonate group; thus the  $\mu_3$ -3-sb extends the structure into a ladder-like chain (Fig. 2) in which the shortest Pb...Pb separations by the sulfonate and the 3-sb are 5.2165 (5) and 8.9811 (7) Å, respectively. O—

**Figure 1**

View of a segment of (I). Displacement ellipsoids are drawn at the 40% probability level. [Symmetry codes: (i)  $-x, 1 - y, -z$ ; (ii)  $x, -1 + y, z$ .]

H $\cdots$ O hydrogen bonds give rise to a two-dimensional layer (Table 2), enhancing the stability of the structure.

## Experimental

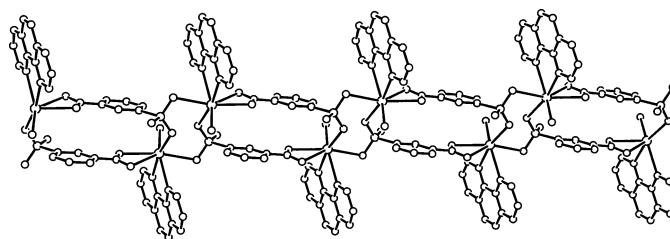
A mixture of  $\text{Pb}(\text{NO}_3)_2$  (0.076 g, 0.23 mmol), sodium hydrogen 3-sulfobenzoate (0.046 g, 0.21 mmol), 1,10-phenanthroline monohydrate (0.041 g, 0.21 mmol) and water (10 ml) was heated at 423 K for 54 h in a 20 ml Teflon-lined stainless steel autoclave. After cooling to room temperature, pale-yellow plate-shaped crystals of (I) were obtained.

### Crystal data

$[\text{Pb}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$	$Z = 2$
$M_r = 605.57$	$D_x = 2.208 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 6.8033$ (6) Å	Cell parameters from 5025 reflections
$b = 11.1687$ (10) Å	$\theta = 2.3\text{--}27.9^\circ$
$c = 12.6787$ (11) Å	$\mu = 9.42 \text{ mm}^{-1}$
$\alpha = 99.684$ (1) $^\circ$	$T = 295$ (2) K
$\beta = 98.109$ (1) $^\circ$	Block, pale yellow
$\gamma = 102.614$ (1) $^\circ$	$0.16 \times 0.12 \times 0.11 \text{ mm}$
$V = 910.76$ (14) Å $^3$	

### Data collection

Bruker APEX area-detector diffractometer	3148 independent reflections
$\varphi$ and $\omega$ scans	2993 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.026$
$T_{\text{min}} = 0.273, T_{\text{max}} = 0.361$	$\theta_{\text{max}} = 25.0^\circ$
6518 measured reflections	$h = -8 \rightarrow 8$
	$k = -13 \rightarrow 12$
	$l = -15 \rightarrow 14$

**Figure 2**

View of the ladder-like chain in (I). H atoms have been omitted for clarity.

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.027$   
 $wR(F^2) = 0.070$   
 $S = 1.14$   
 3148 reflections  
 268 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0409P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.62 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.97 \text{ e \AA}^{-3}$

**Table 1**

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

Pb1—O1	2.565 (4)	Pb1—N1	2.505 (4)
Pb1—O2	2.589 (4)	Pb1—N2	2.539 (4)
Pb1—O3 <sup>i</sup>	3.036 (4)	S1—O3	1.461 (4)
Pb1—O4 <sup>ii</sup>	2.683 (4)	S1—O4	1.466 (4)
Pb1—O6	2.641 (4)	S1—O5	1.444 (4)
N1—Pb1—N2	65.43 (14)	O1—Pb1—O4 <sup>ii</sup>	145.32 (13)
N1—Pb1—O1	97.97 (15)	O2—Pb1—O4 <sup>ii</sup>	150.62 (13)
N2—Pb1—O1	75.17 (14)	O6—Pb1—O4 <sup>ii</sup>	78.71 (15)
N1—Pb1—O2	74.54 (15)	N1—Pb1—O3 <sup>i</sup>	166.16 (13)
N2—Pb1—O2	104.63 (15)	N2—Pb1—O3 <sup>i</sup>	100.75 (13)
O1—Pb1—O2	50.25 (13)	O1—Pb1—O3 <sup>i</sup>	78.26 (14)
N1—Pb1—O6	79.96 (14)	O2—Pb1—O3 <sup>i</sup>	111.53 (12)
N2—Pb1—O6	138.16 (15)	O6—Pb1—O3 <sup>i</sup>	112.21 (13)
O1—Pb1—O6	135.03 (15)	O4 <sup>ii</sup> —Pb1—O3 <sup>i</sup>	97.66 (12)
O2—Pb1—O6	86.97 (15)	O5—S1—O3	113.8 (3)
N1—Pb1—O4 <sup>ii</sup>	77.75 (14)	O5—S1—O4	113.5 (3)
N2—Pb1—O4 <sup>ii</sup>	71.81 (13)	O3—S1—O4	110.9 (3)

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

**Table 2**

Hydrogen-bond geometry (Å,  $^\circ$ ).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O6—H6B $\cdots$ O1 <sup>iii</sup>	0.85 (5)	1.89 (4)	2.729 (6)	170 (7)
O6—H6A $\cdots$ O5 <sup>iv</sup>	0.85 (4)	2.27 (4)	3.054 (7)	153 (6)

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

The C-bound H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The O-bound H atoms were located in difference Fourier maps and refined with a distance restraint of O—H = 0.85 (1) Å and  $U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$ . The deepest peak in the final difference Fourier map was 0.93 Å from atom C3.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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