

Poly[aqua(2,2'-bipyridine)( $\mu_3$ -3-sulfonatobenzoato)-lead(II)]Long-Guan Zhu<sup>a\*</sup> and Hong-Ping Xiao<sup>b</sup><sup>a</sup>Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China, and <sup>b</sup>School of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China

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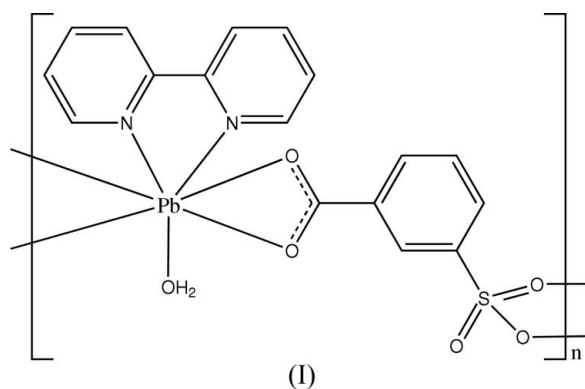
## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.010$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.078  
Data-to-parameter ratio = 12.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title polymeric complex,  $[\text{Pb}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$ , each  $\text{Pb}^{\text{II}}$  atom has a seven-coordinate geometry. The 3-sulfonatobenzoate ligand acts as a  $\mu_3$ -bridging linker, generating a one-dimensional ladder. The packing is further stabilized by an  $\text{O}-\text{H}\cdots\text{O}$  hydrogen-bonding network.

## Comment

Benzenedicarboxylate metal complexes exhibit interesting and diverse topologies (Xiao & Zhu, 2003; Zhu *et al.*, 2004). In order to compare the coordination modes of sulfonate and carboxylate groups, we have recently reported several 4-sulfonatobenzoate (Fan, Xiao, Zhang, Cai & Zhu, 2004; Fan, Xiao, Zhang & Zhu, 2004; Zhang & Zhu, 2005*a,b,c*) and 2-sulfonatobenzoate metal complexes (Xiao, 2005; Xiao, Li & Hu, 2005; Xiao, Shi & Cheng, 2005). As expected, both ligands led to a variety of interesting architectures. We have now synthesized the title 3-sulfonatobenzoate lead(II) complex, (I), and the results are presented here.

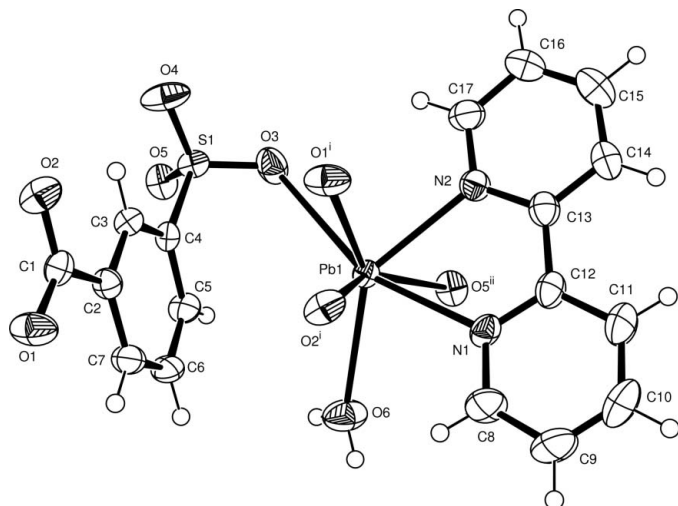


In (I), the  $\text{Pb}^{\text{II}}$  atom adopts a seven-coordinate geometry, involving two N donors from one 2,2'-bipyridine ligand, four O atoms [two from a carboxylate group and two from two sulfonyl groups of three different 3-sulfonatobenzoate (3-sb) ligands] and one O atom from the water molecule (Fig. 1 and Table 1).  $\text{Pb}^{\text{II}}$  coordination geometry is largely affected by the stereochemical activity of valence-shell electron lone pairs (Shimoni-Livny *et al.*, 1998). In our recent work on Pb complexes, we have used a bond-length limit of 3.10 Å (Soudi *et al.*, 2005) to define a reasonable coordination sphere around the  $\text{Pb}^{\text{II}}$  atom. Therefore, in the title compound we have accepted the seven-coordinate geometry for the  $\text{Pb}^{\text{II}}$  atom, even though the  $\text{Pb}1-\text{O}3$  bond, at 2.966 (5) Å, is significantly longer than the other six  $\text{Pb}-\text{O}$  bonds. The carboxylate group of the 3-sb ligand chelates a  $\text{Pb}^{\text{II}}$  atom, while the sulfonate group links two  $\text{Pb}^{\text{II}}$  atoms in a skew-skew bridging mode,

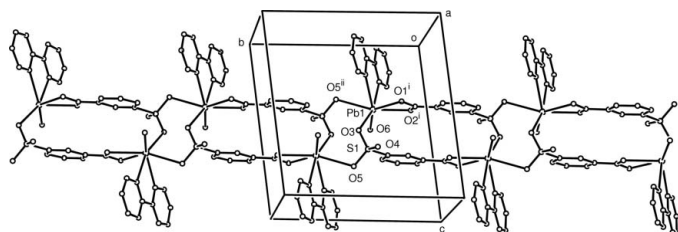
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**Figure 1**  
A view of a segment of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes (i):  $2 - x, -y, 1 - z$ ; (ii):  $2 - x, 1 - y, 1 - z$ .]



**Figure 2**  
A view of the ladder-like chain of (I). H atoms have been omitted for clarity. The symmetry codes are as in Fig. 1.

with a  $\text{Pb} \cdots \text{Pb}$  separation of  $5.2414(4) \text{ \AA}$ . Thus, the bridging 3-sb ligands generate a ladder-like chain (Fig. 2). The packing is further stabilized by an extensive network of  $\text{O} \cdots \text{H} \cdots \text{O}$  hydrogen bonds (Table 2), which links the chains into two-dimensional layers (Fig. 3).

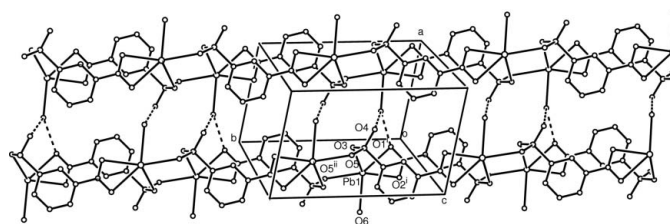
## Experimental

A mixture of  $\text{Pb}(\text{NO}_3)_2$  (0.126 g, 0.38 mmol), sodium hydrogen 3-sulfonatobenzoate (0.063 g, 0.28 mmol), 2,2'-bipyridine (0.053 g, 0.34 mmol) and water (10 ml) was heated at 423 K for 51 h in a 20 ml Teflon-lined stainless steel autoclave. After cooling to room temperature, the mixture was filtered and the resulting solution was put aside. Pale-yellow block-shaped crystals of (I) were obtained after 10 d.

### Crystal data

$[\text{Pb}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$   
 $M_r = 581.55$   
 Triclinic,  $P\bar{1}$   
 $a = 7.0098(4) \text{ \AA}$   
 $b = 11.2360(7) \text{ \AA}$   
 $c = 11.6818(7) \text{ \AA}$   
 $\alpha = 98.227(1)^\circ$   
 $\beta = 98.147(1)^\circ$   
 $\gamma = 102.232(1)^\circ$   
 $V = 875.75(9) \text{ \AA}^3$

$Z = 2$   
 $D_x = 2.205 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 3723 reflections  
 $\theta = 2.8\text{--}28.0^\circ$   
 $\mu = 9.79 \text{ mm}^{-1}$   
 $T = 295(2) \text{ K}$   
 Block, pale yellow  
 $0.18 \times 0.15 \times 0.07 \text{ mm}$



**Figure 3**  
A view of the packing of (I), showing the hydrogen bonds (dashed lines) linking the ladder-like chains in two dimensions. The symmetry codes are as in Fig. 1.

### Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
 $T_{\min} = 0.185, T_{\max} = 0.508$   
 4803 measured reflections

3210 independent reflections  
 3069 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.019$   
 $\theta_{\max} = 25.5^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -13 \rightarrow 13$   
 $l = -14 \rightarrow 13$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.078$   
 $S = 1.05$   
 3210 reflections  
 250 parameters

H-atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0524P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 2.08 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -1.55 \text{ e \AA}^{-3}$

**Table 1**

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

Pb1—O1 <sup>i</sup>	2.607 (4)	Pb1—N2	2.515 (5)
Pb1—O2 <sup>i</sup>	2.543 (4)	S1—O3	1.459 (5)
Pb1—O3	2.966 (5)	S1—O4	1.440 (5)
Pb1—O5 <sup>ii</sup>	2.689 (4)	S1—O5	1.451 (5)
Pb1—O6	2.680 (5)	O1—C1	1.260 (7)
Pb1—N1	2.511 (5)	O2—C1	1.250 (8)
O2 <sup>i</sup> —Pb1—O1 <sup>i</sup>	50.53 (14)	O5 <sup>ii</sup> —Pb1—O3	94.41 (14)
O1 <sup>i</sup> —Pb1—O3	76.52 (15)	O6—Pb1—O3	117.93 (15)
O1 <sup>i</sup> —Pb1—O5 <sup>ii</sup>	143.95 (15)	N1—Pb1—O3	158.46 (15)
O1 <sup>i</sup> —Pb1—O6	136.36 (17)	N2—Pb1—O3	94.25 (15)
N1—Pb1—O1 <sup>i</sup>	98.92 (16)	O6—Pb1—O5 <sup>ii</sup>	78.85 (17)
N2—Pb1—O1 <sup>i</sup>	74.58 (16)	N1—Pb1—O5 <sup>ii</sup>	76.79 (15)
O2 <sup>i</sup> —Pb1—O3	113.63 (14)	N2—Pb1—O5 <sup>ii</sup>	71.37 (15)
O2 <sup>i</sup> —Pb1—O5 <sup>ii</sup>	151.96 (15)	N1—Pb1—O6	80.07 (16)
O2 <sup>i</sup> —Pb1—O6	87.76 (16)	N2—Pb1—O6	137.58 (18)
N1—Pb1—O2 <sup>i</sup>	76.70 (15)	N1—Pb1—N2	64.39 (16)
N2—Pb1—O2 <sup>i</sup>	104.73 (16)		

Symmetry codes: (i)  $-x + 2, -y, -z + 1$ ; (ii)  $-x + 2, -y + 1, -z + 1$ .

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

$D\text{---}H \cdots A$	$D\text{---}H$	$H \cdots A$	$D \cdots A$	$D\text{---}H \cdots A$
O6—H6A $\cdots$ O4 <sup>iii</sup>	0.85 (5)	2.21 (4)	2.982 (8)	151 (6)
O6—H6B $\cdots$ O1 <sup>iv</sup>	0.85 (5)	1.91 (5)	2.756 (7)	175 (7)

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

All aromatic H atoms were placed in calculated positions, with  $C\text{---}H = 0.93 \text{ \AA}$ , and refined as riding atoms, with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ . Water H atoms molecule were located in a difference Fourier map

and refined with a distance restraint of O—H = 0.85 (1) Å and a fixed isotropic displacement parameter of  $U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$ . The highest peak and deepest hole in the final difference Fourier map are 0.93 Å and 1.10 Å from atom Pb1, respectively.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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