

**Zheng Zhang, Yi-Li Zhou and  
Hong-Yin He\***Biological and Chemical Engineering School,  
Jiaxing College, Jiaxing 314001, People's  
Republic of China

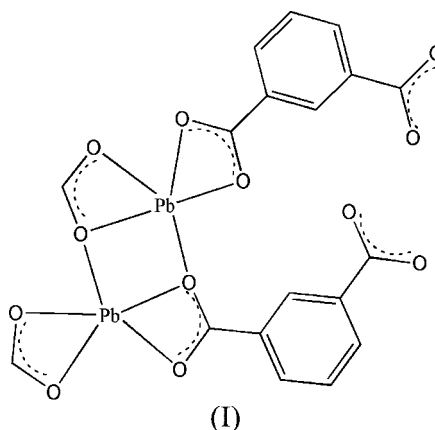
Correspondence e-mail: hhy123@163.com

**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.013$  Å  
 $R$  factor = 0.035  
 $wR$  factor = 0.072  
Data-to-parameter ratio = 11.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Poly[ $\mu$ -isophthalato-lead(II)]**

In the title compound,  $[\text{Pb}(\text{C}_8\text{H}_4\text{O}_4)]_n$ , the  $\text{Pb}^{\text{II}}$  atoms adopt very asymmetric six- and seven-coordinate geometries due to their stereochemically active lone pairs. The isophthalate (benzene-1,3-dicarboxylate) dianions bridge the Pb atoms into a three-dimensional framework. Aromatic  $\pi$ - $\pi$  stacking and a possible  $\text{Pb} \cdots \pi$  interaction are also seen in this structure.

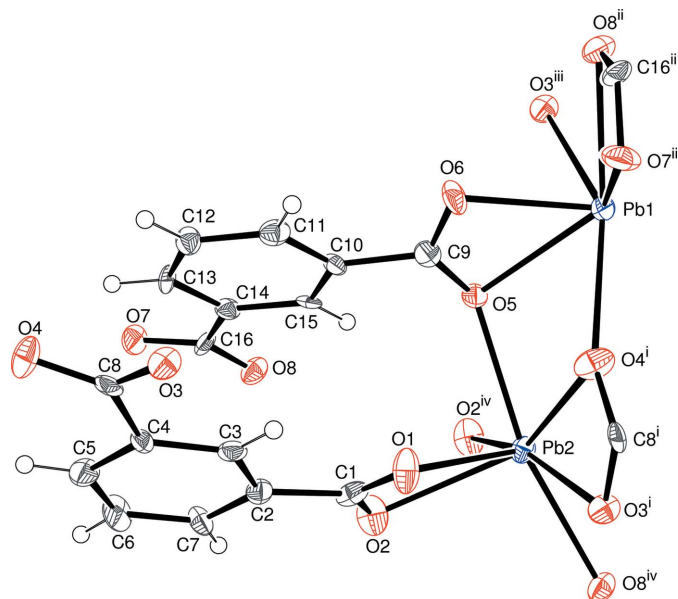
Received 20 June 2006  
Accepted 13 August 2006**Comment**

Coordination polymers containing transition metal cations and isophthalate (benzene-1,3-dicarboxylate; 1,3-bdc) dianions have been extensively studied (*e.g.* Moulton *et al.*, 2003). Conversely, main-group metal-1,3-bdc complexes are rare. Recently a few lead(II) complexes with 1,3-bdc have been synthesized, including  $[\text{Pb}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)]_n$  (Wang *et al.*, 2005). Here, we report the title compound, (I), in which the  $\text{Pb}^{\text{II}}$  atoms adopt two different, irregular, coordination geometries (Fig. 1 and Table 1). The Pb1 and Pb2 species are coordinated by six and seven O atoms, respectively. These asymmetric geometries presumably arise due to the stereochemically active lone pair of electrons on the cation.

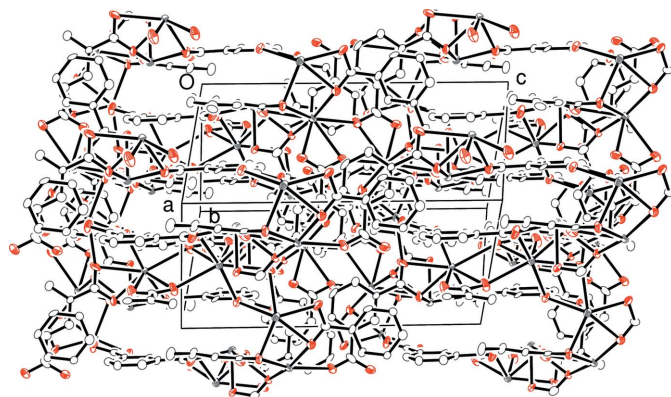


The 1,3-bdc species are normal. Their roughly equal C—O bond lengths for each carboxylate group (Table 1) suggest that the negative charge of these groups is delocalized. The C1/O1/O2 and C8/O3/O4 groups make dihedral angles of 10.3 (17) and 14.2 (9)°, respectively, with their attached benzene ring (C2–C7). C9/O5/O6 and C16/O7/O8 make dihedral angles of 17.7 (13) and 7.2 (8)°, respectively, with the C10–C15 benzene ring.

The 1,3-bdc ligands coordinate to the  $\text{Pb}^{\text{II}}$  atoms, the C1 molecules acting as a  $\mu_5$ -bridge ( $\mu_2$  from one carboxylate group and  $\mu_3$  from the other) and the C9 molecule functions as a  $\mu_4$  ( $\mu_2 + \mu_2$ ) bridge. This bridging mode results in a



**Figure 1**  
View of (I) expanded to show the Pb-atom coordinations. Displacement ellipsoids are drawn at the 50% probability level (H atoms are represented by arbitrary spheres). Symmetry codes: (i)  $\frac{3}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (ii)  $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$ ; (iii)  $x - 1, y, z$ ; (iv)  $1 - x, -y, 1 - z$ .



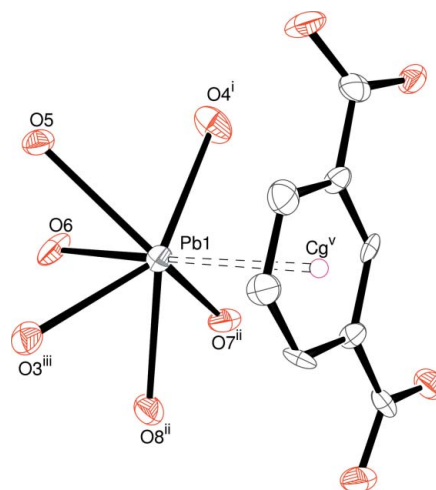
**Figure 2**  
The packing of (I), showing 50% displacement ellipsoids (H atoms have been omitted for clarity).

complex three-dimensional framework (Fig. 2) that appears to possess small squashed channels propagating in [110].

Aromatic  $\pi$ - $\pi$  stacking occurs in (I), the separation between the centroids of the C2–C7 and C10–C15 benzene rings being 3.624 (6) Å. Additionally, an unusual Pb1... $\pi$  interaction (Fig. 3) with a Pb to ring-centroid separation of 3.121 (4) Å is present.

### Experimental

A mixture of Pb(NO<sub>3</sub>)<sub>2</sub> (0.0985 g, 0.3 mmol), benzene-1,3-dicarboxylic acid (0.0575 g, 0.3 mmol), 4-aminopyridine (0.0510 g, 0.54 mmol), 1 ml 0.1 M NaOH and 10 ml water was heated at 393 K for 5 d in a 20 ml Teflon-lined stainless steel autoclave. After cooling, colourless needles of (I) were obtained.



**Figure 3**  
Detail of (I), showing the possible Pb1... $\pi$  interaction (50% displacement ellipsoids and H atoms omitted for clarity). The symmetry codes are as in Fig. 1; additionally, (v)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ . Cg is the centroid of the C9–C15 benzene ring.

### Crystal data

[Pb(C<sub>8</sub>H<sub>4</sub>O<sub>4</sub>)]  
M<sub>r</sub> = 371.30  
Monoclinic, P2<sub>1</sub>/n  
a = 8.6132 (19) Å  
b = 11.032 (2) Å  
c = 17.008 (4) Å  
 $\beta$  = 98.393 (3)°  
V = 1598.8 (6) Å<sup>3</sup>

Z = 8  
D<sub>x</sub> = 3.085 Mg m<sup>-3</sup>  
Mo K $\alpha$  radiation  
 $\mu$  = 21.08 mm<sup>-1</sup>  
T = 293 (2) K  
Needle, colourless  
0.26 × 0.03 × 0.03 mm

### Data collection

Bruker SMART CCD diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 1997)  
T<sub>min</sub> = 0.073, T<sub>max</sub> = 0.570 (expected range = 0.068–0.531)

11038 measured reflections  
2801 independent reflections  
2376 reflections with I > 2 $\sigma$ (I)  
R<sub>int</sub> = 0.066  
 $\theta_{max}$  = 25.0°

### Refinement

Refinement on F<sup>2</sup>  
R[F<sup>2</sup> > 2 $\sigma$ (F<sup>2</sup>)] = 0.035  
wR(F<sup>2</sup>) = 0.072  
S = 1.04  
2801 reflections  
235 parameters

H-atom parameters constrained  
w = 1/[ $\sigma^2(F_o^2) + 2.3602P$ ]  
where P = (F<sub>o</sub><sup>2</sup> + 2F<sub>c</sub><sup>2</sup>)/3  
( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho_{max}$  = 1.34 e Å<sup>-3</sup>  
 $\Delta\rho_{min}$  = -1.77 e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Pb1—O6	2.365 (6)	Pb2—O2	2.756 (7)
Pb1—O7 <sup>i</sup>	2.393 (7)	Pb2—O2 <sup>iv</sup>	2.842 (7)
Pb1—O8 <sup>i</sup>	2.565 (6)	C1—O1	1.261 (12)
Pb1—O4 <sup>ii</sup>	2.597 (7)	C1—O2	1.243 (11)
Pb1—O3 <sup>iii</sup>	2.614 (6)	C8—O3	1.269 (11)
Pb1—O5	2.656 (6)	C8—O4	1.275 (10)
Pb2—O1	2.323 (7)	C9—O5	1.257 (11)
Pb2—O3 <sup>ii</sup>	2.553 (6)	C9—O6	1.263 (10)
Pb2—O5	2.604 (6)	C16—O7	1.263 (11)
Pb2—O8 <sup>iv</sup>	2.639 (6)	C16—O8	1.251 (11)
Pb2—O4 <sup>ii</sup>	2.741 (7)		

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

The H atoms were positioned geometrically (C–H = 0.93 Å) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The distance between the highest peak and the nearest heavy atom Pb1 is 1.05 Å.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; 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*.

## References

- Bruker (1997). *SADABS*, *SAINT*, *SMART* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Moulton, B., Abourahma, H., Bradner, M. W., Lu, J. J., McManus, G. J. & Zaworotko, M. J. (2003). *Chem. Commun.* pp. 1342–1343.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wang, H.-D., He, H.-Y., Wang, Y.-J., Zhu, L.-G. & Ng, S. W. (2005). *Acta Cryst. E61*, m531–m532.