Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[(1,10-phenanthroline)lead(II)]-μ_5-1,3-benzenedicarboxylato]

Hai-Dong Wang,[a] Hong-Yin He,[a] Yue-Jian Wang,[a] Long-Guan Zhu[b]* and Seik Weng Ng[c]

[a]Department of Chemical Engineering, Jiaxing College, Jiaxing 314001, People's Republic of China, [b]Department of Chemistry, Zhejiang University, Hangzhou 310007, People's Republic of China, and [c]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

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

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.028
wR factor = 0.059
Data-to-parameter ratio = 16.0

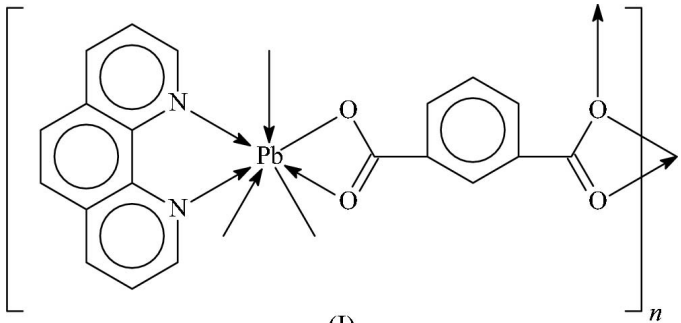
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 February 2005
Accepted 9 February 2005
Online 19 February 2005

The Pb atom in the polymeric title compound, $[Pb(C_8H_4O_4)(C_{12}H_8N_2)]_n$, is chelated by the carboxylate arms of two isophthalate dianions and bridged by one carboxylate O atom. The bridging mode of the dianion gives rise to the formation of a ladder chain.

Comment

Transition metal 1,3-benzenedicarboxylate (1,3-bdc) complexes have been extensively prepared (Moulton *et al.*, 2003), while main group metal 1,3-bdc complexes are rare. In the title compound, (I), the Pb^{II} atom adopts a seven-coordinated geometry (Fig. 1 and Table 1).



(I)

The 1,3-bdc ligand coordinates to the metal atom, acting as a μ_5-bridge. One carboxylate group is in a chelating mode, while the other is in a chelating–bridging mode. The bridging property of the carboxylate group results in a one-dimensional ladder chain (Fig. 2). In the chain, bridged carboxylate groups construct a four-membered ring, $[Pb_2O_2]$, with a Pb···Pb distance of 4.3475 (5) Å and a $[Pb_2(mbdc)_2]$ box. In the box motif, two 1,3-benzenedicarboxylate ligands are parallel and the separation of Pb···Pb by 1,3-bdc is 10.2706 (9) Å. It is worth noting that the coordination sphere can be considered as hemidirected (Shimoni-Livny *et al.*, 1998). The lone pair of electrons on the Pb atom is stereochemically active; it occupies one of the sites of the dodecahedron.

Experimental

A mixture of $Pb(NO_3)_2$ (0.02130 g, 0.64 mmol), 1,3-benzenedicarboxylic acid (0.0504 g, 0.30 mmol), 1,10-phenanthroline (0.0599 g, 0.30 mmol), NaOH (0.0148 g, 0.37 mmol) and water (10 ml) was heated at 433 K for 48 h in a 20 ml Teflon-lined stainless steel autoclave. After cooling, colorless needle-shaped crystals of (I) were obtained.

Crystal data

$[Pb(C_8H_4O_4)(C_{12}H_8N_2)]$	$Z = 2$
$M_r = 551.51$	$D_x = 2.125$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.5493$ (8) Å	Cell parameters from 3925 reflections
$b = 9.786$ (1) Å	$\theta = 2.3$–$26.7°$
$c = 13.148$ (1) Å	$\mu = 9.82$ mm^{-1}
$\alpha = 69.753$ (1)°	$T = 295$ (2) K
$\beta = 80.542$ (1)°	Needle, colorless
$\gamma = 71.340$ (1)°	0.20 × 0.07 × 0.04 mm
$V = 861.8$ (2) Å^3	

Data collection

Bruker SMART APEX area-detector diffractometer	3893 independent reflections
φ and ω scans	3451 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.038$
$T_{min} = 0.317$, $T_{max} = 0.672$	$\theta_{max} = 27.5°$
9956 measured reflections	$h = -9 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.028$	$w = 1/[\sigma^2(F_o^2) + (0.0221P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.059$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.96$	$\Delta\rho_{max} = 0.90$ e Å^{-3}
3893 reflections	$\Delta\rho_{min} = -0.82$ e Å^{-3}
244 parameters	

Table 1
Selected geometric parameters (Å, °).

Pb1—O1	2.706 (3)	Pb1—O4^{i}	2.627 (3)
Pb1—O2	2.385 (3)	Pb1—N1	2.519 (4)
Pb1—O3^{i}	2.461 (3)	Pb1—N2	2.688 (4)
Pb1—O3^{ii}	2.877 (3)		
O1—Pb1—O2	50.9 (1)	O3^{i}—Pb1—O3^{ii}	71.2 (1)
O1—Pb1—O3^{i}	131.9 (1)	O3^{i}—Pb1—O4^{i}	51.4 (1)
O1—Pb1—O3^{ii}	102.5 (1)	O3^{i}—Pb1—N1	75.3 (1)
O1—Pb1—O4^{i}	153.8 (1)	O3^{i}—Pb1—N2	119.9 (1)
O1—Pb1—N1	79.9 (1)	O3^{ii}—Pb1—O4^{i}	102.4 (1)
O1—Pb1—N2	82.4 (1)	O3^{ii}—Pb1—N1	136.3 (1)
O2—Pb1—O3^{i}	82.8 (1)	O3^{ii}—Pb1—N2	160.1 (1)
O2—Pb1—O3^{ii}	73.7 (1)	O4^{i}—Pb1—N1	76.5 (1)
O2—Pb1—O4^{i}	130.9 (1)	O4^{i}—Pb1—N2	77.0 (1)
O2—Pb1—N1	75.1 (1)	N1—Pb1—N2	63.3 (1)
O2—Pb1—N2	122.1 (1)		

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

The aromatic H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

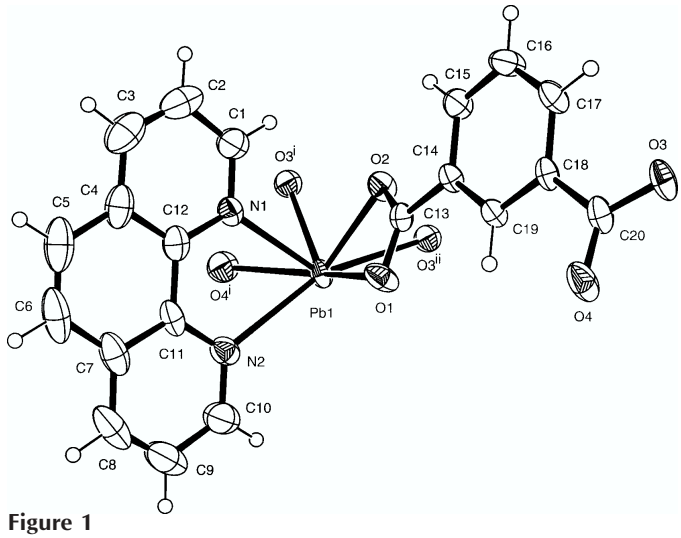


Figure 1
ORTEPII plot (Johnson, 1976) of a portion of the polymeric structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1 + x, y - 1, z$; (ii) $1 - x, 1 - y, 1 - z$.]

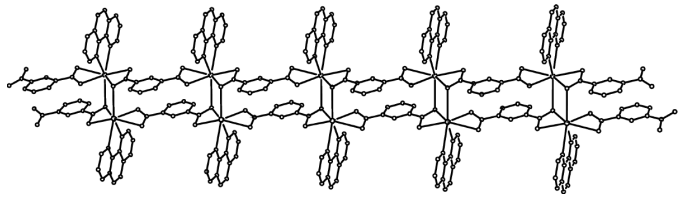


Figure 2
View of the one-dimensional ladder chain of (I). H atoms have been omitted for clarity.

We thank the Analytical and Measurement Fund of Zhejiang Province, the National Natural Science Foundation of China (50073019) and the University of Malaya for supporting this study.

References

Bruker (2002). *SADABS, SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, 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.
Shimoni-Livny, L., Glusker, J. P. & Bock, C. W. (1998). *Inorg. Chem.* **37**, 1853–1867.