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Key indicators

Single-crystal X-ray study

T = 295 K

Mean $\sigma(\text{C}-\text{C}) = 0.008 \text{ \AA}$

R factor = 0.026

wR factor = 0.060

Data-to-parameter ratio = 14.6

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[(2,2'-diamino-4,4'-bi-1,3-thiazole- κ^2N,N')lead(II)]-di- μ -isonicotinato- $\kappa^4O:O'$]**

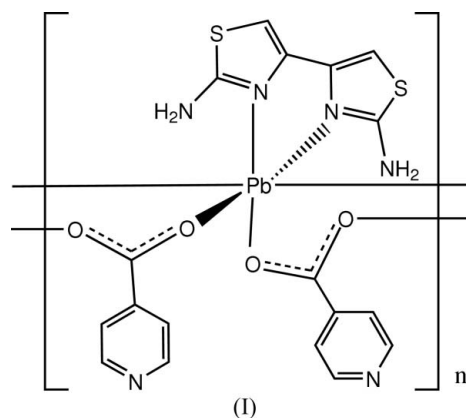
In the polymeric title compound, $[\text{Pb}(\text{C}_6\text{H}_4\text{NO}_2)_2\text{-C}_6\text{H}_6\text{N}_4\text{S}_2]_n$, the Pb^{II} ion is located on a twofold axis and coordinated by one N,N' -bidentate diaminobithiazole (DABT) ligand and four O-monodentate isonicotinate anions in a very distorted $\text{cis-PbN}_2\text{O}_4$ octahedral geometry. The carboxylate group of the isonicotinate anion bridges two Pb^{II} ions, forming a polymeric chain. The complete DABT molecule is generated by twofold symmetry; its two thiazole rings are twisted with a dihedral angle of $9.5 (2)^\circ$. There are no $\pi-\pi$ stacking interactions in the title compound, but $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds help to stabilize the structure.

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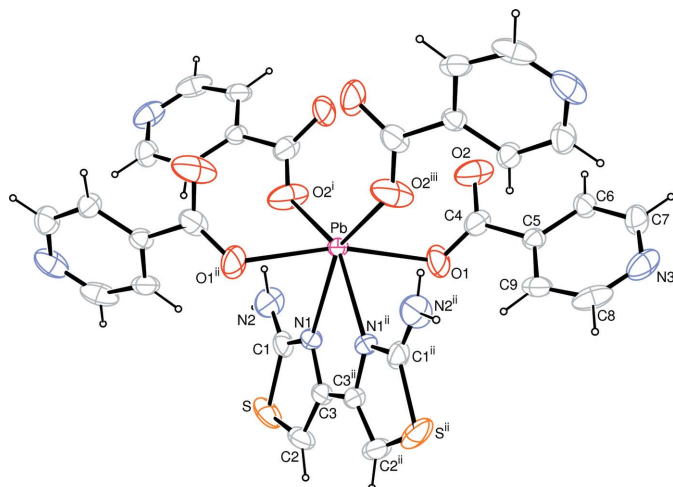
Comment

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential applications in the field of soft magnetic materials (Sun *et al.*, 1997). As a continuation of our investigations of metal complexes with DABT (Liu *et al.*, 2003), the title Pb^{II} complex, (I), has been prepared and its X-ray crystal structure is presented here.

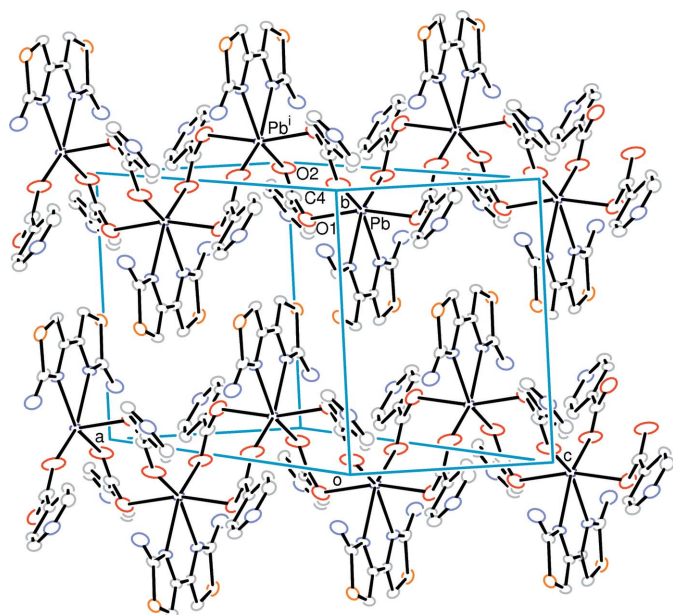


The coordination environment around the Pb^{II} ion in (I) is shown in Fig. 1. The Pb^{II} ion is located on a twofold axis and is coordinated by one DABT ligand and four isonicotinate anions, resulting in a very distorted $\text{cis-PbN}_2\text{O}_4$ octahedral geometry (Table 1). The two unique $\text{Pb}-\text{O}$ distances differ by some 0.11 \AA . The two carboxylate $\text{C}-\text{O}$ distances are approximately equal, implying charge delocalization for the CO_2^- group. The carboxyl group of each isonicotinate anion bridges two Pb^{II} ions, forming a polymeric complex chain, extending along the crystallographic c axis (Fig. 2).

The DABT system possesses twofold symmetry with the mid-point of the $\text{C}3-\text{C}3^{\text{ii}}$ bond located on the rotation axis [symmetry code: (ii) $1-x, y, \frac{3}{2}-z$]. The two thiazole rings of


Figure 1

The molecular structure of (I) expanded to show the coordination environment around the Pb^{II} ion (30% probability displacement ellipsoids; arbitrary spheres for H atoms). [Symmetry codes: (i) $1 - x, 2 - y, 1 - z$; (ii) $1 - x, y, \frac{3}{2} - z$; (iii) $x, 2 - y, \frac{1}{2} + z$.]


Figure 2

The unit-cell packing of (I), showing polymeric complex chains and the parallel arrangement of DABT ligands [symmetry code: (i) $1 - x, 2 - y, 1 - z$]. H atoms have been omitted.

DABT are twisted with respect to each other, with a dihedral angle of $9.5(2)^\circ$; this compares with an equivalent value of $14.7(3)^\circ$ found in a Cd^{II} complex with DABT (Zhang *et al.*, 2006).

The amino group of DABT makes hydrogen bonds to adjacent carboxyl O and pyridine N atoms (Table 2), which help to stabilize the crystal structure. A parallel arrangement of DABT ligands from neighboring polymeric chains is observed (Fig. 2). However, the closest centroid-to-centroid separation of $4.142(3) \text{ \AA}$ between thiazole rings related by an inversion center at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ indicates that there are no significant aromatic π - π stacking interactions between them.

Experimental

An aqueous solution (20 ml) containing DABT (1 mmol) and Pb(NO₃)₂ (1 mmol) was mixed with an aqueous solution (10 ml) of isonicotinic acid (1 mmol) and NaOH (1 mmol). The mixture was refluxed for 5 h. The solution was filtered after cooling to room temperature. Yellow single crystals of (I) were obtained from the filtrate after 10 d.

Crystal data

[Pb(C₆H₄NO₂)₂(C₆H₆N₄S₂)]
 $M_r = 649.66$
 Monoclinic, $C2/c$
 $a = 25.430(3) \text{ \AA}$
 $b = 10.7493(19) \text{ \AA}$
 $c = 7.7480(12) \text{ \AA}$
 $\beta = 104.715(12)^\circ$
 $V = 2048.5(6) \text{ \AA}^3$

$Z = 4$
 $D_x = 2.106 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 8.48 \text{ mm}^{-1}$
 $T = 295(2) \text{ K}$
 Prism, yellow
 $0.12 \times 0.10 \times 0.10 \text{ mm}$

Data collection

Bruker APEX-2 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.355, T_{\max} = 0.430$

5814 measured reflections
 2077 independent reflections
 1939 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\text{max}} = 26.2^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.060$
 $S = 1.07$
 2077 reflections
 142 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2 + 4.0444P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.71 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.65 \text{ e \AA}^{-3}$

Table 1

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

Pb—N1	2.544 (4)	C4—O1	1.259 (7)
Pb—O1	2.510 (4)	C4—O2	1.244 (8)
Pb—O2 ⁱ	2.622 (4)		
O1 ⁱⁱ —Pb—O1	165.1 (2)	N1—Pb—O2 ⁱⁱⁱ	149.69 (14)
O1—Pb—N1	86.01 (13)	O1—Pb—O2 ⁱ	100.2 (2)
O1—Pb—N1 ⁱⁱ	81.49 (16)	N1—Pb—O2 ⁱ	83.46 (14)
N1—Pb—N1 ⁱⁱⁱ	66.4 (2)	O2 ⁱⁱⁱ —Pb—O2 ⁱ	126.8 (2)
O1—Pb—O2 ⁱⁱⁱ	86.55 (18)		

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

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2A \cdots O2 ⁱ	0.86	1.99	2.816 (7)	160
N2—H2B \cdots N3 ^{iv}	0.86	2.12	2.961 (8)	164

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

H atoms were placed in calculated positions, with C—H = 0.93 \AA and N—H = 0.86 \AA , and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); 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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