

catena-Poly[[bis(thiocyanato-*N*)-lead(II)]- μ -1,2-bis(4-pyridyl)-ethane-*N*:*N'*]

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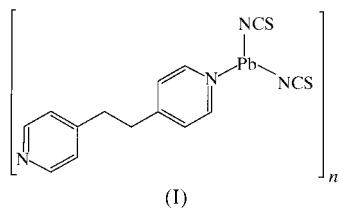
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In the title coordination polymer, [Pb(NCS)₂(C₁₂H₁₂N₂)], the coordination geometry about the Pb^{II} atom is a distorted octahedron, composed of two N atoms from bpe ligands [bpe is 1,2-bis(4-pyridyl)ethane], two other N atoms from NCS⁻ groups and two neighbouring S atoms through short contacts. The *trans*-bpe ligands act as bridges between two Pb^{II} centres resulting in the formation of a linear chain. The terminal S atoms of the NCS⁻ ligands make short contacts with the Pb^{II} atom of neighbouring chains to form an infinite two-dimensional polymeric structure.

Comment

The study of coordination polymers in modern supramolecular chemistry has spawned tremendous interest in the role of multifunctional bridging ligands in determining the final type or topology of the self-assembled product. Among these basic building blocks, 4,4'-bipyridine and its derivatives have been widely employed for their appropriate rigidity and capacity in the construction of solid-state architecture, mostly with linear chain structures (Fujita & Kwon, 1994; Witherly & Blake, 1997; Losier & Zaworotko, 1996; Hennigar *et al.*, 1997; Lu *et al.*, 1997). The main efforts in this field have been devoted to



their reactions with transition metals with different coordination numbers and preferences. However, there are few reports on bivalent main-group metal polymers, such as Pb^{II}

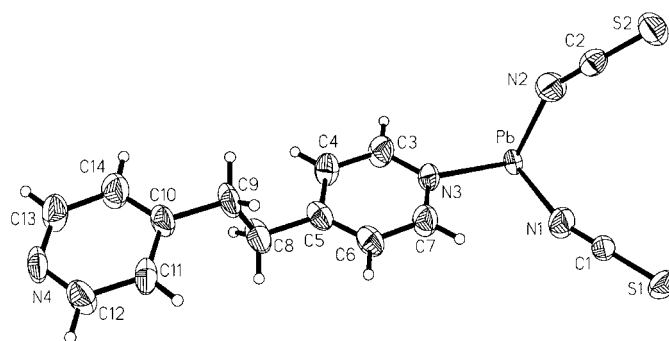


Figure 1

The structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

polymers, with these spacers. We report here the self assembly of a two-dimensional polymer with Pb^{II}, (I).

The Pb^{II} atom adopts a distorted octahedral geometry. The bpe ligand acts as a bridge between two Pb^{II} centers resulting in the formation of a linear Pb–bpe–Pb chain. The terminal S atoms of the NCS⁻ ligands make short contacts with the Pb^{II} atom of a neighbouring polymeric chain to form an infinite two-dimensional polymeric structure (Fig. 2).

The octahedral coordination is defined by four N atoms and two S atoms; two N atoms belong to NCS⁻ anions [Pb–N1 = 2.413 (9) Å and Pb–N2 = 2.415 (9) Å], two other N atoms belong to bpe units [Pb–N3 = 2.570 (7) Å and Pb–N4ⁱ = 2.713 (8) Å] and two S atoms [Pb–S1ⁱⁱ = 3.226 (6) Å and Pb–S2ⁱⁱ = 3.196 (6) Å]. The equatorial plane consists of N1, N2, S1ⁱⁱ and S2ⁱⁱ atoms, and the axial atoms are N3 and N4ⁱ [symmetry codes: (i) 1 + x, 1 + y, 1 + z; (ii) x, –1 + y, z].

The N3–Pb–N4ⁱ angle is 160.7 (3)°, smaller than those found in the related transition metal assemblies exhibiting *M*–*anti*-bpe–*M* bridges (Hong & Do, 1998; Hernandez *et al.*, 1999, 2000; Fujita *et al.*, 1994). The chain exhibits slight zigzag

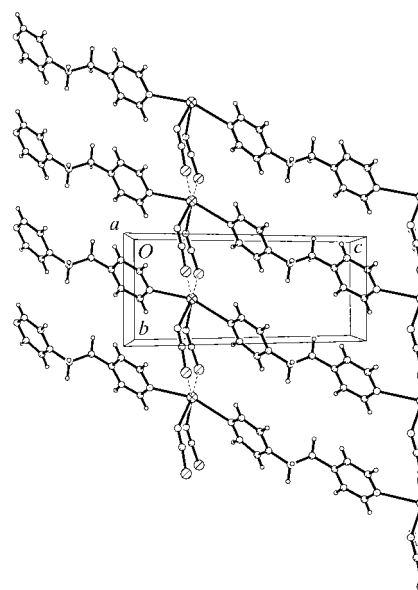


Figure 2

Packing diagram of (I) viewed down the *a* axis.

characteristics. The terminal NCS⁻ groups are almost linear, with N—C—S angles of 176.9 (1) and 179.2 (1)°. The connections between the Pb^{II} atom and the two NCS⁻ groups are bent, with Pb—N—C angles of 145.7 (1) and 153.1 (9)°. It can be deduced that the bivalent main group metals exhibiting different coordination preferences influence the crystal packing and final structure of the self-assembled product.

Experimental

The title compound was synthesized by mixing successively a methanol solution of Pb(NO₃)₂ (0.03 g, 0.1 mmol), bpe (0.02 g, 0.1 mmol) and KNCS (0.02 g, 0.2 mmol) at room temperature. Colourless crystals were obtained by slow evaporation of the solution.

Crystal data

[Pb(NCS) ₂ (C ₁₂ H ₁₂ N ₂)]	$D_x = 2.023 \text{ Mg m}^{-3}$
$M_r = 507.59$	Mo $K\alpha$ radiation
Monoclinic, Pc	Cell parameters from 5094 reflections
$a = 11.6335 (1) \text{ \AA}$	$\theta = 2.0\text{--}28.2^\circ$
$b = 5.6309 (1) \text{ \AA}$	$\mu = 10.37 \text{ mm}^{-1}$
$c = 14.8578 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 121.091 (1)^\circ$	Prism, colourless
$V = 833.48 (2) \text{ \AA}^3$	$0.42 \times 0.28 \times 0.22 \text{ mm}$
$Z = 2$	

Data collection

Siemens SMART CCD area-detector diffractometer	3398 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.050$
Absorption correction: empirical (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 28.2^\circ$
$T_{\text{min}} = 0.042$, $T_{\text{max}} = 0.102$	$h = -15 \rightarrow 15$
5572 measured reflections	$k = -7 \rightarrow 3$
3678 independent reflections	$l = -19 \rightarrow 18$
	Intensity decay: negligible

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2)]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$wR(F^2) = 0.089$	$\Delta\rho_{\text{max}} = 1.38 \text{ e \AA}^{-3}$
$S = 0.92$	$\Delta\rho_{\text{min}} = -1.64 \text{ e \AA}^{-3}$
3678 reflections	Extinction correction: <i>SHELXTL</i> (Sheldrick, 1997)
203 parameters	Extinction coefficient: 0.0199 (10)
H atoms treated by a mixture of independent and constrained refinement	Flack parameter = 0.006 (9)

After checking their presence in the difference map, all H atoms were geometrically fixed, but their displacement parameters were allowed to refine. The C—H distances for H atoms attached to C8 and C9 were set at 0.97 Å; all other C—H distances were set at 0.93 Å. The maximum and minimum electron-density peaks are located 1.03 and 1.16 Å, respectively, from the Pb atom.

Table 1

Selected geometric parameters (Å, °).

Pb—N2	2.415 (9)	Pb—N3	2.570 (7)
Pb—N1	2.413 (9)	Pb—N4 ⁱ	2.713 (8)
N2—Pb—N1	81.1 (3)	N3—Pb—N4 ⁱ	160.7 (3)
N2—Pb—N3	89.6 (4)	C1—N1—Pb	153.1 (9)
N1—Pb—N3	81.2 (3)	C2—N2—Pb	145.7 (10)
N2—Pb—N4 ⁱ	75.7 (4)	N1—C1—S1	179.2 (11)
N1—Pb—N4 ⁱ	84.3 (3)	N2—C2—S2	176.9 (12)

Symmetry code: (i) $1 + x, 1 + y, 1 + z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1453). Services for accessing these data are described at the back of the journal.

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