

Poly[[bis(μ -1,2-bis[[2-(2-pyridyl)-1H-imidazol-1-yl]methyl]benzene)lead(II)] dithiocyanate]

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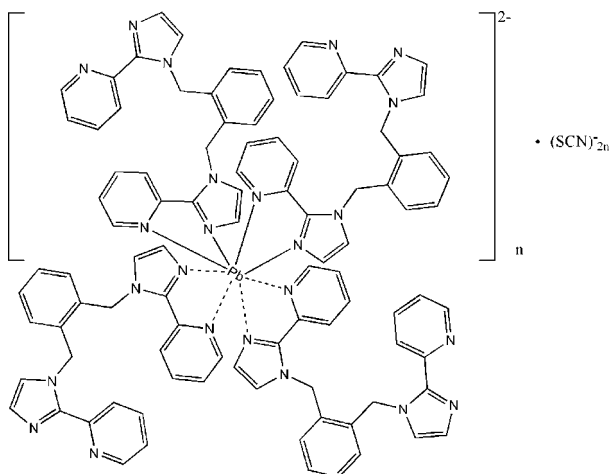
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.034; wR factor = 0.080; data-to-parameter ratio = 17.3.

The title Pb^{II} coordination polymer, $\{[\text{Pb}(\text{C}_{24}\text{H}_{20}\text{N}_6)_2](\text{SCN})_2\}_n$, was obtained by the reaction of $\text{Pb}(\text{CH}_3\text{COO})_2 \cdot 3\text{H}_2\text{O}$, KSCN and 1,2-bis[[2-(2-pyridyl)-1H-imidazol-1-yl]methyl]benzene (hereafter *L*). Each *L* molecule coordinates to two Pb^{II} cations through the four aromatic N atoms, thus acting as a bridging bis-bidentate ligand. The Pb^{II} cations, which lie on inversion centres, are bridged by four *L* molecules, forming a two-dimensional (4,4)-sheet. The SCN^- anions act as counter-ions and are uncoordinated.

Related literature

For related literature, see: Batten & Robson, (1998); Moulton & Zaworotko, (2001); Jack *et al.*, (2004); Carcelli *et al.* (2003).



Experimental

Crystal data

$[\text{Pb}(\text{C}_{24}\text{H}_{20}\text{N}_6)_2](\text{SCN})_2$	$V = 4472.2$ (4) Å ³
$M_r = 1108.27$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 23.9560$ (8) Å	$\mu = 3.92$ mm ⁻¹
$b = 12.6670$ (8) Å	$T = 293$ (2) K
$c = 18.3560$ (9) Å	$0.36 \times 0.31 \times 0.28$ mm
$\beta = 126.593$ (1)°	

Data collection

Bruker APEX CCD area-detector diffractometer	13428 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	5253 independent reflections
$T_{\text{min}} = 0.271$, $T_{\text{max}} = 0.333$	4435 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	303 parameters
$wR(F^2) = 0.080$	H-atom parameters constrained
$S = 0.99$	$\Delta\rho_{\text{max}} = 1.02$ e Å ⁻³
5253 reflections	$\Delta\rho_{\text{min}} = -1.15$ e Å ⁻³

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2062).

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supplementary materials

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Poly[[bis(μ -1,2-bis{[2-(2-pyridyl)-1H-imidazol-1-yl]methyl}benzene)lead(II)] dithiocyanate]

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Comment

In recent years, research into coordination polymers has been expanding rapidly because of their fascinating structural diversity and potential application as functional materials (Batten & Robson, 1998; Moulton & Zaworotko, 2001). As a heavy *p*-block metal ion, lead(II), with its large radius, flexible coordination environment, and variable stereochemical activity, provides unique opportunities for formation of unusual network topologies with interesting properties (Jack *et al.*, 2004). In the present paper, we report the preparation and crystal structure of a novel two-dimensional coordination polymer, namely [Pb(C₂₄H₂₀N₆)₂](SCN)₂, (I).

As shown in Fig. 1, the Pb^{II} cation occupies the inversion centre and is eight-coordinated by eight N atoms from four *L* molecules. The average Pb—N distances are 2.689 (4), 2.717 (3), 2.750 (3) and 2.805 (3) Å, respectively, which are in the normal Pb—N range (Carcelli *et al.*, 2003). As illustrated in Fig. 2, each *L* molecule in (I) coordinates to two Pb^{II} cations through its four aromatic N atoms, thus acting as a bridging bis(bidentate) ligand. The Pb^{II} cations, which lie on the inversion centres, are bridged by four *L* molecules to form a two-dimensional neutral (4,4)-network (Fig. 3). The (SCN)[−] anions act as counterions.

Experimental

A mixture of Pb(CH₃COO)₂·3H₂O (0.121 g, 0.5 mmol), KSCN(0.097 g, 1 mmol) and *L* (0.392 g, 1 mmol) in H₂O (13 ml) was stirred for 0.5 h. The mixture was then transferred and sealed into an 18 ml Teflon-lined autoclave, which was heated at 150 °C for 60 h. After the mixture was cooled to room temperature, colorless blocks of the title complex were filtered off and dried at ambient temperature in air (yield 62% based on Pb).

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 – 0.97 Å, and $U_{\text{iso}}=1.2U_{\text{eq}}(\text{C})$.

Figures

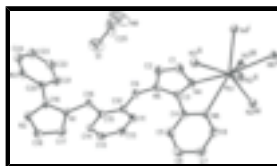


Fig. 1. A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted for clarity.

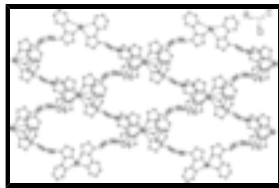


Fig. 2. Ball-stick representation of the two-dimensional structure of (I). All $(\text{SCN})^-$ anions are omitted for clarity.



Fig. 3. View of the (4,4) sheet.

poly[[bis(μ -1,2-bis[[2-(2-pyridyl)-1H-imidazol-1-yl]methyl]benzene)lead(II)] dithiocyanate]

Crystal data

$[\text{Pb}(\text{C}_{24}\text{H}_{20}\text{N}_6)_2](\text{SCN})_2$

$M_r = 1108.27$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 23.9560\ (8)\ \text{\AA}$

$b = 12.6670\ (8)\ \text{\AA}$

$c = 18.3560\ (9)\ \text{\AA}$

$\beta = 126.593\ (1)^\circ$

$V = 4472.2\ (4)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 2208$

$D_x = 1.646\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9825 reflections

$\theta = 1.9\text{--}28.4^\circ$

$\mu = 3.92\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Block, colorless

$0.36 \times 0.31 \times 0.28\ \text{mm}$

Data collection

Bruker APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293\ (2)\ \text{K}$

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.271$, $T_{\max} = 0.333$

13428 measured reflections

5253 independent reflections

4435 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 28.4^\circ$

$\theta_{\min} = 1.9^\circ$

$h = -31\text{--}25$

$k = -16\text{--}16$

$l = -24\text{--}23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.080$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2]$

$S = 0.99$

5253 reflections

303 parameters

Primary atom site location: structure-invariant direct methods

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.02 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.15 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pb1	0.0000	0.369453 (14)	0.7500	0.03277 (8)
S1	0.23584 (15)	0.88594 (17)	0.80144 (19)	0.1210 (8)
C1	0.1039 (3)	0.6026 (3)	0.8718 (3)	0.0527 (11)
H1	0.0700	0.6391	0.8713	0.063*
C2	0.1559 (3)	0.6481 (3)	0.8750 (3)	0.0510 (11)
H2	0.1647	0.7200	0.8774	0.061*
C3	0.1634 (2)	0.4757 (3)	0.8719 (3)	0.0370 (8)
C4	0.1862 (2)	0.3677 (3)	0.8724 (2)	0.0363 (8)
C5	0.2552 (3)	0.3402 (4)	0.9119 (3)	0.0494 (10)
H5	0.2895	0.3919	0.9379	0.059*
C6	0.2721 (3)	0.2370 (4)	0.9124 (4)	0.0581 (12)
H6	0.3179	0.2178	0.9387	0.070*
C7	0.2206 (3)	0.1624 (4)	0.8734 (3)	0.0555 (12)
H7	0.2305	0.0917	0.8722	0.067*
C8	0.1535 (3)	0.1949 (3)	0.8360 (3)	0.0484 (11)
H8	0.1187	0.1439	0.8102	0.058*
C9	0.2509 (2)	0.5851 (3)	0.8679 (3)	0.0401 (9)
H9A	0.2405	0.6467	0.8304	0.048*
H9B	0.2546	0.5250	0.8383	0.048*
C10	0.3202 (2)	0.6016 (3)	0.9593 (3)	0.0338 (8)
C11	0.3293 (2)	0.5842 (3)	1.0405 (3)	0.0417 (9)
H11	0.2916	0.5629	1.0392	0.050*
C12	0.3925 (3)	0.5976 (3)	1.1220 (3)	0.0473 (10)
H12	0.3977	0.5846	1.1756	0.057*
C13	0.4494 (2)	0.6307 (3)	1.1254 (3)	0.0461 (10)
H13	0.4925	0.6400	1.1810	0.055*

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C14	0.4414 (2)	0.6498 (3)	1.0452 (3)	0.0418 (9)
H14	0.4794	0.6719	1.0473	0.050*
C15	0.3770 (2)	0.6362 (3)	0.9617 (2)	0.0344 (8)
C16	0.3669 (2)	0.6580 (3)	0.8735 (3)	0.0406 (9)
H16A	0.3425	0.5989	0.8327	0.049*
H16B	0.3378	0.7200	0.8454	0.049*
C17	0.4706 (3)	0.5944 (4)	0.8856 (3)	0.0531 (12)
H17	0.4635	0.5224	0.8868	0.064*
C18	0.5209 (3)	0.6404 (3)	0.8849 (4)	0.0606 (13)
H18	0.5551	0.6042	0.8858	0.073*
C19	0.4607 (2)	0.7666 (3)	0.8829 (3)	0.0397 (9)
C20	0.4387 (2)	0.8735 (3)	0.8845 (3)	0.0387 (8)
C21	0.4112 (3)	0.9009 (4)	0.9309 (3)	0.0506 (11)
H21	0.4033	0.8496	0.9600	0.061*
C22	0.3959 (3)	1.0061 (4)	0.9329 (3)	0.0568 (12)
H22	0.3772	1.0259	0.9630	0.068*
C23	0.4085 (3)	1.0805 (4)	0.8903 (3)	0.0552 (12)
H23	0.3990	1.1514	0.8913	0.066*
C24	0.4356 (3)	1.0471 (3)	0.8456 (3)	0.0479 (10)
H24	0.4434	1.0977	0.8159	0.057*
C25	0.1601 (5)	0.8640 (6)	0.7079 (9)	0.110 (4)
N1	0.4318 (2)	0.6750 (3)	0.8843 (2)	0.0411 (8)
N2	0.5148 (2)	0.7480 (3)	0.8825 (3)	0.0525 (10)
N3	0.45138 (19)	0.9469 (3)	0.8425 (2)	0.0406 (8)
N4	0.1078 (2)	0.4945 (3)	0.8693 (2)	0.0453 (8)
N5	0.19362 (19)	0.5672 (3)	0.8739 (2)	0.0397 (8)
N6	0.13584 (19)	0.2947 (2)	0.8348 (2)	0.0395 (7)
N8	0.1191 (6)	0.8507 (9)	0.6599 (9)	0.182 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.03127 (11)	0.03239 (11)	0.04649 (12)	0.000	0.02959 (9)	0.000
S1	0.1069 (18)	0.1023 (15)	0.1358 (19)	0.0092 (13)	0.0626 (16)	-0.0211 (12)
C1	0.052 (3)	0.048 (2)	0.077 (3)	0.000 (2)	0.049 (3)	-0.013 (2)
C2	0.053 (3)	0.038 (2)	0.071 (3)	-0.007 (2)	0.042 (3)	-0.013 (2)
C3	0.032 (2)	0.040 (2)	0.045 (2)	-0.0058 (17)	0.0253 (19)	-0.0043 (16)
C4	0.034 (2)	0.041 (2)	0.0406 (18)	0.0007 (19)	0.0257 (16)	0.0017 (16)
C5	0.038 (2)	0.049 (2)	0.065 (3)	-0.001 (2)	0.033 (2)	-0.001 (2)
C6	0.050 (3)	0.054 (3)	0.083 (3)	0.012 (2)	0.046 (3)	0.005 (2)
C7	0.067 (4)	0.043 (2)	0.069 (3)	0.011 (2)	0.047 (3)	0.008 (2)
C8	0.053 (3)	0.042 (2)	0.054 (2)	-0.003 (2)	0.033 (2)	0.0029 (19)
C9	0.038 (2)	0.044 (2)	0.049 (2)	-0.0081 (19)	0.031 (2)	-0.0035 (17)
C10	0.035 (2)	0.0303 (17)	0.0433 (19)	-0.0031 (16)	0.0271 (18)	-0.0027 (15)
C11	0.047 (3)	0.041 (2)	0.049 (2)	-0.0044 (19)	0.035 (2)	-0.0011 (17)
C12	0.057 (3)	0.048 (2)	0.045 (2)	0.005 (2)	0.034 (2)	0.0059 (18)
C13	0.040 (2)	0.052 (2)	0.0383 (19)	0.005 (2)	0.0193 (18)	0.0019 (18)
C14	0.035 (2)	0.042 (2)	0.051 (2)	0.0019 (18)	0.0268 (19)	0.0051 (17)

C15	0.035 (2)	0.0308 (17)	0.0435 (18)	-0.0022 (17)	0.0267 (17)	0.0016 (16)
C16	0.034 (2)	0.048 (2)	0.048 (2)	-0.0022 (18)	0.0284 (19)	0.0052 (17)
C17	0.061 (3)	0.040 (2)	0.079 (3)	0.011 (2)	0.053 (3)	0.016 (2)
C18	0.065 (3)	0.051 (3)	0.096 (4)	0.025 (3)	0.064 (3)	0.024 (2)
C19	0.041 (2)	0.042 (2)	0.051 (2)	0.0016 (18)	0.035 (2)	0.0061 (17)
C20	0.035 (2)	0.046 (2)	0.0424 (19)	0.0030 (19)	0.0273 (17)	0.0031 (17)
C21	0.057 (3)	0.056 (2)	0.060 (3)	0.002 (2)	0.046 (3)	0.003 (2)
C22	0.065 (3)	0.060 (3)	0.071 (3)	0.006 (3)	0.054 (3)	-0.004 (2)
C23	0.061 (3)	0.047 (2)	0.071 (3)	0.002 (2)	0.047 (3)	-0.008 (2)
C24	0.053 (3)	0.043 (2)	0.053 (2)	-0.002 (2)	0.035 (2)	0.0021 (19)
C25	0.094 (6)	0.050 (3)	0.237 (13)	-0.030 (5)	0.125 (8)	-0.057 (6)
N1	0.042 (2)	0.0398 (17)	0.055 (2)	0.0041 (16)	0.0366 (18)	0.0092 (15)
N2	0.053 (3)	0.049 (2)	0.081 (3)	0.0086 (18)	0.054 (2)	0.0153 (18)
N3	0.042 (2)	0.0425 (18)	0.0474 (19)	-0.0031 (16)	0.0318 (17)	-0.0024 (14)
N4	0.044 (2)	0.0426 (18)	0.067 (2)	-0.0085 (16)	0.043 (2)	-0.0125 (16)
N5	0.0315 (19)	0.0409 (18)	0.0497 (19)	-0.0052 (15)	0.0260 (16)	-0.0044 (14)
N6	0.036 (2)	0.0380 (17)	0.0478 (19)	-0.0002 (15)	0.0269 (17)	0.0018 (14)
N8	0.120 (9)	0.134 (8)	0.213 (12)	0.052 (7)	0.057 (8)	-0.044 (7)

Geometric parameters (Å, °)

Pb1—N4	2.689 (4)	C11—C12	1.364 (7)
Pb1—N4 ⁱ	2.689 (4)	C11—H11	0.9300
Pb1—N2 ⁱⁱ	2.717 (3)	C12—C13	1.392 (7)
Pb1—N2 ⁱⁱⁱ	2.717 (3)	C12—H12	0.9300
Pb1—N3 ⁱⁱⁱ	2.750 (3)	C13—C14	1.387 (6)
Pb1—N3 ⁱⁱ	2.750 (3)	C13—H13	0.9300
Pb1—N6	2.805 (3)	C14—C15	1.394 (6)
Pb1—N6 ⁱ	2.805 (3)	C14—H14	0.9300
S1—C25	1.614 (12)	C15—C16	1.512 (5)
C1—C2	1.343 (7)	C16—N1	1.462 (5)
C1—N4	1.376 (5)	C16—H16A	0.9700
C1—H1	0.9300	C16—H16B	0.9700
C2—N5	1.373 (6)	C17—C18	1.347 (7)
C2—H2	0.9300	C17—N1	1.371 (6)
C3—N4	1.326 (5)	C17—H17	0.9300
C3—N5	1.355 (5)	C18—N2	1.368 (5)
C3—C4	1.472 (5)	C18—H18	0.9300
C4—N6	1.341 (5)	C19—N2	1.322 (5)
C4—C5	1.395 (6)	C19—N1	1.359 (5)
C5—C6	1.367 (6)	C19—C20	1.460 (5)
C5—H5	0.9300	C20—N3	1.352 (5)
C6—C7	1.370 (7)	C20—C21	1.396 (5)
C6—H6	0.9300	C21—C22	1.387 (6)
C7—C8	1.382 (7)	C21—H21	0.9300
C7—H7	0.9300	C22—C23	1.368 (7)
C8—N6	1.329 (5)	C22—H22	0.9300
C8—H8	0.9300	C23—C24	1.381 (6)

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C9—N5	1.458 (5)	C23—H23	0.9300
C9—C10	1.515 (6)	C24—N3	1.336 (5)
C9—H9A	0.9700	C24—H24	0.9300
C9—H9B	0.9700	C25—N8	0.858 (13)
C10—C11	1.389 (5)	N2—Pb1 ^{iv}	2.717 (3)
C10—C15	1.405 (5)	N3—Pb1 ^{iv}	2.750 (3)
N4—Pb1—N4 ⁱ	107.83 (16)	C14—C13—H13	120.2
N4—Pb1—N2 ⁱⁱ	127.73 (11)	C12—C13—H13	120.2
N4 ⁱ —Pb1—N2 ⁱⁱ	93.16 (12)	C13—C14—C15	120.5 (4)
N4—Pb1—N2 ⁱⁱⁱ	93.16 (12)	C13—C14—H14	119.8
N4 ⁱ —Pb1—N2 ⁱⁱⁱ	127.73 (11)	C15—C14—H14	119.8
N2 ⁱⁱ —Pb1—N2 ⁱⁱⁱ	111.02 (16)	C14—C15—C10	119.3 (3)
N4—Pb1—N3 ⁱⁱⁱ	80.90 (10)	C14—C15—C16	121.4 (4)
N4 ⁱ —Pb1—N3 ⁱⁱⁱ	74.82 (10)	C10—C15—C16	119.3 (3)
N2 ⁱⁱ —Pb1—N3 ⁱⁱⁱ	151.37 (12)	N1—C16—C15	113.7 (3)
N2 ⁱⁱⁱ —Pb1—N3 ⁱⁱⁱ	61.71 (10)	N1—C16—H16A	108.8
N4—Pb1—N3 ⁱⁱ	74.82 (10)	C15—C16—H16A	108.8
N4 ⁱ —Pb1—N3 ⁱⁱ	80.90 (10)	N1—C16—H16B	108.8
N2 ⁱⁱ —Pb1—N3 ⁱⁱ	61.71 (10)	C15—C16—H16B	108.8
N2 ⁱⁱⁱ —Pb1—N3 ⁱⁱ	151.37 (12)	H16A—C16—H16B	107.7
N3 ⁱⁱⁱ —Pb1—N3 ⁱⁱ	138.22 (14)	C18—C17—N1	106.2 (4)
C2—C1—N4	110.4 (4)	C18—C17—H17	126.9
C2—C1—H1	124.8	N1—C17—H17	126.9
N4—C1—H1	124.8	C17—C18—N2	110.6 (4)
C1—C2—N5	106.3 (4)	C17—C18—H18	124.7
C1—C2—H2	126.8	N2—C18—H18	124.7
N5—C2—H2	126.8	N2—C19—N1	111.1 (4)
N4—C3—N5	110.9 (3)	N2—C19—C20	122.1 (4)
N4—C3—C4	121.9 (3)	N1—C19—C20	126.8 (4)
N5—C3—C4	127.2 (4)	N3—C20—C21	121.7 (4)
N6—C4—C5	121.3 (4)	N3—C20—C19	114.9 (3)
N6—C4—C3	114.9 (4)	C21—C20—C19	123.3 (4)
C5—C4—C3	123.8 (4)	C22—C21—C20	118.8 (4)
C6—C5—C4	119.8 (5)	C22—C21—H21	120.6
C6—C5—H5	120.1	C20—C21—H21	120.6
C4—C5—H5	120.1	C23—C22—C21	119.7 (4)
C5—C6—C7	119.0 (5)	C23—C22—H22	120.2
C5—C6—H6	120.5	C21—C22—H22	120.2
C7—C6—H6	120.5	C22—C23—C24	118.1 (4)
C6—C7—C8	118.3 (4)	C22—C23—H23	121.0
C6—C7—H7	120.9	C24—C23—H23	121.0
C8—C7—H7	120.9	N3—C24—C23	124.1 (4)
N6—C8—C7	123.8 (5)	N3—C24—H24	117.9
N6—C8—H8	118.1	C23—C24—H24	117.9
C7—C8—H8	118.1	N8—C25—S1	177 (2)

N5—C9—C10	113.4 (3)	C19—N1—C17	106.8 (4)
N5—C9—H9A	108.9	C19—N1—C16	129.5 (4)
C10—C9—H9A	108.9	C17—N1—C16	123.2 (4)
N5—C9—H9B	108.9	C19—N2—C18	105.3 (4)
C10—C9—H9B	108.9	C19—N2—Pb1 ^{iv}	107.4 (3)
H9A—C9—H9B	107.7	C18—N2—Pb1 ^{iv}	123.1 (3)
C11—C10—C15	119.2 (4)	C24—N3—C20	117.6 (3)
C11—C10—C9	122.3 (4)	C24—N3—Pb1 ^{iv}	126.9 (3)
C15—C10—C9	118.6 (3)	C20—N3—Pb1 ^{iv}	115.4 (2)
C12—C11—C10	121.2 (4)	C3—N4—C1	105.3 (4)
C12—C11—H11	119.4	C3—N4—Pb1	112.4 (2)
C10—C11—H11	119.4	C1—N4—Pb1	124.2 (3)
C11—C12—C13	120.3 (4)	C3—N5—C2	107.0 (4)
C11—C12—H12	119.9	C3—N5—C9	130.0 (3)
C13—C12—H12	119.9	C2—N5—C9	122.8 (3)
C14—C13—C12	119.6 (4)	C8—N6—C4	117.9 (4)
N4—C1—C2—N5	0.4 (6)	C15—C16—N1—C19	-103.2 (5)
N4—C3—C4—N6	25.5 (5)	C15—C16—N1—C17	86.3 (5)
N5—C3—C4—N6	-154.5 (4)	N1—C19—N2—C18	-0.7 (5)
N4—C3—C4—C5	-151.8 (4)	C20—C19—N2—C18	177.5 (4)
N5—C3—C4—C5	28.2 (6)	N1—C19—N2—Pb1 ^{iv}	132.1 (3)
N6—C4—C5—C6	0.3 (6)	C20—C19—N2—Pb1 ^{iv}	-49.7 (5)
C3—C4—C5—C6	177.5 (4)	C17—C18—N2—C19	0.7 (6)
C4—C5—C6—C7	0.2 (7)	C17—C18—N2—Pb1 ^{iv}	-122.6 (4)
C5—C6—C7—C8	-0.6 (7)	C23—C24—N3—C20	1.2 (7)
C6—C7—C8—N6	0.7 (7)	C23—C24—N3—Pb1 ^{iv}	177.0 (4)
N5—C9—C10—C11	9.7 (6)	C21—C20—N3—C24	-1.1 (6)
N5—C9—C10—C15	-170.0 (3)	C19—C20—N3—C24	-176.8 (4)
C15—C10—C11—C12	-1.6 (6)	C21—C20—N3—Pb1 ^{iv}	-177.4 (3)
C9—C10—C11—C12	178.7 (4)	C19—C20—N3—Pb1 ^{iv}	6.9 (5)
C10—C11—C12—C13	0.9 (7)	N5—C3—N4—C1	-1.4 (5)
C11—C12—C13—C14	-0.1 (6)	C4—C3—N4—C1	178.6 (4)
C12—C13—C14—C15	0.1 (6)	N5—C3—N4—Pb1	136.6 (3)
C13—C14—C15—C10	-0.7 (6)	C4—C3—N4—Pb1	-43.4 (4)
C13—C14—C15—C16	179.2 (4)	C2—C1—N4—C3	0.6 (5)
C11—C10—C15—C14	1.5 (6)	C2—C1—N4—Pb1	-131.0 (4)
C9—C10—C15—C14	-178.8 (4)	N4 ⁱ —Pb1—N4—C3	-122.7 (3)
C11—C10—C15—C16	-178.4 (3)	N2 ⁱⁱ —Pb1—N4—C3	-13.9 (3)
C9—C10—C15—C16	1.3 (5)	N2 ⁱⁱⁱ —Pb1—N4—C3	105.9 (3)
C14—C15—C16—N1	10.4 (5)	N3 ⁱⁱⁱ —Pb1—N4—C3	166.6 (3)
C10—C15—C16—N1	-169.7 (3)	N3 ⁱⁱ —Pb1—N4—C3	-47.7 (3)
N1—C17—C18—N2	-0.4 (6)	N4 ⁱ —Pb1—N4—C1	6.1 (3)
N2—C19—C20—N3	31.1 (6)	N2 ⁱⁱ —Pb1—N4—C1	114.9 (3)
N1—C19—C20—N3	-151.0 (4)	N2 ⁱⁱⁱ —Pb1—N4—C1	-125.3 (3)
N2—C19—C20—C21	-144.5 (5)	N3 ⁱⁱⁱ —Pb1—N4—C1	-64.7 (3)

supplementary materials

N1—C19—C20—C21	33.4 (7)	N3 ⁱⁱ —Pb1—N4—C1	81.0 (3)
N3—C20—C21—C22	0.8 (7)	N4—C3—N5—C2	1.6 (5)
C19—C20—C21—C22	176.1 (5)	C4—C3—N5—C2	-178.4 (4)
C20—C21—C22—C23	-0.5 (8)	N4—C3—N5—C9	-173.1 (4)
C21—C22—C23—C24	0.6 (8)	C4—C3—N5—C9	6.9 (7)
C22—C23—C24—N3	-1.0 (8)	C1—C2—N5—C3	-1.2 (5)
N2—C19—N1—C17	0.5 (5)	C1—C2—N5—C9	174.0 (4)
C20—C19—N1—C17	-177.6 (4)	C10—C9—N5—C3	-98.8 (5)
N2—C19—N1—C16	-171.2 (4)	C10—C9—N5—C2	87.2 (5)
C20—C19—N1—C16	10.7 (7)	C7—C8—N6—C4	-0.2 (6)
C18—C17—N1—C19	0.0 (5)	C5—C4—N6—C8	-0.3 (5)
C18—C17—N1—C16	172.3 (4)	C3—C4—N6—C8	-177.6 (3)

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

Fig. 1

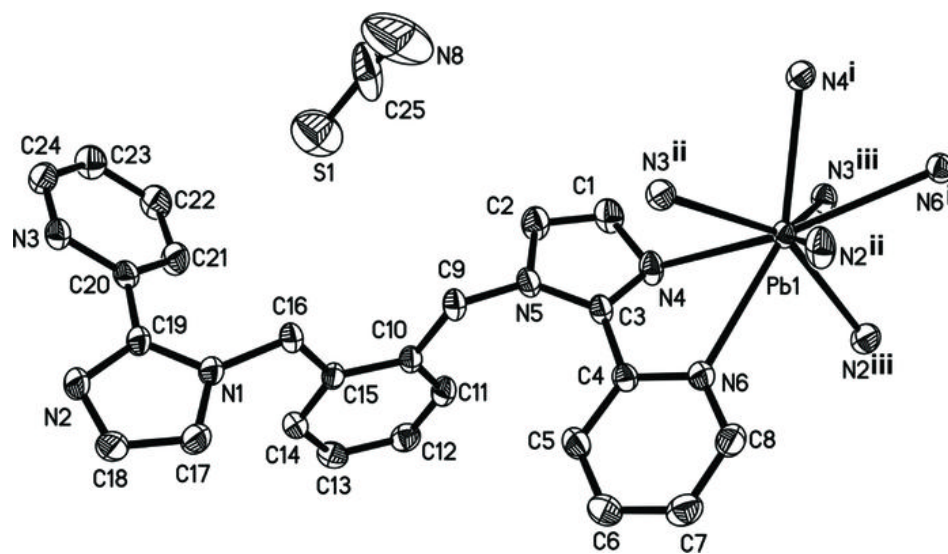


Fig. 2

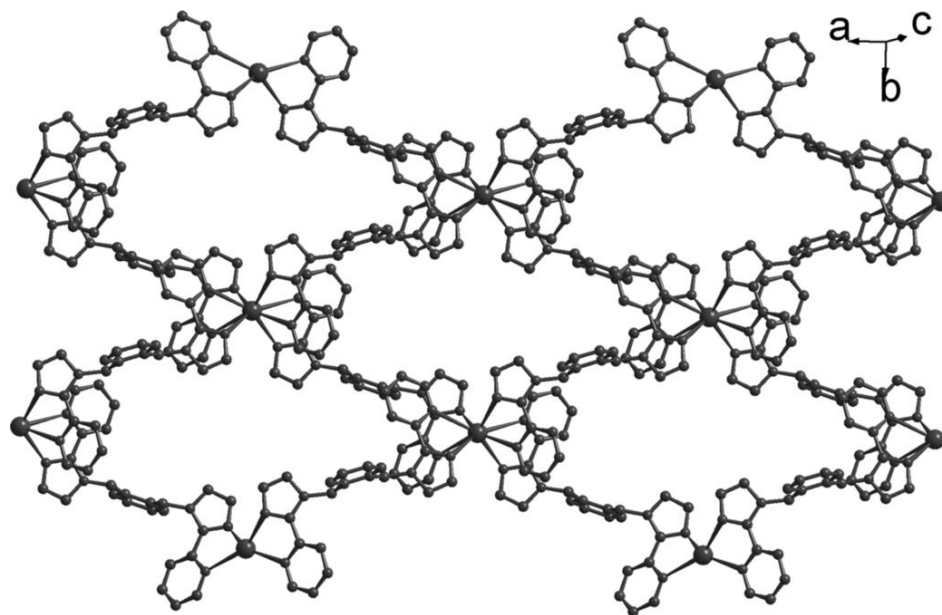


Fig. 3

