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catena-Poly[lead(II)-bis(μ -2-amino-1,3-benzothiazole-6-carboxylato)]

Ke-Ke Zhang, Xin Fang, Hai-Yang Yu, Hua Ke and Jun-Dong Wang*

College of Chemistry and Chemical Engineering, Fuzhou University, Fuzhou, Fujian 350108, People's Republic of China

Correspondence e-mail: wangjd@fzu.edu.cn

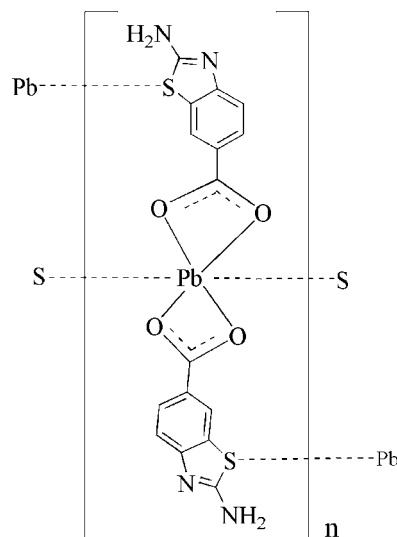
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.037; wR factor = 0.096; data-to-parameter ratio = 15.4.

The title complex, $[\text{Pb}(\text{C}_8\text{H}_5\text{N}_2\text{O}_2\text{S})_2]_n$, consists of one Pb^{II} ion located on a crystallographic twofold axis and two symmetry-related 2-amino-1,3-benzothiazole-6-carboxylate (ABTC) ligands. The central Pb^{II} ion has a (4 + 2) coordination by four O atoms of the two ABTC ligands and two weaker Pb—S bonding interactions (Pb—S secondary bonds) from S atoms of other two neighbouring ABTC ligands. These bonds link the metal ions into zigzag chains along the c axis, which, in turn, aggregate through π – π interactions [centroid–centroid distance = 3.7436 Å] between ABTC rings and N—H...O and N—H...N hydrogen bonds.

Related literature

For applications of benzothiazole and its derivatives, see: Petkova *et al.* (2000); Leng *et al.* (2001); Karlsson *et al.* (2003); Čaleta *et al.* (2009); Tzanopoulou *et al.* (2010). For the use of benzothiazoles in building novel complexes, see: Vuoti *et al.* (2007); Zou *et al.* (2004); Ng *et al.* (2008); Chen *et al.* (2010); For our recent work on the design and synthesis of benzothiazole derivatives, see: Fang *et al.* (2010); Lei *et al.* (2010). For secondary Pb—S bonds, see: Chan & Rossi (1997); Turner *et al.* (2008). For van der Waals radii, see: Bondi (1964). For (4 + 2) coordination, see: Chan & Rossi (1997); Calatayud *et al.* (2007); Turner *et al.* (2008); Pena-Hueso *et al.* (2008). For π – π interactions, see: Sredojević *et al.* (2010). For the preparation of the 2-aminobenzothiazole-6-carboxylic acid ligand, see: Das *et al.* (2003). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$[\text{Pb}(\text{C}_8\text{H}_5\text{N}_2\text{O}_2\text{S})_2]$

$M_r = 593.59$

Monoclinic, $P2_1/c$

$a = 10.909$ (2) Å

$b = 4.8271$ (10) Å

$c = 15.980$ (3) Å

$\beta = 100.02$ (3)°

$V = 828.6$ (3) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 10.47$ mm⁻¹

$T = 293$ K

$0.39 \times 0.29 \times 0.15$ mm

Data collection

Rigaku Saturn 724 CCD area-detector diffractometer

Absorption correction: numerical

(NUMABS; Higashi, 2000)

$T_{\text{min}} = 0.378$, $T_{\text{max}} = 1.000$

6088 measured reflections

1890 independent reflections

1871 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.096$

$S = 1.11$

1890 reflections

123 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 2.13$ e Å⁻³

$\Delta\rho_{\text{min}} = -2.56$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1B}\cdots\text{O1}^{\text{i}}$	0.86	2.11	2.973 (7)	179
$\text{N1}-\text{H1A}\cdots\text{N2}^{\text{ii}}$	0.86	2.09	2.934 (7)	168

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

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP* (McArdle, 1995); 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: BG2378).

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supporting information

Acta Cryst. (2010). E66, m1700–m1701 [https://doi.org/10.1107/S1600536810049330]

catena-Poly[lead(II)-bis(μ -2-amino-1,3-benzothiazole-6-carboxylato)]**Ke-Ke Zhang, Xin Fang, Hai-Yang Yu, Hua Ke and Jun-Dong Wang****S1. Comment**

In recent years, benzothiazole and its derivatives have been attracting more attention because they exhibit interesting optical and biological activities, which made them widely used in many fields, such as fluorescent materials, nonlinear optical materials, pesticides, anti-tumor and anti-microbial drugs, *etc.* (Petkova *et al.*, 2000; Leng *et al.*, 2001; Karlsson *et al.*, 2003; Čaleta *et al.*, 2009). Related structural studies are partly focused on the fact that the benzothiazole ring contains N, S and O as potential donor atoms, which exhibit good coordination capacity, and so are propitious to build novel complexes (Zou *et al.*, 2004; Vuoti *et al.*, 2007; Ng *et al.*, 2008; Chen *et al.*, 2010;). By reviewing their metal complexes (Cambridge Structural Database, Version of 5.31 of August 2010; Allen, 2002), it was found that most metal atoms only match with N atom of thiazole ring, but not the S atom (because the coordination capacity of S is much weaker than N), as long as these metal atoms have interaction with the thiazole ring. In our recent work, accompanied with the design and synthesis of benzothiazole derivatives (Lei *et al.*, 2010; Fang *et al.*, 2010), complexes of benzothiazole derivatives with metal atoms were composed and structurally analyzed to explore their coordination behaviors. In this paper, we report the structure of a coordination polymer of lead and 2-amino-1,3-benzothiazole-6-carboxylate ligand (ABTC), where the coordination mode of S with Pb is seen as a secondary Pb—S bond (Chan *et al.*, 1997; Turner *et al.*, 2008).

The asymmetric unit of the complex contains a Pb^{II} ion located on a two fold axis and one independent 2-amino-1,3-benzothiazole-6-carboxylate (ABTC) ligand (Figure 1). The central Pb^{II} ion is coordinated by four O atoms of two ABTC ligands in a pyramid fashion with the Pb^{II} ion at the apex, covalently bounded to the four O atoms making up the base of the pyramid. The four Pb—O bonds are Pb1—O1 and Pb1—O1ⁱⁱⁱ, (iii): $-x+1, -y, -z+1$, with a distance of 2.395 (5) Å, and Pb1—O2 and Pb1—O2ⁱⁱ, (ii) $-x+1, y, -z+3/2$; with a distance of 2.366 (4) Å. The stereochemistry of the distorted pyramid is described by angles of O1—Pb—O1ⁱⁱⁱ, 106.4 (3)°, and O2—Pb—O2ⁱⁱⁱ, 102.8 (3)°, and the sides of the base defined by O1—O2 and O1ⁱⁱⁱ—O2ⁱⁱⁱ, distanced 2.1708 (60) Å, and O1—O2ⁱⁱⁱ and O2—O1ⁱⁱⁱ, distanced 3.081 (7) Å.

In the crystal, two S atoms also interact with the apical Pb^{II} ion with so-called secondary bonds, where the Pb—S distance [Pb1—S1ⁱ (i) $x, -y, z+1/2$] and Pb1—S1ⁱⁱ, with a distance of 3.3894 (17) Å] is shorter than the corresponding sum of the van der Waals radii (3.80 Å) of Pb and S atoms (Bondi, 1964). So the Pb^{II} ion in this structure should be described as (4 + 2) coordinated (Chan *et al.*, 1997; Calatayud *et al.*, 2007; Turner *et al.*, 2008; Pena-Hueso *et al.*, 2008). Under this coordination mode, each ABTC ligand acts as a linear linker to coordinate two metal centers, while each metal ion is linked to four ABTC ligands, then, along the *c* axis, one-dimensional zigzag chains are formed (Figure 2).

Along the *b* axis, neighboring chains are linked by N—H \cdots O H-bonds and π - π interactions between the thiazole and benzene rings [with perpendicular distance of 3.4184 Å and centroid-centroid distance of 3.7436 Å]. Simultaneously, there is an interaction between the benzene ring and the carboxyl group coordinated on the Pb^{II} ion, described by the 4-membered ring of O1—C8—O2—Pb1, with a perpendicular distance of 3.5021 Å and centroid-centroid distance of 3.5740 Å (Sredojević *et al.*, 2010).

Finally, along the *a* axis, neighboring chains are further connected to each other by N—H···N hydrogen bonds which complete an infinite three-dimensional framework of the structure (Table 1 and Figure 3).

It is worth noting that S secondary bonds were also present in the previously reported complex of Ag and a benzothiazole derivative (Zou *et al.*, 2004) through the weak interaction between Ag and the S atom of the thiazole ring. Also here these secondary Ag—S bonds play an important role in building the crystal framework, cooperating with the hydrogen bonds and π - π interactions to build the supramolecular structure.

S2. Experimental

The 2-aminobenzothiazole-6-carboxylic acid ligand was obtained by hydrolyzing ethyl 2-amino-1,3-benzothiazole-6-carboxylate (Das *et al.* 2003). The mixture of lead acetate (0.0379 g, 0.10 mmol), 2-aminobenzothiazole-6-carboxylic acid (0.0194 g, 0.1 mmol), and H₂O (5 ml) was sealed in a 15 ml stainless-steel reactor with Teflon liner and heated (10°C per hour) from room temperature to 140°C and kept at 140°C for 96 h, then cooled to room temperature again at a similar rate. Brown crystals suitable for X-ray diffraction analysis were obtained.

S3. Refinement

All H atoms bound to C and N atoms were located in difference Fourier syntheses and were refined as riding, with C—H distances of 0.93 Å and N—H distances of 0.86 Å. All $U_{\text{iso}}(\text{H})$ were kept at $1.2U_{\text{eq}}(\text{Host})$.

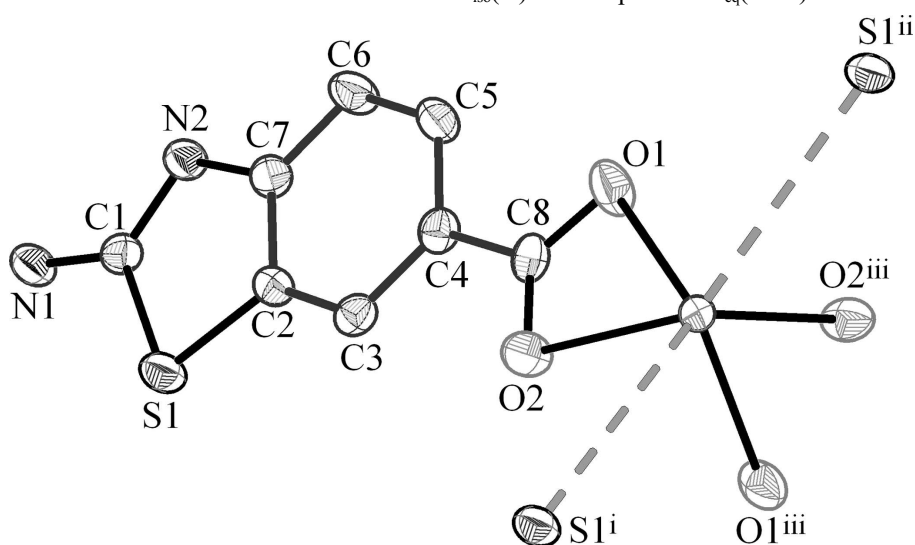
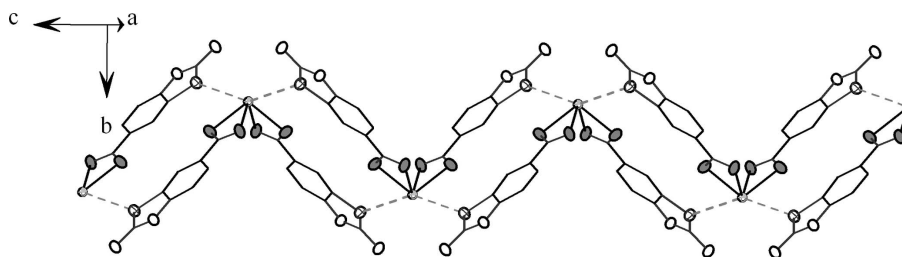
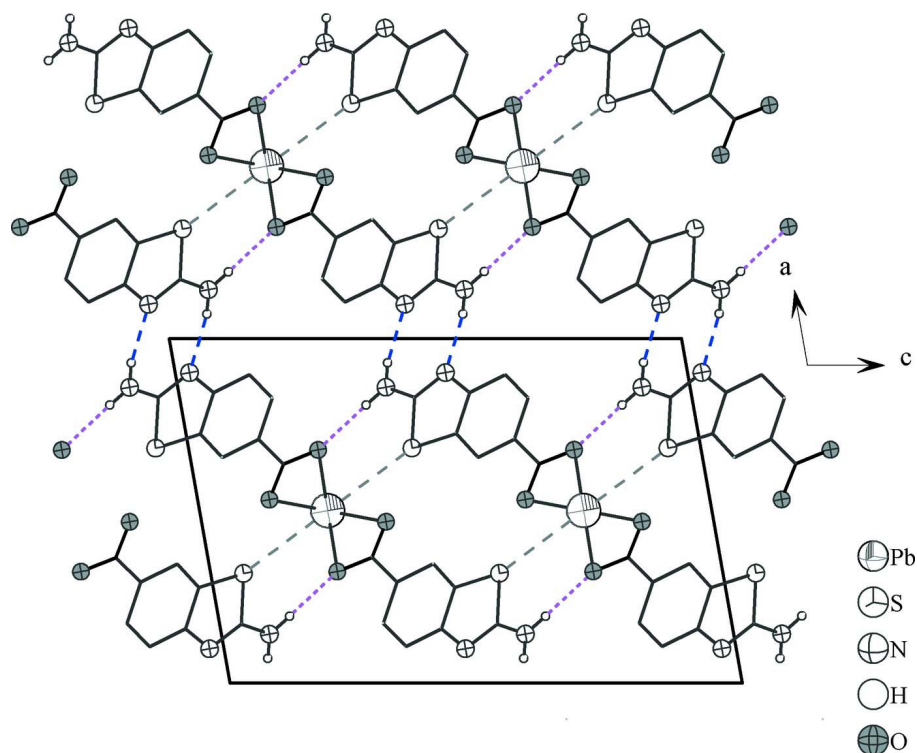


Figure 1

The crystal structure of (I), drawn with 40% probability displacement ellipsoids. H atoms have been omitted for clarity. Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $x, -y, 1/2 + z$; (iii) $1 - x, y, 3/2 - z$.


Figure 2

A view of the one-dimensional chain formed by Pb—S secondary bonds in (I). All H atoms have been omitted and all C atoms are shown as wires or sticks for clarify.


Figure 3

A packing diagram for (I), showing some of the hydrogen bonds (blue and red dashed lines) and π - π interactions along the b direction. Most of the H atoms have been omitted except those involved in the weak interactions. All C atoms are shown as wires or sticks for clarify.

catena-Poly[lead(II)-bis(μ -2-amino-1,3-benzothiazole-6-carboxylato)]

Crystal data

[Pb(C₈H₅N₂O₂S)₂]

$M_r = 593.59$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 10.909 (2) \text{ \AA}$

$b = 4.8271 (10) \text{ \AA}$

$c = 15.980 (3) \text{ \AA}$

$\beta = 100.02 (3)^\circ$

$V = 828.6 (3) \text{ \AA}^3$

$Z = 2$

$F(000) = 560$

$D_x = 2.379 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3030 reflections

$\theta = 3.5\text{--}27.6^\circ$

$\mu = 10.47 \text{ mm}^{-1}$

$T = 293$ K $0.39 \times 0.29 \times 0.15$ mm
 Prism, brown

Data collection

Rigaku Saturn 724 CCD area-detector diffractometer	6088 measured reflections
Radiation source: fine-focus sealed tube	1890 independent reflections
Graphite monochromator	1871 reflections with $I > 2\sigma(I)$
Detector resolution: 28.5714 pixels mm ⁻¹	$R_{\text{int}} = 0.075$
dtprofit.ref scans	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.5^\circ$
Absorption correction: numerical (NUMABS; Higashi, 2000)	$h = -14 \rightarrow 12$
$T_{\text{min}} = 0.378$, $T_{\text{max}} = 1.000$	$k = -6 \rightarrow 6$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 0.8091P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
1890 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
123 parameters	$\Delta\rho_{\text{max}} = 2.13 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -2.56 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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	0.5000	0.46437 (5)	0.7500	0.02893 (13)
S1	0.68171 (12)	-0.6475 (3)	0.43591 (9)	0.0341 (3)
N1	0.8579 (6)	-1.0111 (11)	0.4062 (4)	0.0358 (12)
H1A	0.9286	-1.0940	0.4177	0.043*
H1B	0.8061	-1.0545	0.3611	0.043*
N2	0.9003 (4)	-0.7340 (11)	0.5281 (3)	0.0314 (10)
O1	0.6764 (4)	0.1672 (12)	0.7523 (3)	0.0456 (12)
O2	0.5321 (4)	0.1587 (10)	0.6401 (3)	0.0400 (10)
C1	0.8286 (5)	-0.8158 (13)	0.4580 (3)	0.0293 (10)
C2	0.7228 (6)	-0.4520 (10)	0.5281 (4)	0.0269 (11)
C3	0.6541 (5)	-0.2540 (12)	0.5620 (3)	0.0293 (11)
H3	0.5754	-0.2021	0.5341	0.035*
C4	0.7070 (5)	-0.1345 (12)	0.6396 (3)	0.0303 (11)
C5	0.8264 (5)	-0.2125 (15)	0.6806 (4)	0.0382 (13)

H5	0.8603	-0.1325	0.7324	0.046*
C6	0.8940 (6)	-0.4066 (16)	0.6445 (4)	0.0401 (14)
H6	0.9740	-0.4530	0.6712	0.048*
C7	0.8425 (6)	-0.5332 (12)	0.5682 (4)	0.0301 (12)
C8	0.6357 (6)	0.0758 (12)	0.6796 (4)	0.0295 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.03445 (19)	0.02334 (18)	0.0291 (2)	0.000	0.00589 (12)	0.000
S1	0.0295 (6)	0.0391 (8)	0.0308 (7)	0.0058 (6)	-0.0030 (5)	-0.0049 (6)
N1	0.033 (3)	0.042 (3)	0.030 (3)	0.005 (2)	-0.001 (2)	-0.010 (2)
N2	0.0270 (19)	0.036 (3)	0.030 (2)	0.0052 (19)	0.0017 (17)	-0.0053 (19)
O1	0.052 (3)	0.055 (3)	0.028 (2)	0.021 (2)	0.0025 (18)	-0.007 (2)
O2	0.034 (2)	0.042 (3)	0.042 (2)	0.0081 (19)	0.0009 (17)	-0.013 (2)
C1	0.026 (2)	0.033 (3)	0.029 (2)	0.004 (2)	0.0043 (19)	0.003 (2)
C2	0.028 (3)	0.027 (3)	0.025 (3)	-0.0007 (19)	0.002 (2)	0.0008 (19)
C3	0.026 (2)	0.030 (3)	0.032 (3)	0.003 (2)	0.0063 (19)	0.005 (2)
C4	0.032 (2)	0.028 (3)	0.032 (3)	0.005 (2)	0.009 (2)	0.000 (2)
C5	0.035 (3)	0.050 (4)	0.027 (3)	0.008 (3)	0.000 (2)	-0.009 (3)
C6	0.032 (3)	0.050 (3)	0.034 (3)	0.012 (3)	-0.005 (2)	-0.009 (3)
C7	0.029 (3)	0.032 (3)	0.029 (3)	0.005 (2)	0.004 (2)	0.001 (2)
C8	0.037 (3)	0.025 (2)	0.030 (3)	0.002 (2)	0.014 (2)	0.003 (2)

Geometric parameters (Å, °)

Pb1—O2	2.366 (4)	N2—C7	1.375 (7)
Pb1—O2 ⁱ	2.366 (4)	O1—C8	1.251 (8)
Pb1—O1 ⁱ	2.395 (5)	O2—C8	1.259 (8)
Pb1—O1	2.395 (5)	C2—C3	1.382 (8)
Pb1—C8	2.749 (6)	C2—C7	1.406 (8)
Pb1—C8 ⁱ	2.749 (6)	C3—C4	1.399 (8)
Pb1—S1 ⁱⁱ	3.3894 (17)	C3—H3	0.9300
Pb1—S1 ⁱⁱⁱ	3.3894 (17)	C4—C5	1.404 (8)
S1—C2	1.741 (6)	C4—C8	1.489 (8)
S1—C1	1.776 (5)	C5—C6	1.378 (9)
N1—C1	1.330 (8)	C5—H5	0.9300
N1—H1A	0.8600	C6—C7	1.392 (9)
N1—H1B	0.8600	C6—H6	0.9300
N2—C1	1.310 (7)		
O2—Pb1—O2 ⁱ	102.8 (3)	H1A—N1—H1B	120.0
O2—Pb1—O1 ⁱ	80.64 (17)	C1—N2—C7	110.9 (5)
O2 ⁱ —Pb1—O1 ⁱ	54.26 (15)	C8—O1—Pb1	92.4 (4)
O2—Pb1—O1	54.26 (15)	C8—O2—Pb1	93.6 (4)
O2 ⁱ —Pb1—O1	80.64 (17)	N2—C1—N1	125.0 (5)
O1 ⁱ —Pb1—O1	106.4 (3)	N2—C1—S1	114.6 (4)
O2—Pb1—C8	27.21 (17)	N1—C1—S1	120.4 (4)

O2 ⁱ —Pb1—C8	92.19 (17)	C3—C2—C7	122.5 (5)
O1 ⁱ —Pb1—C8	94.21 (19)	C3—C2—S1	129.0 (5)
O1—Pb1—C8	27.04 (17)	C7—C2—S1	108.5 (4)
O2—Pb1—C8 ⁱ	92.19 (17)	C2—C3—C4	117.7 (5)
O2 ⁱ —Pb1—C8 ⁱ	27.21 (17)	C2—C3—H3	121.2
O1 ⁱ —Pb1—C8 ⁱ	27.04 (17)	C4—C3—H3	121.2
O1—Pb1—C8 ⁱ	94.21 (19)	C3—C4—C5	120.6 (5)
C8—Pb1—C8 ⁱ	93.9 (2)	C3—C4—C8	119.7 (5)
O2—Pb1—S1 ⁱⁱ	132.35 (10)	C5—C4—C8	119.7 (5)
O2 ⁱ —Pb1—S1 ⁱⁱ	69.61 (11)	C6—C5—C4	120.5 (6)
O1 ⁱ —Pb1—S1 ⁱⁱ	121.04 (10)	C6—C5—H5	119.7
O1—Pb1—S1 ⁱⁱ	78.27 (11)	C4—C5—H5	119.7
C8—Pb1—S1 ⁱⁱ	105.21 (14)	C5—C6—C7	120.1 (6)
C8 ⁱ —Pb1—S1 ⁱⁱ	95.37 (14)	C5—C6—H6	120.0
O2—Pb1—S1 ⁱⁱⁱ	69.61 (11)	C7—C6—H6	120.0
O2 ⁱ —Pb1—S1 ⁱⁱⁱ	132.35 (11)	N2—C7—C6	124.8 (6)
O1 ⁱ —Pb1—S1 ⁱⁱⁱ	78.27 (11)	N2—C7—C2	116.7 (6)
O1—Pb1—S1 ⁱⁱⁱ	121.04 (10)	C6—C7—C2	118.6 (6)
C8—Pb1—S1 ⁱⁱⁱ	95.37 (14)	O1—C8—O2	119.7 (5)
C8 ⁱ —Pb1—S1 ⁱⁱⁱ	105.21 (14)	O1—C8—C4	120.8 (6)
S1 ⁱⁱ —Pb1—S1 ⁱⁱⁱ	149.76 (6)	O2—C8—C4	119.5 (6)
C2—S1—C1	89.4 (3)	O1—C8—Pb1	60.5 (3)
C1—N1—H1A	120.0	O2—C8—Pb1	59.2 (3)
C1—N1—H1B	120.0	C4—C8—Pb1	178.7 (5)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B \cdots O1 ^{iv}	0.86	2.11	2.973 (7)	179
N1—H1A \cdots N2 ^v	0.86	2.09	2.934 (7)	168

Symmetry codes: (iv) $x, -y-1, z-1/2$; (v) $-x+2, -y-2, -z+1$.