

Bis(μ -iminodiacetato)bis[(2,2'-diamino-4,4'-bi-1,3-thiazole)lead(II)] tetrahydrate

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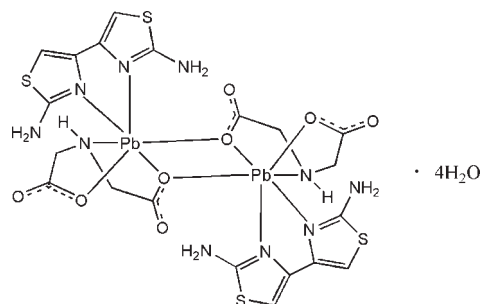
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 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.020; wR factor = 0.048; data-to-parameter ratio = 11.8.

In the crystal structure of the title compound, $[\text{Pb}_2(\text{C}_4\text{H}_5\text{NO}_4)_2(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)_2] \cdot 4\text{H}_2\text{O}$, the dinuclear Pb^{II} complex molecule is centrosymmetric. The Pb atom is chelated by a tridentate iminodiacetate anion (IDA) and a diaminobithiazole (DABT) ligand, while a carboxylate O atom from an adjacent IDA anion further bridges the Pb atom with a longer Pb—O bond [2.892 (3) Å]. The lone-pair electrons of the Pb atom occupy an axial site in the Ψ -pentagonal-bipyramidal coordination polyhedron. The IDA anion displays a facial configuration: its chelating five-membered rings assume an envelope configuration. Within the DABT ligand, the two thiazole rings are twisted relative to each other, making a dihedral angle of 9.51 (17)°. Extensive N—H...O, O—H...O and weak C—H...O hydrogen bonding helps to stabilize the crystal structure.

Related literature

For the potential applications of metal complexes of diaminobithiazole in the field of biology, see: Waring (1981); Fisher *et al.* (1985). For Pb^{II} complexes with a similar coordination geometry, see: Lacouture *et al.* (2001); Jones *et al.* (1988). For a complex with a longer Pb—O bond distance [2.968 (4) Å], see: Inoue *et al.* (1993). For the dihedral angles between thiazole rings in diaminobithiazole complexes, see: Liu *et al.* (2006); Zhang *et al.* (2006).



Experimental

Crystal data

$[\text{Pb}_2(\text{C}_4\text{H}_5\text{NO}_4)_2(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)_2] \cdot 4\text{H}_2\text{O}$	$\beta = 67.4141$ (15)°
$M_r = 1145.16$	$\gamma = 69.0690$ (12)°
Triclinic, $P\bar{1}$	$V = 829.54$ (14) Å ³
$a = 9.2241$ (8) Å	$Z = 1$
$b = 9.8526$ (9) Å	Mo $K\alpha$ radiation
$c = 10.6380$ (11) Å	$\mu = 10.46$ mm ⁻¹
$\alpha = 77.0732$ (12)°	$T = 295$ K
	$0.20 \times 0.12 \times 0.10$ mm

Data collection

Rigaku R-Axis RAPID diffractometer	5960 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	2878 independent reflections
$T_{\min} = 0.132$, $T_{\max} = 0.350$	2745 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.048$	$\Delta\rho_{\max} = 0.54$ e Å ⁻³
$S = 1.07$	$\Delta\rho_{\min} = -0.70$ e Å ⁻³
2878 reflections	
244 parameters	
9 restraints	

Table 1

Selected bond lengths (Å).

Pb—O1	2.546 (3)	Pb—N1	2.593 (3)
Pb—O1 ⁱ	2.892 (3)	Pb—N3	2.594 (3)
Pb—O3	2.536 (3)	Pb—N5	2.402 (4)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N2—H2A...O3	0.86 (6)	2.05 (5)	2.880 (6)	162 (5)
N2—H2B...O1W	0.86 (3)	2.16 (4)	2.959 (6)	153 (6)
N4—H4A...O1	0.86 (5)	2.15 (5)	2.946 (5)	155 (5)
N4—H4B...O4 ⁱⁱⁱ	0.86 (3)	2.07 (5)	2.885 (7)	159 (6)
N5—H5N...O2W	0.87 (5)	2.01 (6)	2.809 (7)	153 (4)
O1W—H11...O2 ⁱⁱⁱ	0.82 (2)	1.97 (2)	2.783 (6)	171 (5)
O1W—H12...O3 ^{iv}	0.82 (5)	2.11 (4)	2.819 (6)	144 (5)
O2W—H21...O1W ^v	0.82 (7)	2.10 (7)	2.892 (7)	161 (6)
O2W—H22...O4 ^{vi}	0.82 (5)	1.95 (5)	2.766 (6)	168 (7)
C5—H5...O2 ^{vii}	0.93	2.56	3.476 (6)	167

 Symmetry codes: (ii) $x, y, z + 1$; (iii) $x, y + 1, z - 1$; (iv) $-x + 1, -y + 2, -z$; (v) $-x + 2, -y + 2, -z$; (vi) $-x + 2, -y + 1, -z$; (vii) $x, y + 1, z$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2733).

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supporting information

Acta Cryst. (2010). E66, m343–m344 [doi:10.1107/S1600536810006926]

Bis(μ -iminodiacetato)bis[(2,2'-diamino-4,4'-bi-1,3-thiazole)lead(II)] tetrahydrate

Mei Du, Bing-Xin Liu, Jing-Jing Nie and Duan-Jun Xu

S1. Comment

Some metal complexes with 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown the potential application in the biological field (Waring, 1981; Fisher *et al.*, 1985). As a part of serial structural investigation of metal complexes with DABT, the title Pb^{II} complex was prepared in the laboratory and its X-ray structure is presented here.

The molecular structure of the title compound is shown in Fig. 1. The dinuclear Pb^{II} complex molecule is centrosymmetric. Each Pb atom is chelated by a tridentate iminodiacetate anion (IDA) and a diaminobithiazole (DABT) ligand, and one carboxyl O atom from the adjacent IDA anion further bridges the Pb atom. The lone-pair electrons of the Pb atom occupy an axial site in the distorted Ψ -pentagonal bipyramidal coordination geometry, which is similar to that found in Pb^{II} complexes reported previously (Lacouture *et al.*, 2001; Jones *et al.*, 1988). The longer Pb—O(bridge) bond distance (Table 1) is comparable to 2.968 (4) Å found in a related Pb complex (Inoue *et al.*, 1993). The IDA displays a facial configuration, its both chelating five-membered rings assume the envelope configuration. Within the DABT ligand, the two thiazole rings are twisted to each other with a dihedral angle of 9.51 (17)°, it agrees with 14.7 (3) and 9.5 (2)° found in transition metal complexes of DABT (Liu *et al.*, 2006; Zhang *et al.*, 2006).

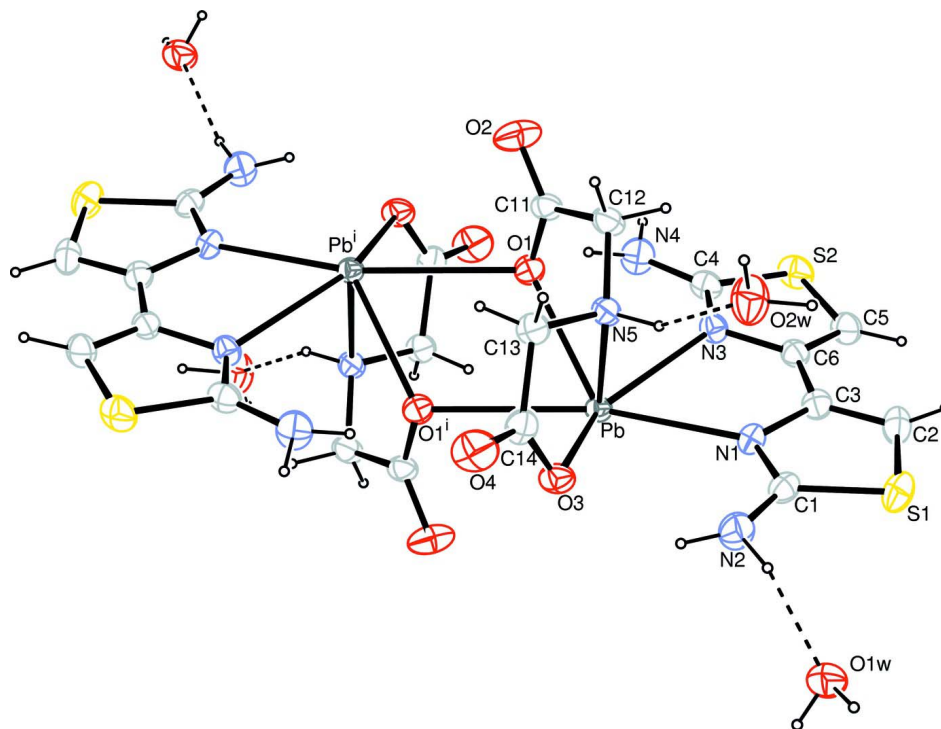
The extensive N—H \cdots O, O—H \cdots O and weak C—H \cdots O hydrogen bonding helps to stabilize the crystal structure (Table 2).

S2. Experimental

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and Pb(NO₃)₂ (0.33 g, 1 mmol) was mixed with another aqueous solution (10 ml) of H₂IDA (0.13 g, 1 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 5 h. The solution was filtered after cooling to room temperature. Single crystals were obtained from the filtrate after one week.

S3. Refinement

H atoms bonded to N and O atoms were located in a difference Fourier map and were refined with distance constraints [O—H = 0.82±0.03 and N—H = 0.86±0.03 Å] and $U_{\text{iso}}(\text{H}) = 0.08 \text{ \AA}^2$. H atoms on carbon atoms were placed in calculated positions with C—H = 0.97 Å (methylene) and 0.93 Å (aromatic), and included in the final cycles of refinement in the riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

The dinuclear molecular structure with 30% probability displacement ellipsoids. Dashed lines indicate the hydrogen bonding [symmetric code: (i) $-x, -y, 1-z$].

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Crystal data

$[\text{Pb}_2(\text{C}_4\text{H}_5\text{NO}_4)_2(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)_2] \cdot 4\text{H}_2\text{O}$

$M_r = 1145.16$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.2241$ (8) Å

$b = 9.8526$ (9) Å

$c = 10.6380$ (11) Å

$\alpha = 77.0732$ (12)°

$\beta = 67.4141$ (15)°

$\gamma = 69.0690$ (12)°

$V = 829.54$ (14) Å³

$Z = 1$

$F(000) = 544$

$D_x = 2.292$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4336 reflections

$\theta = 2.1\text{--}24.6^\circ$

$\mu = 10.46$ mm⁻¹

$T = 295$ K

Block, yellow

$0.20 \times 0.12 \times 0.10$ mm

Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.00 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.132$, $T_{\max} = 0.350$

5960 measured reflections

2878 independent reflections

2745 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.020$
 $wR(F^2) = 0.048$
 $S = 1.07$
 2878 reflections
 244 parameters
 9 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.019P)^2 + 0.7917P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.54 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.70 \text{ e } \text{Å}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pb	0.545731 (18)	0.724630 (15)	0.424338 (14)	0.02919 (7)
S1	0.85653 (18)	1.10157 (14)	0.16319 (14)	0.0551 (3)
S2	0.70556 (17)	0.84111 (15)	0.78711 (13)	0.0513 (3)
O1	0.6288 (4)	0.4760 (3)	0.5554 (3)	0.0400 (7)
O2	0.8401 (5)	0.2774 (4)	0.5652 (4)	0.0696 (11)
O3	0.5809 (4)	0.7154 (3)	0.1777 (3)	0.0431 (7)
O4	0.6770 (6)	0.5550 (4)	0.0268 (4)	0.0714 (12)
O1W	0.7380 (5)	1.1758 (4)	-0.1588 (4)	0.0577 (9)
O2W	1.0741 (5)	0.6671 (5)	0.1186 (5)	0.0717 (11)
N1	0.7119 (4)	0.9098 (4)	0.3108 (4)	0.0359 (8)
N2	0.7160 (6)	0.9566 (5)	0.0832 (4)	0.0541 (11)
N3	0.6755 (4)	0.7770 (4)	0.5787 (3)	0.0357 (8)
N4	0.5919 (6)	0.6270 (5)	0.7807 (4)	0.0563 (11)
N5	0.8084 (4)	0.5688 (4)	0.2998 (4)	0.0355 (8)
C1	0.7507 (5)	0.9781 (5)	0.1862 (4)	0.0382 (10)
C2	0.8435 (6)	1.0598 (5)	0.3335 (5)	0.0494 (12)
H2	0.8841	1.1027	0.3770	0.059*
C3	0.7666 (5)	0.9569 (5)	0.3947 (4)	0.0372 (10)
C4	0.6525 (6)	0.7362 (5)	0.7099 (4)	0.0399 (10)
C5	0.7564 (6)	0.9461 (5)	0.6339 (5)	0.0461 (11)
H5	0.7934	1.0262	0.6206	0.055*
C6	0.7354 (5)	0.8967 (4)	0.5350 (5)	0.0368 (10)
C11	0.7810 (6)	0.4004 (5)	0.5131 (4)	0.0370 (10)
C12	0.8948 (6)	0.4667 (5)	0.3912 (5)	0.0418 (10)

H12A	0.9443	0.5183	0.4229	0.050*
H12B	0.9827	0.3892	0.3400	0.050*
C13	0.7855 (6)	0.4939 (5)	0.2072 (4)	0.0408 (10)
H13A	0.7393	0.4162	0.2599	0.049*
H13B	0.8919	0.4499	0.1420	0.049*
C14	0.6733 (6)	0.5959 (5)	0.1303 (4)	0.0427 (11)
H11	0.768 (8)	1.197 (7)	-0.2418 (10)	0.080*
H12	0.6393 (18)	1.220 (6)	-0.132 (6)	0.080*
H21	1.124 (7)	0.724 (5)	0.113 (7)	0.080*
H22	1.147 (6)	0.594 (4)	0.086 (7)	0.080*
H2A	0.662 (6)	0.895 (5)	0.101 (6)	0.080*
H2B	0.751 (8)	0.997 (6)	0.001 (2)	0.080*
H4A	0.582 (7)	0.570 (5)	0.736 (5)	0.080*
H4B	0.595 (7)	0.598 (6)	0.862 (2)	0.080*
H5N	0.865 (6)	0.626 (5)	0.247 (5)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb	0.03072 (10)	0.03010 (10)	0.02682 (10)	-0.00792 (7)	-0.01080 (7)	-0.00292 (6)
S1	0.0619 (9)	0.0475 (7)	0.0531 (7)	-0.0305 (6)	-0.0092 (6)	0.0054 (6)
S2	0.0594 (8)	0.0592 (8)	0.0430 (7)	-0.0105 (6)	-0.0248 (6)	-0.0183 (6)
O1	0.0430 (19)	0.0399 (17)	0.0384 (17)	-0.0150 (15)	-0.0159 (14)	0.0016 (13)
O2	0.070 (3)	0.051 (2)	0.064 (2)	-0.0008 (19)	-0.025 (2)	0.0136 (19)
O3	0.051 (2)	0.0448 (18)	0.0352 (16)	-0.0102 (15)	-0.0218 (15)	-0.0005 (14)
O4	0.110 (3)	0.068 (2)	0.049 (2)	-0.016 (2)	-0.046 (2)	-0.0134 (19)
O1W	0.063 (2)	0.059 (2)	0.054 (2)	-0.0169 (19)	-0.030 (2)	0.0050 (19)
O2W	0.062 (3)	0.076 (3)	0.074 (3)	-0.035 (2)	-0.002 (2)	-0.013 (2)
N1	0.040 (2)	0.0315 (18)	0.0362 (19)	-0.0136 (16)	-0.0107 (16)	-0.0017 (15)
N2	0.068 (3)	0.058 (3)	0.039 (2)	-0.030 (2)	-0.019 (2)	0.010 (2)
N3	0.038 (2)	0.041 (2)	0.0309 (18)	-0.0143 (16)	-0.0126 (16)	-0.0041 (15)
N4	0.081 (3)	0.066 (3)	0.032 (2)	-0.033 (3)	-0.026 (2)	0.007 (2)
N5	0.034 (2)	0.039 (2)	0.035 (2)	-0.0125 (16)	-0.0138 (16)	-0.0001 (16)
C1	0.038 (2)	0.033 (2)	0.037 (2)	-0.0107 (19)	-0.0072 (19)	-0.0009 (18)
C2	0.050 (3)	0.046 (3)	0.058 (3)	-0.024 (2)	-0.013 (2)	-0.010 (2)
C3	0.034 (2)	0.035 (2)	0.040 (2)	-0.0065 (19)	-0.0086 (19)	-0.0115 (19)
C4	0.043 (3)	0.047 (3)	0.032 (2)	-0.008 (2)	-0.015 (2)	-0.010 (2)
C5	0.052 (3)	0.044 (3)	0.051 (3)	-0.012 (2)	-0.024 (2)	-0.014 (2)
C6	0.033 (2)	0.034 (2)	0.045 (2)	-0.0053 (18)	-0.015 (2)	-0.0113 (19)
C11	0.043 (3)	0.038 (2)	0.034 (2)	-0.008 (2)	-0.021 (2)	-0.0024 (19)
C12	0.038 (3)	0.048 (3)	0.042 (2)	-0.012 (2)	-0.021 (2)	0.001 (2)
C13	0.049 (3)	0.040 (2)	0.036 (2)	-0.009 (2)	-0.019 (2)	-0.0080 (19)
C14	0.054 (3)	0.045 (3)	0.032 (2)	-0.020 (2)	-0.014 (2)	0.000 (2)

Geometric parameters (Å, °)

Pb—O1	2.546 (3)	N2—H2A	0.86 (6)
Pb—O1 ⁱ	2.892 (3)	N2—H2B	0.86 (3)

Pb—O3	2.536 (3)	N3—C4	1.318 (5)
Pb—N1	2.593 (3)	N3—C6	1.391 (5)
Pb—N3	2.594 (3)	N4—C4	1.335 (6)
Pb—N5	2.402 (4)	N4—H4A	0.86 (5)
S1—C2	1.732 (5)	N4—H4B	0.86 (3)
S1—C1	1.739 (4)	N5—C13	1.468 (5)
S2—C5	1.718 (5)	N5—C12	1.475 (5)
S2—C4	1.741 (4)	N5—H5N	0.86 (5)
O1—C11	1.283 (5)	C2—C3	1.348 (6)
O2—C11	1.237 (5)	C2—H2	0.9300
O3—C14	1.259 (5)	C3—C6	1.435 (6)
O4—C14	1.239 (5)	C5—C6	1.354 (6)
O1W—H11	0.819 (16)	C5—H5	0.9300
O1W—H12	0.82 (5)	C11—C12	1.509 (6)
O2W—H21	0.82 (7)	C12—H12A	0.9700
O2W—H22	0.82 (5)	C12—H12B	0.9700
N1—C1	1.321 (5)	C13—C14	1.513 (6)
N1—C3	1.403 (5)	C13—H13A	0.9700
N2—C1	1.331 (6)	C13—H13B	0.9700
N5—Pb—O3	66.12 (11)	N1—C1—S1	114.6 (3)
N5—Pb—O1	67.04 (11)	N2—C1—S1	120.7 (3)
O3—Pb—O1	114.56 (10)	C3—C2—S1	110.9 (4)
N5—Pb—N1	78.68 (11)	C3—C2—H2	124.5
O3—Pb—N1	81.95 (10)	S1—C2—H2	124.5
O1—Pb—N1	128.64 (10)	C2—C3—N1	115.0 (4)
N5—Pb—N3	90.68 (12)	C2—C3—C6	125.7 (4)
O3—Pb—N3	143.48 (11)	N1—C3—C6	119.3 (4)
O1—Pb—N3	77.56 (10)	N3—C4—N4	124.6 (4)
N1—Pb—N3	65.44 (11)	N3—C4—S2	113.7 (3)
C2—S1—C1	89.0 (2)	N4—C4—S2	121.7 (3)
C5—S2—C4	89.4 (2)	C6—C5—S2	111.0 (4)
C11—O1—Pb	116.9 (3)	C6—C5—H5	124.5
C14—O3—Pb	114.4 (3)	S2—C5—H5	124.5
H11—O1W—H12	105 (6)	C5—C6—N3	114.7 (4)
H21—O2W—H22	104 (6)	C5—C6—C3	126.4 (4)
C1—N1—C3	110.4 (4)	N3—C6—C3	119.0 (4)
C1—N1—Pb	132.4 (3)	O2—C11—O1	124.6 (4)
C3—N1—Pb	117.1 (3)	O2—C11—C12	118.1 (4)
C1—N2—H2A	116 (4)	O1—C11—C12	117.3 (4)
C1—N2—H2B	122 (4)	N5—C12—C11	112.3 (4)
H2A—N2—H2B	121 (6)	N5—C12—H12A	109.1
C4—N3—C6	111.2 (4)	C11—C12—H12A	109.1
C4—N3—Pb	128.8 (3)	N5—C12—H12B	109.1
C6—N3—Pb	116.8 (3)	C11—C12—H12B	109.1
C4—N4—H4A	118 (4)	H12A—C12—H12B	107.9
C4—N4—H4B	119 (4)	N5—C13—C14	112.6 (4)
H4A—N4—H4B	119 (6)	N5—C13—H13A	109.1

C13—N5—C12	112.7 (3)	C14—C13—H13A	109.1
C13—N5—Pb	109.0 (3)	N5—C13—H13B	109.1
C12—N5—Pb	112.3 (3)	C14—C13—H13B	109.1
C13—N5—H5N	105 (4)	H13A—C13—H13B	107.8
C12—N5—H5N	111 (4)	O4—C14—O3	124.8 (5)
Pb—N5—H5N	106 (4)	O4—C14—C13	117.8 (4)
N1—C1—N2	124.7 (4)	O3—C14—C13	117.4 (4)

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

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2 <i>A</i> \cdots O3	0.86 (6)	2.05 (5)	2.880 (6)	162 (5)
N2—H2 <i>B</i> \cdots O1 <i>W</i>	0.86 (3)	2.16 (4)	2.959 (6)	153 (6)
N4—H4 <i>A</i> \cdots O1	0.86 (5)	2.15 (5)	2.946 (5)	155 (5)
N4—H4 <i>B</i> \cdots O4 ⁱⁱ	0.86 (3)	2.07 (5)	2.885 (7)	159 (6)
N5—H5 <i>N</i> \cdots O2 <i>W</i>	0.87 (5)	2.01 (6)	2.809 (7)	153 (4)
O1 <i>W</i> —H11 \cdots O2 ⁱⁱⁱ	0.82 (2)	1.97 (2)	2.783 (6)	171 (5)
O1 <i>W</i> —H12 \cdots O3 ^{iv}	0.82 (5)	2.11 (4)	2.819 (6)	144 (5)
O2 <i>W</i> —H21 \cdots O1 <i>W</i> ^v	0.82 (7)	2.10 (7)	2.892 (7)	161 (6)
O2 <i>W</i> —H22 \cdots O4 ^{vi}	0.82 (5)	1.95 (5)	2.766 (6)	168 (7)
C5—H5 \cdots O2 ^{vii}	0.93	2.56	3.476 (6)	167

Symmetry codes: (ii) $x, y, z+1$; (iii) $x, y+1, z-1$; (iv) $-x+1, -y+2, -z$; (v) $-x+2, -y+2, -z$; (vi) $-x+2, -y+1, -z$; (vii) $x, y+1, z$.