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Bis(2,2′-diamino-4,4′-bi-1,3-thiazole-$\kappa^2N^3,N^{3'}$)bis(nitrato-κO)lead(II) dihydrate

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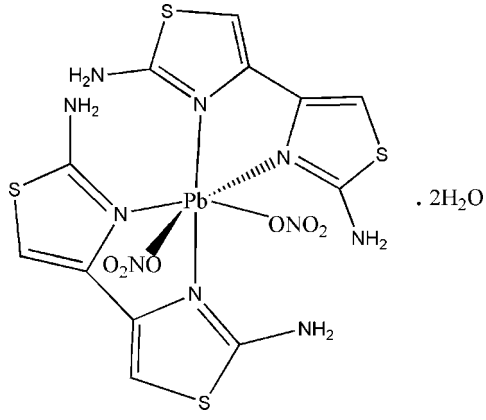
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.025; wR factor = 0.065; data-to-parameter ratio = 12.6.

In the title compound, $[Pb(NO_3)_2(C_6H_6N_4S_2)_2]\cdot 2H_2O$, the Pb^{II} cation is N,N'-chelated by two 2,2′-diamino-4,4′-bi-1,3-thiazole (DABT) ligands and further is *cis* coordinated by two nitrate anions in a distorted PbN_4O_2 octahedral geometry. One of the uncoordinated water molecules is close to an inversion center and is disordered equally over two sites. Intramolecular N—H···N and N—H···O interactions are present. An extensive hydrogen-bonding network of types N—H···O, O—H···O, O—H···N and O—H···S consolidates the crystal structure.

Related literature

For the application of 2,2′-diamino-4,4′-bi-1,3-thiazole complexes as soft magnetic materials, see: Sun *et al.* (1997). For general background to the structures of complexes of 2,2′-diamino-4,4′-bi-1,3-thiazole, see: Liu *et al.* (2003). For Pb—N bond distances in 2,2′-diamino-4,4′-bi-1,3-thiazole complexes, see: Abedini *et al.* (2005); Liu *et al.* (2006). H atoms bonded to the disordered O atoms were placed in calculated positions, see: Nardelli (1999)



. $2H_2O$

Experimental

Crystal data

$[Pb(NO_3)_2(C_6H_6N_4S_2)_2]\cdot 2H_2O$
M_r = 1527.66
Triclinic, $P\overline{1}$
a = 9.2387 (8) Å
b = 9.6962 (9) Å
c = 13.5636 (6) Å
α = 105.731 (4)°
β = 90.377 (3)°
γ = 97.072 (5)°
V = 1159.61 (16) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 7.70 mm^{-1}
T = 294 K
0.21 × 0.16 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.215, T_{max} = 0.340
6095 measured reflections
4012 independent reflections
3705 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.08
4012 reflections
319 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pb—N1	2.656 (4)	Pb—N7	2.692 (4)
Pb—N3	2.563 (4)	Pb—O1	2.704 (4)
Pb—N5	2.535 (5)	Pb—O4	2.803 (5)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.92	2.08	2.884 (8)	145
N2—H2B···O4^{i}	0.90	2.33	3.209 (7)	165
N2—H2B···O6^{i}	0.90	2.31	3.057 (7)	140
N4—H4A···N7	0.99	2.19	3.168 (7)	166
N4—H4B···O1W^{ii}	0.88	2.29	3.015 (8)	141
N4—H4B···O2WA^{iii}	0.88	2.26	2.98 (9)	140
N6—H6A···N1	0.93	2.22	3.119 (8)	160
N6—H6B···O2WA^{iv}	0.96	2.29	3.12 (10)	145
N6—H6B···O1W^{iv}	0.96	2.10	2.929 (10)	144
N8—H8A···O3^{v}	0.90	2.17	3.027 (7)	159
N8—H8B···O4	0.84	2.13	2.916 (7)	156
O1W—H1A···O3	0.85	1.94	2.782 (8)	168
O1W—H1B···O2WA	0.83	1.97	2.54 (9)	125
O1W—H1B···O2WB	0.83	2.14	2.93 (4)	160
O2WA—H2C···N4^{iii}	0.85	2.42	2.98 (9)	124
O2WA—H2D···O1W^{vi}	0.85	2.17	2.85 (9)	136
O2WB—H2E···S4^{iii}	0.85	2.27	3.09 (5)	164
O2WB—H2F···S3^{vii}	0.85	2.80	3.53 (5)	144
O2WB—H2F···N6^{vii}	0.85	1.91	2.67 (5)	148

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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: HK2747).

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supporting information

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Bis(2,2′-diamino-4,4′-bi-1,3-thiazole-$\kappa^2N^3,N^{3'}$)bis(nitrato-κO)lead(II) dihydrate

Bing-Xin Liu and Duan-Jun Xu

S1. Comment

Some metal complexes of 2,2′-diamino-4,4′-bi-1,3-thiazole (DABT) have shown potential application in the field of soft magnetic material (Sun *et al.*, 1997). As part of the ongoing structural investigation of metal complexes with DABT ligand (Liu *et al.*, 2003), the title Pb^{II} complex has recently been prepared and its crystal structure is reported herein.

In the title compound, the Pb^{II} cation is N,*N*′-chelated by two DABT ligands and further is *cis*-coordinated by two nitrate anions in a distorted PbN_4O_2 octahedral geometry (Fig. 1). The Pb—N bond distances (Table 1) are somewhat longer than those [2.527, 2.544 and 2.551 Å] found in other two Pb complexes with DABT ligand (Abedini *et al.* 2005; Liu *et al.* 2006). One of the lattice water molecules is close to an inversion center and is disordered equally over two sites. The extensive hydrogen bonding network of types N—H···O, O—H···O, O—H···N and O—H···S is present in the crystal structure.

S2. Experimental

An aqueous solution (15 ml) of DABT (0.20 g, 1 mmol) and $Pb(NO_3)_2$ (0.33 g, 1 mmol) was refluxed for 4 h. The solution was filtered after cooling to room temperature. Yellow single crystals were obtained from the filtrate after 4 d.

S3. Refinement

One of the lattice water molecules [O2W] is close to an inversion center and is disordered equally over two sites. H atoms bonded to the disordered O atoms are placed in calculated position (Nardelli, 1999). H atoms bonded to the O1W and N atoms were located in a difference Fourier map. All H atoms bonded to O and N atoms were refined as riding in as-found relative positions. Aromatic H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode. U_{iso}(H) = 1.2U_{eq}(carrier) for all H atoms.

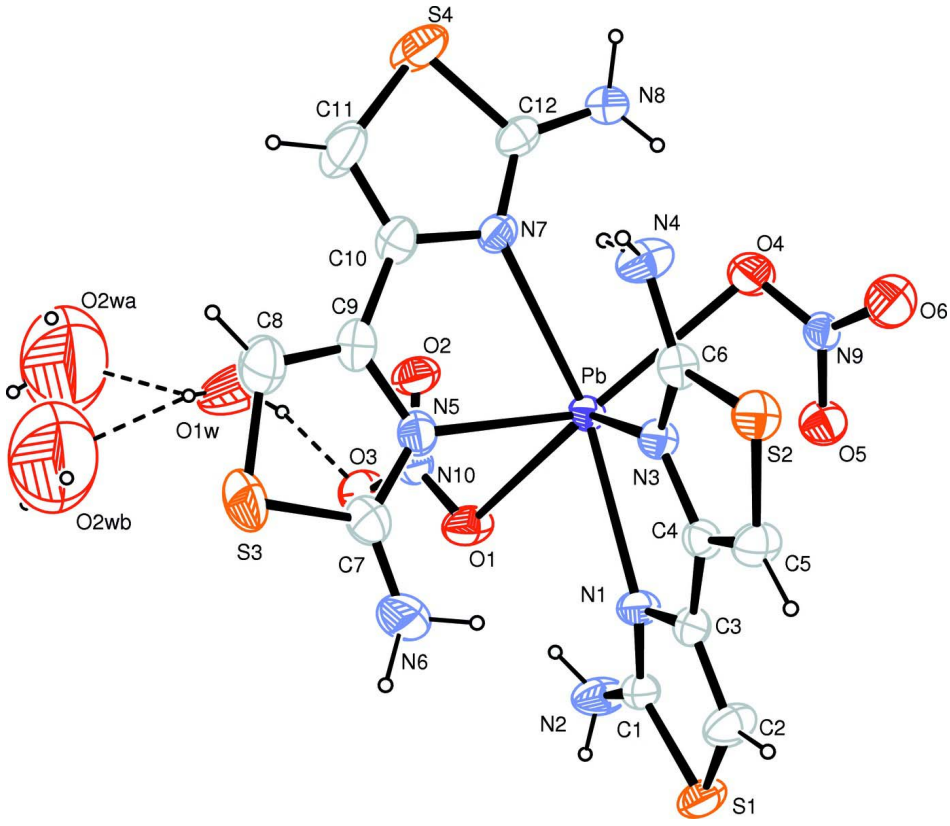

Figure 1

The molecular structure of the title compound with 30% probability displacement ellipsoids (arbitrary spheres for H atoms); dashed lines indicate the hydrogen bonding.

Bis(2,2′-diamino-4,4′-bi-1,3-thiazole- $\kappa^2N^3,N^{3'}$)bis(nitrato-κO)lead(II) dihydrate

Crystal data

$[Pb(NO_3)_2(C_6H_6N_4S_2)_2]\cdot 2H_2O$
$M_r = 1527.66$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.2387\ (8)$ Å
$b = 9.6962\ (9)$ Å
$c = 13.5636\ (6)$ Å
$\alpha = 105.731\ (4)°$
$\beta = 90.377\ (3)°$
$\gamma = 97.072\ (5)°$
$V = 1159.61\ (16)$ Å^3
$Z = 1$
$F(000) = 736$
$D_x = 2.187$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4246 reflections
$\theta = 2.2–25.0°$
$\mu = 7.70$ mm^{-1}
$T = 294$ K
Block, yellow
0.21 × 0.16 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.215$, $T_{max} = 0.340$
6095 measured reflections
4012 independent reflections
3705 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$

θ_{max} = 25.0°, θ_{min} = 1.6°
h = −9→10
k = −9→11
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.08
4012 reflections
319 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 1.6634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Pb	0.51296 (2)	0.384529 (19)	0.321343 (15)	0.03622 (8)	
S1	0.86425 (18)	0.07481 (19)	0.43924 (14)	0.0634 (4)	
S2	0.20076 (16)	−0.09836 (15)	0.28488 (12)	0.0527 (4)	
S3	0.6251 (3)	0.1416 (2)	−0.04539 (14)	0.0887 (6)	
S4	0.1267 (3)	0.5374 (2)	0.10337 (14)	0.0845 (6)	
N1	0.6815 (5)	0.2053 (5)	0.3667 (3)	0.0462 (11)	
N2	0.9129 (5)	0.3416 (6)	0.4149 (5)	0.0660 (15)	
H2A	0.9059	0.4168	0.3862	0.079*	
H2B	1.0104	0.3441	0.4233	0.079*	
N3	0.3856 (4)	0.1266 (4)	0.2963 (3)	0.0395 (9)	
N4	0.1501 (5)	0.1384 (5)	0.2314 (4)	0.0614 (14)	
H4A	0.1852	0.2369	0.2254	0.074*	
H4B	0.0971	0.0753	0.1816	0.074*	
N5	0.5432 (6)	0.2735 (5)	0.1318 (3)	0.0537 (12)	
N6	0.7467 (8)	0.1533 (8)	0.1351 (5)	0.101 (2)	
H6A	0.7241	0.1444	0.2003	0.121*	
H6B	0.8060	0.0773	0.1133	0.121*	
N7	0.3075 (5)	0.4293 (5)	0.1959 (3)	0.0450 (10)	
N8	0.1492 (5)	0.5684 (5)	0.3050 (4)	0.0566 (12)	
H8A	0.0613	0.5979	0.3009	0.068*	
H8B	0.1761	0.5443	0.3564	0.068*	
N9	0.2813 (5)	0.3333 (5)	0.4915 (3)	0.0417 (10)	
N10	0.7714 (5)	0.5968 (5)	0.2504 (4)	0.0499 (11)	

O1	0.7860 (4)	0.4915 (5)	0.2859 (4)	0.0662 (12)	
O2	0.6464 (4)	0.6191 (5)	0.2306 (3)	0.0637 (11)	
O3	0.8811 (5)	0.6758 (5)	0.2381 (4)	0.0757 (13)	
O4	0.2622 (5)	0.4100 (5)	0.4368 (4)	0.0767 (14)	
O5	0.4074 (4)	0.3241 (4)	0.5214 (3)	0.0583 (10)	
O6	0.1759 (5)	0.2579 (6)	0.5126 (4)	0.0799 (14)	
C1	0.8164 (6)	0.2223 (6)	0.4046 (4)	0.0465 (13)	
C2	0.6914 (7)	−0.0124 (7)	0.4019 (5)	0.0649 (17)	
H2	0.6586	−0.1055	0.4053	0.078*	
C3	0.6101 (6)	0.0701 (5)	0.3673 (4)	0.0417 (11)	
C4	0.4582 (6)	0.0295 (5)	0.3302 (4)	0.0406 (11)	
C5	0.3759 (6)	−0.0963 (6)	0.3282 (5)	0.0536 (14)	
H5	0.4097	−0.1719	0.3476	0.064*	
C6	0.2493 (6)	0.0720 (5)	0.2691 (4)	0.0433 (12)	
C7	0.6410 (8)	0.1928 (7)	0.0868 (5)	0.0664 (17)	
C8	0.4800 (9)	0.2367 (9)	−0.0394 (5)	0.082 (2)	
H8	0.4276	0.2442	−0.0961	0.099*	
C9	0.4521 (7)	0.2994 (6)	0.0586 (4)	0.0565 (15)	
C10	0.3355 (7)	0.3902 (6)	0.0933 (4)	0.0528 (14)	
C11	0.2503 (10)	0.4381 (8)	0.0331 (5)	0.084 (2)	
H11	0.2573	0.4198	−0.0375	0.100*	
C12	0.2007 (6)	0.5091 (6)	0.2119 (4)	0.0479 (13)	
O1W	0.8919 (7)	0.9099 (6)	0.1556 (7)	0.143 (3)	
H1A	0.8768	0.8420	0.1848	0.172*	
H1B	0.9025	0.8687	0.0946	0.172*	
O2WA	0.952 (12)	0.968 (9)	−0.012 (7)	0.46 (3)	0.50
H2C	0.8712	0.9381	−0.0459	0.553*	0.50
H2D	1.0193	0.9627	−0.0553	0.553*	0.50
O2WB	1.007 (6)	0.784 (5)	−0.045 (3)	0.46 (3)	0.50
H2E	0.9815	0.6950	−0.0507	0.553*	0.50
H2F	1.0980	0.7961	−0.0538	0.553*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb	0.03230 (12)	0.03302 (12)	0.04414 (12)	0.00269 (8)	0.00326 (8)	0.01255 (8)
S1	0.0507 (9)	0.0742 (11)	0.0805 (11)	0.0126 (8)	−0.0077 (8)	0.0450 (9)
S2	0.0488 (8)	0.0411 (7)	0.0670 (9)	−0.0075 (6)	0.0027 (7)	0.0187 (7)
S3	0.1077 (16)	0.1029 (15)	0.0530 (10)	0.0293 (13)	0.0292 (10)	0.0096 (10)
S4	0.1085 (16)	0.0875 (13)	0.0631 (11)	0.0429 (12)	−0.0244 (10)	0.0174 (9)
N1	0.038 (2)	0.045 (2)	0.060 (3)	0.010 (2)	0.002 (2)	0.021 (2)
N2	0.035 (3)	0.062 (3)	0.109 (5)	−0.001 (2)	−0.009 (3)	0.041 (3)
N3	0.038 (2)	0.036 (2)	0.045 (2)	0.0012 (18)	0.0018 (18)	0.0118 (18)
N4	0.047 (3)	0.051 (3)	0.091 (4)	−0.007 (2)	−0.019 (3)	0.033 (3)
N5	0.063 (3)	0.055 (3)	0.047 (3)	0.016 (2)	0.013 (2)	0.018 (2)
N6	0.114 (6)	0.131 (6)	0.068 (4)	0.079 (5)	0.023 (4)	0.017 (4)
N7	0.044 (3)	0.049 (3)	0.047 (3)	0.004 (2)	−0.002 (2)	0.022 (2)
N8	0.047 (3)	0.071 (3)	0.061 (3)	0.018 (2)	0.005 (2)	0.028 (3)

N9	0.035 (2)	0.052 (3)	0.038 (2)	0.001 (2)	0.0006 (18)	0.014 (2)
N10	0.047 (3)	0.053 (3)	0.053 (3)	0.005 (2)	0.005 (2)	0.020 (2)
O1	0.047 (2)	0.061 (3)	0.104 (4)	0.005 (2)	0.003 (2)	0.047 (3)
O2	0.050 (3)	0.075 (3)	0.076 (3)	0.013 (2)	−0.006 (2)	0.034 (2)
O3	0.054 (3)	0.075 (3)	0.113 (4)	−0.003 (2)	0.013 (3)	0.055 (3)
O4	0.069 (3)	0.078 (3)	0.112 (4)	0.033 (3)	0.034 (3)	0.064 (3)
O5	0.047 (2)	0.066 (3)	0.057 (2)	0.0002 (19)	−0.0071 (19)	0.012 (2)
O6	0.050 (3)	0.100 (4)	0.098 (4)	−0.015 (3)	−0.006 (2)	0.052 (3)
C1	0.039 (3)	0.055 (3)	0.053 (3)	0.011 (3)	0.004 (2)	0.024 (3)
C2	0.057 (4)	0.057 (4)	0.093 (5)	0.003 (3)	−0.007 (3)	0.042 (3)
C3	0.043 (3)	0.042 (3)	0.044 (3)	0.006 (2)	0.005 (2)	0.017 (2)
C4	0.041 (3)	0.037 (3)	0.045 (3)	0.006 (2)	0.008 (2)	0.013 (2)
C5	0.051 (3)	0.041 (3)	0.074 (4)	0.003 (3)	0.001 (3)	0.026 (3)
C6	0.046 (3)	0.038 (3)	0.042 (3)	−0.002 (2)	0.002 (2)	0.008 (2)
C7	0.075 (5)	0.069 (4)	0.055 (4)	0.022 (4)	0.014 (3)	0.012 (3)
C8	0.092 (6)	0.101 (6)	0.050 (4)	0.014 (5)	0.003 (4)	0.013 (4)
C9	0.068 (4)	0.055 (3)	0.046 (3)	−0.001 (3)	0.006 (3)	0.016 (3)
C10	0.068 (4)	0.045 (3)	0.045 (3)	0.006 (3)	−0.001 (3)	0.011 (2)
C11	0.123 (7)	0.090 (5)	0.044 (3)	0.032 (5)	−0.010 (4)	0.021 (3)
C12	0.048 (3)	0.042 (3)	0.055 (3)	−0.002 (3)	−0.010 (3)	0.020 (3)
O1W	0.117 (5)	0.087 (4)	0.240 (9)	−0.022 (4)	−0.075 (6)	0.087 (5)
O2WA	0.66 (8)	0.50 (7)	0.31 (4)	0.30 (6)	0.16 (4)	0.17 (4)
O2WB	0.66 (8)	0.50 (7)	0.31 (4)	0.30 (6)	0.16 (4)	0.17 (4)

Geometric parameters (Å, º)

Pb—N1	2.656 (4)	N7—C12	1.311 (7)
Pb—N3	2.563 (4)	N7—C10	1.375 (7)
Pb—N5	2.535 (5)	N8—C12	1.354 (7)
Pb—N7	2.692 (4)	N8—H8A	0.8999
Pb—O1	2.704 (4)	N8—H8B	0.8393
Pb—O4	2.803 (5)	N9—O4	1.210 (6)
S1—C2	1.717 (7)	N9—O6	1.227 (6)
S1—C1	1.726 (5)	N9—O5	1.252 (5)
S2—C5	1.714 (6)	N10—O3	1.233 (6)
S2—C6	1.728 (5)	N10—O2	1.242 (6)
S3—C8	1.709 (8)	N10—O1	1.262 (6)
S3—C7	1.726 (7)	C2—C3	1.330 (7)
S4—C11	1.710 (8)	C2—H2	0.9300
S4—C12	1.720 (5)	C3—C4	1.458 (7)
N1—C1	1.319 (7)	C4—C5	1.349 (7)
N1—C3	1.395 (6)	C5—H5	0.9300
N2—C1	1.345 (7)	C8—C9	1.344 (9)
N2—H2A	0.9230	C8—H8	0.9300
N2—H2B	0.9039	C9—C10	1.474 (8)
N3—C6	1.313 (6)	C10—C11	1.338 (9)
N3—C4	1.390 (6)	C11—H11	0.9300
N4—C6	1.355 (7)	O1W—H1A	0.8534

N4—H4A	0.9949	O1W—H1B	0.8279
N4—H4B	0.8762	O2WA—O2WA^{i}	1.0 (2)
N5—C7	1.313 (8)	O2WA—H2C	0.8498
N5—C9	1.391 (8)	O2WA—H2D	0.8500
N6—C7	1.323 (9)	O2WB—H2E	0.8502
N6—H6A	0.9337	O2WB—H2F	0.8500
N6—H6B	0.9558		

N5—Pb—N3	78.40 (14)	O3—N10—O1	119.2 (5)
N5—Pb—N1	90.14 (15)	O2—N10—O1	118.7 (5)
N3—Pb—N1	65.73 (13)	N10—O1—Pb	105.8 (3)
N5—Pb—N7	64.98 (15)	N1—C1—N2	124.6 (5)
N3—Pb—N7	89.39 (13)	N1—C1—S1	114.4 (4)
N1—Pb—N7	148.47 (14)	N2—C1—S1	121.0 (4)
N5—Pb—O1	75.24 (16)	C3—C2—S1	111.4 (5)
N3—Pb—O1	132.73 (13)	C3—C2—H2	124.3
N1—Pb—O1	75.77 (13)	S1—C2—H2	124.3
N7—Pb—O1	113.10 (13)	C2—C3—N1	115.0 (5)
C2—S1—C1	89.0 (3)	C2—C3—C4	125.6 (5)
C5—S2—C6	89.2 (3)	N1—C3—C4	119.4 (4)
C8—S3—C7	89.4 (3)	C5—C4—N3	114.7 (5)
C11—S4—C12	88.7 (3)	C5—C4—C3	125.5 (5)
C1—N1—C3	110.2 (4)	N3—C4—C3	119.7 (4)
C1—N1—Pb	133.5 (4)	C4—C5—S2	111.0 (4)
C3—N1—Pb	115.4 (3)	C4—C5—H5	124.5
C1—N2—H2A	127.5	S2—C5—H5	124.5
C1—N2—H2B	123.9	N3—C6—N4	125.3 (5)
H2A—N2—H2B	102.7	N3—C6—S2	114.5 (4)
C6—N3—C4	110.5 (4)	N4—C6—S2	120.2 (4)
C6—N3—Pb	130.0 (3)	N5—C7—N6	124.9 (6)
C4—N3—Pb	118.7 (3)	N5—C7—S3	114.5 (5)
C6—N4—H4A	115.8	N6—C7—S3	120.6 (5)
C6—N4—H4B	109.5	C9—C8—S3	110.7 (6)
H4A—N4—H4B	120.6	C9—C8—H8	124.7
C7—N5—C9	110.0 (5)	S3—C8—H8	124.7
C7—N5—Pb	129.2 (4)	C8—C9—N5	115.4 (6)
C9—N5—Pb	120.7 (4)	C8—C9—C10	126.0 (6)
C7—N6—H6A	114.4	N5—C9—C10	118.7 (5)
C7—N6—H6B	131.4	C11—C10—N7	115.5 (6)
H6A—N6—H6B	100.3	C11—C10—C9	125.7 (6)
C12—N7—C10	109.9 (5)	N7—C10—C9	118.8 (5)
C12—N7—Pb	132.8 (4)	C10—C11—S4	110.9 (5)
C10—N7—Pb	115.3 (3)	C10—C11—H11	124.5
C12—N8—H8A	112.9	S4—C11—H11	124.5
C12—N8—H8B	120.1	N7—C12—N8	124.8 (5)
H8A—N8—H8B	121.3	N7—C12—S4	115.0 (4)
O4—N9—O6	119.0 (5)	N8—C12—S4	120.3 (4)
O4—N9—O5	120.7 (5)	H1A—O1W—H1B	105.1

O6—N9—O5	120.1 (5)	H2C—O2WA—H2D	107.7
O3—N10—O2	122.1 (5)	H2E—O2WB—H2F	107.7

Symmetry code: (i) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1	0.92	2.08	2.884 (8)	145
N2—H2*B*···O4^{ii}	0.90	2.33	3.209 (7)	165
N2—H2*B*···O6^{ii}	0.90	2.31	3.057 (7)	140
N4—H4*A*···N7	0.99	2.19	3.168 (7)	166
N4—H4*B*···O1*W*^{iii}	0.88	2.29	3.015 (8)	141
N4—H4*B*···O2*WA*^{iv}	0.88	2.26	2.98 (9)	140
N6—H6*A*···N1	0.93	2.22	3.119 (8)	160
N6—H6*B*···O2*WA*^{v}	0.96	2.29	3.12 (10)	145
N6—H6*B*···O1*W*^{v}	0.96	2.10	2.929 (10)	144
N8—H8*A*···O3^{vi}	0.90	2.17	3.027 (7)	159
N8—H8*B*···O4	0.84	2.13	2.916 (7)	156
O1*W*—H1*A*···O3	0.85	1.94	2.782 (8)	168
O1*W*—H1*B*···O2*WA*	0.83	1.97	2.54 (9)	125
O1*W*—H1*B*···O2*WB*	0.83	2.14	2.93 (4)	160
O2*WA*—H2*C*···N4^{iv}	0.85	2.42	2.98 (9)	124
O2*WA*—H2*D*···O1*W*^{i}	0.85	2.17	2.85 (9)	136
O2*WB*—H2*E*···S4^{iv}	0.85	2.27	3.09 (5)	164
O2*WB*—H2*F*···S3^{vii}	0.85	2.80	3.53 (5)	144
O2*WB*—H2*F*···N6^{vii}	0.85	1.91	2.67 (5)	148

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