

## [Bis(1*H*-benzimidazol-2-ylmethyl)amine- $\kappa^3$ N,N',N'']dinitratolead(II)

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Received 13 May 2007; accepted 25 May 2007

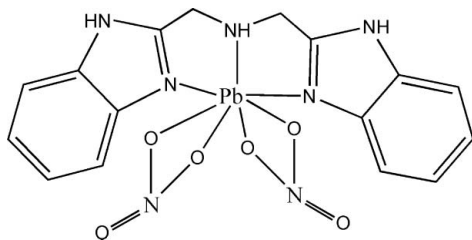
Key indicators: single-crystal X-ray study;  $T = 292$  K; mean  $\sigma(\text{C}-\text{C}) = 0.014$  Å;  $R$  factor = 0.045;  $wR$  factor = 0.126; data-to-parameter ratio = 14.8.

In the title compound,  $[\text{Pb}(\text{NO}_3)_2(\text{C}_{16}\text{H}_{15}\text{N}_5)]$ , the  $\text{Pb}^{\text{II}}$  ion is chelated by three N atoms of a bis(1*H*-benzimidazol-2-ylmethyl)amine (IDB) ligand and two O atoms from each of two nitrate ligands, resulting in an asymmetric seven-coordinate configuration. The crystal structure is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\pi-\pi$  interactions, with ring-centroid separations of 3.578 (5) and 3.686 (5) Å, leading to a three-dimensional network.

### Related literature

Studies of lead(II) complexes with N-donor ligands have been reported previously (Ali & Ali, 2002; Ali *et al.*, 2005). We have recently determined the structure of a potential ligand containing multi-benzimidazole groups (Zhang *et al.* 2005).

For related literature, see: Adams *et al.* (1990); Byriel *et al.* (1992).



### Experimental

#### Crystal data

$[\text{Pb}(\text{NO}_3)_2(\text{C}_{16}\text{H}_{15}\text{N}_5)]$   
 $M_r = 608.54$

Triclinic,  $P\bar{1}$   
 $a = 8.9865$  (4) Å

$b = 10.4501$  (5) Å  
 $c = 11.3544$  (5) Å  
 $\alpha = 98.296$  (1)°  
 $\beta = 102.842$  (1)°  
 $\gamma = 104.642$  (1)°  
 $V = 982.88$  (8) Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 8.63$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
 $0.20 \times 0.16 \times 0.10$  mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)  
 $T_{\text{min}} = 0.277$ ,  $T_{\text{max}} = 0.479$   
(expected range = 0.244–0.422)

9540 measured reflections  
4007 independent reflections  
3723 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.126$   
 $S = 1.12$   
4007 reflections

271 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 2.79$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -2.37$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3}\cdots\text{O6}^{\text{i}}$	0.86	2.04	2.895 (9)	170
$\text{C4}-\text{H4}\cdots\text{O2}^{\text{i}}$	0.93	2.58	3.332 (13)	138
$\text{C4}-\text{H4}\cdots\text{O5}^{\text{i}}$	0.93	2.52	3.248 (12)	136
$\text{N3}-\text{H3}\cdots\text{O5}^{\text{i}}$	0.86	2.50	3.165 (10)	135
$\text{N5}-\text{H5A}\cdots\text{O3}^{\text{ii}}$	0.86	2.11	2.876 (9)	149
$\text{C12}-\text{H12}\cdots\text{O1}^{\text{iii}}$	0.93	2.53	3.242 (11)	133
$\text{N1}-\text{H1}\cdots\text{O4}^{\text{iv}}$	0.91	2.27	3.099 (9)	151

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2392).

### References

- Adams, H., Bailey, N. A., Carane, J. D. & Fenton, D. E. (1990). *J. Chem. Soc. Dalton Trans.* pp. 1727–1735.  
Ali, A. S., Farzin, M. & Ali, M. (2005). *Inorg. Chem. Commun.* **8**, 773–776.  
Ali, R. M. & Ali, M. (2002). *Polyhedron*, **21**, 197–203.  
Bruker (2001). SAINT-Plus (Version 6.45) and SMART (Version 5.628). Bruker AXS, Inc., Madison, Wisconsin, USA.  
Byriel, K., Dunster, K. R. & Gahan, L. R. (1992). *Polyhedron*, **10**, 1205–1208.  
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
Sheldrick, G. M. (2001). SADABS. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.  
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
Zhang, Y., Liao, Z.-R., Li, D.-F. & Meng, X.-G. (2005). *Acta Cryst. E* **61**, o3396–o3397.

**supplementary materials**

*Acta Cryst.* (2007). E63, m1792 [ doi:10.1107/S1600536807025615 ]

## [Bis(1*H*-benzimidazol-2-ylmethyl)amine- $\kappa^3$ N,N',N'']dinitratolead(II)

Y. Zhang, X.-Y. Xia, X.-Q. Liu, X.-M. Chen and T. Liu

### Comment

The lead(II) complexes with N-donor ligands have been widely studied in recent years (Ali & Ali, 2002; Ali *et al.*, 2005). As part of our continuing studies on the ligands or metal complexes containing multi-benzimidazole groups (Zhang *et al.* 2005), We report herein the crystal structure of the title compound, [Bis(1*H*-benzimidazol-2-ylmethyl)amine]dinitratolead(II), (I).

In (I) (Fig. 1), the Pb atom is seven-coordinated by three nitrogen atoms of IDB and four oxygen atoms of two nitrates, resulting a rather asymmetric configuration. The seven donor atoms occupy half of the space environment around the lead ion, leaving a zone free from co-ordinated donor atoms, which is occupied by the lone pair of Pb around the lead ion (Byriel *et al.*, 1992).

In the crystal structure, the molecules are linked into a three-dimensional framework by intermolecular N—H—O and C—H—O hydrogen bonds (Table 1 and Fig. 2).  $\pi$ - $\pi$  stacking interactions are also observed between the adjacent imidazole rings. The imidazole ring of N2/N3/C2/C3/C8 at (*x,y,z*) and (1 - *x*, 1 - *y*, 1 - *z*) have a ring centroid separation of 3.578 (5) Å and an interplanar spacing of *ca* 3.521 Å. Similarly, the N4/N5/C10/C11/C16 rings at (*x,y,z*) and (-*x*, -*y*, -*z*) have a centroid separation of 3.686 (5) Å, with an interplanar spacing of 3.479 Å, corresponding to a plane slippage of 1.217 Å.

### Experimental

All reagents and solvents were used as obtained without further purification. Bis(benzimidazol-2-yl-methyl)amine (IDB) was prepared according to the method described by Adams *et al.* (1990). Compound (I) was synthesized by reaction of IDB (0.27 g, 1 mmol) and Pb(NO<sub>3</sub>)<sub>2</sub> (0.33 g, 1 mmol) in methanol (40 ml) at 333 K for 8 h. The resulting solution was filtered and yellow crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of the filtrate at room temperature after one week.

### Refinement

All the H atoms were located at their idealized positions [*C*—*H*(methylene) = 0.97 Å, N—H = 0.86 Å (imine) or 0.91 Å (amine), *C*—H(aromatic) = 0.93 Å], with the *U*<sub>iso</sub>(H) value being set 1.2 times of their carrier atoms for all the H atoms. The largest peak in the final difference Fourier map of 2.79 e Å<sup>-3</sup> is 1.00 Å from atom Pb1, and the deepest hole of 2.36 e Å<sup>-3</sup> is 0.93 Å from atom Pb1.

## Figures

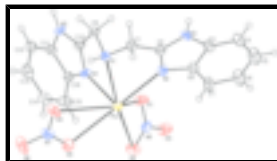


Fig. 1. Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

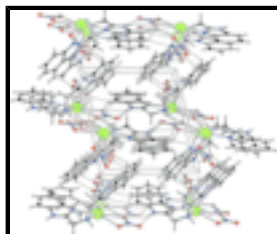


Fig. 2. Part of the crystal structure of (I), showing the formation of the three-dimensional network. Hydrogen bonding are shown as dashed lines.

## [Bis(1*H*-benzimidazol-2-ylmethyl)amine- $\kappa^3 N, N', N''$ ]dinitratolead(II)

### Crystal data

[Pb(NO<sub>3</sub>)<sub>2</sub>(C<sub>16</sub>H<sub>15</sub>N<sub>5</sub>)]

$M_r = 608.54$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 8.9865$  (4) Å

$b = 10.4501$  (5) Å

$c = 11.3544$  (5) Å

$\alpha = 98.296$  (1)°

$\beta = 102.842$  (1)°

$\gamma = 104.642$  (1)°

$V = 982.88$  (8) Å<sup>3</sup>

$Z = 2$

$F_{000} = 580$

$D_x = 2.056$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 6445 reflections

$\theta = 2.4$ – $28.1$ °

$\mu = 8.63$  mm<sup>-1</sup>

$T = 292$  (2) K

Block, yellow

$0.20 \times 0.16 \times 0.10$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer

4007 independent reflections

Radiation source: fine focus sealed Siemens Mo tube

3723 reflections with  $I > 2s(I)$

Monochromator: graphite

$R_{\text{int}} = 0.037$

$T = 298$ (2) K

$\theta_{\text{max}} = 26.5$ °

$0.3$ ° wide  $\omega$  exposures scans

$\theta_{\text{min}} = 1.9$ °

Absorption correction: multi-scan (SADABS; Sheldrick, 2001)

$h = -11 \rightarrow 11$

$T_{\text{min}} = 0.277$ ,  $T_{\text{max}} = 0.479$

$k = -13 \rightarrow 13$

9540 measured reflections

$l = -14 \rightarrow 12$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.126$	$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 3.4147P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
4007 reflections	$(\Delta/\sigma)_{\max} < 0.001$
271 parameters	$\Delta\rho_{\max} = 2.79 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -2.36 \text{ e } \text{\AA}^{-3}$
	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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pb1	0.35209 (3)	0.12463 (3)	0.37567 (3)	0.03271 (13)
C1	0.1658 (10)	0.3633 (8)	0.4442 (8)	0.0355 (17)
H1A	0.2099	0.3855	0.5333	0.043*
H1B	0.0748	0.3979	0.4250	0.043*
C2	0.2885 (9)	0.4286 (8)	0.3853 (8)	0.0337 (17)
C3	0.4516 (11)	0.5856 (8)	0.3237 (8)	0.0355 (17)
C4	0.5364 (13)	0.7010 (10)	0.2973 (9)	0.050 (2)
H4	0.5150	0.7831	0.3157	0.060*
C5	0.6561 (16)	0.6891 (13)	0.2415 (12)	0.066 (3)
H5	0.7179	0.7655	0.2230	0.080*
C6	0.6864 (15)	0.5644 (11)	0.2121 (11)	0.060 (3)
H6	0.7663	0.5600	0.1732	0.073*
C7	0.6012 (12)	0.4492 (9)	0.2394 (10)	0.049 (2)
H7	0.6233	0.3675	0.2211	0.059*
C8	0.4802 (10)	0.4589 (9)	0.2954 (8)	0.0339 (17)
C9	-0.0145 (8)	0.1762 (8)	0.2844 (7)	0.0308 (15)
H9A	-0.0012	0.2472	0.2380	0.037*
H9B	-0.1171	0.1628	0.3027	0.037*

## supplementary materials

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C10	-0.0116 (8)	0.0482 (9)	0.2085 (7)	0.0306 (16)
C11	-0.0887 (9)	-0.1419 (8)	0.0670 (7)	0.0312 (16)
C12	-0.1692 (11)	-0.2562 (9)	-0.0261 (8)	0.0408 (19)
H12	-0.2747	-0.2713	-0.0701	0.049*
C13	-0.0867 (13)	-0.3455 (10)	-0.0501 (9)	0.049 (2)
H13	-0.1389	-0.4270	-0.1067	0.058*
C14	0.0767 (12)	-0.3150 (10)	0.0100 (9)	0.047 (2)
H14	0.1325	-0.3736	-0.0135	0.057*
C15	0.1570 (11)	-0.2016 (10)	0.1023 (8)	0.043 (2)
H15	0.2636	-0.1855	0.1441	0.052*
C16	0.0727 (9)	-0.1120 (8)	0.1309 (7)	0.0292 (15)
N1	0.1139 (7)	0.2177 (7)	0.4010 (6)	0.0323 (14)
H1	0.0735	0.1803	0.4591	0.039*
N2	0.3766 (8)	0.3627 (7)	0.3384 (7)	0.0330 (14)
N3	0.3254 (8)	0.5588 (6)	0.3798 (6)	0.0330 (14)
H3	0.2802	0.6164	0.4058	0.040*
N4	0.1155 (7)	0.0067 (6)	0.2194 (6)	0.0278 (13)
N5	-0.1368 (7)	-0.0350 (7)	0.1195 (6)	0.0321 (14)
H5A	-0.2303	-0.0245	0.0983	0.039*
N6	0.5429 (8)	0.0792 (7)	0.1767 (7)	0.0391 (16)
N7	0.2026 (10)	-0.1607 (8)	0.4578 (8)	0.0439 (18)
O1	0.4232 (8)	0.1232 (8)	0.1732 (7)	0.0541 (17)
O2	0.5790 (10)	0.0167 (9)	0.2572 (9)	0.068 (2)
O3	0.6224 (8)	0.1029 (8)	0.1037 (7)	0.0583 (19)
O4	0.1378 (9)	-0.0720 (7)	0.4771 (7)	0.0521 (17)
O5	0.3208 (8)	-0.1363 (8)	0.4138 (7)	0.0523 (17)
O6	0.1556 (12)	-0.2715 (8)	0.4820 (10)	0.081 (3)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pb1	0.02497 (17)	0.0335 (2)	0.0372 (2)	0.01051 (12)	0.00101 (12)	0.00779 (13)
C1	0.037 (4)	0.024 (4)	0.045 (5)	0.009 (3)	0.015 (4)	0.001 (3)
C2	0.030 (3)	0.031 (4)	0.038 (4)	0.010 (3)	0.006 (3)	0.004 (3)
C3	0.047 (4)	0.032 (4)	0.030 (4)	0.013 (3)	0.012 (3)	0.008 (3)
C4	0.068 (6)	0.045 (5)	0.045 (5)	0.019 (5)	0.021 (5)	0.022 (4)
C5	0.086 (8)	0.063 (7)	0.065 (7)	0.017 (6)	0.049 (7)	0.029 (6)
C6	0.078 (7)	0.049 (6)	0.067 (7)	0.017 (5)	0.045 (6)	0.017 (5)
C7	0.056 (5)	0.033 (5)	0.069 (7)	0.010 (4)	0.039 (5)	0.013 (4)
C8	0.035 (4)	0.035 (4)	0.032 (4)	0.009 (3)	0.012 (3)	0.006 (3)
C9	0.026 (3)	0.030 (4)	0.034 (4)	0.009 (3)	0.002 (3)	0.005 (3)
C10	0.024 (3)	0.046 (5)	0.024 (4)	0.013 (3)	0.004 (3)	0.012 (3)
C11	0.033 (4)	0.040 (4)	0.025 (4)	0.013 (3)	0.009 (3)	0.016 (3)
C12	0.046 (5)	0.040 (5)	0.031 (4)	0.010 (4)	0.003 (4)	0.011 (4)
C13	0.065 (6)	0.041 (5)	0.034 (5)	0.007 (4)	0.012 (4)	0.009 (4)
C14	0.057 (5)	0.046 (5)	0.046 (5)	0.024 (4)	0.013 (4)	0.016 (4)
C15	0.047 (5)	0.055 (6)	0.035 (5)	0.031 (4)	0.011 (4)	0.009 (4)
C16	0.029 (3)	0.033 (4)	0.026 (4)	0.007 (3)	0.009 (3)	0.009 (3)

N1	0.027 (3)	0.037 (4)	0.035 (4)	0.011 (3)	0.010 (3)	0.012 (3)
N2	0.033 (3)	0.032 (4)	0.035 (4)	0.009 (3)	0.012 (3)	0.005 (3)
N3	0.039 (3)	0.023 (3)	0.040 (4)	0.013 (3)	0.009 (3)	0.007 (3)
N4	0.023 (3)	0.030 (3)	0.026 (3)	0.009 (2)	0.000 (2)	-0.001 (3)
N5	0.021 (3)	0.045 (4)	0.028 (3)	0.009 (3)	0.003 (2)	0.009 (3)
N6	0.026 (3)	0.033 (4)	0.054 (5)	0.006 (3)	0.009 (3)	0.003 (3)
N7	0.048 (4)	0.047 (5)	0.048 (5)	0.022 (4)	0.022 (4)	0.017 (4)
O1	0.042 (3)	0.070 (5)	0.064 (4)	0.035 (3)	0.019 (3)	0.017 (4)
O2	0.061 (5)	0.070 (5)	0.089 (6)	0.035 (4)	0.022 (4)	0.038 (5)
O3	0.048 (4)	0.084 (5)	0.061 (4)	0.034 (4)	0.029 (3)	0.022 (4)
O4	0.070 (4)	0.047 (4)	0.063 (4)	0.036 (3)	0.035 (4)	0.025 (3)
O5	0.047 (4)	0.062 (4)	0.067 (5)	0.025 (3)	0.033 (3)	0.031 (4)
O6	0.103 (6)	0.051 (5)	0.134 (8)	0.037 (4)	0.092 (7)	0.045 (5)

*Geometric parameters (Å, °)*

Pb1—N4	2.357 (6)	C9—H9A	0.9700
Pb1—O1	2.519 (7)	C9—H9B	0.9700
Pb1—N2	2.546 (7)	C10—N4	1.307 (9)
Pb1—N1	2.618 (6)	C10—N5	1.338 (10)
Pb1—O4	2.988 (7)	C11—C12	1.388 (12)
C1—N1	1.448 (10)	C11—N5	1.399 (10)
C1—C2	1.486 (11)	C11—C16	1.402 (10)
C1—H1A	0.9700	C12—C13	1.364 (13)
C1—H1B	0.9700	C12—H12	0.9300
C2—N2	1.320 (10)	C13—C14	1.407 (14)
C2—N3	1.332 (10)	C13—H13	0.9300
C3—C4	1.366 (13)	C14—C15	1.377 (14)
C3—N3	1.407 (11)	C14—H14	0.9300
C3—C8	1.418 (11)	C15—C16	1.391 (11)
C4—C5	1.386 (15)	C15—H15	0.9300
C4—H4	0.9300	C16—N4	1.387 (10)
C5—C6	1.407 (16)	N1—H1	0.9100
C5—H5	0.9300	N3—H3	0.8600
C6—C7	1.370 (14)	N5—H5A	0.8600
C6—H6	0.9300	N6—O3	1.221 (10)
C7—C8	1.393 (11)	N6—O2	1.231 (11)
C7—H7	0.9300	N6—O1	1.267 (9)
C8—N2	1.410 (11)	N7—O6	1.221 (11)
C9—N1	1.474 (10)	N7—O4	1.232 (9)
C9—C10	1.492 (11)	N7—O5	1.257 (10)
N4—Pb1—O1	73.5 (2)	N5—C10—C9	124.0 (6)
N4—Pb1—N2	98.9 (2)	C12—C11—N5	132.5 (7)
O1—Pb1—N2	74.9 (2)	C12—C11—C16	123.2 (7)
N4—Pb1—N1	68.2 (2)	N5—C11—C16	104.4 (7)
O1—Pb1—N1	117.3 (2)	C13—C12—C11	117.0 (8)
N2—Pb1—N1	64.6 (2)	C13—C12—H12	121.5
N4—Pb1—O4	70.6 (2)	C11—C12—H12	121.5
O1—Pb1—O4	135.3 (2)	C12—C13—C14	120.5 (9)

## supplementary materials

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N2—Pb1—O4	136.02 (18)	C12—C13—H13	119.8
N1—Pb1—O4	72.04 (19)	C14—C13—H13	119.8
N1—C1—C2	110.9 (6)	C15—C14—C13	122.4 (9)
N1—C1—H1A	109.5	C15—C14—H14	118.8
C2—C1—H1A	109.5	C13—C14—H14	118.8
N1—C1—H1B	109.5	C14—C15—C16	117.6 (8)
C2—C1—H1B	109.5	C14—C15—H15	121.2
H1A—C1—H1B	108.1	C16—C15—H15	121.2
N2—C2—N3	113.7 (7)	N4—C16—C15	132.0 (7)
N2—C2—C1	122.4 (7)	N4—C16—C11	108.8 (6)
N3—C2—C1	123.8 (7)	C15—C16—C11	119.1 (8)
C4—C3—N3	132.5 (8)	C1—N1—C9	111.1 (6)
C4—C3—C8	123.1 (8)	C1—N1—Pb1	111.7 (4)
N3—C3—C8	104.4 (7)	C9—N1—Pb1	110.7 (4)
C3—C4—C5	116.3 (9)	C1—N1—H1	107.7
C3—C4—H4	121.8	C9—N1—H1	107.7
C5—C4—H4	121.8	Pb1—N1—H1	107.7
C4—C5—C6	121.6 (10)	C2—N2—C8	105.3 (7)
C4—C5—H5	119.2	C2—N2—Pb1	116.9 (5)
C6—C5—H5	119.2	C8—N2—Pb1	136.9 (5)
C7—C6—C5	121.7 (9)	C2—N3—C3	107.8 (6)
C7—C6—H6	119.2	C2—N3—H3	126.1
C5—C6—H6	119.2	C3—N3—H3	126.1
C6—C7—C8	117.6 (9)	C10—N4—C16	106.5 (6)
C6—C7—H7	121.2	C10—N4—Pb1	120.6 (5)
C8—C7—H7	121.2	C16—N4—Pb1	132.7 (5)
C7—C8—N2	131.6 (8)	C10—N5—C11	107.9 (6)
C7—C8—C3	119.6 (8)	C10—N5—H5A	126.0
N2—C8—C3	108.7 (7)	C11—N5—H5A	126.0
N1—C9—C10	110.8 (6)	O3—N6—O2	121.6 (7)
N1—C9—H9A	109.5	O3—N6—O1	119.9 (8)
C10—C9—H9A	109.5	O2—N6—O1	118.5 (8)
N1—C9—H9B	109.5	O6—N7—O4	121.3 (8)
C10—C9—H9B	109.5	O6—N7—O5	119.2 (7)
H9A—C9—H9B	108.1	O4—N7—O5	119.4 (8)
N4—C10—N5	112.3 (7)	N6—O1—Pb1	109.6 (6)
N4—C10—C9	123.6 (7)	N7—O4—Pb1	93.5 (5)
N1—C1—C2—N2	-22.6 (12)	C3—C8—N2—Pb1	-166.3 (6)
N1—C1—C2—N3	160.7 (8)	N4—Pb1—N2—C2	80.7 (6)
N3—C3—C4—C5	179.3 (11)	O1—Pb1—N2—C2	150.8 (6)
C8—C3—C4—C5	-0.8 (15)	N1—Pb1—N2—C2	20.0 (6)
C3—C4—C5—C6	1.0 (19)	O4—Pb1—N2—C2	9.5 (8)
C4—C5—C6—C7	-1(2)	N4—Pb1—N2—C8	-111.9 (8)
C5—C6—C7—C8	1.3 (19)	O1—Pb1—N2—C8	-41.8 (8)
C6—C7—C8—N2	-177.4 (10)	N1—Pb1—N2—C8	-172.6 (9)
C6—C7—C8—C3	-1.1 (16)	O4—Pb1—N2—C8	176.9 (7)
C4—C3—C8—C7	0.8 (15)	N2—C2—N3—C3	-0.1 (10)
N3—C3—C8—C7	-179.2 (9)	C1—C2—N3—C3	176.9 (8)
C4—C3—C8—N2	178.0 (9)	C4—C3—N3—C2	-178.7 (10)



N3—C3—C8—N2	-2.1 (9)	C8—C3—N3—C2	1.4 (9)
N1—C9—C10—N4	-23.1 (11)	N5—C10—N4—C16	0.4 (9)
N1—C9—C10—N5	158.8 (7)	C9—C10—N4—C16	-177.8 (7)
N5—C11—C12—C13	-176.5 (8)	N5—C10—N4—Pb1	-176.5 (5)
C16—C11—C12—C13	3.6 (12)	C9—C10—N4—Pb1	5.2 (10)
C11—C12—C13—C14	-5.6 (13)	C15—C16—N4—C10	-177.9 (9)
C12—C13—C14—C15	5.8 (15)	C11—C16—N4—C10	-1.2 (9)
C13—C14—C15—C16	-3.4 (14)	C15—C16—N4—Pb1	-1.5 (13)
C14—C15—C16—N4	177.7 (8)	C11—C16—N4—Pb1	175.3 (5)
C14—C15—C16—C11	1.2 (13)	O1—Pb1—N4—C10	-121.6 (6)
C12—C11—C16—N4	-178.7 (7)	N2—Pb1—N4—C10	-50.4 (6)
N5—C11—C16—N4	1.4 (8)	N1—Pb1—N4—C10	7.6 (6)
C12—C11—C16—C15	-1.4 (12)	O4—Pb1—N4—C10	85.4 (6)
N5—C11—C16—C15	178.6 (7)	O1—Pb1—N4—C16	62.3 (7)
C2—C1—N1—C9	-85.2 (8)	N2—Pb1—N4—C16	133.6 (7)
C2—C1—N1—Pb1	38.9 (8)	N1—Pb1—N4—C16	-168.4 (7)
C10—C9—N1—C1	151.1 (6)	O4—Pb1—N4—C16	-90.6 (7)
C10—C9—N1—Pb1	26.4 (7)	N4—C10—N5—C11	0.4 (9)
N4—Pb1—N1—C1	-142.9 (6)	C9—C10—N5—C11	178.7 (7)
O1—Pb1—N1—C1	-86.3 (6)	C12—C11—N5—C10	178.9 (8)
N2—Pb1—N1—C1	-31.0 (5)	C16—C11—N5—C10	-1.1 (8)
O4—Pb1—N1—C1	141.4 (6)	O3—N6—O1—Pb1	-160.6 (7)
N4—Pb1—N1—C9	-18.6 (5)	O2—N6—O1—Pb1	17.1 (10)
O1—Pb1—N1—C9	38.1 (6)	N4—Pb1—O1—N6	-127.9 (6)
N2—Pb1—N1—C9	93.4 (5)	N2—Pb1—O1—N6	127.8 (6)
O4—Pb1—N1—C9	-94.3 (5)	N1—Pb1—O1—N6	178.2 (5)
N3—C2—N2—C8	-1.2 (10)	O4—Pb1—O1—N6	-90.2 (6)
C1—C2—N2—C8	-178.3 (8)	O6—N7—O4—Pb1	-178.5 (10)
N3—C2—N2—Pb1	169.9 (5)	O5—N7—O4—Pb1	2.4 (9)
C1—C2—N2—Pb1	-7.2 (10)	N4—Pb1—O4—N7	94.9 (6)
C7—C8—N2—C2	178.7 (10)	O1—Pb1—O4—N7	56.6 (7)
C3—C8—N2—C2	2.1 (9)	N2—Pb1—O4—N7	177.5 (5)
C7—C8—N2—Pb1	10.4 (16)	N1—Pb1—O4—N7	167.5 (6)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3 $\cdots$ O6 <sup>i</sup>	0.86	2.04	2.895 (9)	170
C4—H4 $\cdots$ O2 <sup>i</sup>	0.93	2.58	3.332 (13)	138
C4—H4 $\cdots$ O5 <sup>i</sup>	0.93	2.52	3.248 (12)	136
N3—H3 $\cdots$ O5 <sup>i</sup>	0.86	2.50	3.165 (10)	135
N5—H5A $\cdots$ O3 <sup>ii</sup>	0.86	2.11	2.876 (9)	149
C12—H12 $\cdots$ O1 <sup>iii</sup>	0.93	2.53	3.242 (11)	133
N1—H1 $\cdots$ O4 <sup>iv</sup>	0.91	2.27	3.099 (9)	151

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

Fig. 1

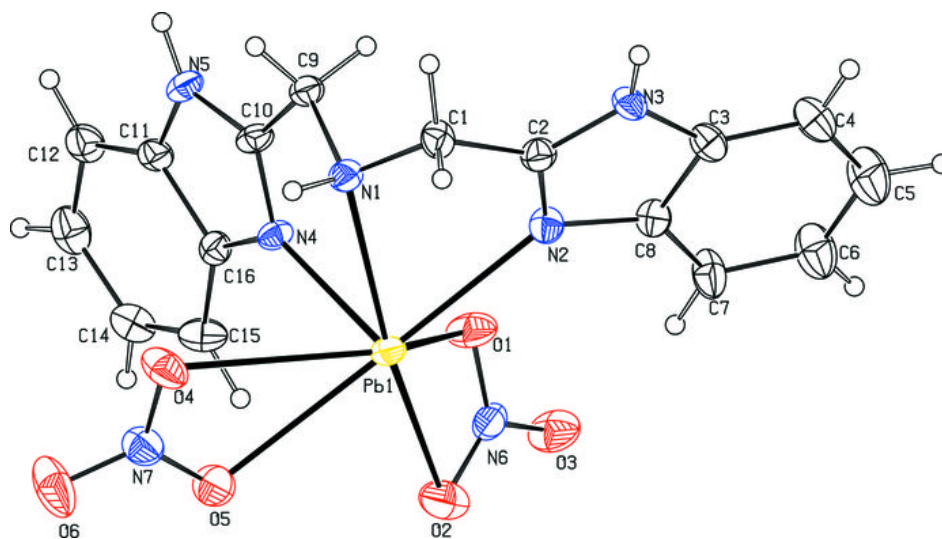


Fig. 2

