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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.019 \text{ \AA}$   
 R factor = 0.036  
 wR factor = 0.079  
 Data-to-parameter ratio = 19.8

For details of how these key indicators were  
 automatically derived from the article, see  
<http://journals.iucr.org/e>.

# 1-Naphthylammonium triiodoplumbate(II)

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The title compound,  $(\text{C}_{10}\text{H}_{10}\text{N})[\text{PbI}_3]$ , crystallizes as an organic–inorganic hybrid. As such, the structure contains extended chains of  $[\text{PbI}_3]^-$  units running along the *b* axis. Each Pb atom is octahedrally coordinated by six iodides, arranged as chains of face-sharing octahedra. These inorganic chains are separated by the isolated organic cations.

## Comment

In recent years a significant number of organic–inorganic hybrid materials based on metal halide units have been prepared and studied; for reviews see Papavassiliou (1997) and Mitzi (1999). Haloplumbates in particular have demonstrated a propensity for forming a great variety of crystalline structures by self-assembly from suitable solution mixtures. It has been shown that their structures can vary considerably, ranging from systems based on isolated molecules to ones containing extended chains as in  $[\text{Me}_4\text{N}][\text{PbI}_3]$  (Contreras *et al.*, 1983) and right up to two- or three-dimensional networks (Mitzi, 1999). For systems containing extended chains, the extended chains may be formed by one, two or three bridging halides. A search of the Cambridge Structural Database (Version 5.27, November 2005 release; Allen 2002) revealed that the crystal structure of the unprotonated amine itself was reported only in 1945. Only the cell parameters and space group were determined, but no three-dimensional coordinates (Kitaigorodskii, 1945). A more recent structure incorporating the 1-naphthylamine system is seen in the ternary  $\pi$ – $\pi^*$  charge-transfer salt pyridinium–1-naphthylamine–picrate (Bernstein *et al.*, 1980).

Having previously reported the structure of an organic–inorganic hybrid containing lead bromide face-sharing chains and the cation (*S*)- $\beta$ -phenylethylammonium (Billing & Lemmerer, 2003), we present here the room temperature structure of the title compound,  $(\text{C}_{10}\text{H}_7\text{NH}_3)[\text{PbI}_3]$  (I).

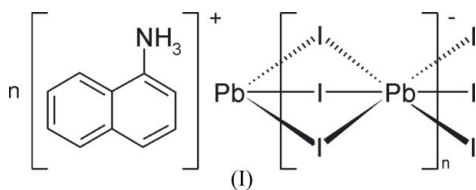
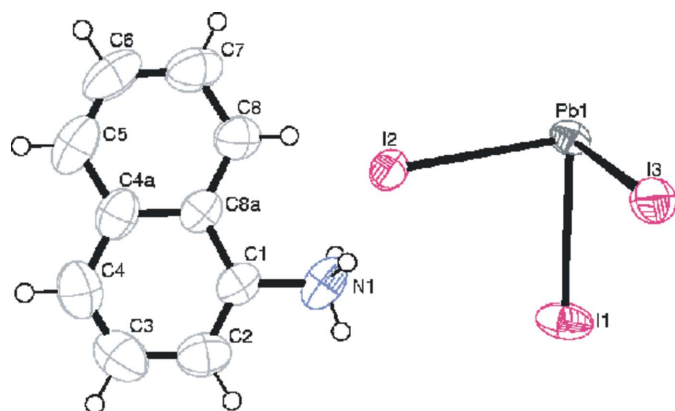
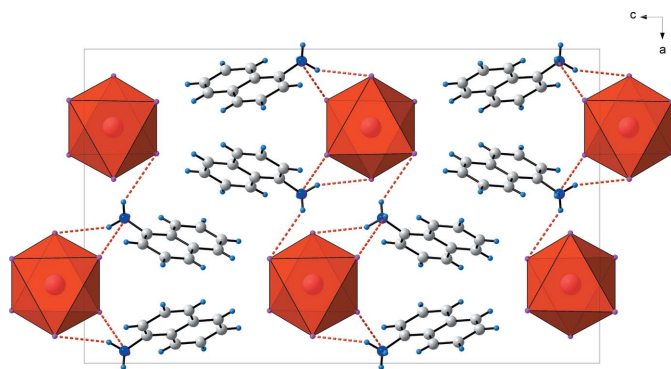


Fig. 2 clearly underlines the one-dimensional arrangement in which four chains of face-sharing  $\text{PbI}_6$  octahedra extend through the unit cell, parallel to the *b* axis. The channels between the chains are occupied by 1-naphthylammonium cations. In the direction perpendicular to the chains, the crystal cohesion is achieved by  $\text{N}-\text{H}\cdots\text{I}$  hydrogen bonds,



**Figure 1**  
The asymmetric unit of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
Packing of (I), viewed along the *b* axis. The hydrogen bonds between the ammonium ions and the iodine atoms are shown as dashed red lines.

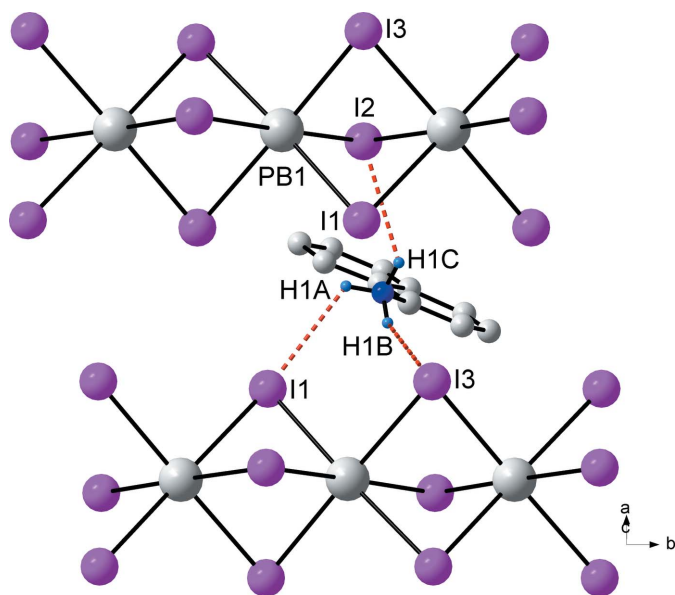
related to the  $\text{NH}_3$  polar groups, and by weak van der Waals forces between the ring systems as the nearest  $\text{C}\cdots\text{C}$  distance is 3.891 (1) Å.

The inorganic motif is built up from characteristic face-sharing  $\text{PbI}_6$  octahedra that form chains along the *b* axis. Two chains are at approximately  $x \sim 0.25$  and the other two at  $x \sim 0.75$ . The octahedra are severely distorted, with all lead Pb—I distances different (Table 1). The bond angles between *cis* ligands vary from 74.98 (3)° to 95.13 (4)° and *trans* angles from 177.41 (2)° to 178.57 (3)°.

Within the organic component, adjacent naphthalene ring systems are separated by a centroid-to-centroid distance of 4.905 (7) Å, which is probably too large to be considered as representing  $\pi$ - $\pi$  stacking interactions.

## Experimental

0.038 g  $\text{PbI}_2$  (0.082 mmol) was dissolved in 2 ml 47% HI in a sample vial. Thereafter, 0.016 g  $\text{C}_{10}\text{H}_9\text{N}_1$  (0.112 mmol) was added and the precipitate dissolved by refluxing for 12 h at 373 K. The solution was slowly cooled at 2K/hour to room temperature. A yellow single crystal suitable for X-ray diffraction analysis was selected and studied. Analysis calculated for  $\text{C}_{10}\text{H}_{10}\text{I}_3\text{N}_1\text{Pb}$ : C 16.41, H 1.38 N 1.91%; found: C 16.50, H 1.64, N 2.04%



**Figure 3**  
Magnified view of the face-sharing  $[\text{Pb}_6]$  octahedra and hydrogen-bonding (dashed lines) scheme.

### Crystal data

$(\text{C}_{10}\text{H}_{10}\text{N})[\text{PbI}_3]$   
 $M_r = 732.08$   
Orthorhombic,  $Pbca$   
 $a = 15.546$  (4) Å  
 $b = 7.8944$  (19) Å  
 $c = 25.522$  (7) Å  
 $V = 3132.2$  (14) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 3.105$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 796 reflections  
 $\theta = 3.5$ –28.1°  
 $\mu = 16.66$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Rhomboid, yellow  
0.18 × 0.14 × 0.04 mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: integration (*XPREP*; Bruker, 1999)  
 $T_{\min} = 0.067$ ,  $T_{\max} = 0.526$   
9144 measured reflections

2729 independent reflections  
1618 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.072$   
 $\theta_{\max} = 25^\circ$   
 $h = -18 \rightarrow 15$   
 $k = -9 \rightarrow 9$   
 $l = -29 \rightarrow 25$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.079$   
 $S = 0.96$   
2729 reflections  
138 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.88$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.97$  e Å<sup>-3</sup>  
Extinction correction: *SHELXL97*  
Extinction coefficient: 0.00082 (3)

**Table 1**

Selected bond lengths (Å).

I3—Pb1	3.1443 (10)	I2—Pb1 <sup>i</sup>	3.2903 (10)
I3—Pb1 <sup>i</sup>	3.2347 (9)	I1—Pb1	3.2146 (10)
I2—Pb1	3.1938 (10)	I1—Pb1 <sup>i</sup>	3.2401 (10)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots I2^{ii}$	0.89	2.7	3.554 (8)	161
$N1-H1B\cdots I1^{iii}$	0.89	2.89	3.719 (10)	156
$N1-H1C\cdots I3$	0.89	2.74	3.606 (9)	166

Symmetry codes: (ii)  $-x + 1, -y + 2, -z + 1$ ; (iii)  $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$ .

H atoms were refined in idealized positions in the riding-model approximation, with  $C-H = 0.93$  Å and  $N-H = 0.89$  Å and  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.5U_{eq}(N)$ . The highest residual peak was  $1.03$  Å from Pb1.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999) and *PLATON* (Spek, 2003).

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