NaPb Structure: AB_tI64_142_ef_g-001

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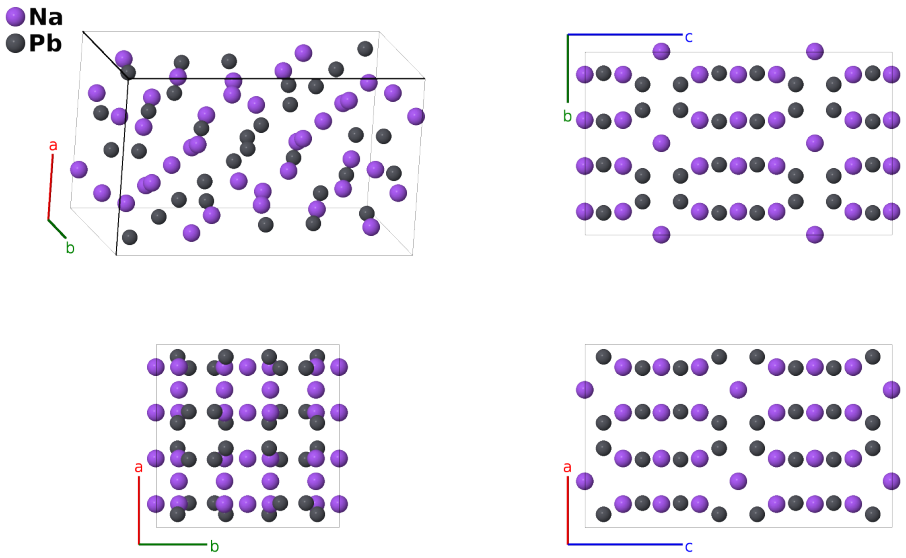
https://aflow.org/p/X6RS

https://aflow.org/p/AB_tI64_142_ef_g-001



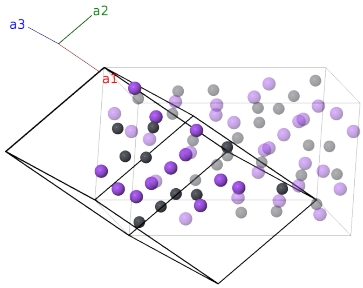
Prototype	NaPb
AFLOW prototype label	AB_tI64_142_ef_g-001
ICSD	105156
Pearson symbol	tI64
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	`aflow --proto=AB_tI64_142_ef_g-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

Other compounds with this structure
CsPb, CsSn, KPb, KSn, RbPb, RbSn

- (Marsh, 1953) describe the structure in the first setting of space group $I4_1/acd$ #142. We used FINDSYM to translate this into the standard second setting.

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_3}$	=	$\left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_4}$	=	$-\left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}}$	(16e)	Na I
$\mathbf{B_5}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_7}$	=	$-\left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_8}$	=	$\left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_9}$	=	$\left(x_2 + \frac{3}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{3}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{11}}$	=	$\left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{13}}$	=	$-\left(x_2 - \frac{5}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{5}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{15}}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{5}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{16}}$	=	$\left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{5}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	Na II
$\mathbf{B_{17}}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{18}}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{19}}$	=	$(x_3 + z_3)\,\mathbf{a}_1 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{20}}$	=	$-(x_3 - z_3)\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{21}}$	=	$(y_3 - z_3)\,\mathbf{a}_1 - \left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{22}}$	=	$-\left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I

$\mathbf{B_{23}}$	=	$\left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 - z_3\right)\,\mathbf{a}_2 + \left(x_3 + y_3\right)\,\mathbf{a}_3$	=	$a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{24}}$	=	$-\left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{25}}$	=	$-\left(y_3 + z_3\right)\,\mathbf{a}_1 - \left(x_3 + z_3\right)\,\mathbf{a}_2 - \left(x_3 + y_3\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{26}}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - z_3\right)\,\mathbf{a}_2 + \left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{27}}$	=	$-\left(x_3 + z_3\right)\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - y_3\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{28}}$	=	$\left(x_3 - z_3\right)\,\mathbf{a}_1 - \left(y_3 + z_3\right)\,\mathbf{a}_2 + \left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{29}}$	=	$-\left(y_3 - z_3\right)\,\mathbf{a}_1 + \left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{30}}$	=	$\left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - y_3\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{31}}$	=	$\left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - z_3\right)\,\mathbf{a}_2 - \left(x_3 + y_3\right)\,\mathbf{a}_3$	=	$-a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I
$\mathbf{B_{32}}$	=	$\left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	Pb I

References

[1] R. E. Marsh and D. P. Shoemaker, *The crystal structure of NaPb*, Acta Cryst. **6**, 197–205 (1953), doi:10.1107/S0365110X53000570.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).