

PtPb₄ (*D*1_d) Structure:

A4B_tP10_125_m_a-001

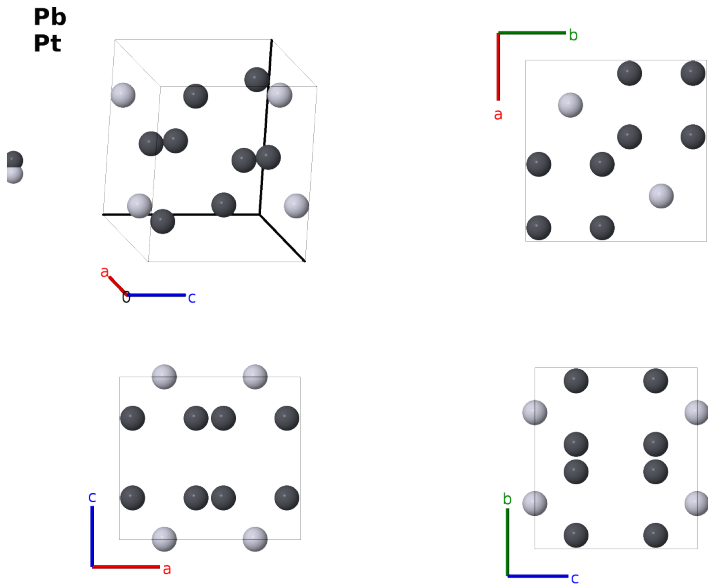
This structure previously used the label(s) **A4B_tP10_125_m_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/0BXW>

https://aflow.org/prototype-encyclopedia/A4B_tP10_125_m_a-001



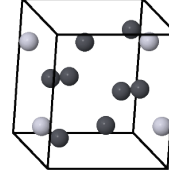
Prototype	Pb ₄ Pt
AFLOW prototype label	A4B_tP10_125_m_a-001
<i>Strukturbericht</i> designation	<i>D</i> 1 _d
ICSD	648397
CCDC	1763188
Pearson symbol	tP10
Space group number	125
Space group symbol	<i>P</i> 4/ <i>nbm</i>
AFLOW prototype command	<code>aflow --proto=A4B_tP10_125_m_a-001</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>x</i>₂, <i>z</i>₂</code>

- (Rösler, 1951) give the structure in setting 1 of space group *P*4/*nbm* #125. We have shifted this to our standard setting 2.
- (Pearson, 1958) states that this structure is related to *C*16 khatyrkite (Al₂Cu).

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$

$\mathbf{a}_1$ $\mathbf{a}_2$ $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	Pt I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	Pt I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_4$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_5$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_7$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_8$	$= x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8m)	Pb I
$\mathbf{B}_{10}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8m)	Pb I

References

- [1] U. Rösler and K. Schubert, *Kristallstruktur von $PtPb_4$* , *Naturwissenschaften* **38**, 331 (1951), doi:10.1007/BF00638136.

Found in

- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

First cited in

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