

Hexagonal PuAl₃ Structure:

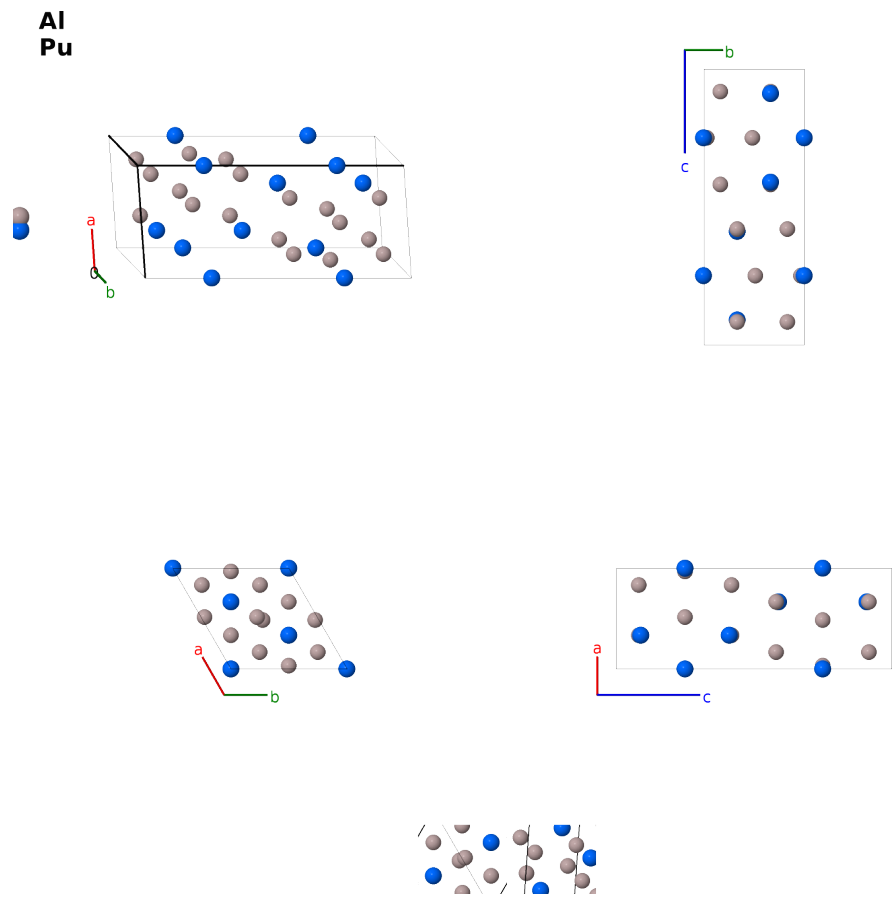
A3B_hP24_194_hk_bf-002

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<https://aflow.org/prototype-encyclopedia/E109>

https://aflow.org/prototype-encyclopedia/A3B_hP24_194_hk_bf-002

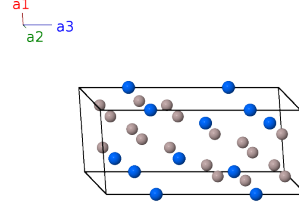


Prototype	Al ₃ Pu
AFLOW prototype label	A3B_hP24_194_hk_bf-002
ICSD	58141
CCDC	1622170
Pearson symbol	hP24
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A3B_hP24_194_hk_bf-002</code> <code>--params=a, c/a, z₂, x₃, x₄, z₄</code>

- PuAl₃ can also be found in a rhombohedral form which is isostructural with BaPb₃. (Runnals, 1965)
- Hexagonal PuAl₃ and VCo₃ have the same AFLOW prototype label, A3B_hP24_194_hk_bf. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Pu I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Pu I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4f)	Pu II
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_2 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Pu II
$\mathbf{B}_5$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4f)	Pu II
$\mathbf{B}_6$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Pu II
$\mathbf{B}_7$	$= x_3\mathbf{a}_1 + 2x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_8$	$= -2x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_9$	$= x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_{10}$	$= -x_3\mathbf{a}_1 - 2x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_{11}$	$= 2x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_{12}$	$= -x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_{13}$	$= x_4\mathbf{a}_1 + 2x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{14}$	$= -2x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{15}$	$= x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$-\sqrt{3}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{16}$	$= -x_4\mathbf{a}_1 - 2x_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{17}$	$= 2x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{18}$	$= -x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$\sqrt{3}ax_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{19}$	$= 2x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{20}$	$= -x_4\mathbf{a}_1 - 2x_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{21}$	$= -x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\sqrt{3}ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{22}$	$= -2x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{23}$	$= x_4\mathbf{a}_1 + 2x_4\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{24}$	$= x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-\sqrt{3}ax_4\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Al II

References

- [1] A. C. Larson, D. T. Cromer, and C. K. Stambaugh, *The Crystal Structure of PuAl_3* , Acta Cryst. **10**, 443–446 (1957), doi:10.1107/S0365110X57001504.
- [2] O. J. C. Runnalls and R. R. Boucher, *The crystal structure of rhombohedral PuAl_3* , Acta Cryst. **19**, 184–186 (1965), doi:10.1107/S0365110X65003055.

Found in

- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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