

α -Pu Structure:

A_mP16_11_8e-001

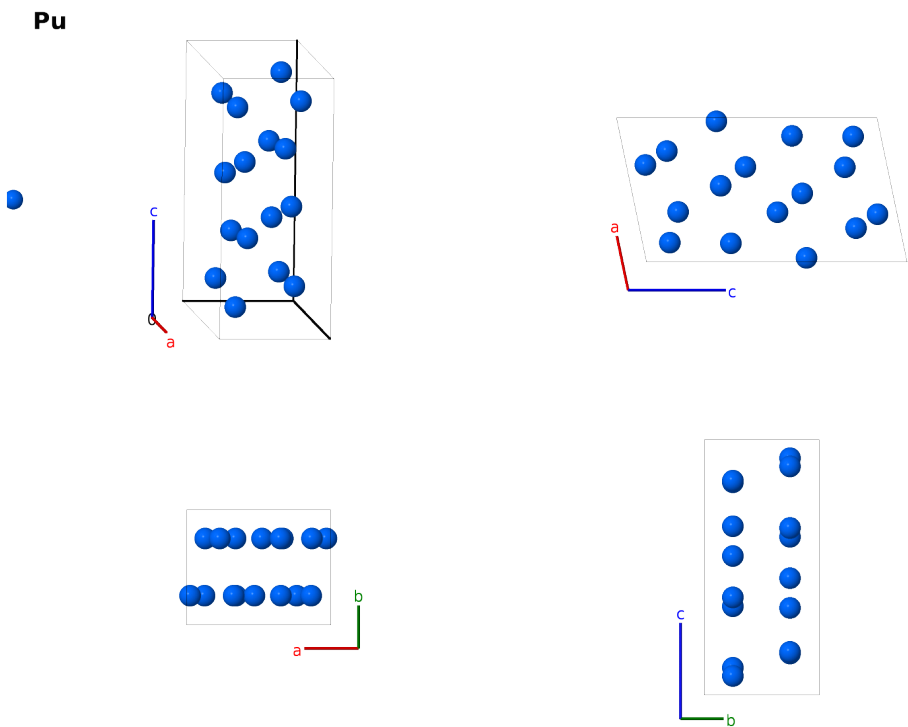
This structure previously used the label(s) **A_mP16_11_8e**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/2MX7>

https://aflow.org/prototype-encyclopedia/A_mP16_11_8e-001

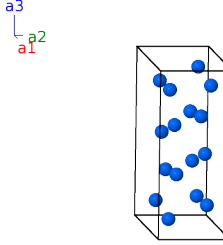


Prototype	Pu
AFLOW prototype label	A_mP16_11_8e-001
ICSD	43335
CCDC	1612844
Pearson symbol	mP16
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	<code>aflow --proto=A_mP16_11_8e-001</code> <code>--params=$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8$</code>

- Plutonium has been found in a variety of structures (Donohue, 1982):

- α -Pu (this structure)
- β -Pu
- γ -Pu
- δ -Pu is in the face-centered cubic $A1$ structure
- δ' -Pu is in the body-centered tetragonal $A6$ (In) structure
- ϵ -Pu is in the body-centered cubic $A2$ structure

Simple Monoclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$


The diagram shows a 3D coordinate system with axes labeled a1 (red), a2 (green), and a3 (blue). To the right is a 3D representation of a monoclinic unit cell, a rectangular prism with blue spheres representing atoms at various lattice points.

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu IV
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu V
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu V
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu VI
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu VI
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu VII
$\mathbf{B}_{14}$	$= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu VII
$\mathbf{B}_{15}$	$= x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu VIII
$\mathbf{B}_{16}$	$= -x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	Pu VIII

References

- [1] W. H. Zachariasen and F. H. Ellinger, *The Crystal Structure of Alpha Plutonium Metal*, Acta Cryst. **16**, 777–783 (1963), doi:10.1107/S0365110X63002012.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017