β-Pu Structure: A_mC34_12_ah3i2j-001
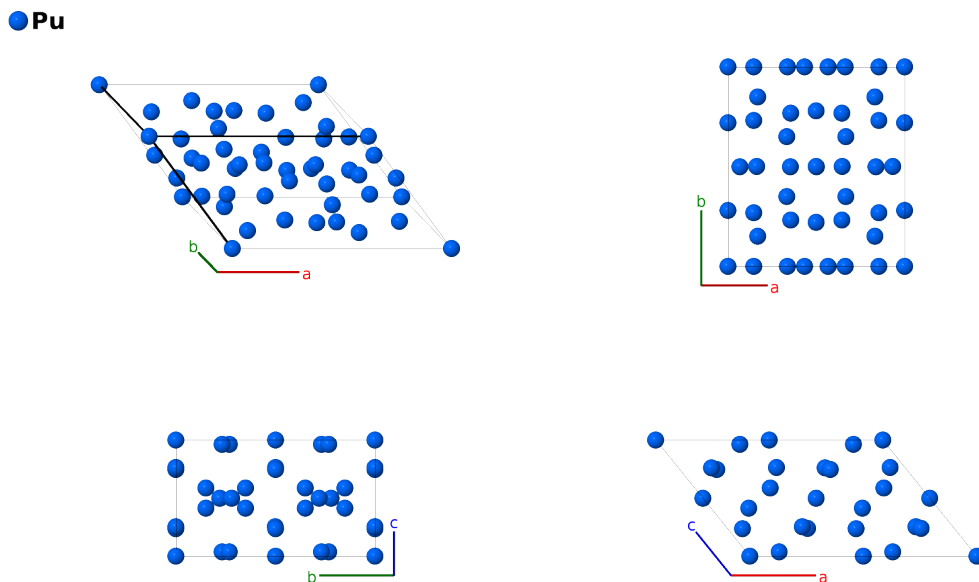
This structure originally had the label `A_mC34_12_ah3i2j`. Calls to that address will be redirected here.

https://aflow.org/p/VV4N

https://aflow.org/p/A_mC34_12_ah3i2j-001

Prototype	Pu
AFLOW prototype label	A_mC34_12_ah3i2j-001
ICSD	43336
Pearson symbol	mC34
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A_mC34_12_ah3i2j-001` `--params=`$a, b/a, c/a, \beta, y_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

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

    - α-Pu

    - β-Pu (this structure)

    - 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

- (Zachariasen, 1963) give the coordinates of this structure in the $I2/m$ setting of space group #12. We used FINDSYM to transform this to the standard $C2/m$ setting.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
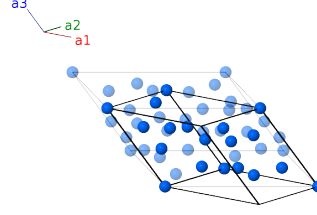
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Pu I
$\mathbf{B_2}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \tfrac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Pu II
$\mathbf{B_3}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \tfrac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Pu II
$\mathbf{B_4}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pu III
$\mathbf{B_5}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pu III
$\mathbf{B_6}$	$=$	$x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pu IV
$\mathbf{B_7}$	$=$	$-x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pu IV
$\mathbf{B_8}$	$=$	$x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pu V
$\mathbf{B_9}$	$=$	$-x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pu V
$\mathbf{B_{10}}$	$=$	$(x_6 - y_6)\,\mathbf{a_1} + (x_6 + y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VI
$\mathbf{B_{11}}$	$=$	$-(x_6 + y_6)\,\mathbf{a_1} - (x_6 - y_6)\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VI
$\mathbf{B_{12}}$	$=$	$-(x_6 - y_6)\,\mathbf{a_1} - (x_6 + y_6)\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VI
$\mathbf{B_{13}}$	$=$	$(x_6 + y_6)\,\mathbf{a_1} + (x_6 - y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VI
$\mathbf{B_{14}}$	$=$	$(x_7 - y_7)\,\mathbf{a_1} + (x_7 + y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VII
$\mathbf{B_{15}}$	$=$	$-(x_7 + y_7)\,\mathbf{a_1} - (x_7 - y_7)\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VII
$\mathbf{B_{16}}$	$=$	$-(x_7 - y_7)\,\mathbf{a_1} - (x_7 + y_7)\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VII
$\mathbf{B_{17}}$	$=$	$(x_7 + y_7)\,\mathbf{a_1} + (x_7 - y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pu VII

References

[1] W. H. Zachariasen and F. H. Ellinger, *The Crystal Structure of Beta Plutonium Metal*, Acta Cryst. **16**, 369–375 (1963), doi:10.1107/S0365110X63000992.

Found in

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