γ-Pu Structure: A_oF8_70_a-001

This structure originally had the label `A_oF8_70_a`. Calls to that address will be redirected here.

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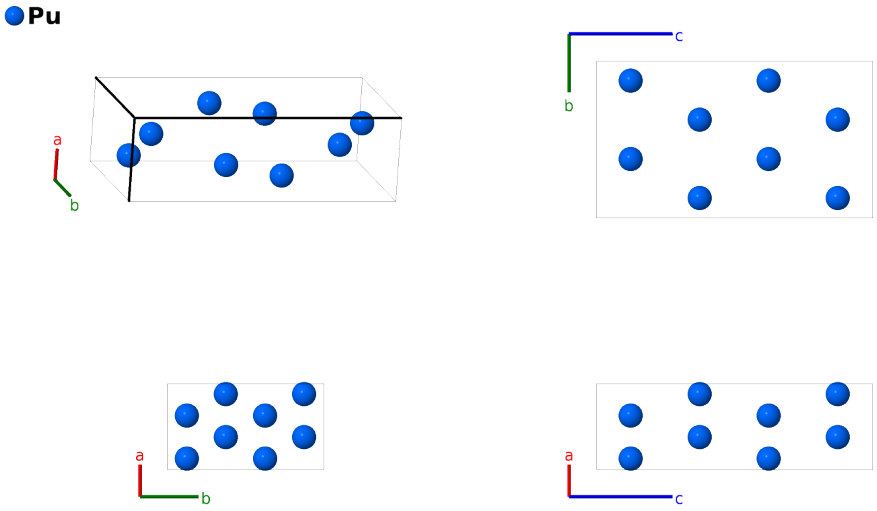
https://aflow.org/p/7VYN

https://aflow.org/p/A_oF8_70_a-001



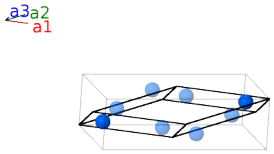
Prototype	Pu
AFLOW prototype label	A_oF8_70_a-001
ICSD	44866
Pearson symbol	oF8
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=A_oF8_70_a-001 --params=`$a, b/a, c/a$

- Plutonium has been found in a variety of structures (Donohue, 1982):
  - α-Pu
  - β-Pu
  - γ-Pu (this structure)
  - 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

- It is obvious from the coordinates that this is an extremely distorted diamond ($A4$) structure, but, as noted by (Donohue, 1982), it can also be considered as a distorted hcp ($A3$) structure.

Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8a)	Pu I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}b\,\hat{\mathbf{y}} + \frac{7}{8}c\,\hat{\mathbf{z}}$	(8a)	Pu I

References

[1] W. H. Zachariasen and F. H. Ellinger, *Crystal chemical studies of the 5f-series of elements. XXIV. The crystal structure and thermal expansion of γ-plutonium*, Acta Cryst. **8**, 431–433 (1955), doi:10.1107/S0365110X55001357.

Found in

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