Pa (A_a) Structure: A_tI2_139_a-002

This structure originally had the label `A_tI2_139_a.alpha-Pa`. Calls to that address will be redirected here.

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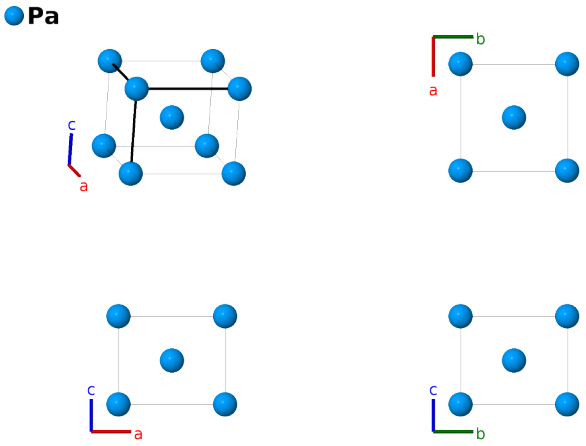
https://aflow.org/p/YF8N

https://aflow.org/p/A_tI2_139_a-002

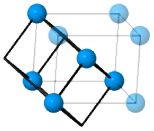


Prototype	Pa
AFLOW prototype label	A_tI2_139_a-002
***Strukturbericht* designation**	A_a
ICSD	648333
Pearson symbol	tI2
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A_tI2_139_a-002 --params=`$a, c/a$

- This is an example of a body-centered tetragonal (bct) lattice, a distortion of the bcc lattice.
- $A6$ and A_a structures have the same AFLOW prototype label, A_tI2_139_a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files. When $c/a = \sqrt{2/3} \approx 0.861$ the coordination number of this system is 10. In Pa the c/a ratio is 0.823.
- We take our data from (Zachariasen, 1959), but the ICSD entry is from the later work of (Benedict, 1982).

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Pa I

References

[1] W. H. Zachariasen, *On the crystal structure of protactinium metal*, Acta Cryst. **12**, 698–700 (1959), doi:10.1107/S0365110X59002043.

[2] U. Benedict, J. C. Spirlet, C. Doufour, I. Birkel, W. B. Holzapfle, and J. R. Petersen, *X-ray diffraction study of protactinium metal to 53 GPa*, J. Magn. Magn. Mater. **29**, 287–290 (1982), doi:10.1016/0304-8853(82)90252-9.

Found in

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