High Pressure Californium (Cf) Structure: A_aP4_2_aci-001

This structure previously used the label(s) `A_aP4_2_aci`. Calls to these addresses will be redirected here.

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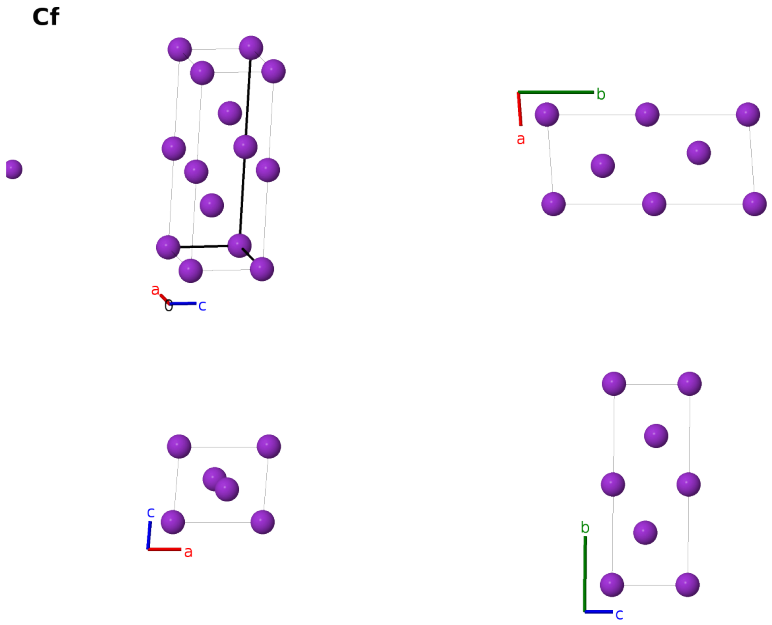
https://aflow.org/prototype-encyclopedia/G18C

https://aflow.org/prototype-encyclopedia/A_aP4_2_aci-001

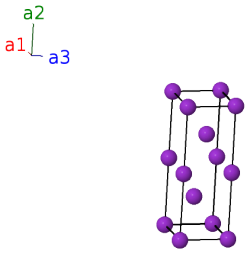


Prototype	Cf
AFLOW prototype label	A_aP4_2_aci-001
ICSD	52913
CCDC	1617626
Pearson symbol	aP4
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=A_aP4_2_aci-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_3, y_3, z_3$

- This is a high-pressure phase of californium, observed between 30 and 40 GPa.
- The pressure at which the X-ray data was taken was not specified by (Roof, 1986).

Triclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}} \\
c_x &= c\cos\beta \\
c_y &= c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cf I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\cos\gamma\,\hat{\mathbf{x}} + \frac{1}{2}b\sin\gamma\,\hat{\mathbf{y}}$	(1c)	Cf II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(2i)	Cf III
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} - c_z z_3\,\hat{\mathbf{z}}$	(2i)	Cf III

References

[1] R. B. Roof, *Concerning the Structure of a High Pressure Phase in Californium Metal*, J. Less-Common Met. **120**, 345–349 (1986), doi:10.1016/0022-5088(86)90660-0.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, vol. 2 (ASM International, Materials Park, OH, 1991), 2nd edn.

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