

Cf Structure:

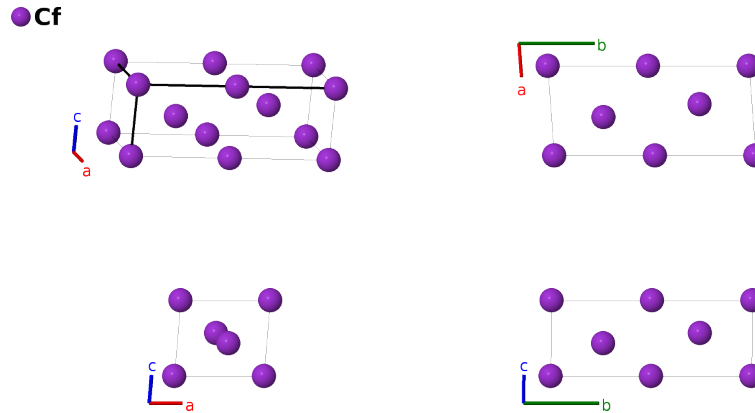
A_aP4_2_aci-001

This structure originally had the label **A_aP4_2_aci**. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. 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

<https://aflow.org/p/G18C>

https://aflow.org/p/A_aP4_2_aci-001

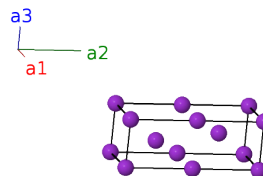


Prototype	Cf
AFLOW prototype label	A_aP4_2_aci-001
ICSD	52913
Pearson symbol	aP4
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<code>aflow --proto=A_aP4_2_aci-001 --params=a, b/a, c/a, α, β, γ, x_3, y_3, z_3</code>

- This is a high-pressure phase, 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.