

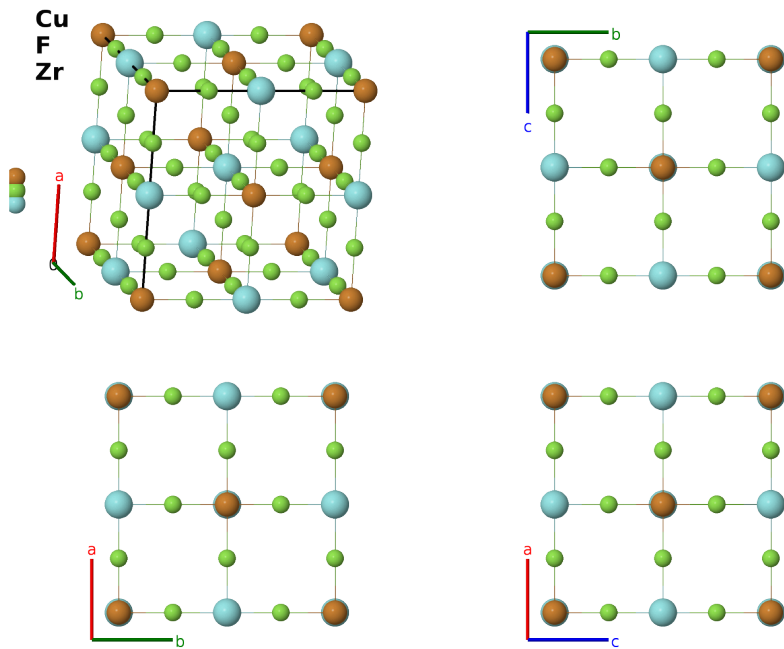
α' -CuZrF₆ Structure: AB6C_cF32_225_a_e_b-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/2016>

https://aflow.org/prototype-encyclopedia/AB6C_cF32_225_a_e_b-001



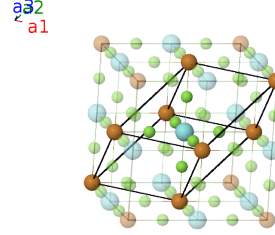
Prototype	CuF ₆ Zr
AFLOW prototype label	AB6C_cF32_225_a_e_b-001
Pearson symbol	cF32
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB6C_cF32_225_a_e_b-001 --params=a, x₃</code>

- CuZrF₆ exists in four forms, depending on the temperature. Structures below 500K show evidence of a Jahn-Teller distortion.
 - α' -CuZrF₆ (this structure) is the high temperature cubic form. Evidence from (Propach, 1978) shows this to be stable above ≈ 450 K. We use the lattice constant at 500K.
 - α -CuZrF₆ is stable above 383K. The fluorine (6f) sites are doubled, with only one of each pair occupied. We use data taken at 393K.

- β -CuZrF₆ is stable between 353 and 383K. In this case the Jahn-Teller distortion is locked in, so there are only six fluorine sites, all fully occupied.
- γ -CuZrF₆ is stable below 353K. Again each fluorine site is only half-filled.
- Although the other entries for CuZrF₆ have ICSD entries, the α' phase does not.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Cu I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(4b) Zr I
$\mathbf{B}_3$	=	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}}$	(24e) F I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}}$	(24e) F I
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{y}}$	(24e) F I
$\mathbf{B}_6$	=	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{y}}$	(24e) F I
$\mathbf{B}_7$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{z}}$	(24e) F I
$\mathbf{B}_8$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{z}}$	(24e) F I

First cited in

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