α'-$CuZrF_6$ Structure: AB6C_cF32_225_a_e_b-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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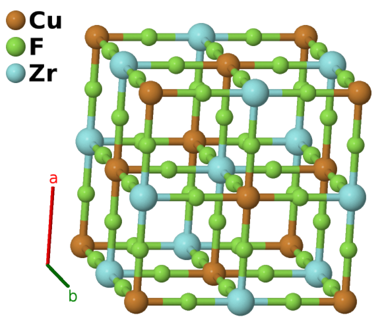
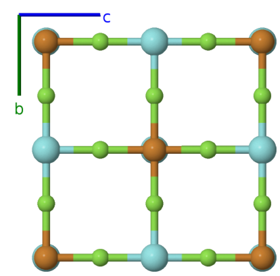
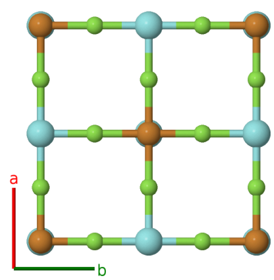
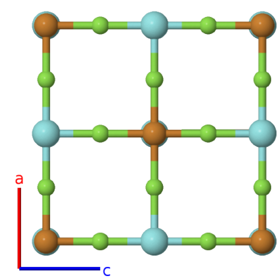
https://aflow.org/p/2016

https://aflow.org/p/AB6C_cF32_225_a_e_b-001









Prototype	CuF_6Zr
AFLOW prototype label	AB6C_cF32_225_a_e_b-001
ICSD	none
Pearson symbol	cF32
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB6C_cF32_225_a_e_b-001` `--params=`a, x_3

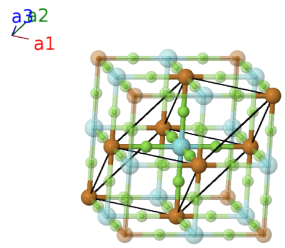
- $CuZrF_6$ exists in four forms, depending on the temperature. Structures below 500K show evidence of a Jahn-Teller distortion.
  - α'-$CuZrF_6$ (this structure) is the high temperature cubic form. Evidence from (Propach, 1978) shows this to be stable above $\approx$ 450K. We use the lattice constant at 500K.
  - α-$CuZrF_6$ is stable above 383K. The fluorine (6f) sites are doubled, with only one of each pair occupied. We use data taken at 393K.
  - β-$CuZrF_6$ 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-$CuZrF_6$ is stable below 353K. Again each fluorine site is only half-filled.

- Although the other entries for $CuZrF_6$ have ICSD entries, the α' phase does not.

Face-centered Cubic primitive vectors

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



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