α-$CuZrF_6$ Structure: AB12C_cF56_202_a_h_b-001

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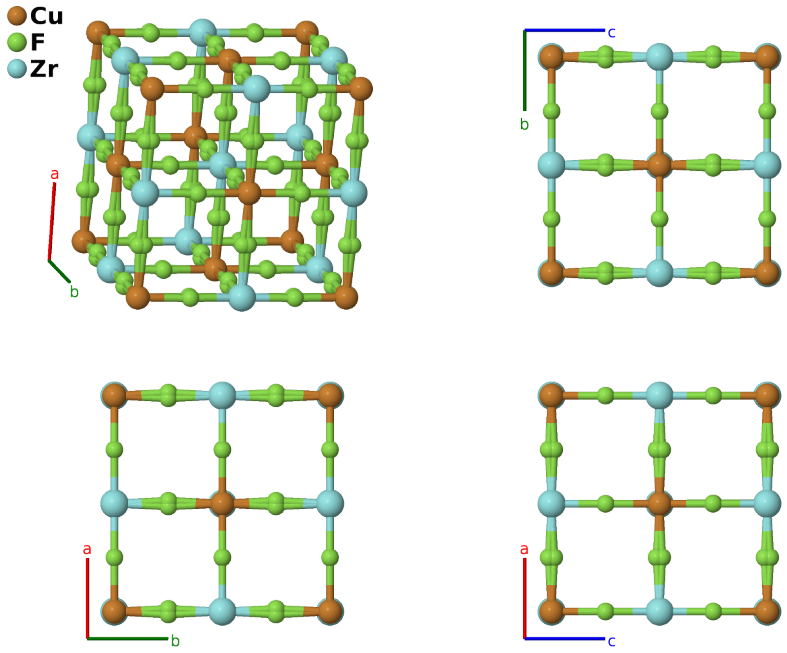
https://aflow.org/p/G65V

https://aflow.org/p/AB12C_cF56_202_a_h_b-001



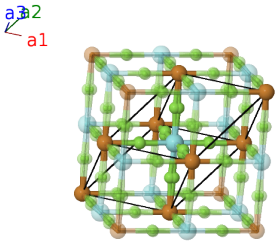
Prototype	CuF_6Zr
AFLOW prototype label	AB12C_cF56_202_a_h_b-001
ICSD	30115
Pearson symbol	cF56
Space group number	202
Space group symbol	$Fm\overline{3}$
AFLOW prototype command	`aflow --proto=AB12C_cF56_202_a_h_b-001 --params=`a, y_3, z_3

- $CuZrF_6$ exists in four forms, depending on the temperature. Structures below 500K show evidence of a Jahn-Teller distortion.
  - α'-$CuZrF_6$ 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-$CuZrF_6$ (this structure) 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.

Face-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}$$



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
$\mathbf{B_3}$	=	$(y_3 + z_3)\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 + (y_3 - z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_4}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 - (y_3 + z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_5}$	=	$(y_3 - z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_6}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_7}$	=	$(y_3 - z_3)\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_8}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_9}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (y_3 + z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_{10}}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 + (y_3 - z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(48h)	F I
$\mathbf{B_{11}}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(48h)	F I
$\mathbf{B_{12}}$	=	$(y_3 + z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(48h)	F I
$\mathbf{B_{13}}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + (y_3 - z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(48h)	F I
$\mathbf{B_{14}}$	=	$(y_3 - z_3)\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 - (y_3 + z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(48h)	F I

References

[1] V. Propach and F. Steffens, *Über die Strukturen der $CuZrF_6$-Modifikationen - Neutronenbeugungsuntersuchungen an den Kristallpulvern*, Z. Krystallogr. **33**, 268–274 (1978), doi:10.1515/znb-1978-0304.