

β -CuZrF₆ Structure:

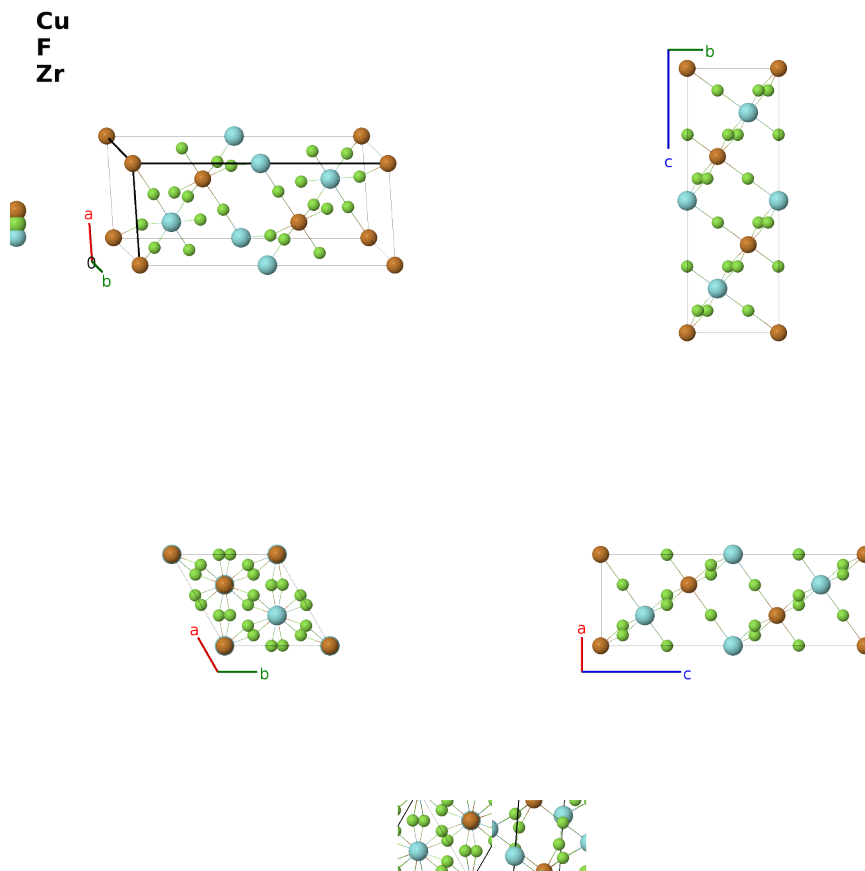
AB6C_hR8_148_a_f_b-001

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<https://aflow.org/prototype-encyclopedia/7RW9>

https://aflow.org/prototype-encyclopedia/AB6C_hR8_148_a_f_b-001

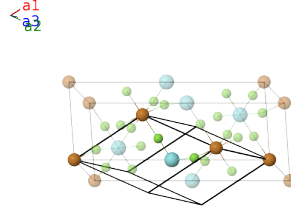


Prototype	CuF_6Zr
AFLOW prototype label	AB6C_hR8_148_a_f_b-001
ICSD	30116
CCDC	1604561
Pearson symbol	hR8
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=AB6C_hR8_148_a_f_b-001</code> <code>--params=a, c/a, x₃, y₃, z₃</code>

- 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 $\approx 450\text{K}$. 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 (this structure) 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.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(1a)	Cu I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Zr I
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	F I
$\mathbf{B}_4$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	F I
$\mathbf{B}_5$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	F I
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	F I
$\mathbf{B}_7$	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	F I
$\mathbf{B}_8$	$-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	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.

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