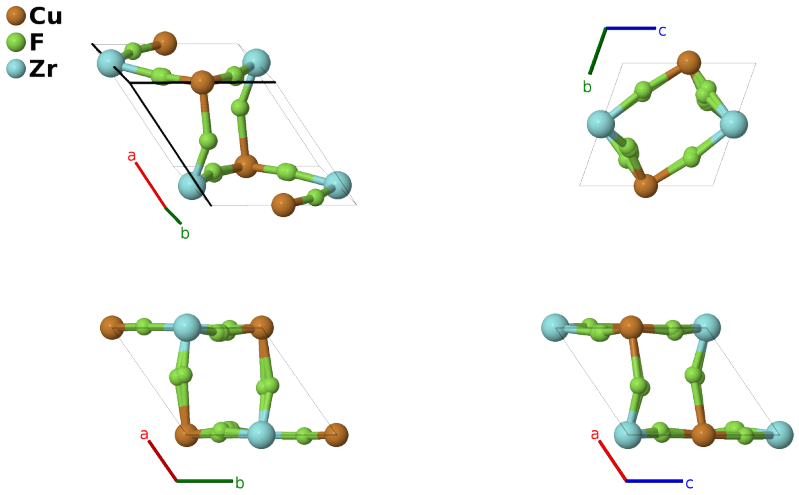
γ-$CuZrF_6$ Structure: AB12C_aP14_2_b_6i_c-001

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.

https://aflow.org/p/5H3G

https://aflow.org/p/AB12C_aP14_2_b_6i_c-001

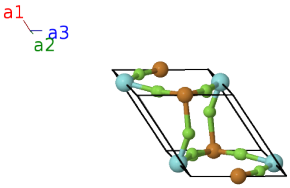


Prototype	CuF_6Zr
AFLOW prototype label	AB12C_aP14_2_b_6i_c-001
ICSD	30117
Pearson symbol	aP14
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=AB12C_aP14_2_b_6i_c-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- $CuZrF_6$ 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-$CuZrF_6$ 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-$CuZrF_6$ (this structure) is stable below 353K. Again each fluorine site is only half-filled, but the ICSD entry only picks one site from each pair.
- The primitive vectors here are equivalent to, but substantially different from, those used by (Propach, 1978).

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
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c_x\,\hat{\mathbf{x}} + \frac{1}{2}c_y\,\hat{\mathbf{y}} + \frac{1}{2}c_z\,\hat{\mathbf{z}}$	(1b)	Cu 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)	Zr I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(2i)	F I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} - c_z z_3\,\hat{\mathbf{z}}$	(2i)	F I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(2i)	F II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} - c_z z_4\,\hat{\mathbf{z}}$	(2i)	F II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(2i)	F III
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} - c_z z_5\,\hat{\mathbf{z}}$	(2i)	F III
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(2i)	F IV
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} - c_z z_6\,\hat{\mathbf{z}}$	(2i)	F IV
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} + c_z z_7\,\hat{\mathbf{z}}$	(2i)	F V
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} - (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} - c_z z_7\,\hat{\mathbf{z}}$	(2i)	F V
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} + c_z z_8\,\hat{\mathbf{z}}$	(2i)	F VI
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} - (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} - c_z z_8\,\hat{\mathbf{z}}$	(2i)	F VI

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.