

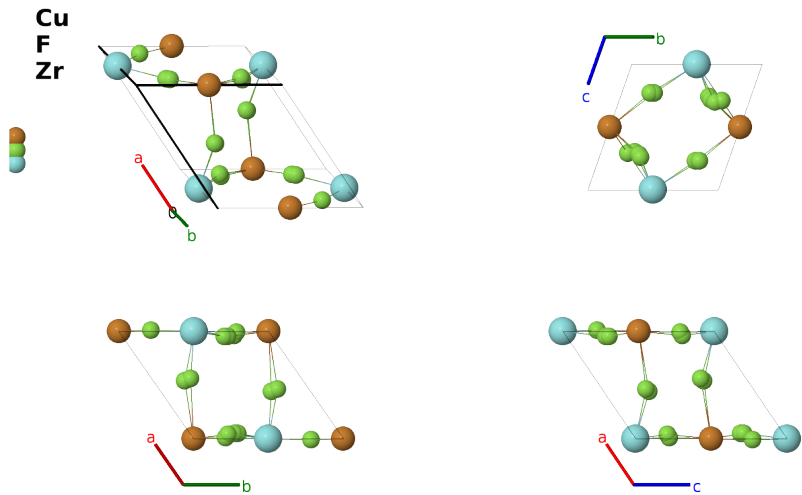
γ -CuZrF₆ Structure: AB12C_aP14_2_b_6i_c-001

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<https://aflow.org/prototype-encyclopedia/5H3G>

https://aflow.org/prototype-encyclopedia/AB12C_aP14_2_b_6i_c-001



Prototype	CuF ₆ Zr
AFLOW prototype label	AB12C_aP14_2_b_6i_c-001
ICSD	30117
CCDC	1604562
Pearson symbol	aP14
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=AB12C_aP14_2_b_6i_c-001 --params=a,b/a,c/a,alpha,beta,gamma,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8</pre>

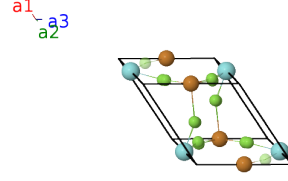
- CuZrF₆ exists in four forms, depending on the temperature. Structures below 500K show evidence of a Jahn-Teller distortion.
 - α' -CuZrF₆ is the high temperature cubic form. Evidence from (Propach, 1978) shows this to be stable above $\approx$ 450K. We use the lattice constant at 500K.
 - α -CuZrF₆ 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 (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 CuZrF₆-Modifikationen - Neutronenbeugungsuntersuchungen an den Kristallpulvern*, Z. Krystallogr. **33**, 268–274 (1978), doi:10.1515/znb-1978-0304.

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