θ-Zr_2CuAu Structure: ABC2_oP8_59_a_b_e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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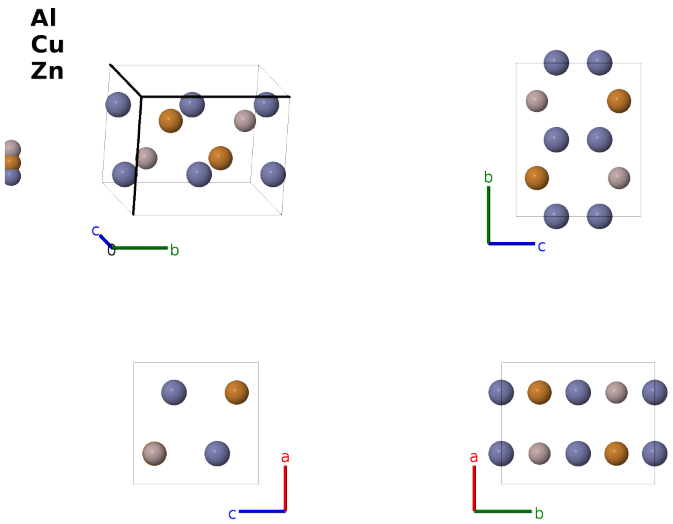
https://aflow.org/prototype-encyclopedia/X1YG

https://aflow.org/prototype-encyclopedia/ABC2_oP8_59_a_b_e-001



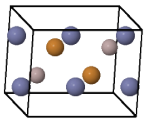
Prototype	$AuCuZr_2$
AFLOW prototype label	ABC2_oP8_59_a_b_e-001
ICSD	150572
CCDC	1667734
Pearson symbol	oP8
Space group number	59
Space group symbol	$Pmmn$
AFLOW prototype command	`aflow --proto=ABC2_oP8_59_a_b_e-001 --params=`$a, b/a, c/a, z_1, z_2, y_3, z_3$

Other compounds with this structure
Cu_3Al

- At low temperatures, the heusler structure β-Zr_2CuAu has a martensitic transformation to this phase. The data was taken at 78K.
- (Duggin, 1966) places this in the $P2mm$ setting of polar space group #25 (standard setting $Pmm2$), but the numerical values of the Wyckoff positions place it in the centrosymmetric space group $Pmmn$. We used AFLOW to determine the transformation.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Zn I

References

[1] M. J. Duggin, *Further studies of martensitic transformations in gold-copper-zinc and copper-aluminium-nickel alloys*, Acta Metall. **14**, 123–129 (1966), doi:10.1016/0001-6160(66)90293-8.

Found in

[1] The Materials Project, *Materials Data on Zn2CuAu* (2020), doi:10.17188/1189168. mp-12759.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).