Al_3Zr ($D0_{23}$) Structure: A3B_tI16_139_cde_e-001

This structure previously used the label(s) `A3B_tI16_139_cde_e`. Calls to these addresses will be redirected here.

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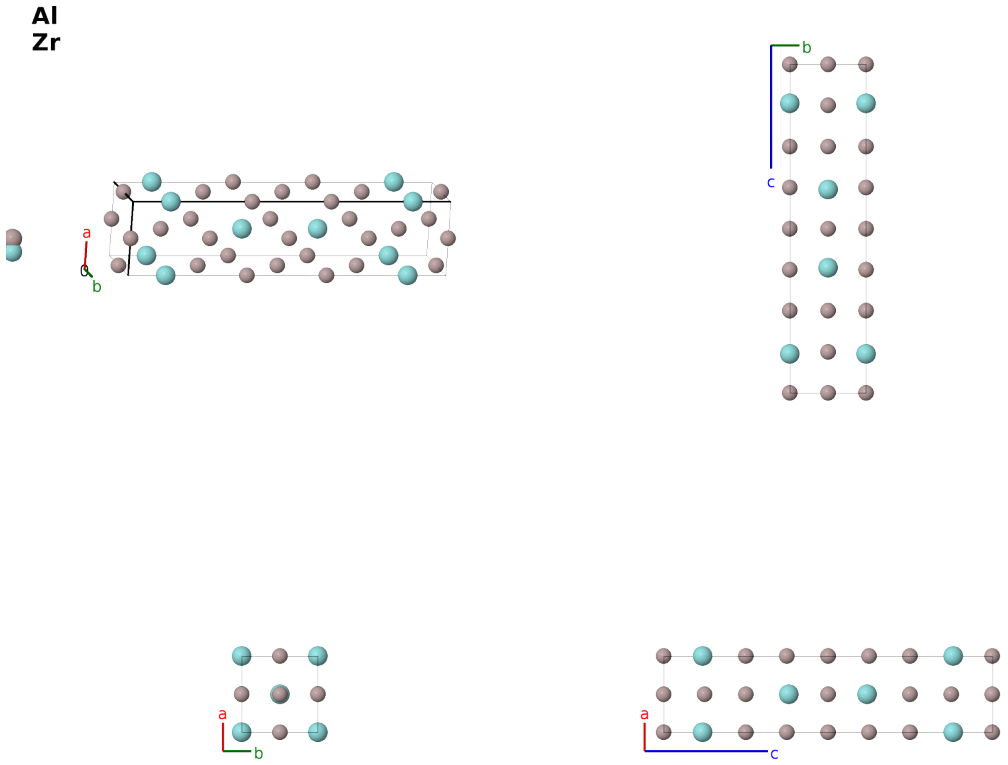
https://aflow.org/prototype-encyclopedia/CSTH

https://aflow.org/prototype-encyclopedia/A3B_tI16_139_cde_e-001



Prototype	Al_3Zr
AFLOW prototype label	A3B_tI16_139_cde_e-001
***Strukturbericht* designation**	$D0_{23}$
ICSD	107130
CCDC	1664860
Pearson symbol	tI16

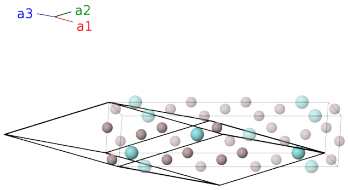
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A3B_tI16_139_cde_e-001 --params=`$a, c/a, z_3, z_4$

Other compounds with this structure
Al_3Hf, Al_3Zn, Au_3Mg, Ga_3Zr, Pd_3In, Pd_3Mg, Pd_3Mn, Pd_3Tl, Pt_3Sb, Ti_3Cu, Zn_3Ru

- When c=4a, z_3=3/8 and z_4=1/8 the atoms are on the sites of a face-centered cubic lattice. This phase can also be described as a set of alternating $L1_2$ and $D0_{22}$ lattices.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Al I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B_6}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Zr I
$\mathbf{B_8}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Zr I

References

[1] Y. Ma, C. Romming, B. Lebech, J. Gjonnes, and J. Tafto, *Structure Refinement of AI3Zr using Single-Crystal X-ray Diffraction, Powder Neutron Diffraction and CBED*, Acta Crystallogr. Sect. B **48**, 11–16 (1992), doi:10.1107/S0108768191010467.

Found in

[1] G. Ghosh and M. Asta, *First-principles calculation of structural energetics of Al-TM (TM = Ti, Zr, Hf) intermetallics*, Acta Mater. **53**, 3225–3252 (2005), doi:10.1016/j.actamat.2005.03.028.

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