

Zr₃Al₂ Structure:

A2B3_tP20_136_j_dfg-001

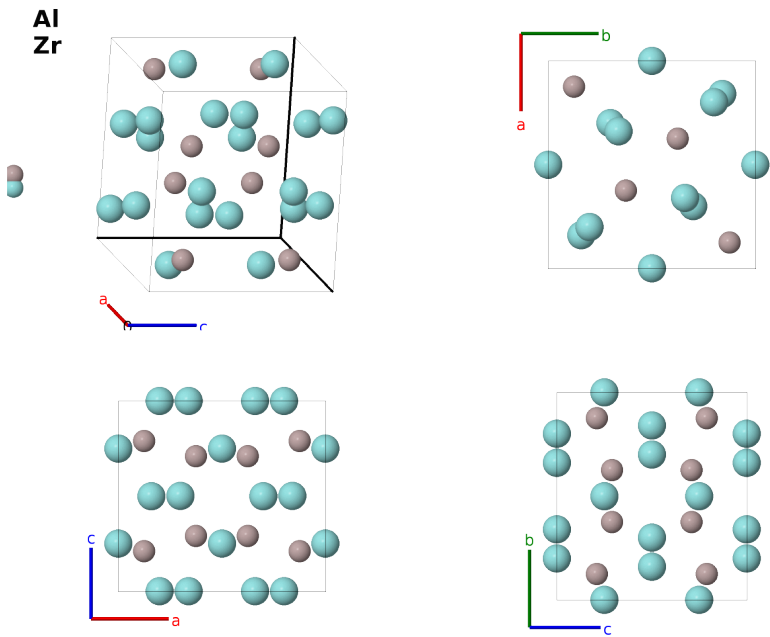
This structure previously used the label(s) **A2B3_tP20_136_j_dfg**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/QSNP>

https://aflow.org/prototype-encyclopedia/A2B3_tP20_136_j_dfg-001



Prototype	Al ₂ Zr ₃
AFLOW prototype label	A2B3_tP20_136_j_dfg-001
ICSD	58231
CCDC	1622257
Pearson symbol	tP20
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<code>aflow --proto=A2B3_tP20_136_j_dfg-001</code> <code>--params=a, c/a, x₂, x₃, x₄, z₄</code>

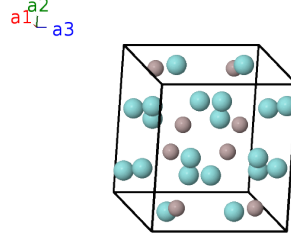
Other compounds with this structure

Dy₃Al₂, Er₃Al₂, Ga₃Hf₂, Ga₃Zr₂, Gd₃Al₂, Hf₃Al₂, Ho₃Al₂, Tb₃Al₂, Y₃Al₂

- The Gd_3Al_2 structure is similar to this one, but that structure does not have an inversion center.

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Zr I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Zr I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Zr I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Zr I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(4f)	Zr II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(4f)	Zr II
$\mathbf{B}_7$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Zr II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Zr II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4g)	Zr III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4g)	Zr III
$\mathbf{B}_{11}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Zr III
$\mathbf{B}_{12}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Zr III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{15}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{17}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{18}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8j)	Al I
$\mathbf{B}_{20}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8j)	Al I

References

- [1] C. G. Wilson and F. J. Spooner, *The Crystal Structure of Zr_3Al_2* , Acta Cryst. **13**, 358–359 (1960), doi:10.1107/S0365110X60000844.

Found in

- [1] L.-E. Edshammar, *Crystal Structure Investigations on the Zr-Al and Hf-Al Systems*, Acta Chem. Scand. **14**, 20–30 (1962), doi:10.3891/acta.chem.scand.16-0020.

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