Zr_2Al_3 Structure: A3B2_oF40_43_ab_b-001

This structure originally had the label `A3B2_oF40_43_ab_b`. Calls to that address will be redirected here.

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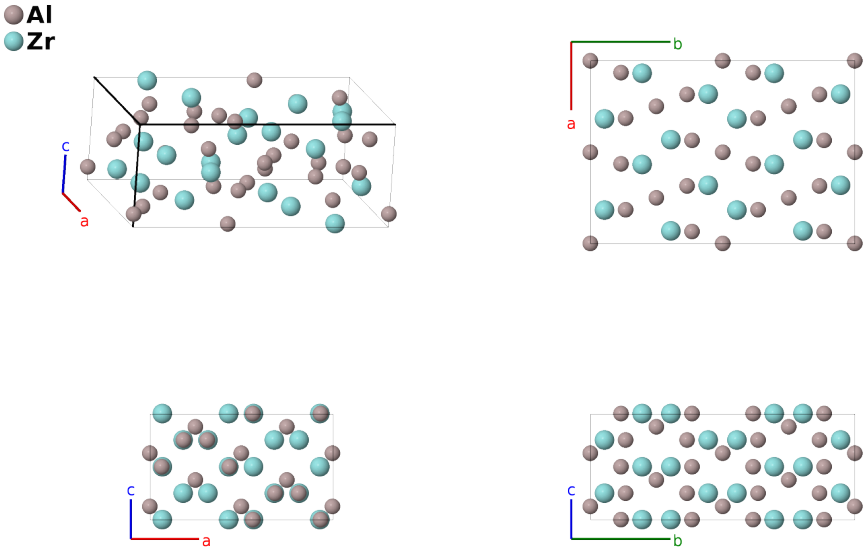
https://aflow.org/p/7D48

https://aflow.org/p/A3B2_oF40_43_ab_b-001



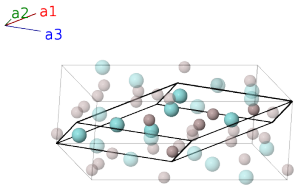
Prototype	Al_3Zr_2
AFLOW prototype label	A3B2_oF40_43_ab_b-001
ICSD	58233
Pearson symbol	oF40
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=A3B2_oF40_43_ab_b-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

Other compounds with this structure
Ga_2Al_3, Ga_2Zr_3, Hf_2Al_3

- The $z = 0$ plane is not fixed in space group $Fdd2$ #43. Here it is arbitrarily set so that $z_3 = 0$ for the zirconium atom.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(8a)	Al I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 - \left(z_1-\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8a)	Al I
$\mathbf{B_3}$	=	$(-x_2+y_2+z_2)\,\mathbf{a}_1 + (x_2-y_2+z_2)\,\mathbf{a}_2 + (x_2+y_2-z_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_4}$	=	$(x_2-y_2+z_2)\,\mathbf{a}_1 + (-x_2+y_2+z_2)\,\mathbf{a}_2 - (x_2+y_2+z_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_5}$	=	$-\left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_2-y_2-z_2+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_2-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_6}$	=	$\left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_2-y_2+z_2-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_2+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_7}$	=	$(-x_3+y_3+z_3)\,\mathbf{a}_1 + (x_3-y_3+z_3)\,\mathbf{a}_2 + (x_3+y_3-z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	Zr I
$\mathbf{B_8}$	=	$(x_3-y_3+z_3)\,\mathbf{a}_1 + (-x_3+y_3+z_3)\,\mathbf{a}_2 - (x_3+y_3+z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	Zr I
$\mathbf{B_9}$	=	$-\left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_3-y_3-z_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Zr I
$\mathbf{B_{10}}$	=	$\left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_3-y_3+z_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Zr I

References

[1] T. J. Renouf and C. A. Beevers, *The Crystal Structure of Zr_2Al_3*, Acta Cryst. **14**, 469–472 (1961), doi:10.1107/S0365110X61001510.

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.