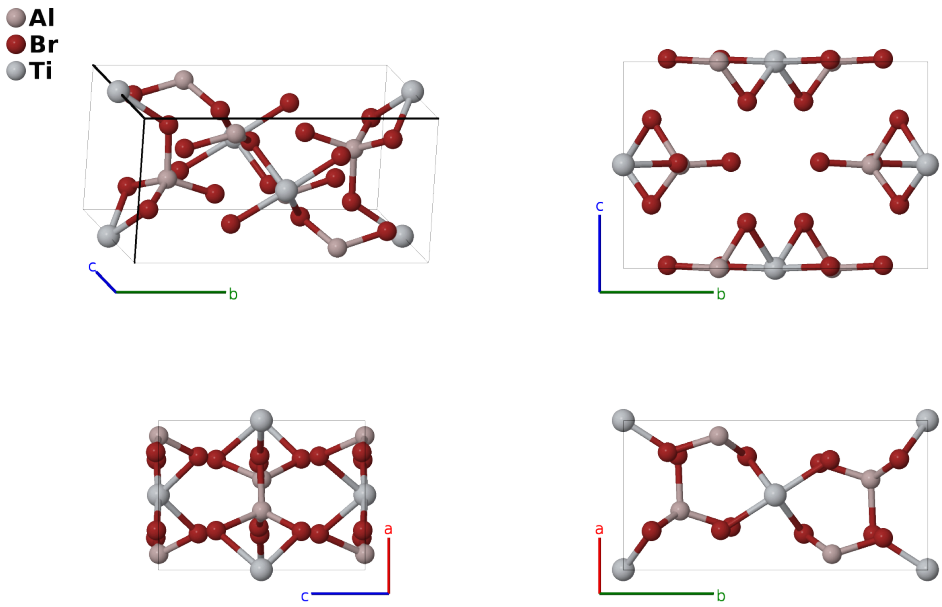
$TiAl_2Br_8$ Structure: A2B8C_oP22_34_c_4c_a-001

This structure originally had the label `A2B8C_oP22_34_c_4c_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

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

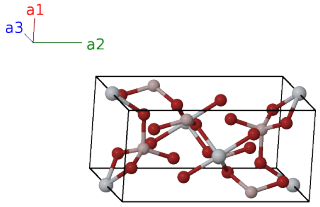
https://aflow.org/p/A2B8C_oP22_34_c_4c_a-001



Prototype	Al_2Br_8Ti
AFLOW prototype label	A2B8C_oP22_34_c_4c_a-001
ICSD	39243
Pearson symbol	oP22
Space group number	34
Space group symbol	$Pnn2$
AFLOW prototype command	`aflow --proto=A2B8C_oP22_34_c_4c_a-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}b\,\hat{\mathbf{y}}+c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_5}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_6}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4c)	Br I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4c)	Br I
$\mathbf{B_9}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br I
$\mathbf{B_{10}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4c)	Br II
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4c)	Br II
$\mathbf{B_{13}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br II
$\mathbf{B_{14}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br II
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4c)	Br III
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4c)	Br III
$\mathbf{B_{17}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br III
$\mathbf{B_{18}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br III
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(4c)	Br IV
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(4c)	Br IV
$\mathbf{B_{21}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br IV
$\mathbf{B_{22}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Br IV

References

[1] S. I. Troyanov, V. B. Rybakov, and V. M. Ionov, *Synthesis and Crystal Structure of $TiBr_4$, $TiBr_3$ and $Ti(AlBr_4)_2$*, Russ. J. Inorg. Chem. **35**, 882–887 (1990).

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.