

Cr₄AlB₆ Structure:

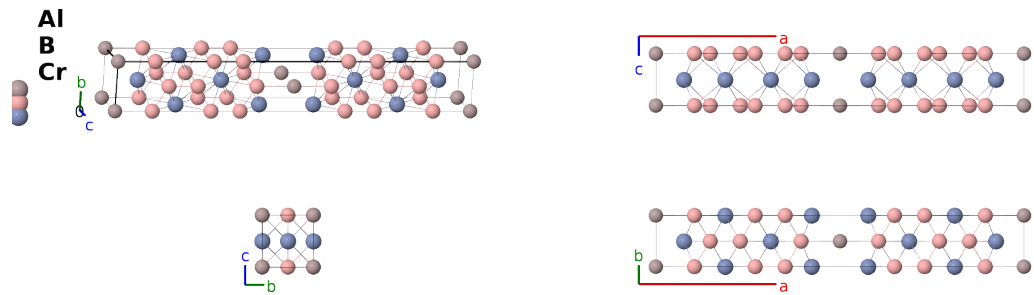
AB6C4_oC22_65_a_3g_2h-001

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- 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.

<https://aflow.org/prototype-encyclopedia/6ZPS>

https://aflow.org/prototype-encyclopedia/AB6C4_oC22_65_a_3g_2h-001

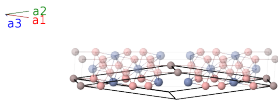


Prototype	AlB ₆ Cr ₄
AFLOW prototype label	AB6C4_oC22_65_a_3g_2h-001
ICSD	251807
CCDC	1717272
Pearson symbol	oC22
Space group number	65
Space group symbol	<i>Cmmm</i>
AFLOW prototype command	<code>aflow --proto=AB6C4_oC22_65_a_3g_2h-001</code> <code>--params=a, b/a, c/a, x₂, x₃, x₄, x₅, x₆</code>

- (Ade, 2015) put set the origin so that the aluminum atoms were at the (2c) Wyckoff position. We shifted this so that the aluminum atoms are at the (2a) Wyckoff position, placing an aluminum atom at the origin.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Al I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}}$	(4g) B I
$\mathbf{B}_3$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$	(4g) B I
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	(4g) B II
$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(4g) B II
$\mathbf{B}_6$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}}$	(4g) B III
$\mathbf{B}_7$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}}$	(4g) B III
$\mathbf{B}_8$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h) Cr I
$\mathbf{B}_9$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h) Cr I
$\mathbf{B}_{10}$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h) Cr II
$\mathbf{B}_{11}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h) Cr II

References

- [1] M. Ade and H. Hillebrecht, *Ternary Borides Cr_2AlB_2 , Cr_2AlB_4 , and Cr_4AlB_6 : The First Members of the Series $(\text{CrB}_2)_n\text{CrAl}$ with $n = 1, 2, 3$ and a Unifying Concept for Ternary Borides as MAB-Phases*, Inorg. Chem. **54**, 6122–6135 (2015), doi:10.1021/acs.inorgchem.5b00049.
- [2] D. Hicks, C. Toher, D. C. Ford, F. Rose, C. D. Santo, O. Levy, M. J. Mehl, and S. Curtarolo, *AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes* **7**, 30 (2021), doi:10.1038/s41524-020-00483-4.

Found in

- [1] H. Zhang, J. Kim, R. Su, P. Richardson, J. Xi, E. Kisi, J. O’Connor, L. Shi, and I. Szlufarska, *Defect behavior and radiation tolerance of MAB phases (MoAlB and Fe_2AlB_2) with comparison to MAX phases*, Acta Mater. **196**, 505–515 (2020), doi:10.1016/j.actamat.2020.07.002.

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