Cr_4AlB_6 Structure: AB6C4_oC22_65_a_3g_2h-001

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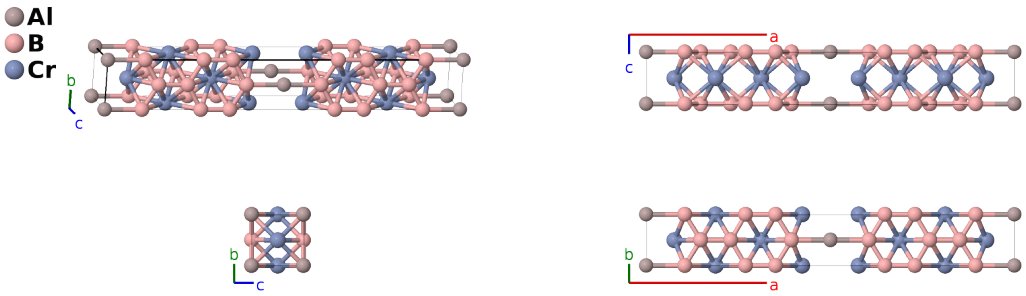
https://aflow.org/p/6ZPS

https://aflow.org/p/AB6C4_oC22_65_a_3g_2h-001

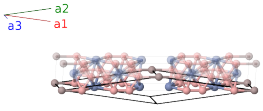


Prototype	AlB_6Cr_4
AFLOW prototype label	AB6C4_oC22_65_a_3g_2h-001
ICSD	251807
Pearson symbol	oC22
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=AB6C4_oC22_65_a_3g_2h-001 --params=`$a, b/a, c/a, x_2, x_3, x_4, x_5, x_6$

- (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

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



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

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[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.

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