Mn_2AlB_2 Structure: AB2C2_oC10_65_a_g_h-001

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https://aflow.org/p/XPEY

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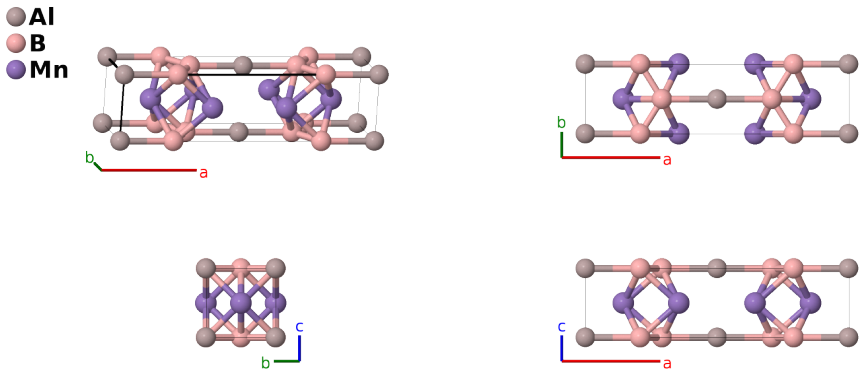


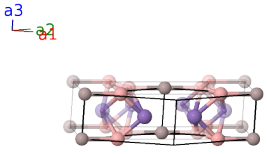
Prototype	AlB_2Mn_2
AFLOW prototype label	AB2C2_oC10_65_a_g_h-001
ICSD	25518
Pearson symbol	oC10
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=AB2C2_oC10_65_a_g_h-001 --params=`$a, b/a, c/a, x_2, x_3$

Other compounds with this structure
Cr_2AlB_2, Fe_2AlB_2

- (Becher, 1966) give the space group as $C222$ #20, but their Wyckoff positions are obviously from space group $Cmmm$ #65, a result which was confirmed by (Ade, 2015).

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
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mn I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mn I

References

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[2] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.

[3] M. Ade and H. Hillebrecht, *Ternary Borides Cr_2AlB_2, Cr_2AlB_4, and Cr_4AlB_6: The First Members of the Series $(CrB_2)_nCrAl$ 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.

Found in

[1] M. Ade and H. Hillebrecht, *Ternary Borides Cr_2AlB_2, Cr_2AlB_4, and Cr_4AlB_6: The First Members of the Series $(CrB_2)_nCrAl$ 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.