MoAlB Structure: ABC_oC12_63_c_c_c-005

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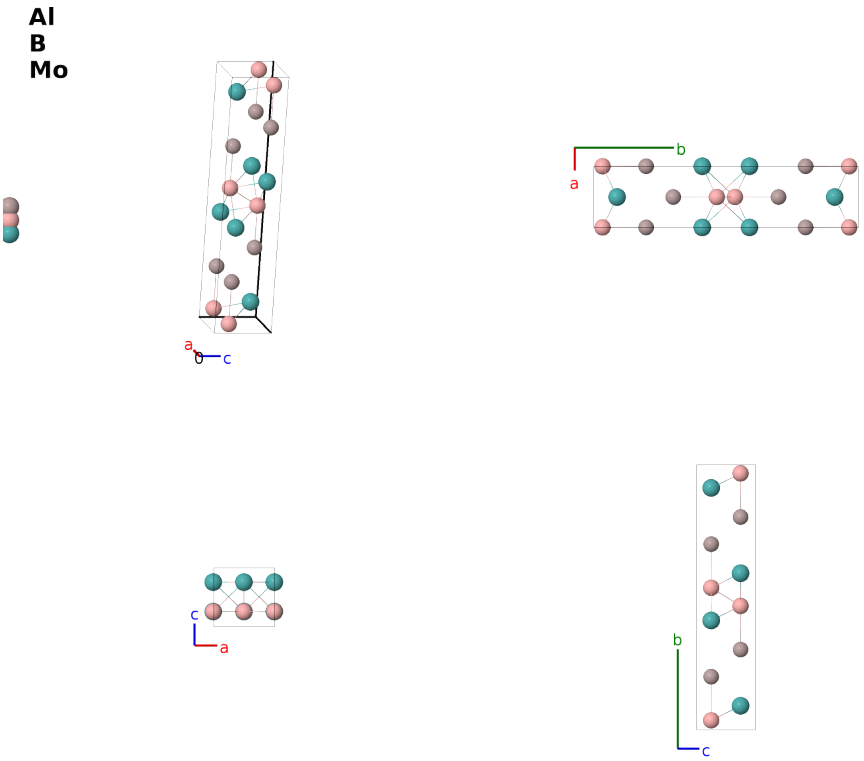
https://aflow.org/prototype-encyclopedia/XSM0

https://aflow.org/prototype-encyclopedia/ABC_oC12_63_c_c_c-005



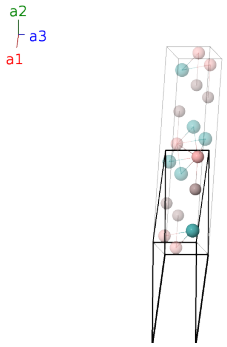
Prototype	AlBMo
AFLOW prototype label	ABC_oC12_63_c_c_c-005
ICSD	251808
CCDC	1786967
Pearson symbol	oC12
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=ABC_oC12_63_c_c_c-005 --params=`$a, b/a, c/a, y_1, y_2, y_3$

Other compounds with this structure
NbNiB, MgNiTb, WAlB

- (Ade, 2015) give atomic positions for WAlB that do not reproduce their interatomic distances and make the W-B distance far too small. We find that the parameters $(y_{Al}, y_B, y_W) = (0.19950, 0.03547, 0.41002)$ reproduce the reported distances.
- The ICSD entry gives the structure type as UBC, but XtalFinder (Hicks, 2021) finds that the structures are essentially unmatchable.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Mo I

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.

Found in

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