Mo_2FeB_2 Structure: A2BC2_tP10_127_g_a_h-002

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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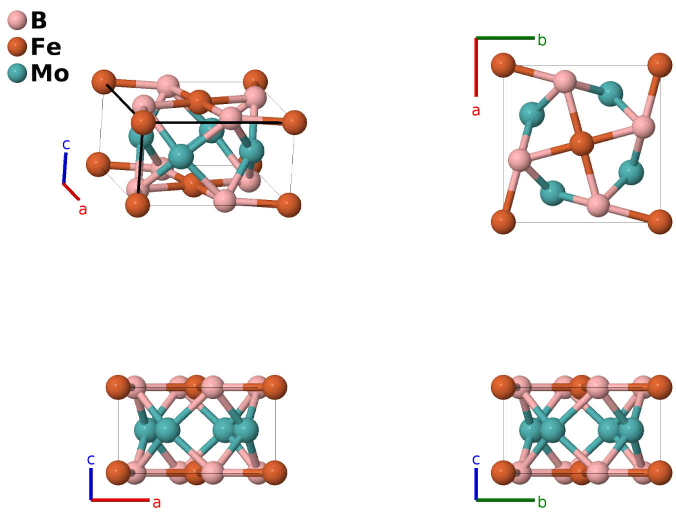
https://aflow.org/p/5SWM

https://aflow.org/p/A2BC2_tP10_127_g_a_h-002



Prototype	B_2FeMo_2
AFLOW prototype label	A2BC2_tP10_127_g_a_h-002
ICSD	5431
Pearson symbol	tP10
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=A2BC2_tP10_127_g_a_h-002` `--params=`$a, c/a, x_2, x_3$

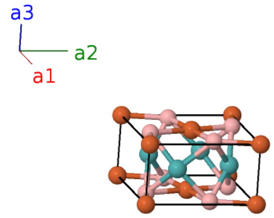
Other compounds with this structure

Al_2CrB_2, Al_2FeB_2, Al_2NiB_2, Ce_2InPd_2, Dy_2CdPd_2, Dy_2InPd_2, Er_2CdPd_2, Er_2InPd_2, Gd_2CdPd_2, Gd_2InPd_2, Ho_2CdPd_2, Ho_2InNi_2, Ho_2InPd_2, La_2InCu_2, La_2InPd_2, Lu_2CdPd_2, Lu_2InPd_2, Mo_2CrB_2, Mo_2NiB_2, Nb_2FeB_2, Nd_2InPd_2, Ni_2SnZr_2, Pr_2CdPd_2, Pr_2InPd_2, Sm_2CdPd_2, Sm_2InPd_2, Ta_2FeB_2, Tb_2CdPd_2, Tb_2InPd_2, Th_2InPd_2, Ti_2CrB_2, Ti_2FeB_2, Ti_2NiB_2, Tm_2CdPd_2, Tm_2InCu_2, Tm_2InPd_2, U_2PbRh_2, Yb_2PbPt_2

- This is the ternary form of the Si_2U_3 ($D5_a$ structure).

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	Fe I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mo I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mo I
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mo I
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mo I

References

[1] W. Rieger, H. Nowotny, and F. Benesovsky, *Die Kristallstruktur von Mo_2FeB_2*, Monatsh. Chem. **95**, 1502–1503 (1964), doi:10.1007/BF00901704.

Found in

[1] Y. Jian, Z. Huang, X. Liu, and J. Xing, *Comparative investigation on the stability, electronic structures and mechanical properties of Mo_2FeB_2 and Mo_2NiB_2 ternary borides by first-principles calculations*, Results in Physics **15**, 102698 (2019), doi:10.1016/j.rinp.2019.102698.