MoB (B_g) Structure: AB_tI16_141_e_e-001

This structure originally had the label `AB_tI16_141_e_e`. Calls to that address will be redirected here.

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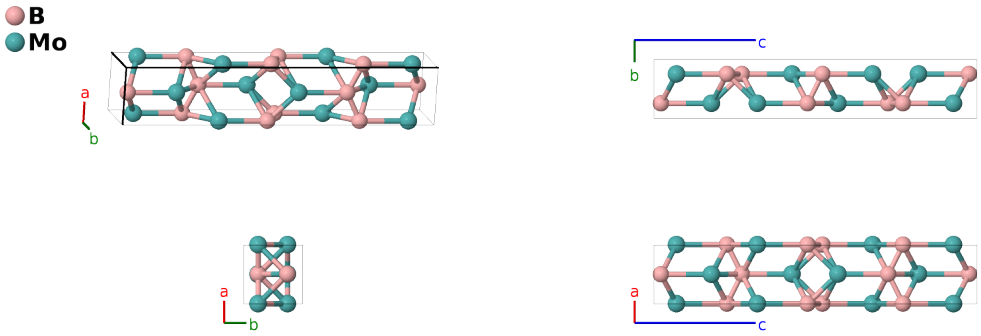
https://aflow.org/p/B9A8

https://aflow.org/p/AB_tI16_141_e_e-001



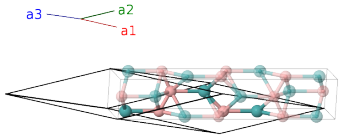
Prototype	BMo
AFLOW prototype label	AB_tI16_141_e_e-001
***Strukturbericht* designation**	B_g
ICSD	24280
Pearson symbol	tI16
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=AB_tI16_141_e_e-001 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure

BCr, BW, GaZr, $B_5Re_3V_2$, $Co_3Er_5Ni_2$, Ga_3Hf_2Sc

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$= \left(z_1 + \frac{1}{4}\right)\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8e)	B I

$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B_3}$	=	$-\left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B_4}$	=	$-z_1\,\mathbf{a}_1 - \left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B_5}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	Mo I
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Mo I
$\mathbf{B_7}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	Mo I
$\mathbf{B_8}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Mo I

References

[1] R. Kiessling, *The Crystal Structure of Molybdenum and Tungsten Borides*, Acta Chem. Scand. **1**, 893–916 (1947), doi:10.3891/acta.chem.scand.01-0893.