Mo_2B_5 ($D8_i$) Structure: A5B2_hR7_166_a2c_c-001

This structure originally had the label `A5B2_hR7_166_a2c_c`. Calls to that address will be redirected here.

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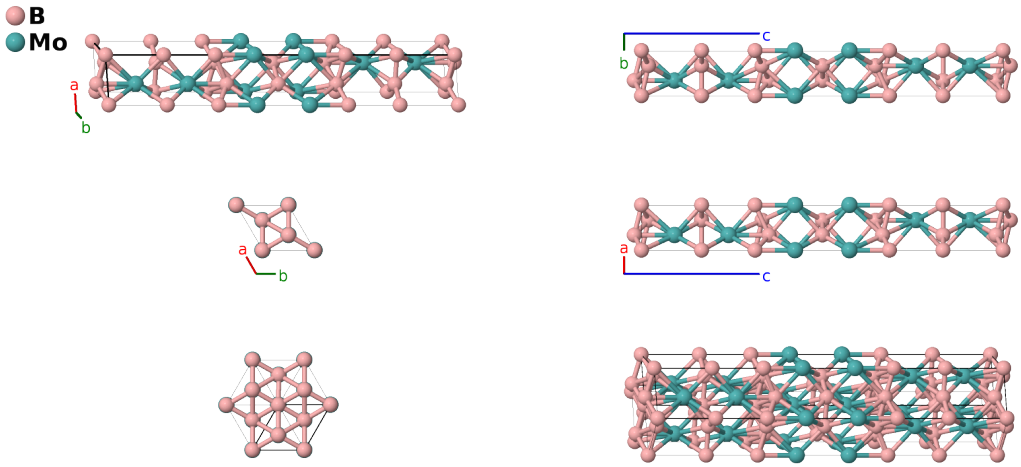
https://aflow.org/p/WZKM

https://aflow.org/p/A5B2_hR7_166_a2c_c-001



Prototype	B_5Mo_2
AFLOW prototype label	A5B2_hR7_166_a2c_c-001
***Strukturbericht* designation**	$D8_i$
ICSD	24282
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A5B2_hR7_166_a2c_c-001 --params=`$a, c/a, x_2, x_3, x_4$

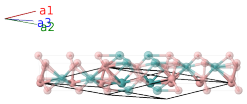
Other compounds with this structure
$InTlLi_5$, Pb_2Na_5, Sn_2Li_5, Tl_2Li_5, V_2B_5

- The B-I and B-III atoms form buckled graphitic sheets, making this the rhombohedral form of $D8_h$. (Frotscher, 2007) suggest that the stable composition in this part of the molybdenum nitride system might be Mo_2B_4, which they describe as having a flattened $C12$ ($CaSi_2$) structure. Here we will describe the $D8_i$ structure, with the warning that this might not be the true structure.
- We have shifted the origin of this lattice so that the B-I atoms are at the (1a) Wyckoff positions. An earlier version of this page, included in (Mehl, 2017), shifted the B-I atom but neglected to shift the remaining atoms.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	B I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	B II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	B II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	B III
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	B III
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Mo I
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Mo I

References

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

[2] M. Frotscher, W. Klein, J. Bauer, C.-M. F., J.-F. Halet, A. Senyshyn, C. Baehtz, and B. Albert, *M_2B_5 or M_2B_4? A Reinvestigation of the Mo/B and W/B System*, Z. Anorganische und Allgemeine Chemie **633**, 2626–2630 (2007), doi:10.1002/zaac.200700376.

[3] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. H., G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.