

Mo₂B₅ (*D*8_i) Structure: A5B2_hR7_166_a2c_c-001

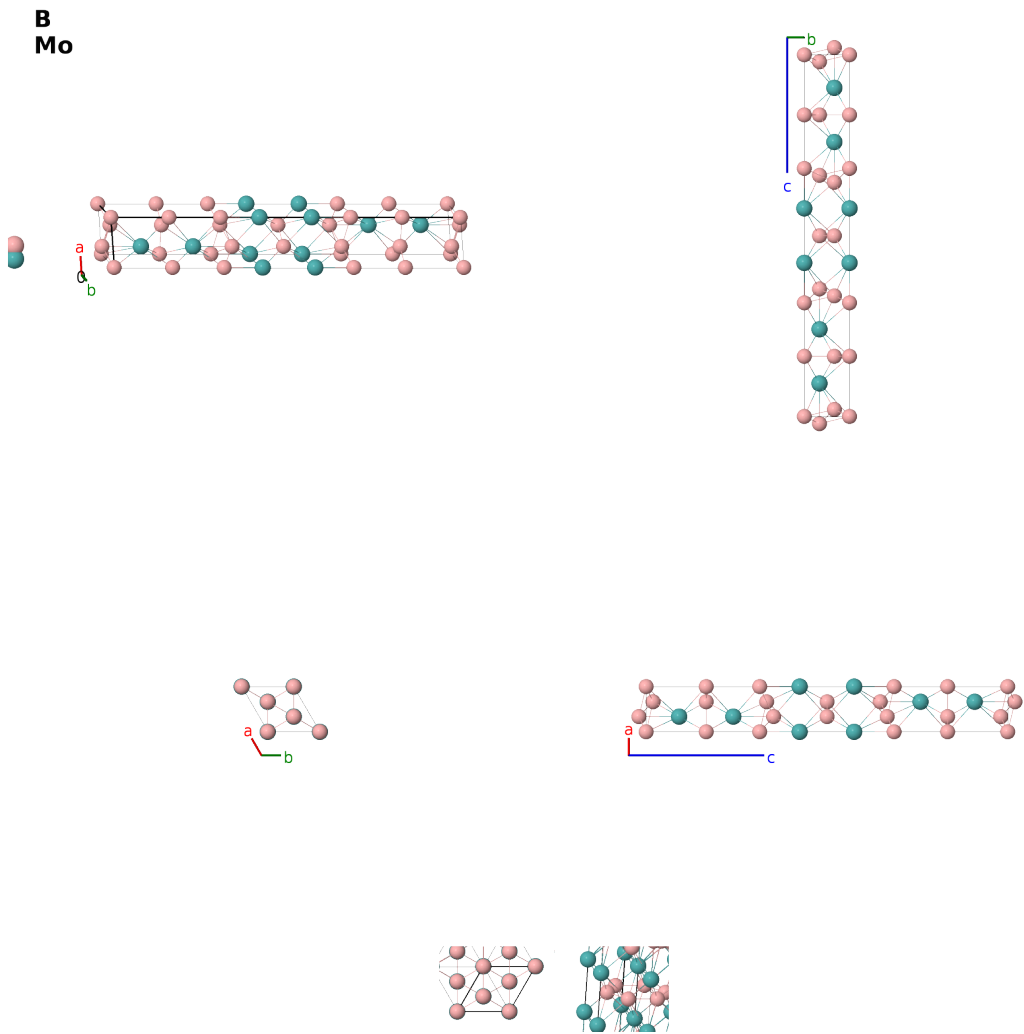
This structure previously used the label(s) **A5B2_hR7_166_a2c_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/WZKM>

https://aflow.org/prototype-encyclopedia/A5B2_hR7_166_a2c_c-001



Prototype	B ₅ Mo ₂
AFLOW prototype label	A5B2_hR7_166_a2c_c-001
<i>Strukturbericht</i> designation	<i>D</i> 8 _i
ICSD	24282

CCDC	1600327
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A5B2_hR7_166_a2c_c-001</code> <code>--params=a, c/a, x₂, x₃, x₄</code>

Other compounds with this structure

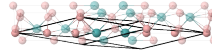
InTlLi₅, Pb₂Na₅, Sn₂Li₅, Tl₂Li₅, V₂B₅

- 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 Mo₂B₄, which they describe as having a flattened $C12$ (CaSi₂) 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

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
 \end{aligned}$$

$\leftarrow \mathbf{a}_1$
 $\mathbf{a}_2$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	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.

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