

Mo₈P₅ Structure: A8B5_mP13_6_5a3b_2a3b-001

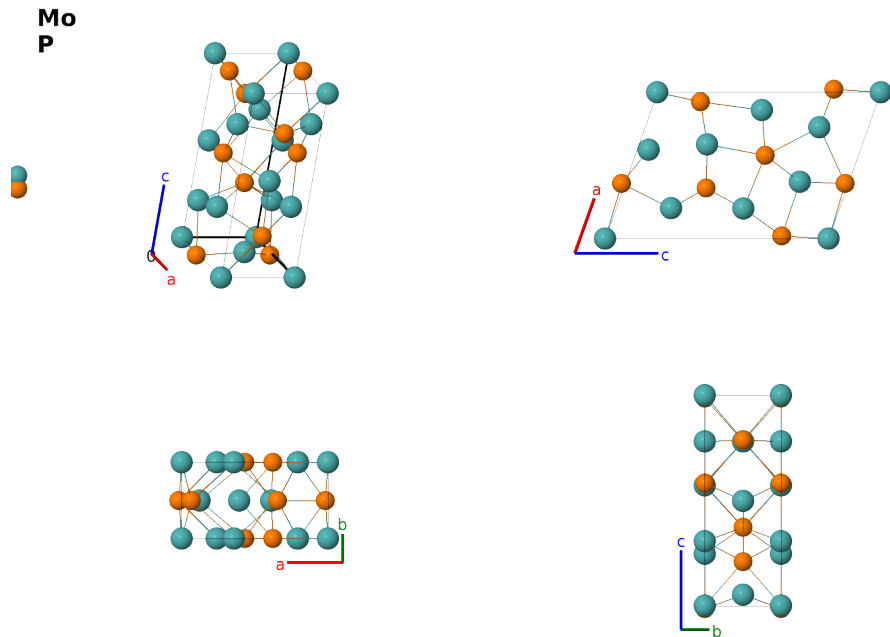
This structure previously used the label(s) **A8B5_mP13_6_a7b_3a2b**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/LEL6>

https://aflow.org/prototype-encyclopedia/A8B5_mP13_6_5a3b_2a3b-001



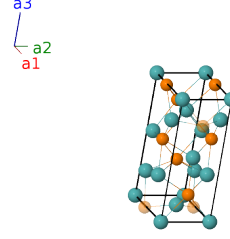
Prototype	Mo ₈ P ₅
AFLOW prototype label	A8B5_mP13_6_5a3b_2a3b-001
ICSD	15058
CCDC	1595841
Pearson symbol	mP13
Space group number	6
Space group symbol	<i>Pm</i>
AFLOW prototype command	<pre>aflow --proto=A8B5_mP13_6_5a3b_2a3b-001 --params=a, b/a, c/a, β, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈, x₉, z₉, x₁₀, z₁₀, x₁₁, z₁₁, x₁₂, z₁₂, x₁₃, z₁₃</pre>

- Our original reconstruction of this prototype (Hicks, 2019) placed two of the Mo (1b) sites on (1a) sites. We have corrected that here.

- This high-temperature phase of the Mo-P system is observed in the range 1580 – 1680°C (Johnsson, 1972).

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(1a)	Mo I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(1a)	Mo II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(1a)	Mo III
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(1a)	Mo IV
$\mathbf{B}_5$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(1a)	Mo V
$\mathbf{B}_6$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(1a)	P I
$\mathbf{B}_7$	$= x_7 \mathbf{a}_1 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(1a)	P II
$\mathbf{B}_8$	$= x_8 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(1b)	Mo VI
$\mathbf{B}_9$	$= x_9 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(1b)	Mo VII
$\mathbf{B}_{10}$	$= x_{10} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(1b)	Mo VIII
$\mathbf{B}_{11}$	$= x_{11} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(1b)	P III
$\mathbf{B}_{12}$	$= x_{12} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(1b)	P IV
$\mathbf{B}_{13}$	$= x_{13} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(1b)	P V

References

- [1] T. Johnsson, *The Crystal Structure of Mo_8P_5 from Twin-crystal Data*, Acta Chem. Scand. **26**, 365–382 (1972), doi:10.3891/acta.chem.scand.26-0365.
- [2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043