Mo_8P_5 Structure: A8B5_mP13_6_5a3b_2a3b-001

This structure originally had the label `A8B5_mP13_6_a7b_3a2b`. Calls to that address will be redirected here.

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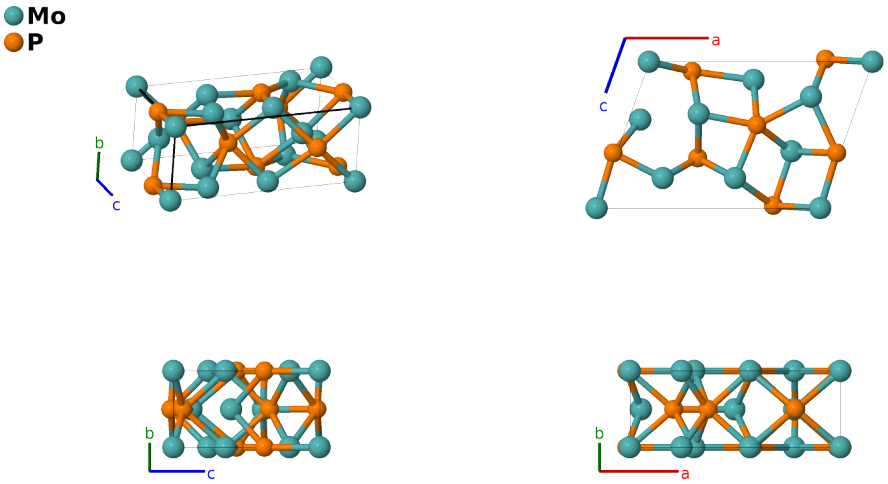
https://aflow.org/p/LEL6

https://aflow.org/p/A8B5_mP13_6_5a3b_2a3b-001

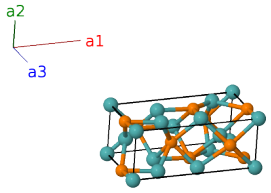


Prototype	Mo_8P_5
AFLOW prototype label	A8B5_mP13_6_5a3b_2a3b-001
ICSD	15058
Pearson symbol	mP13
Space group number	6
Space group symbol	Pm
AFLOW prototype command	`aflow --proto=A8B5_mP13_6_5a3b_2a3b-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}$

- 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.