MoP_2 Structure: AB2_oC12_36_a_2a-002

This structure previously used the label(s) `AB2_oC12_36_a_2a`. Calls to these addresses will be redirected here.

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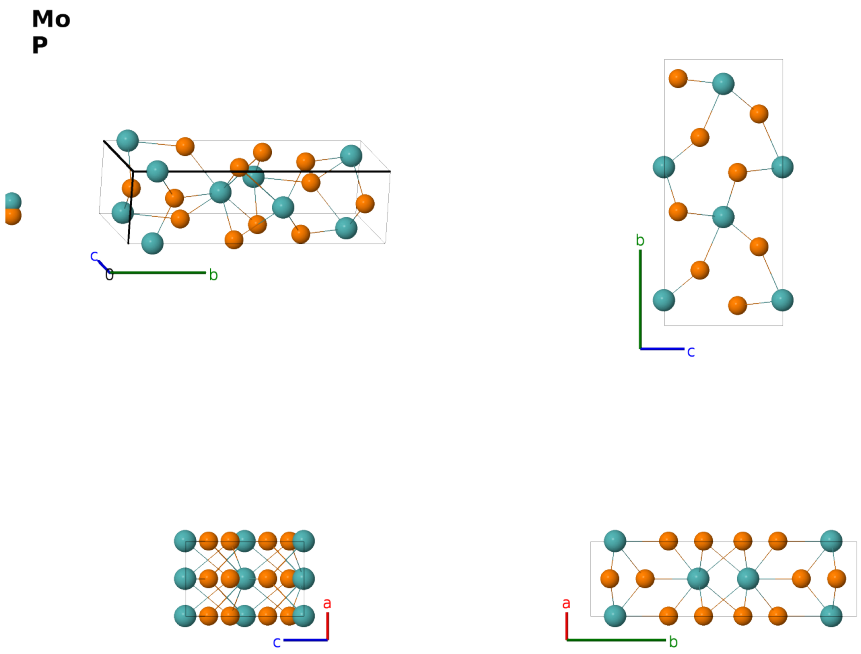
https://aflow.org/prototype-encyclopedia/JTSA

https://aflow.org/prototype-encyclopedia/AB2_oC12_36_a_2a-002



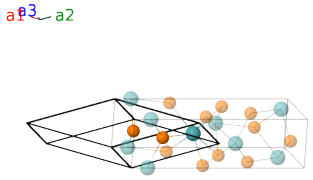
Prototype	MoP_2
AFLOW prototype label	AB2_oC12_36_a_2a-002
ICSD	43331
CCDC	1612842
Pearson symbol	oC12
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=AB2_oC12_36_a_2a-002 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3$

Other compounds with this structure
$HgBr_2$, WP_2

- An earlier version of this page had the wrong value for the length c. We have corrected that in this version.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Mo I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Mo I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P II

References

[1] S. Rundqvist and T. Lundström, *X-Ray Studies of Molybdenum and Tungsten Phosphides*, Acta Chem. Scand. **17**, 37–46 (1962), doi:10.3891/acta.chem.scand.17-0037.

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