$MoPt_2$ Structure: AB2_oI6_71_a_e-001

This structure originally had the label `AB2_oI6_71_a_g`. Calls to that address will be redirected here.

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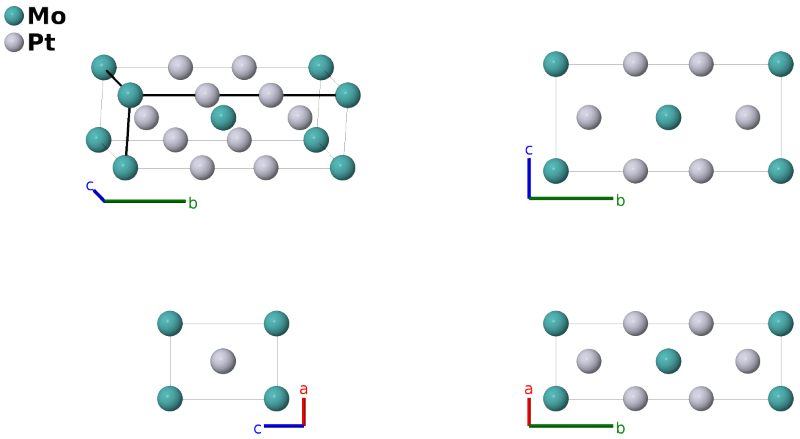
https://aflow.org/p/EKX0

https://aflow.org/p/AB2_oI6_71_a_e-001



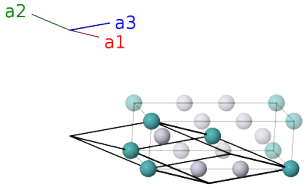
Prototype	$MoPt_2$
AFLOW prototype label	AB2_oI6_71_a_e-001
ICSD	105070
Pearson symbol	oI6
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=AB2_oI6_71_a_e-001 --params=`$a, b/a, c/a, x_2$

Other compounds with this structure
$NbPd_2$, $NbPt_2$, $TaPd_2$, VNi_2, VPd_2, VPt_2

- The original references describe $MoPt_2$ and $ReSi_2$ in different orientations, so they have nominally different AFLOW prototype labels, AB2_oI6_71_a_g and AB2_oI6_71_a_i, respectively. When we apply our AFLOW prototype label rules, however, the label for both structures becomes AB2_oI6_71_a_e. The two structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mo I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(4e)	Pt I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(4e)	Pt I

References

[1] K. Schubert, W. Burkhardt, P. Esslinger, E. Günzel, H. G. Meissner, W. Schütt, J. Wegst, and M. Wilkens, *Einige strukturelle Ergebnisse an metallischen Phasen*, Naturwissenschaften **43**, 248–249 (1956).

Found in

[1] P. Villars, *MoPt2 Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.