Ni_4Mo ($D1_a$) Structure: AB4_tI10_87_a_h-001

This structure previously used the label(s) `AB4_tI10_87_a_h`. Calls to these addresses will be redirected here.

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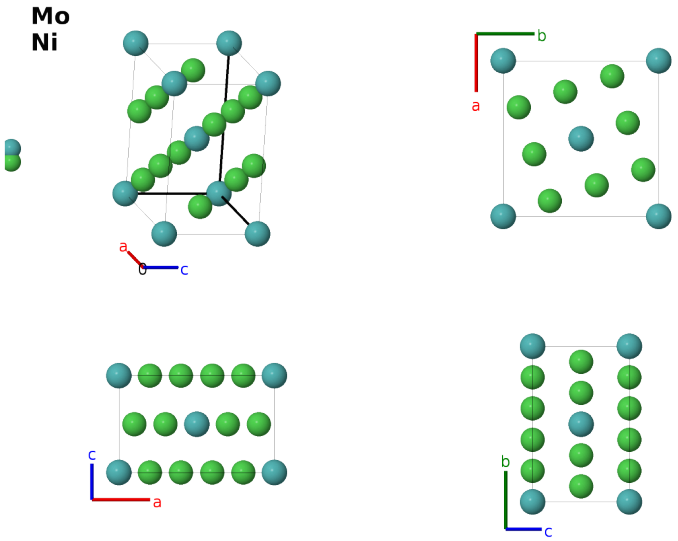
https://aflow.org/prototype-encyclopedia/VMNQ

https://aflow.org/prototype-encyclopedia/AB4_tI10_87_a_h-001



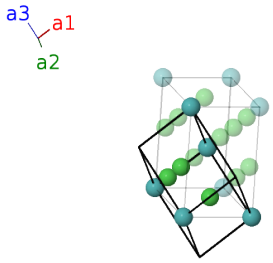
Prototype	$MoNi_4$
AFLOW prototype label	AB4_tI10_87_a_h-001
***Strukturbericht* designation**	$D1_a$
ICSD	105047
CCDC	1662946
Pearson symbol	tI10
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=AB4_tI10_87_a_h-001 --params=`$a, c/a, x_2, y_2$

Other compounds with this structure

Ag_4Lu, Ag_4Sc, Au_4Cr, Au_4Er, Au_4Ho, Au_4Lu, Au_4Mn, Au_4Ti, Au_4V, Au_4Yb, Ni_4W

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mo I
$\mathbf{B_2}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + (x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - (x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + (x_2-y_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - (x_2-y_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Ni I

References

[1] D. Harker, *The Crystal Structure of Ni_4Mo*, J. Chem. Phys. **12**, 315 (1944), doi:10.1063/1.1723945.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017