

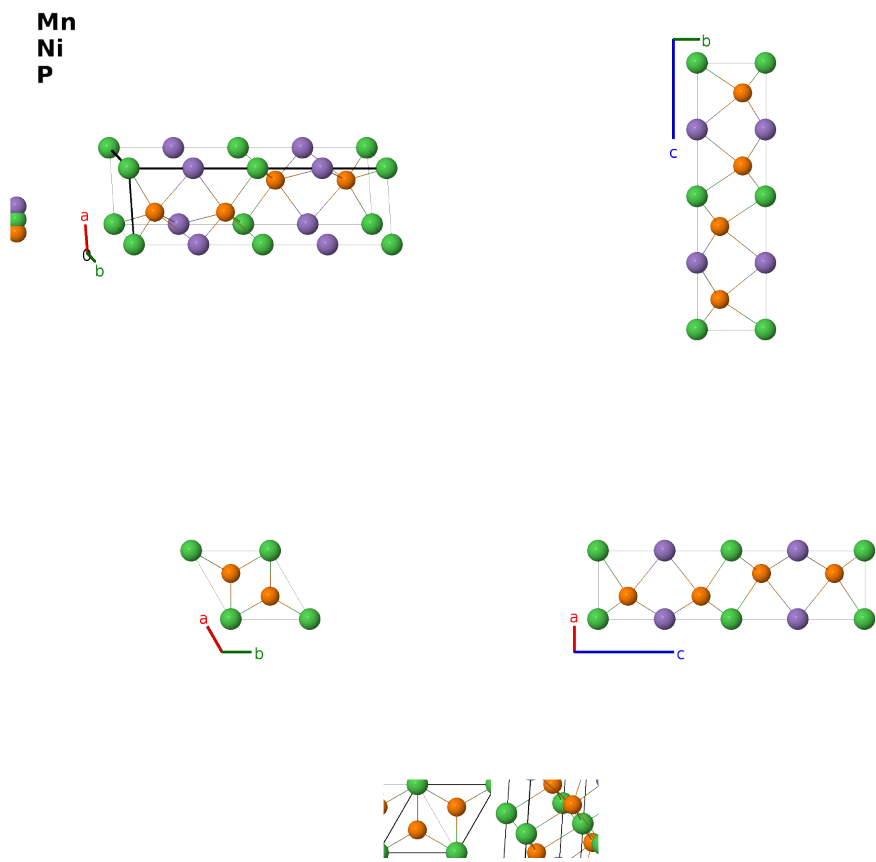
NiMoP₂ Structure: ABC2_hP8_194_b_a_f-001

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<https://aflow.org/prototype-encyclopedia/D1PM>

https://aflow.org/prototype-encyclopedia/ABC2_hP8_194_b_a_f-001



Prototype	MoNiP ₂
AFLOW prototype label	ABC2_hP8_194_b_a_f-001
ICSD	76283
CCDC	1636890
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=ABC2_hP8_194_b_a_f-001</code> <code>--params=a, c/a, z₃</code>

Other compounds with this structure

CoMoP₂, CoWP₂, NiWP₂

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}} \end{aligned}$$





Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	= 0	=	0	(2a)	Ni I
$\mathbf{B}_2$	= $\frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}c\hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B}_3$	= $\frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Mn I
$\mathbf{B}_4$	= $\frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Mn I
$\mathbf{B}_5$	= $\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(4f)	P I
$\mathbf{B}_6$	= $\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_3 + \frac{1}{2})\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_3 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	P I
$\mathbf{B}_7$	= $\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(4f)	P I
$\mathbf{B}_8$	= $\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_3 - \frac{1}{2})\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_3 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	P I

References

- [1] R. Guérin and M. Sergent, *Nouveau phosphure ternaire: NiMoP₂, a chaîne linéaire infinie -Mo-Ni-Mo- et composés isotopes: NiWP₂, CoMoP₂ et CoWP₂*, J. Solid State Chem. **18**, 317–323 (1976), doi:10.1016/0022-4596(76)90113-4.

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