

PrNiO₃ Rhombohedral Perovskite Structure: AB3C_hR10_167_b_e_a-001

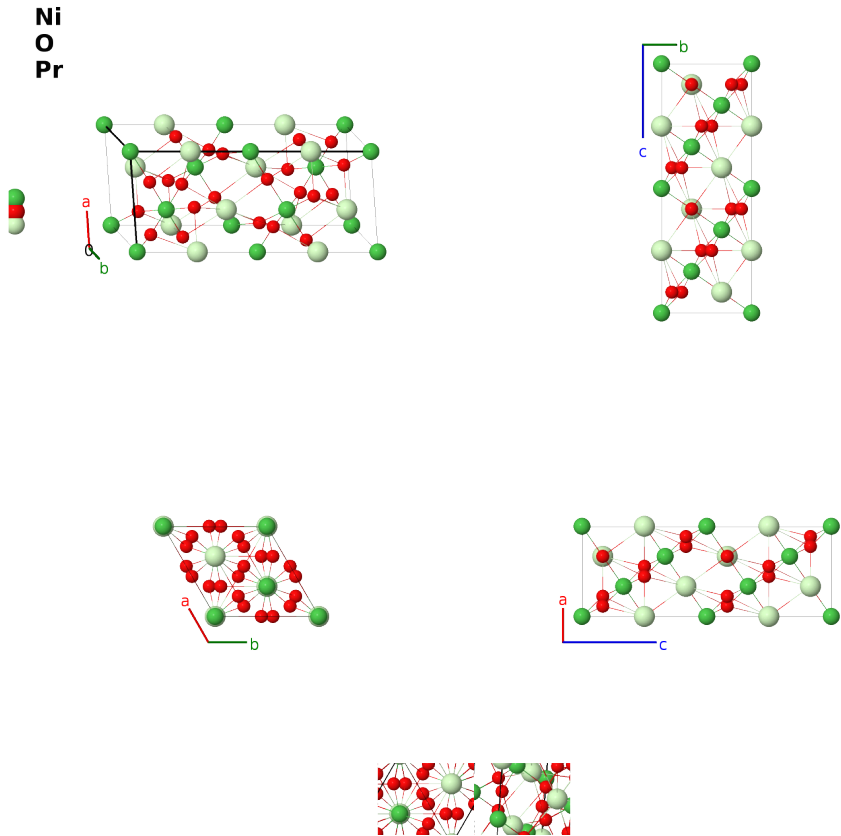
This structure previously used the label(s) **AB3C_hR10_167_b_e_a**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB3C_hR10_167_b_e_a-001



Prototype	NiO ₃ Pr
AFLOW prototype label	AB3C_hR10_167_b_e_a-001
ICSD	69186
CCDC	1631063
Pearson symbol	hR10
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	<code>aflow --proto=AB3C_hR10_167_b_e_a-001 --params=a, c/a, x₃</code>

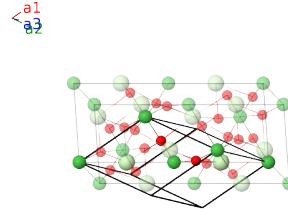
Other compounds with this structure

HgMnO₃, LaAlO₃, LaNiO₃

- This structure has the same crystal structure and occupies the same Wyckoff positions as Calcite (CaCO₃, *G*0₁, ABC3_hR10_167_a_b_e), but *c/a* and *x*₃ are different enough to warrant calling this a new structure.
- This is the high-temperature form of PrNiO₃, and we present the data collected at 500°C, below which it transforms into the orthorhombic perovskite structure (AB3C_oP20_62_c_cd_a).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2a)	Pr I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2a)	Pr I
$\mathbf{B}_3$	$= 0$	$=$	0	(2b)	Ni I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Ni I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_7$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_3 + 3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a (12x_3 + 1) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_1 - x_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a (12x_3 + 5) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{10}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O I

References

- [1] T. C. Huang, W. Parrish, H. Toraya, P. Lacorre, and J. B. Torrance, *High-Temperature Crystal Structures of Orthorhombic and Rhombohedral PrNiO₃*, Mater. Res. Bull. **25**, 1091–1098 (1990), doi:10.1016/0025-5408(90)90138-R.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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