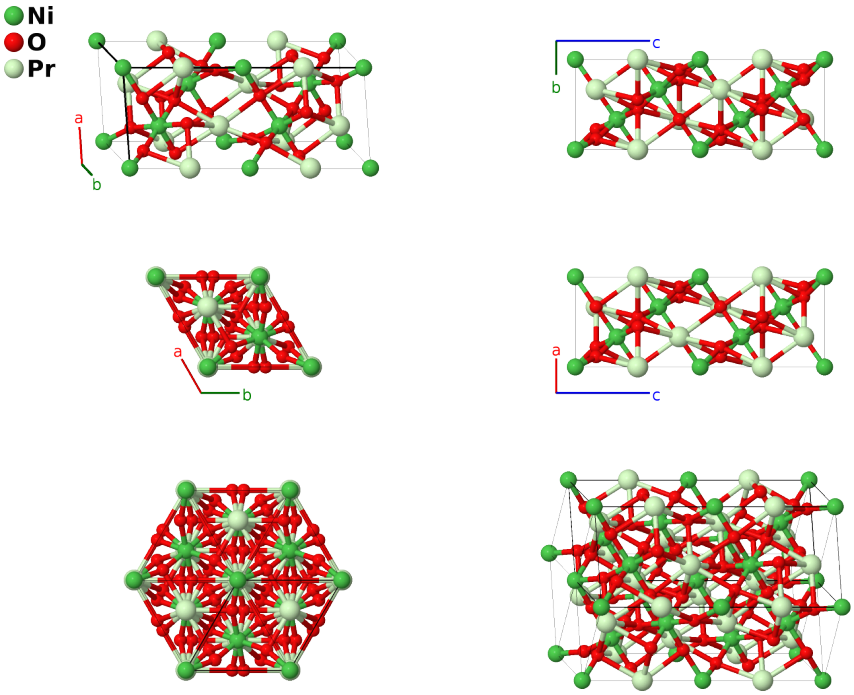
# $PrNiO_3$ Structure: AB3C_hR10_167_b_e_a-001

This structure originally had the label `AB3C_hR10_167_b_e_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/XMCY

https://aflow.org/p/AB3C_hR10_167_b_e_a-001




| | |
|---|---|
| **Prototype** | $NiO_3Pr$ |
| **AFLOW prototype label** | AB3C_hR10_167_b_e_a-001 |
| **ICSD** | 69186 |
| **Pearson symbol** | hR10 |
| **Space group number** | 167 |
| **Space group symbol** | $R\bar{3}c$ |
| **AFLOW prototype command** | `aflow --proto=AB3C_hR10_167_b_e_a-001 --params=`$a, c/a, x_3$ |

**Other compounds with this structure**
$LaAlO_3$, $LaNiO_3$

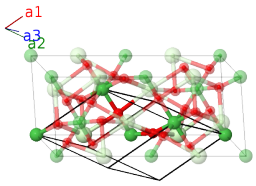
- This structure has the same crystal structure and occupies the same Wyckoff positions as Calcite ($CaCO_3$, $G0_1$, ABC3_hR10_167_a_b_e), but $c/a$ and $x_3$ are different enough to warrant calling this a new structure.

- This is the high-temperature form of $PrNiO_3$, 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**

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$




---

**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 |
| $\mathbf{B_5}$ | = | $x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6e) | O I |
| $\mathbf{B_6}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6e) | O I |
| $\mathbf{B_7}$ | = | $-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6e) | O I |
| $\mathbf{B_8}$ | = | $-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-\frac{1}{8}a\,(4x_3 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_3 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$ | (6e) | O I |
| $\mathbf{B_9}$ | = | $\frac{3}{4}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_3 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$ | (6e) | O I |
| $\mathbf{B_{10}}$ | = | $\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$ | (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 PrNiO$_3$*, 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).