

BaNiO₃ Structure:

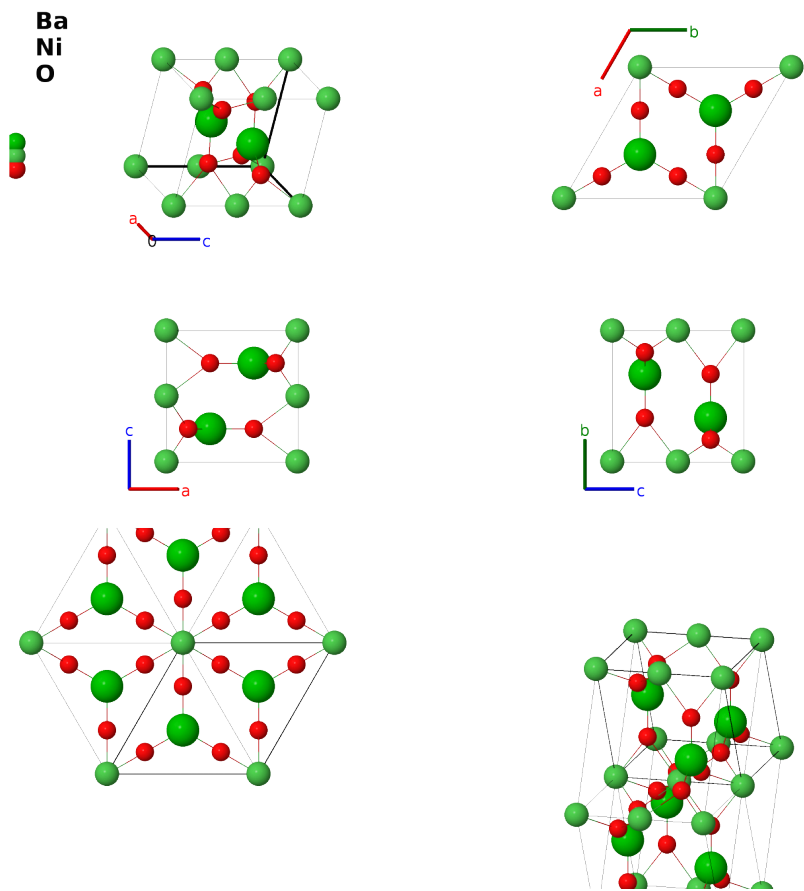
ABC3_hP10_194_c_a_h-001

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

https://aflow.org/prototype-encyclopedia/ABC3_hP10_194_c_a_h-001



Prototype	BaNiO ₃
AFLOW prototype label	ABC3_hP10_194_c_a_h-001
ICSD	30661
CCDC	1604905
Pearson symbol	hP10
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=ABC3_hP10_194_c_a_h-001 --params=a, c/a, x₃</code>

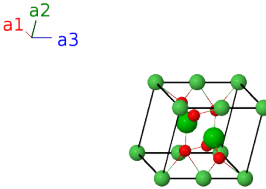
Other compounds with this structure

BaMnO₃, BaRuS₃, BaTiS₃, CeCrO₃, CeTiGe₃, CeTiO₃, CeVO₃, CsCuCl₃, CsMnBr₃, CsVlIr₃, LaCrO₃, LaTiGe₃, LaTiO₃, LaVO₃, NdCrO₃, NdVO₃, PrCrO₃, PrTiGe₃, PrTiO₃, PrVO₃, RbCoCl₃, RbCuCl₃, SmCrO₃, TlCoCl₃

- This structure has the same AFLOW label, ABC3_hP10_194_c_a_h, as the high-temperature GdBO₃ structure, but the c/a ration of GdBO₃ is more than twice that of BaNiO₃, so we treat them as different structures. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Note that the ICSD entry for this structure places the barium atom on the (2d) site rather than the (2c) site as given by (Lander, 1951). This results in a rather profound difference in the structure.

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
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	Ba I
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	Ba I
$\mathbf{B}_5$	$= x_3\mathbf{a}_1 + 2x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B}_6$	$= -2x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B}_7$	$= x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B}_8$	$= -x_3\mathbf{a}_1 - 2x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B}_9$	$= 2x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B}_{10}$	$= -x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	O I

References

- [1] J. J. Lander, *The crystal structures of NiO.3BaO, NiO.BaO, BaNiO₃ and intermediate phases with composition near Ba₂Ni₂O₅; with a note on NiO*, Acta Cryst. **4**, 148–156 (1951), doi:10.1107/S0365110X51000441.

Found in

- [1] T. Negas and R. S. Roth, *Phase equilibria and structural relations in the system BaMnO_{3-x}*, J. Solid State Chem. **3**, 323–329 (1971), doi:10.1016/0022-4596(71)90068-5.

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