$BaNiO_3$ Structure: ABC3_hP10_194_c_a_h-001

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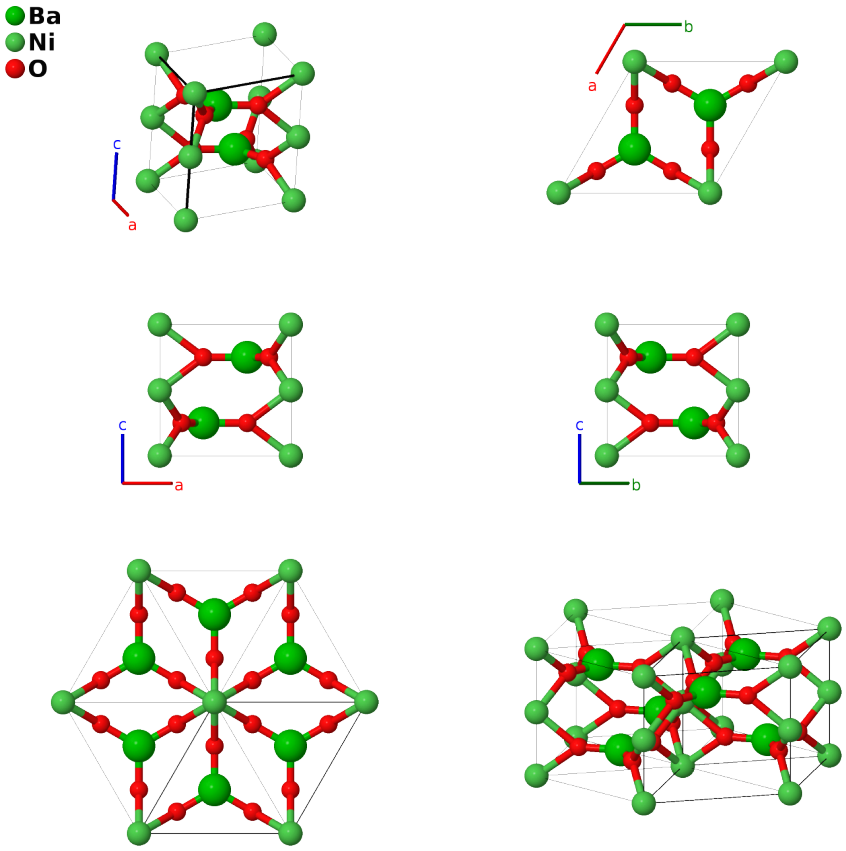
https://aflow.org/p/ABC3_hP10_194_c_a_h-001



Prototype	$BaNiO_3$
AFLOW prototype label	ABC3_hP10_194_c_a_h-001
ICSD	30661
Pearson symbol	hP10
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=ABC3_hP10_194_c_a_h-001 --params=`$a, c/a, x_3$

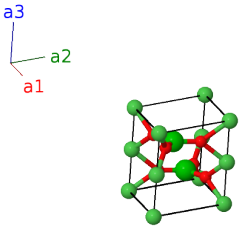
Other compounds with this structure

$BaMnO_3$, $BaTiS_3$, $CeCrO_3$, $CeTiGe_3$, $CeTiO_3$, $CeVO_3$, $CsCuCl_3$, $CsMnBr_3$, $CsVIr_3$, $LaCrO_3$, $LaTiGe_3$, $LaTiO_3$, $LaVO_3$, $NdCrO_3$, $NdVO_3$, $PrCrO_3$, $PrTiGe_3$, $PrTiO_3$, $PrVO_3$, $RbCoCl_3$, $RbCuCl_3$, $SmCrO_3$, $TlCoCl_3$

- This structure has the same AFLOW label, ABC3_hP10_194_c_a_h, as the high-temperature $GdBO_3$ structure, but the c/a ration of $GdBO_3$ is more than twice that of $BaNiO_3$, 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

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



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, $BaNiO_3$ and intermediate phases with composition near $Ba_2Ni_2O_5$; 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.