Orthorhombic La_2NiO_4 Structure: A2BC4_oP28_50_gh_ac_ghm-001

This structure originally had the label `A2BC4_oP28_50_ij_ac_ijm`. Calls to that address will be redirected here.

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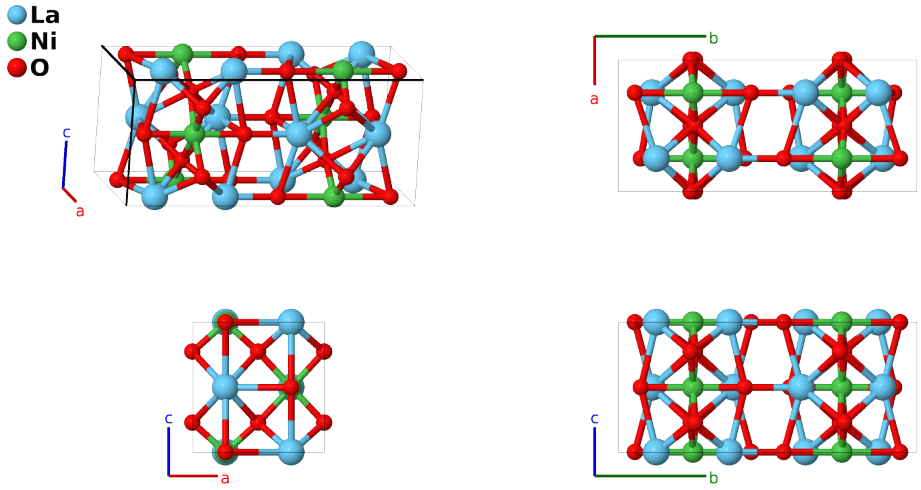
https://aflow.org/p/69JP

https://aflow.org/p/A2BC4_oP28_50_gh_ac_ghm-001

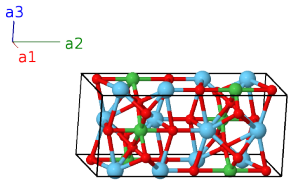


Prototype	La_2NiO_4
AFLOW prototype label	A2BC4_oP28_50_gh_ac_ghm-001
ICSD	201940
Pearson symbol	oP28
Space group number	50
Space group symbol	*Pban*
AFLOW prototype command	`aflow --proto=A2BC4_oP28_50_gh_ac_ghm-001 --params=`$a, b/a, c/a, x_3, x_4, x_5, x_6, x_7, y_7, z_7$

- La_2NiO_4 exhibits several temperature-driven structural phase transitions:
  - The ground state, a low-temperature tetragonal structure.
  - Above 70K it transforms into the orthorhombic La_2CuO_4 structure.
  - At 694K it transforms to the parent Ruddlesden-Popper structure, K_2NiF_4 (Villars,2016).
  - It has also been observed in this orthorhombic space group *Pban* #50 (Odier, 1986).
- (Odier, 1986) give the structure in the *Pncb* setting of space group #50, but we present it in the standard *Pban* setting.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(2a)	Ni I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(2a)	Ni I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Ni II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Ni II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4g)	La I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4g)	La I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4g)	La I
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4g)	La I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{10}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{12}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	La II
$\mathbf{B_{14}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	La II
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	La II
$\mathbf{B_{16}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	La II
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_{18}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_{20}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{22}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{23}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{24}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{25}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{26}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{27}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{28}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8m)	O III

References

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[2] G. H. Lander, P. J. Brown, J. Spałek, and J. M. Honig, *Structural and magnetization density studies of La_2NiO_4*, Phys. Rev. B **40**, 4463–4471 (1989), doi:10.1103/PhysRevB.40.4463.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.