

Orthorhombic La_2NiO_4 Structure: A2BC4_oP28_50_gh_ac_ghm-001

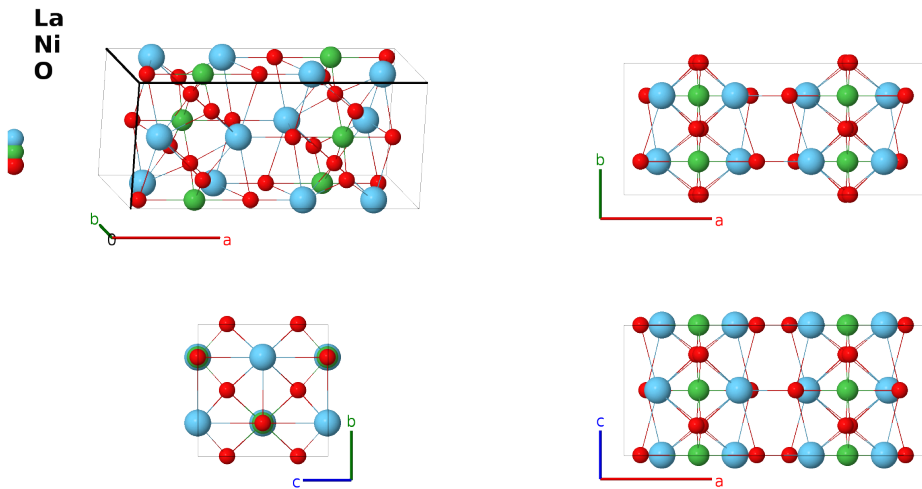
This structure previously used the label(s) **A2BC4.oP28.50.ij.ac.ijm**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/69JP>

https://aflow.org/prototype-encyclopedia/A2BC4.oP28.50_gh_ac_ghm-001



Prototype	La_2NiO_4
AFLOW prototype label	A2BC4_oP28_50_gh_ac_ghm-001
ICSD	201940
CCDC	1706556
Pearson symbol	oP28
Space group number	50
Space group symbol	$Pban$
AFLOW prototype command	<code>aflow --proto=A2BC4_oP28_50_gh_ac_ghm-001</code> <code>--params=a, b/a, c/a, x3, x4, x5, x6, x7, y7, z7</code>

- 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).

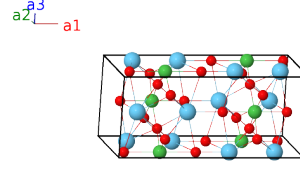
- (Odier, 1986) give the structure in the $Pn\bar{c}b$ setting of space group #50, but we present it in the standard $Pban$ setting.

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
$\mathbf{B}_6$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}}$	(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
$\mathbf{B}_8$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}}$	(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
$\mathbf{B}_{10}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}}$	(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
$\mathbf{B}_{12}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}}$	(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
$\mathbf{B}_{14}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{20}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B}_{23}$	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B}_{24}$	$= x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{26}$	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B}_{27}$	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B}_{28}$	$= -x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8m)	O III

References

- [1] P. Odier, M. Leblanc, and J. Choisnet, *Structural characterization of an orthorhombic form of La_2NiO_4* , Mater. Res. Bull. **21**, 787–796 (1986), doi:10.1016/0025-5408(86)90163-7.
- [2] G. H. Lander, P. J. Brown, J. Spalek, 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.

First cited in

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