Orthorhombic $La_3Ni_2O_7$ Structure: A3B2C7_oF48_69_ag_g_bgl-001

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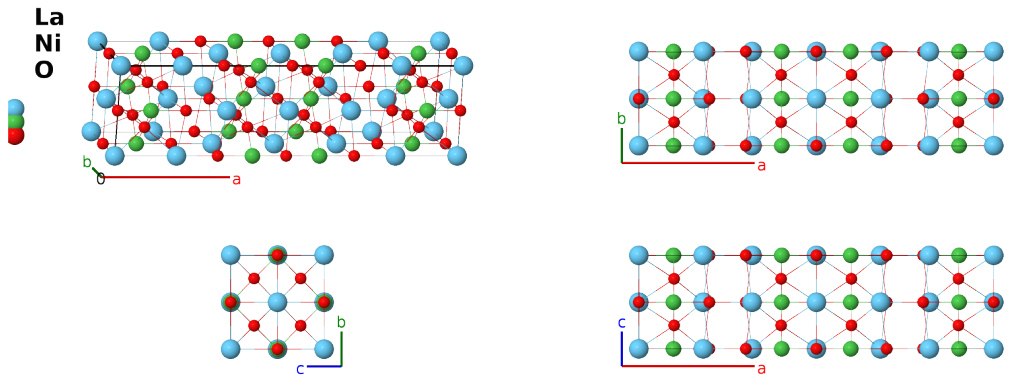
https://aflow.org/prototype-encyclopedia/KRB7

https://aflow.org/prototype-encyclopedia/A3B2C7_oF48_69_ag_g_bgl-001



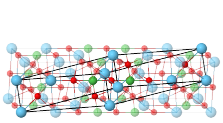
Prototype	$La_3Ni_2O_7$
AFLOW prototype label	A3B2C7_oF48_69_ag_g_bgl-001
ICSD	93920
CCDC	1653370
Pearson symbol	oF48
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=A3B2C7_oF48_69_ag_g_bgl-001 --params=`$a, b/a, c/a, x_3, x_4, x_5, x_6$

- $La_3Ni_2O_{7-\delta}$ is a Ruddlesden-Popper compound with a bilayer NiO_6 structure. The exact structure depends on the pressure and/or oxygen deficiency. (Park, 2001; Lin, 2024)
  - Under ambient pressure the fully stoichiometric compound is in the Sr_3SnO_7 structure.
  - At pressures above ≈ 10 GPa or when $\delta \approx 0.06$ it is in the current structure.
  - As δ increases the system transforms into the tetragonal $Sr_3Ti_2O_7$ structure.
- (Sun, 2023) report "signatures" of superconductivity in this structure at 80 K at pressures between 14 and 43.5 GPa.
- The data for this structure was taken from (Park, 2001) at ambient pressure, and the oxygen (2b) site has 4% vacancies.
- The AFLOW prototype label algorithm swaps the a and c axis compared to experiment, and moves the origin from the O I site to the La I site.

- This structure is a ternary form of the $SrLa_2Sc_2O_7$ structure.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	La I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_3}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8g)	La II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8g)	La II
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(8g)	Ni I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(8g)	Ni I
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}$	(8g)	O II
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}$	(8g)	O II
$\mathbf{B_9}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O III
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O III
$\mathbf{B_{11}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O III
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O III

References

[1] J.-C. Park, D.-K. Kim, S.-H. Byeon, and D. Kim, *XANES study on Ruddlesden-Popper phase, $La_{n+1}Ni_nO_{3n+1}$ (n = 1, 2, and ∞)*, J. Synchrotron Rad. **8**, 704–706 (2001), doi:10.1107/S0909049500015983.

[2] L.-F. Lin, Y. Zhang, N. Kaushal, G. Alvarez, T. A. Maier, A. Moreo, and E. Dagotto, *Magnetic phase diagram of a two-orbital model for bilayer nickelates varying doping*, Physical Review B **110**, 195135 (2024), doi:10.1103/PhysRevB.110.195135.

[3] H. Sun, M. Huo, X. Hu, J. Li, Z. Liu, Y. Han, L. Tang, Z. Mao, P. Yang, B. Wang, J. Cheng, D.-X. Yao, G.-M. Zhang, and M. Wang, *Signatures of superconductivity near 80 K in a nickelate under high pressure*, Nature **621**, 493–498 (2023), doi:10.1038/s41586-023-06408-7.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 93920 (La3Ni2O7).

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