$LiNiO_2$ Structure: ABC2_hR4_166_a_b_c-010

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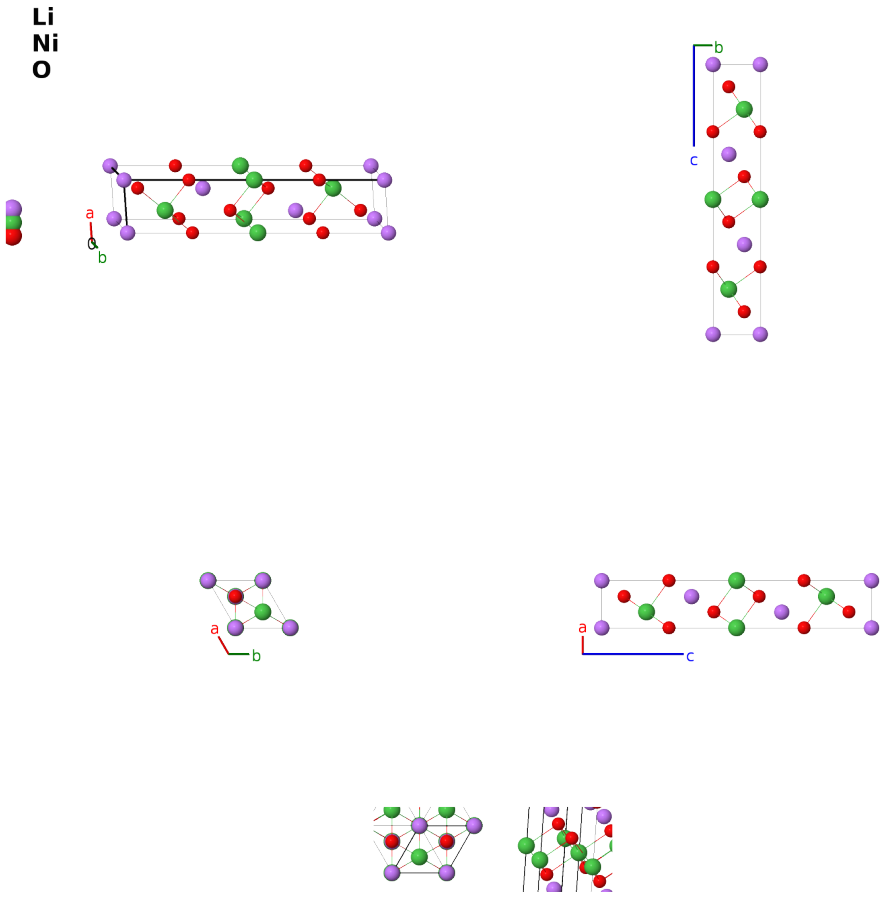
https://aflow.org/prototype-encyclopedia/0R3A

https://aflow.org/prototype-encyclopedia/ABC2_hR4_166_a_b_c-010



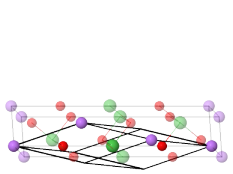
Prototype	$LiNiO_2$
AFLOW prototype label	ABC2_hR4_166_a_b_c-010
ICSD	26608
CCDC	1601998
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC2_hR4_166_a_b_c-010 --params=`$a, c/a, x_3$

Other compounds with this structure
$NaNiO_2$

- α-$NaFeO_2$, rhombohedral delafossite, $CuFeO_2$, caswellsilverite (α-$NaFeO_2$, $F5_1$), $LiNiO_2$ and $Li_2Mn_3O_7$ have the same prototype label, ABC2_hR4_166_a_b_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ni I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	O I

References

[1] L. D. Dyer, B. S. B. Jr., and G. P. Smith, *Alkali Metal-Nickel Oxides of the Type $MNiO_2$*, J. Am. Chem. Soc. **76**, 1499–1503 (1954), doi:10.1021/ja01635a012.

Found in

[1] M. Sofin and M. Jansen, *New Route of Preparation and Properties of $NaNiO_2$*, Z. Naturforsch. B **60**, 701–704 (2005), doi:10.1515/znb-2005-0615.

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