$Nd_4Ni_3O_8$ Structure: A4B3C8_tI30_139_2e_ae_cdg-002

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https://aflow.org/p/W8GW

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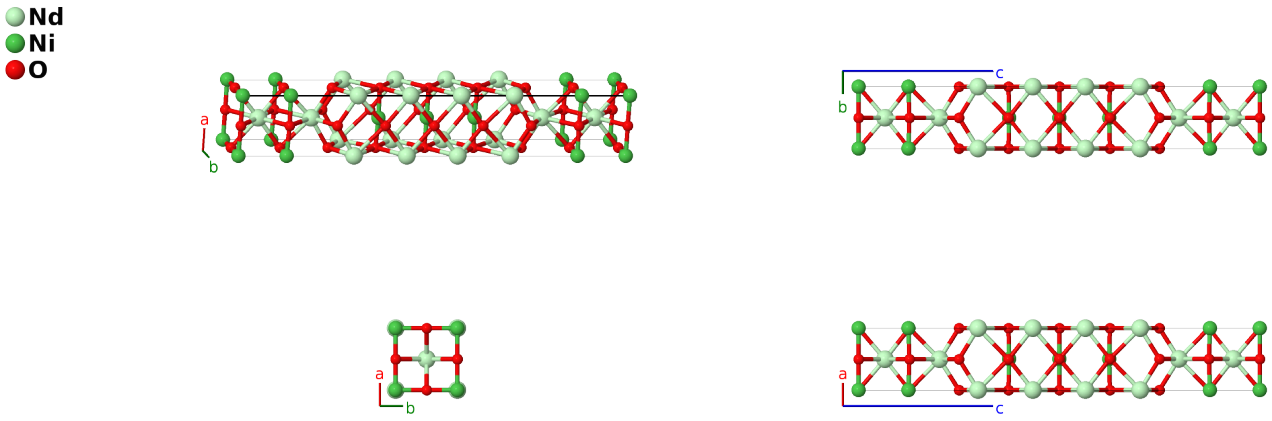
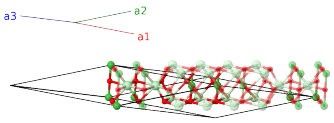


Prototype	$Nd_4Ni_3O_8$
AFLOW prototype label	A4B3C8_tI30_139_2e_ae_cdg-002
ICSD	173372
Pearson symbol	tI30
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A4B3C8_tI30_139_2e_ae_cdg-002 --params=`$a, c/a, z_4, z_5, z_6, z_7$

Other compounds with this structure
$La_4Ni_3O_8$, $Pr_4Ni_3O_8$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ni I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	O I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Nd I
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Nd I
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	Nd II
$\mathbf{B_9}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	Nd II
$\mathbf{B_{10}}$	=	$z_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2$	=	$cz_6\,\hat{\mathbf{z}}$	(4e)	Ni II
$\mathbf{B_{11}}$	=	$-z_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2$	=	$-cz_6\,\hat{\mathbf{z}}$	(4e)	Ni II
$\mathbf{B_{12}}$	=	$\left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{13}}$	=	$z_7\,\mathbf{a}_1 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{14}}$	=	$-\left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{15}}$	=	$-z_7\,\mathbf{a}_1 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_7\,\hat{\mathbf{z}}$	(8g)	O III

References

[1] V. V. Poltavets, K. A. Lokshin, M. Croft, T. K. Mandal, T. Egami, and M. Greenblatt, *Crystal Structures of $Ln_4Ni_3O_8$ (Ln = La, Nd) Triple Layer T'-type Nickelates*, Inorg. Chem. **46**, 10887–10891 (2007), doi:10.1016/j.intermet.2008.04.018.