

Nd₄Co₃O₁₀ Structure:

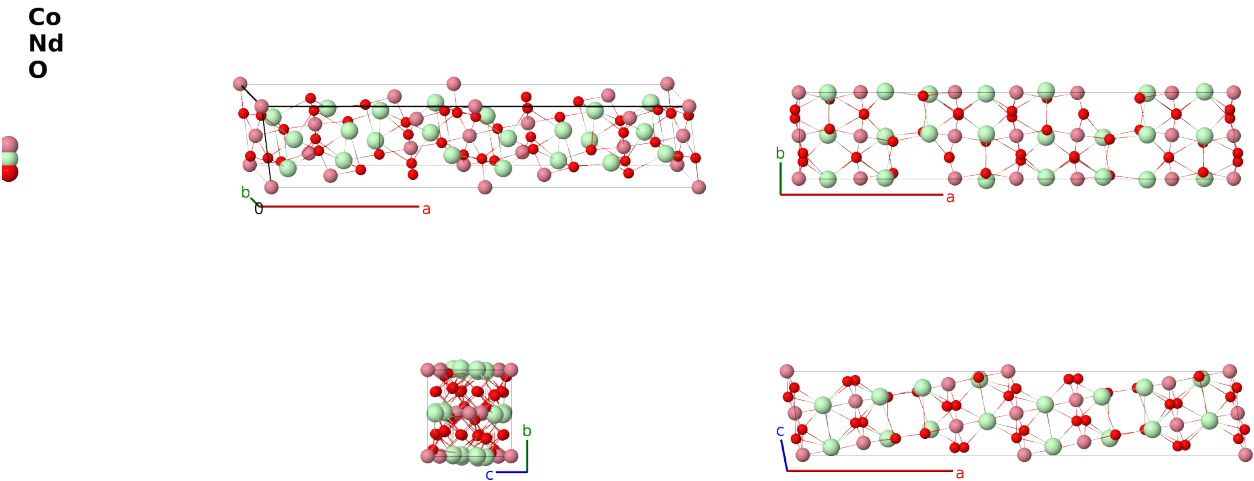
A3B4C10_mP68_14_ab2e_4e_10e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/JXXS>

https://aflow.org/prototype-encyclopedia/A3B4C10_mP68_14_ab2e_4e_10e-001



Prototype	Co ₃ Nd ₄ O ₁₀
AFLOW prototype label	A3B4C10_mP68_14_ab2e_4e_10e-001
ICSD	91099
CCDC	1650666
Pearson symbol	mP68
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A3B4C10_mP68_14_ab2e_4e_10e-001 --params=a,b/a,c/a,β,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈,x₉, y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅,y₁₅,z₁₅,x₁₆,y₁₆,z₁₆, x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈</pre>

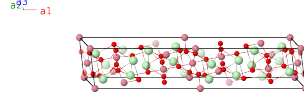
Other compounds with this structure

La₄Co₃O₁₀, La₄Ni₃O₁₀, Nd₄Ni₃O₁₀, Pr₄Ni₃O₁₀

- (Olafsen, 2000) give the structure in the $P2_1/a$ setting of space group #14. We used AFLOW to transform it into the standard $P2_1/c$ setting. This involves a redefinition of the primitive vectors.

Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Co I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(2b)	Co II
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} (a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2b)	Co II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	Co III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Co III
$\mathbf{B}_7$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	Co III
$\mathbf{B}_8$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Co III
$\mathbf{B}_9$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	Co IV
$\mathbf{B}_{10}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Co IV
$\mathbf{B}_{11}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	Co IV
$\mathbf{B}_{12}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Co IV
$\mathbf{B}_{13}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd I
$\mathbf{B}_{14}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd I
$\mathbf{B}_{15}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd I
$\mathbf{B}_{16}$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd I
$\mathbf{B}_{17}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd II
$\mathbf{B}_{18}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd II
$\mathbf{B}_{19}$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd II
$\mathbf{B}_{20}$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd II
$\mathbf{B}_{21}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd III
$\mathbf{B}_{22}$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd III
$\mathbf{B}_{23}$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd III
$\mathbf{B}_{24}$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd III
$\mathbf{B}_{25}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd IV

$\mathbf{B}_{26} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd IV
$\mathbf{B}_{27} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4e)	Nd IV
$\mathbf{B}_{28} =$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Nd IV
$\mathbf{B}_{29} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{30} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{31} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{32} =$	$x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{33} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{34} =$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{10} + c(z_{10} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{35} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{36} =$	$x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{37} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{38} =$	$-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{11} + c(z_{11} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{39} =$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{40} =$	$x_{11} \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{41} =$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{42} =$	$-x_{12} \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{12} + c(z_{12} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{43} =$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{44} =$	$x_{12} \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{12} + c(z_{12} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{45} =$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B}_{46} =$	$-x_{13} \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{13} + c(z_{13} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B}_{47} =$	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B}_{48} =$	$x_{13} \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{13} + c(z_{13} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B}_{49} =$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B}_{50} =$	$-x_{14} \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{14} + c(z_{14} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B}_{51} =$	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - cz_{14} \sin \beta \hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B}_{52} =$	$x_{14} \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{14} + c(z_{14} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O VI

$\mathbf{B}_{53} =$	$x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{54} =$	$-x_{15} \mathbf{a}_1 + (y_{15} + \frac{1}{2}) \mathbf{a}_2 - (z_{15} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{15} + c(z_{15} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{15} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{55} =$	$-x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} - cz_{15} \sin \beta \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{56} =$	$x_{15} \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{15} + c(z_{15} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{57} =$	$x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{58} =$	$-x_{16} \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 - (z_{16} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{16} + c(z_{16} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{16} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{59} =$	$-x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} - cz_{16} \sin \beta \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{60} =$	$x_{16} \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{16} + c(z_{16} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{61} =$	$x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{62} =$	$-x_{17} \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{17} + c(z_{17} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{63} =$	$-x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{64} =$	$x_{17} \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{17} + c(z_{17} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{65} =$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{66} =$	$-x_{18} \mathbf{a}_1 + (y_{18} + \frac{1}{2}) \mathbf{a}_2 - (z_{18} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{18} + c(z_{18} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{18} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{18} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{67} =$	$-x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{68} =$	$x_{18} \mathbf{a}_1 - (y_{18} - \frac{1}{2}) \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{18} + c(z_{18} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{18} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O X

References

- [1] A. Olafsen, H. Fjellvåg, and B. C. Hauback, *Crystal Structure and Properties of $\text{Nd}_4\text{Co}_3\text{O}_{10+\delta}$ and $\text{Nd}_4\text{Ni}_3\text{O}_{10-\delta}$* , J. Solid State Chem. **151**, 46–55 (2000), doi:10.1006/jssc.2000.8620.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).