

NiBi Structure:

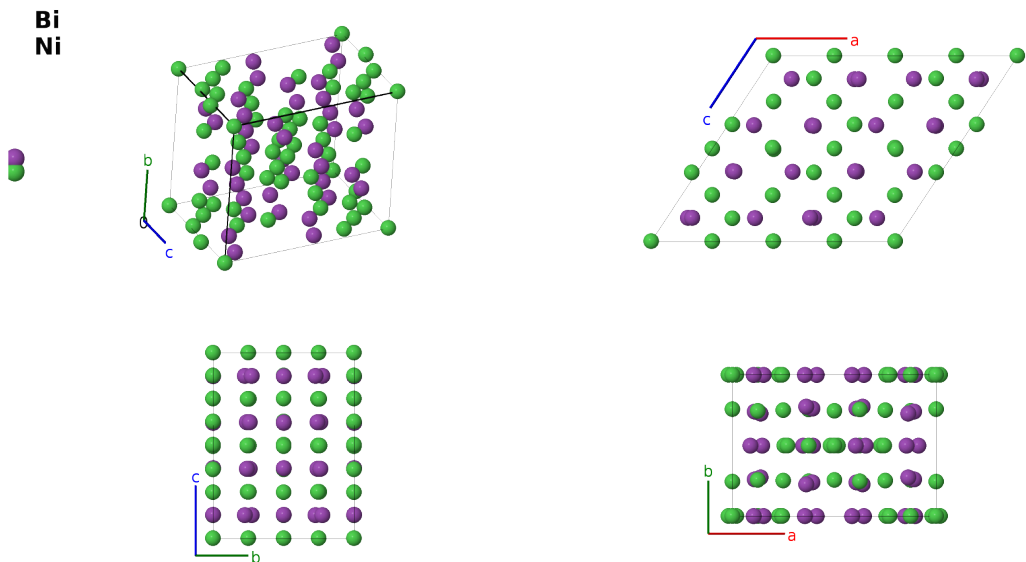
A16B17_mC66_12_4i2j_aeh4ij-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/V4P2>

https://aflow.org/prototype-encyclopedia/A16B17_mC66_12_4i2j_aeh4ij-001

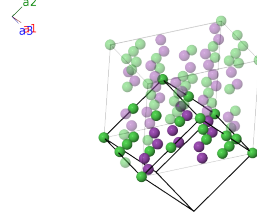


Prototype	BiNi
AFLOW prototype label	A16B17_mC66_12_4i2j_aeh4ij-001
ICSD	410878
CCDC	1726625
Pearson symbol	mC66
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A16B17_mC66_12_4i2j_aeh4ij-001 --params=a,b/a,c/a,β,y₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀,z₁₀,x₁₁,z₁₁, x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄</pre>

- In the ideal stoichiometry half of the Ni-VII sites are occupied. Similar structures have compositions $\text{Ni}_x\text{Bi}_{1-x}$ with $x > 1/2$, so it is likely the some of the excess nickel atoms sit on this site.
- (Ruck, 1999) and the ICSD entry put this structure in the $F2/m$ setting of space-group #12, where we can see that it is pseudo-orthorhombic. We used FINDSYM to place this in the standard $C2/m$ setting.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Ni I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	Ni II
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	Ni II
$\mathbf{B}_4$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Ni III
$\mathbf{B}_5$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Ni III
$\mathbf{B}_6$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	Bi I
$\mathbf{B}_7$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	Bi I
$\mathbf{B}_8$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	Bi II
$\mathbf{B}_9$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	Bi II
$\mathbf{B}_{10}$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	Bi III
$\mathbf{B}_{11}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	Bi III
$\mathbf{B}_{12}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	Bi IV
$\mathbf{B}_{13}$	$=$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	Bi IV
$\mathbf{B}_{14}$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	Ni IV
$\mathbf{B}_{15}$	$=$	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	Ni IV
$\mathbf{B}_{16}$	$=$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	Ni V
$\mathbf{B}_{17}$	$=$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	Ni V
$\mathbf{B}_{18}$	$=$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	Ni VI
$\mathbf{B}_{19}$	$=$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	Ni VI
$\mathbf{B}_{20}$	$=$	$x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	Ni VII
$\mathbf{B}_{21}$	$=$	$-x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	Ni VII
$\mathbf{B}_{22}$	$=$	$(x_{12} - y_{12}) \mathbf{a}_1 +$ $(x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Bi V
$\mathbf{B}_{23}$	$=$	$-(x_{12} + y_{12}) \mathbf{a}_1 -$ $(x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Bi V
$\mathbf{B}_{24}$	$=$	$-(x_{12} - y_{12}) \mathbf{a}_1 -$ $(x_{12} + y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Bi V
$\mathbf{B}_{25}$	$=$	$(x_{12} + y_{12}) \mathbf{a}_1 +$ $(x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Bi V
$\mathbf{B}_{26}$	$=$	$(x_{13} - y_{13}) \mathbf{a}_1 +$ $(x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j) Bi VI

$$\begin{aligned}
\mathbf{B}_{27} &= \begin{matrix} -(x_{13} + y_{13}) \mathbf{a}_1 - \\ (x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - \\ cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Bi VI} \\
\mathbf{B}_{28} &= \begin{matrix} -(x_{13} - y_{13}) \mathbf{a}_1 - \\ (x_{13} + y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - \\ cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Bi VI} \\
\mathbf{B}_{29} &= \begin{matrix} (x_{13} + y_{13}) \mathbf{a}_1 + \\ (x_{13} - y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Bi VI} \\
\mathbf{B}_{30} &= \begin{matrix} (x_{14} - y_{14}) \mathbf{a}_1 + \\ (x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Ni VIII} \\
\mathbf{B}_{31} &= \begin{matrix} -(x_{14} + y_{14}) \mathbf{a}_1 - \\ (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - \\ cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Ni VIII} \\
\mathbf{B}_{32} &= \begin{matrix} -(x_{14} - y_{14}) \mathbf{a}_1 - \\ (x_{14} + y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - \\ cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Ni VIII} \\
\mathbf{B}_{33} &= \begin{matrix} (x_{14} + y_{14}) \mathbf{a}_1 + \\ (x_{14} - y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8j) & \text{Ni VIII}
\end{aligned}$$

References

- [1] M. Ruck, *Die Kristallstruktur von BiNi: eine komplexe Ausdünnungsvariante des InNi₂-Typs*, Z. Anorganische und Allgemeine Chemie **625**, 2050–2054 (1999), doi:10.1002/(SICI)1521-3749(199912)625:12<2050::AID-ZAAC2050>3.0.CO;2-R.

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First cited in

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