

La₄₃Ni₁₇Mg₅ Structure:

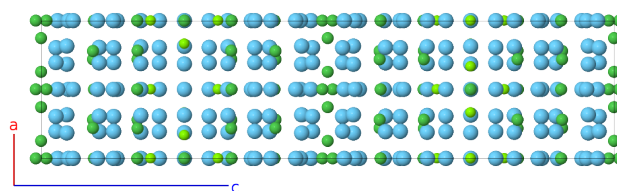
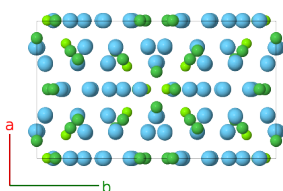
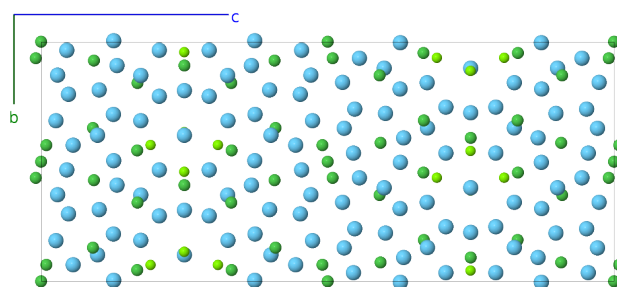
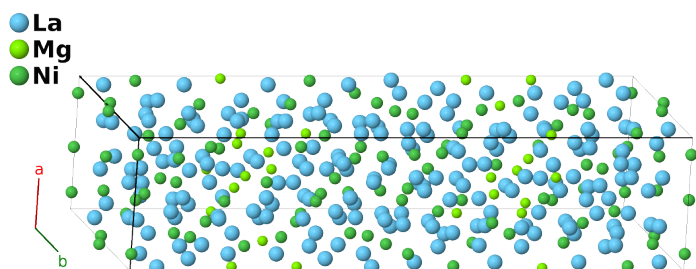
A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h-001

This structure originally had the label A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/Z34R>

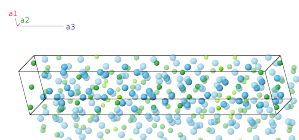
https://aflow.org/p/A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h-001



Prototype	La ₄₃ Mg ₅ Ni ₁₇
AFLOW prototype label	A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h-001
ICSD	249963
Pearson symbol	oC260
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	aflow --proto=A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h-001 --params=a, b/a, c/a, y ₁ , y ₂ , y ₃ , x ₄ , y ₅ , z ₅ , y ₆ , z ₆ , y ₇ , z ₇ , y ₈ , z ₈ , y ₉ , z ₉ , y ₁₀ , z ₁₀ , y ₁₁ , z ₁₁ , y ₁₂ , z ₁₂ , y ₁₃ , z ₁₃ , y ₁₄ , z ₁₄ , y ₁₅ , z ₁₅ , y ₁₆ , z ₁₆ , x ₁₇ , y ₁₇ , x ₁₈ , y ₁₈ , x ₁₉ , y ₁₉ , z ₁₉ , x ₂₀ , y ₂₀ , z ₂₀ , x ₂₁ , y ₂₁ , z ₂₁ , x ₂₂ , y ₂₂ , z ₂₂ , x ₂₃ , y ₂₃ , z ₂₃ , x ₂₄ , y ₂₄ , z ₂₄ , x ₂₅ , y ₂₅ , z ₂₅ , x ₂₆ , y ₂₆ , z ₂₆

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	La I
\mathbf{B}_2	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	La I
\mathbf{B}_3	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_4	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_5	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Ni I
\mathbf{B}_6	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Ni I
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}}$	(8e)	Ni II
\mathbf{B}_8	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Ni II
\mathbf{B}_9	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}}$	(8e)	Ni II
\mathbf{B}_{10}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Ni II
\mathbf{B}_{11}	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	La II
\mathbf{B}_{12}	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La II
\mathbf{B}_{13}	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La II
\mathbf{B}_{14}	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f)	La II
\mathbf{B}_{15}	$= -y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8f)	La III
\mathbf{B}_{16}	$= y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La III
\mathbf{B}_{17}	$= -y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La III
\mathbf{B}_{18}	$= y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8f)	La III
\mathbf{B}_{19}	$= -y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8f)	La IV
\mathbf{B}_{20}	$= y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La IV
\mathbf{B}_{21}	$= -y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La IV
\mathbf{B}_{22}	$= y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8f)	La IV
\mathbf{B}_{23}	$= -y_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8f)	La V
\mathbf{B}_{24}	$= y_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La V
\mathbf{B}_{25}	$= -y_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La V
\mathbf{B}_{26}	$= y_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8f)	La V
\mathbf{B}_{27}	$= -y_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8f)	La VI
\mathbf{B}_{28}	$= y_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La VI
\mathbf{B}_{29}	$= -y_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La VI
\mathbf{B}_{30}	$= y_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8f)	La VI
\mathbf{B}_{31}	$= -y_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8f)	La VII
\mathbf{B}_{32}	$= y_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La VII
\mathbf{B}_{33}	$= -y_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La VII
\mathbf{B}_{34}	$= y_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8f)	La VII
\mathbf{B}_{35}	$= -y_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8f)	La VIII
\mathbf{B}_{36}	$= y_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La VIII
\mathbf{B}_{37}	$= -y_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La VIII
\mathbf{B}_{38}	$= y_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8f)	La VIII

$$\begin{aligned}
\mathbf{B}_{119} &= \begin{matrix} -(x_{25} - y_{25}) \mathbf{a}_1 - \\ (x_{25} + y_{25}) \mathbf{a}_2 - z_{25} \mathbf{a}_3 \end{matrix} &= & -ax_{25} \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}} & (16h) & \text{Ni VI} \\
\mathbf{B}_{120} &= \begin{matrix} (x_{25} - y_{25}) \mathbf{a}_1 + \\ (x_{25} + y_{25}) \mathbf{a}_2 - (z_{25} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & ax_{25} \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} - c(z_{25} - \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{Ni VI} \\
\mathbf{B}_{121} &= \begin{matrix} (x_{25} + y_{25}) \mathbf{a}_1 + \\ (x_{25} - y_{25}) \mathbf{a}_2 + (z_{25} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & ax_{25} \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} + c(z_{25} + \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{Ni VI} \\
\mathbf{B}_{122} &= \begin{matrix} -(x_{25} + y_{25}) \mathbf{a}_1 - \\ (x_{25} - y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 \end{matrix} &= & -ax_{25} \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} & (16h) & \text{Ni VI} \\
\mathbf{B}_{123} &= \begin{matrix} (x_{26} - y_{26}) \mathbf{a}_1 + \\ (x_{26} + y_{26}) \mathbf{a}_2 + z_{26} \mathbf{a}_3 \end{matrix} &= & ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{124} &= \begin{matrix} -(x_{26} - y_{26}) \mathbf{a}_1 - \\ (x_{26} + y_{26}) \mathbf{a}_2 + (z_{26} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & -ax_{26} \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + c(z_{26} + \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{125} &= \begin{matrix} -(x_{26} + y_{26}) \mathbf{a}_1 - \\ (x_{26} - y_{26}) \mathbf{a}_2 - (z_{26} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & -ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} - c(z_{26} - \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{126} &= \begin{matrix} (x_{26} + y_{26}) \mathbf{a}_1 + \\ (x_{26} - y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3 \end{matrix} &= & ax_{26} \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} - cz_{26} \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{127} &= \begin{matrix} -(x_{26} - y_{26}) \mathbf{a}_1 - \\ (x_{26} + y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3 \end{matrix} &= & -ax_{26} \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} - cz_{26} \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{128} &= \begin{matrix} (x_{26} - y_{26}) \mathbf{a}_1 + \\ (x_{26} + y_{26}) \mathbf{a}_2 - (z_{26} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} - c(z_{26} - \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{129} &= \begin{matrix} (x_{26} + y_{26}) \mathbf{a}_1 + \\ (x_{26} - y_{26}) \mathbf{a}_2 + (z_{26} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & ax_{26} \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + c(z_{26} + \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\
\mathbf{B}_{130} &= \begin{matrix} -(x_{26} + y_{26}) \mathbf{a}_1 - \\ (x_{26} - y_{26}) \mathbf{a}_2 + z_{26} \mathbf{a}_3 \end{matrix} &= & -ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \hat{\mathbf{z}} & (16h) & \text{Ni VII}
\end{aligned}$$

References

- [1] P. Solokha, S. D. Negri, V. Pavlyuk, and A. Saccone, *Anti-Mackay Polyicosahedral Clusters in La-Ni-Mg Ternary Compounds: Synthesis and Crystal Structure of the La₄₃Ni₁₇Mg₅ New Intermetallic Phase*, Inorg. Chem. **48**, 11586–11593 (2009), doi:10.1021/ic901422v.