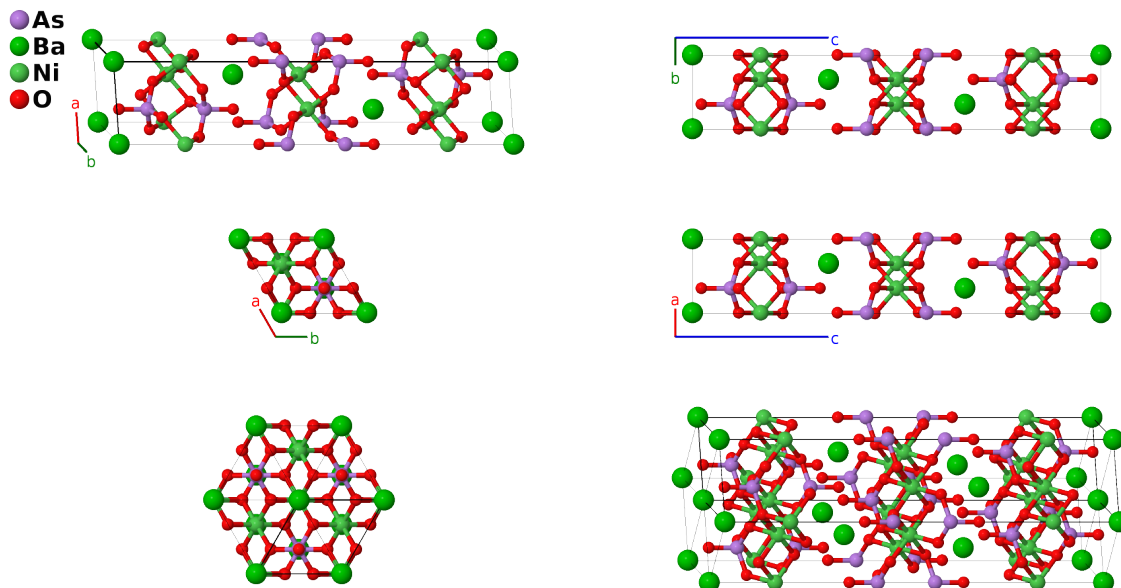


BaNi₂As₂O₈ Structure: A2BC2D8_hR13_148_c_a_c_cf-001

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

https://aflow.org/p/A2BC2D8_hR13_148_c_a_c_cf-001



Prototype	As ₂ BaNi ₂ O ₈
AFLOW prototype label	A2BC2D8_hR13_148_c_a_c_cf-001
ICSD	27014
Pearson symbol	hR13
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	aflow --proto=A2BC2D8_hR13_148_c_a_c_cf-001 --params=a, c/a, x ₂ , x ₃ , x ₄ , x ₅ , y ₅ , z ₅

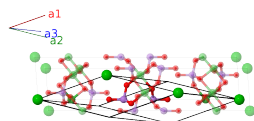
Other compounds with this structure

BaCo₂As₂O₈, BaMg₂As₂O₈, BaCo₂P₂O₈, BaNi₂P₂O₈, BaNi₂V₂O₈

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(1a) Ba I
\mathbf{B}_2	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c) As I
\mathbf{B}_3	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c) As 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) Ni I
\mathbf{B}_5	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c) Ni I
\mathbf{B}_6	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(2c) O I
\mathbf{B}_7	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-cx_4 \hat{\mathbf{z}}$	(2c) O I
\mathbf{B}_8	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f) O II
\mathbf{B}_9	$=$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f) O II
\mathbf{B}_{10}	$=$	$y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f) O II
\mathbf{B}_{11}	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f) O II
\mathbf{B}_{12}	$=$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f) O II
\mathbf{B}_{13}	$=$	$-y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f) O II

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- [1] S. Eymond, C. Martin, and A. Durif, , C. R. Acad. Sci. C **268**, 1694–1696 (1969).

Found in

- [1] S. Eymond, C. Martin, and A. Durif, *Donnees cristallographiques sur quelques composees isomorphes du monoarseniate de baryum-nickel : BaNi₂(AsO₄)₂*, Mater. Res. Bull. **4**, 595–599 (1969), doi:10.1016/0025-5408(69)90120-2.