

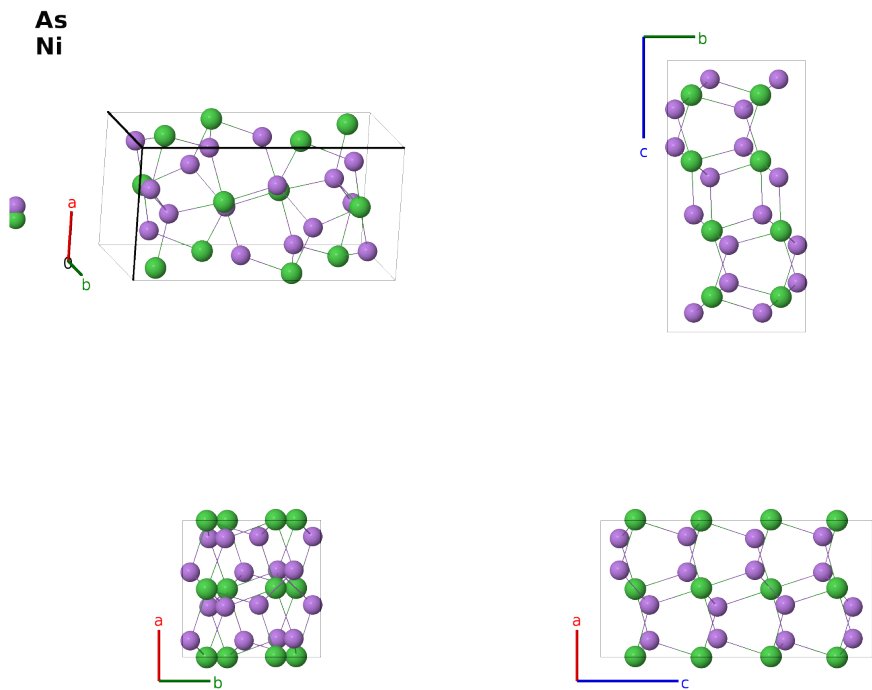
Pararammelsbergite (α -NiAs₂) Structure: A2B_oP24_61_2c_c-003

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<https://aflow.org/prototype-encyclopedia/ZBG0>

https://aflow.org/prototype-encyclopedia/A2B_oP24_61_2c_c-003

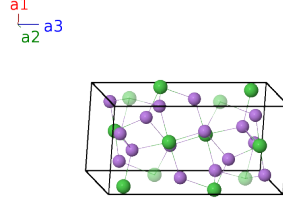


Prototype	As ₂ Ni
AFLOW prototype label	A2B_oP24_61_2c_c-003
Mineral name	pararammelsbergite
ICSD	34851
CCDC	1607130
Pearson symbol	oP24
Space group number	61
Space group symbol	<i>Pbca</i>
AFLOW prototype command	<code>aflow --proto=A2B_oP24_61_2c_c-003</code> <code>--params=a, b/a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃</code>

- This is the room temperature structure of NiAs₂. Above 871K it transforms into rammelsbergite, β -NiAs₂, which has the marcasite (*C*18) structure. (Predel, 1991; Downs, 2003).
- Pararammelsbergite (NiAs₂), β -TeO₂ and brookite (*C*21, TiO₂) have the same AFLOW prototype label, A2B_oP24_61_2c.c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_8$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{12}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{16}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	As II
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B}_{18}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ni I

$$\begin{aligned}
\mathbf{B}_{19} &= \begin{matrix} -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (z_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{Ni I} \\
\mathbf{B}_{20} &= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3 = a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (8c) & \text{Ni I} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (8c) & \text{Ni I} \\
\mathbf{B}_{22} &= (x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{Ni I} \\
\mathbf{B}_{23} &= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 = ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{Ni I} \\
\mathbf{B}_{24} &= - (x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ & \quad z_3 \mathbf{a}_3 = -a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (8c) & \text{Ni I}
\end{aligned}$$

References

- [1] M. E. Fleet, *The crystal structure of pararammelsbergite (NiAs₂)*, Am. Mineral. **57**, 1–9 (1972).
- [2] B. Predel and O. Madelung, *Landolt-Börnstein - Group IV Physical Chemistry* (Springer-Verlag, Berlin, Heidelberg, 1991), vol. 5A: “Ac-Au – Au-Zr”, chap. As-Ni (Arsenic-Nickel).

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