

GeAs₂ Structure:

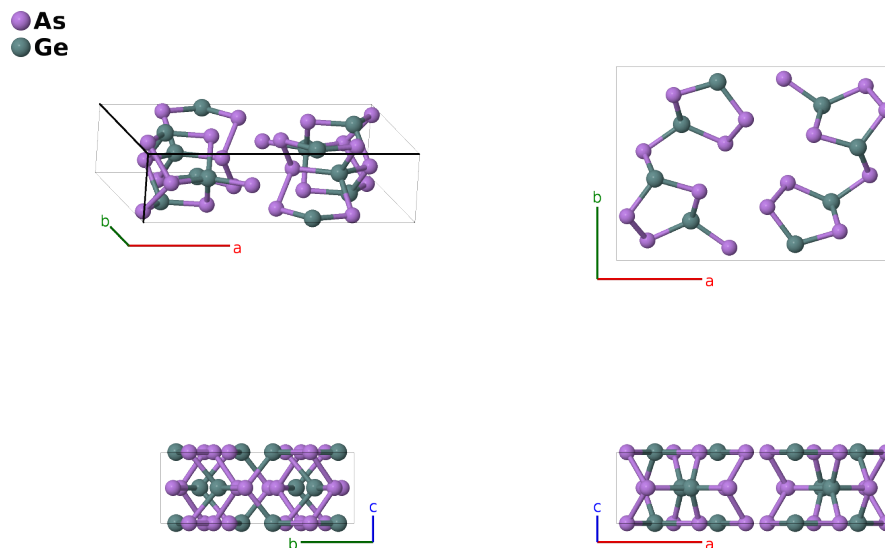
A2B_oP24_55_2g2h_gh-001

This structure originally had the label **A2B_oP24_55_2g2h_gh**. Calls to that address will be redirected here.

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<https://aflow.org/p/X52Z>

https://aflow.org/p/A2B_oP24_55_2g2h_gh-001



Prototype	As ₂ Ge
AFLOW prototype label	A2B_oP24_55_2g2h_gh-001
ICSD	23872
Pearson symbol	oP24
Space group number	55
Space group symbol	<i>Pbam</i>
AFLOW prototype command	<code>aflow --proto=A2B_oP24_55_2g2h_gh-001 --params=a, b/a, c/a, x1, y1, x2, y2, x3, y3, x4, y4, x5, y5, x6, y6</code>

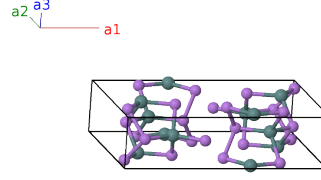
Other compounds with this structure

SiAs₂, SiP₂

- The original report of this structure (Hicks, 2019) referenced a paper that did not contain the details of the structure. We now reference the correct structure.

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	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	=	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}}$	(4g)	As I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	=	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}}$	(4g)	As I
\mathbf{B}_3	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	As I
\mathbf{B}_4	$(x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	As I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	=	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g)	As II
\mathbf{B}_6	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g)	As II
\mathbf{B}_7	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	As II
\mathbf{B}_8	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	As II
\mathbf{B}_9	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	=	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g)	Ge I
\mathbf{B}_{10}	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g)	Ge I
\mathbf{B}_{11}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Ge I
\mathbf{B}_{12}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Ge I
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As III
\mathbf{B}_{14}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As III
\mathbf{B}_{15}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As III
\mathbf{B}_{16}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As III
\mathbf{B}_{17}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As IV
\mathbf{B}_{18}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As IV
\mathbf{B}_{19}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As IV
\mathbf{B}_{20}	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	As IV
\mathbf{B}_{21}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Ge II
\mathbf{B}_{22}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Ge II
\mathbf{B}_{23}	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Ge II
\mathbf{B}_{24}	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Ge II

References

- [1] J. H. Bryden, *The crystal structures of the germanium-arsenic compounds: I. Germanium diarsenide, GeAs₂*, *Acta Cryst.* **15**, 167–171 (1962), doi:10.1107/S0365110X62000407.
- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

- [1] P. Villars, *GeAs₂ Crystal Structure* (2016). PAULING FILE in: *Inorganic Solid Phases*, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.