

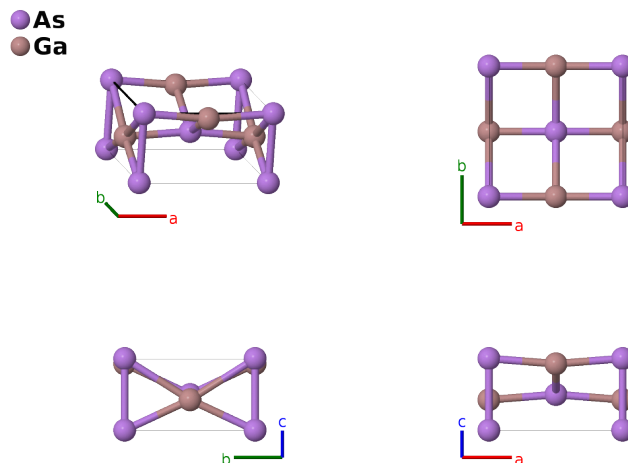
High-pressure GaAs Structure: AB_oI4_44_a_b-001

This structure originally had the label **AB_oI4_44_a_b**. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

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

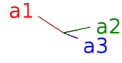
https://aflow.org/p/AB_oI4_44_a_b-001



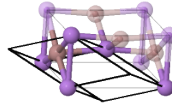
Prototype	AsGa
AFLOW prototype label	AB_oI4_44_a_b-001
ICSD	43950
Pearson symbol	oI4
Space group number	44
Space group symbol	<i>Imm</i> 2
AFLOW prototype command	<code>aflow --proto=AB_oI4_44_a_b-001 --params=a,b/a,c/a,z₁,z₂</code>

- This is a high-pressure phase of GaAs, stable above 24 GPa. The experimental data used here was taken at a pressure of 28.1 GPa. Without loss of generality we can take $z_1 = 0$. When $a = b$ and $z_2 = z_1 + 1/4$ this structure becomes the β -Sn (A5) structure.

Body-centered Orthorhombic primitive vectors



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



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	As I
\mathbf{B}_2	$(z_2 + \frac{1}{2}) \mathbf{a}_1 + z_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	Ga I

References

- [1] S. T. Weir, Y. K. Vohra, C. A. Vanderborgh, and A. L. Ruoff, *Structural phase transitions in GaAs to 108 GPa*, Phys. Rev. B **39**, 1280–1285 (1989), doi:10.1103/PhysRevB.39.1280.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.