High-pressure GaAs Structure: AB_oI4_44_a_b-001

This structure previously used the label(s) `AB_oI4_44_a_b`. Calls to these addresses will be redirected here.

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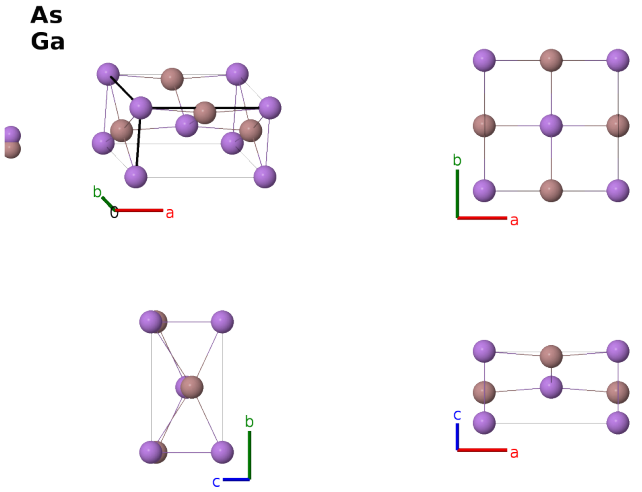
https://aflow.org/prototype-encyclopedia/JZUV

https://aflow.org/prototype-encyclopedia/AB_oI4_44_a_b-001

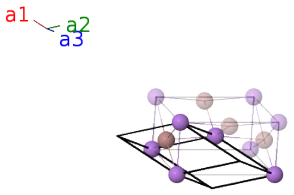


Prototype	AsGa
AFLOW prototype label	AB_oI4_44_a_b-001
ICSD	43950
CCDC	1613400
Pearson symbol	oI4
Space group number	44
Space group symbol	$Imm2$
AFLOW prototype command	`aflow --proto=AB_oI4_44_a_b-001 --params=`$a, b/a, c/a, z_1, z_2$

- 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

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



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
$\mathbf{B_2}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(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.

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