

GaSb (II) Structure: AB_tI4_119_c_a-001

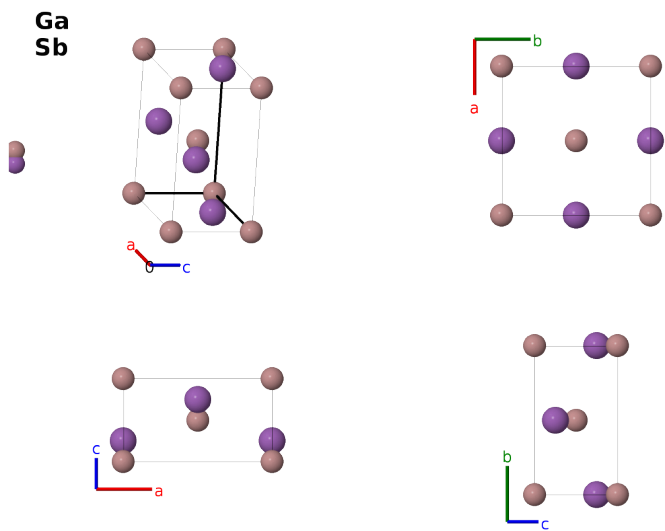
This structure previously used the label(s) **AB_tI4_119_c_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/K2V9>

https://aflow.org/prototype-encyclopedia/AB_tI4_119_c_a-001

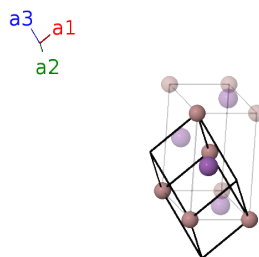


Prototype	GaSb
AFLOW prototype label	AB_tI4_119_c_a-001
Pearson symbol	tI4
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	<code>aflow --proto=AB_tI4_119_c_a-001 --params=a, c/a</code>

- This is the high-pressure phase of GaSb, stable above 60 kBar. The ground state of GaSb has the zincblende (*B3*) structure. This sample remained metastable after cooling to 90K and releasing the pressure.
- If the atomic species are identical this becomes the β -Sn (*A5*) structure.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Ga I
$\mathbf{B}_2$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c) Sb I

References

- [1] T. R. R. McDonald, R. Sard, and E. Gregory, *Retention of GaSb (II) at Low Temperatures and One Atmosphere Pressure*, J. Appl. Phys. **36**, 1498–1499 (2004), doi:10.1063/1.1714346.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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