GaSb (II) Structure: AB_tI4_119_c_a-001

This structure originally had the label `AB_tI4_119_c_a`. Calls to that address will be redirected here.

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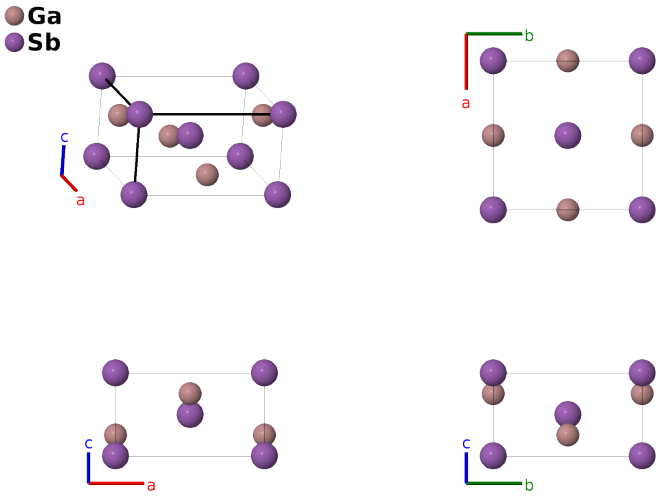
https://aflow.org/p/K2V9

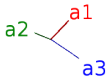
https://aflow.org/p/AB_tI4_119_c_a-001



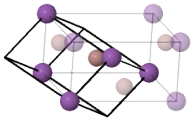
Prototype	GaSb
AFLOW prototype label	AB_tI4_119_c_a-001
ICSD	none
Pearson symbol	tI4
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	`aflow --proto=AB_tI4_119_c_a-001 --params=`$a, c/a$

- 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



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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Sb 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)	Ga 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.