

γ -Ag₃SI (Low-Temperature) Structure: A3BC_hR5_146_b_a_a-001

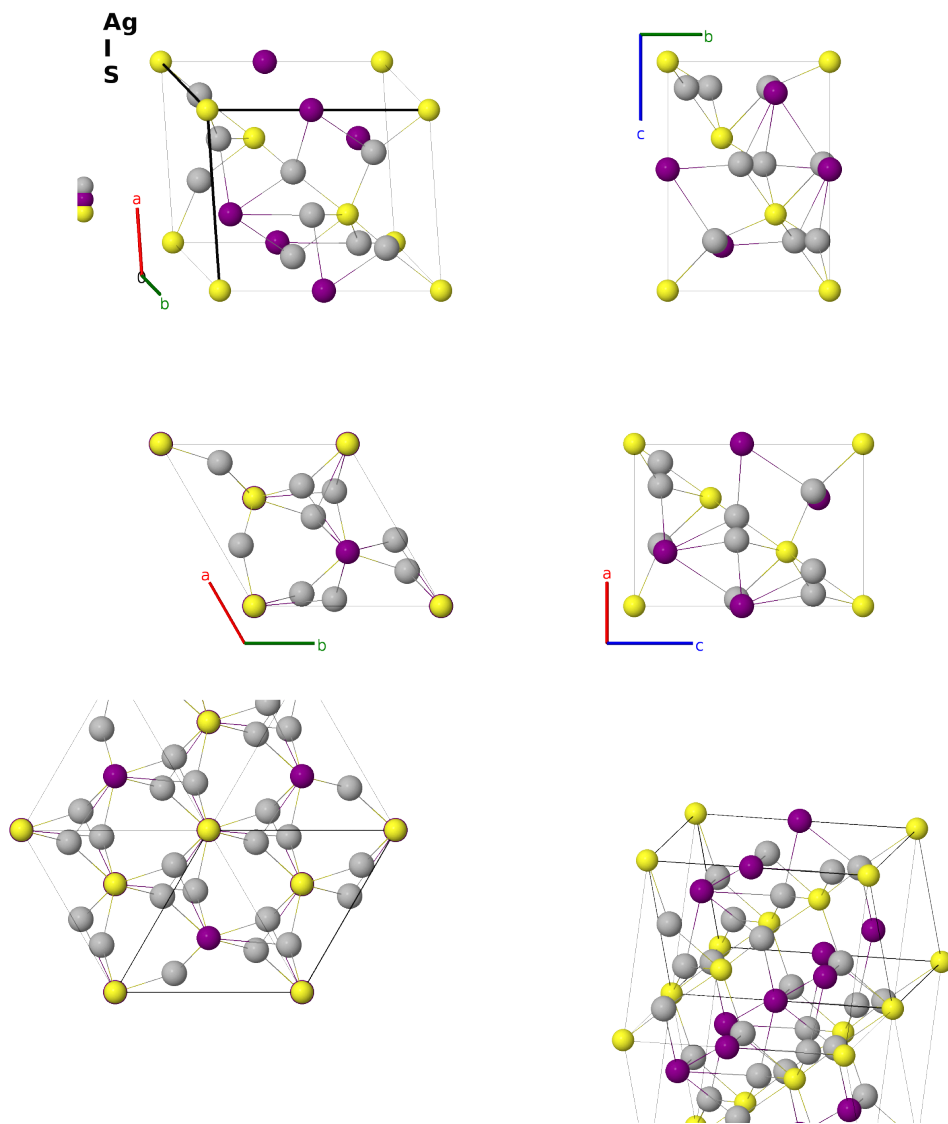
This structure previously used the label(s) **A3BC_hR5_146_b_a_a**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A3BC_hR5_146_b_a_a-001



Prototype

Ag₃IS

AFLOW prototype label

A3BC_hR5_146_b_a_a-001

ICSD

174095

CCDC	1688987
Pearson symbol	hR5
Space group number	146
Space group symbol	$R\bar{3}$
AFLOW prototype command	aflow --proto=A3BC_hR5_146_b_a_a-001 --params= $a, c/a, x_1, x_2, x_3, y_3, z_3$

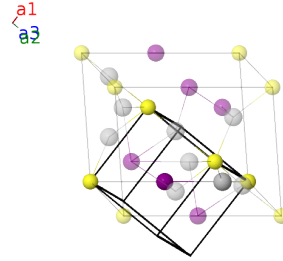
Other compounds with this structure

CsGeCl₃

- γ -Ag₃SI is the low temperature structure. Above 157K it transforms into β -Ag₃SI, a variation of the cubic perovskite ($E2_1$) structure.
- Space group $R\bar{3}$ #146 allows an arbitrary placement of the origin of the z -axis. We use this freedom to place a sulfur atom at the origin, $z_2 = 0$.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a)	I I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(3b)	Ag I
$\mathbf{B}_4$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(3b)	Ag I
$\mathbf{B}_5$	$= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(3b)	Ag I

References

- [1] S. Hoshino, T. Sakuma, and Y. Fujii, *A Structural Phase Transition in Superionic Conductor Ag₃SI*, J. Phys. Soc. Jpn. **47**, 1252–1259 (1979), doi:10.1143/JPSJ.47.1252.

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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