γ-Ag_3SI (Low-Temperature) Structure: A3BC_hR5_146_b_a_a-001

This structure originally had the label `A3BC_hR5_146_b_a_a`. Calls to that address will be redirected here.

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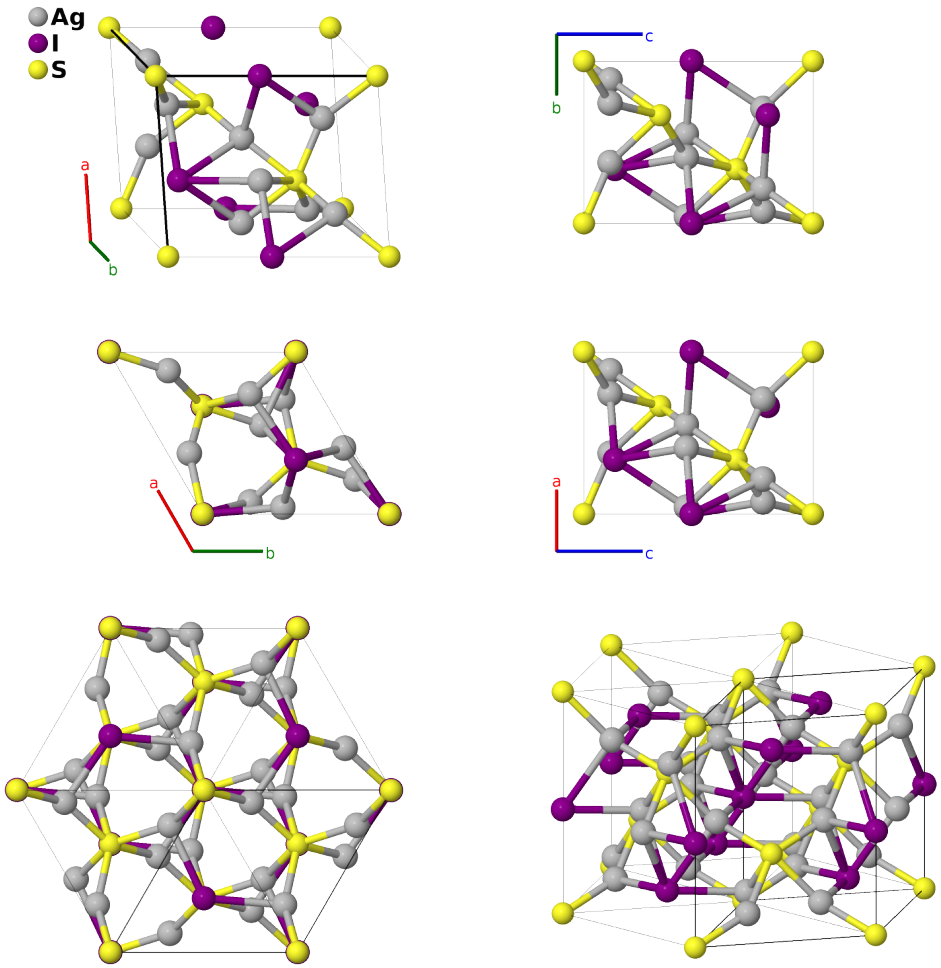
https://aflow.org/p/YGSU

https://aflow.org/p/A3BC_hR5_146_b_a_a-001



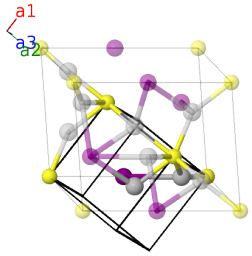
Prototype	Ag_3IS
AFLOW prototype label	A3BC_hR5_146_b_a_a-001
ICSD	174095
Pearson symbol	hR5
Space group number	146
Space group symbol	$R3$
AFLOW prototype command	`aflow --proto=A3BC_hR5_146_b_a_a-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

Other compounds with this structure
$CsGeCl_3$

- γ-Ag_3SI is the low temperature structure. Above 157K it transforms into β-Ag_3SI, a variation of the cubic perovskite ($E2_1$) structure.
- Space group $R3$ #146 allows an arbitary 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



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 Ag_3SI*, 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.