

γ -AgZn (B_b) Structure: A2B_hP9_147_g_ad-001

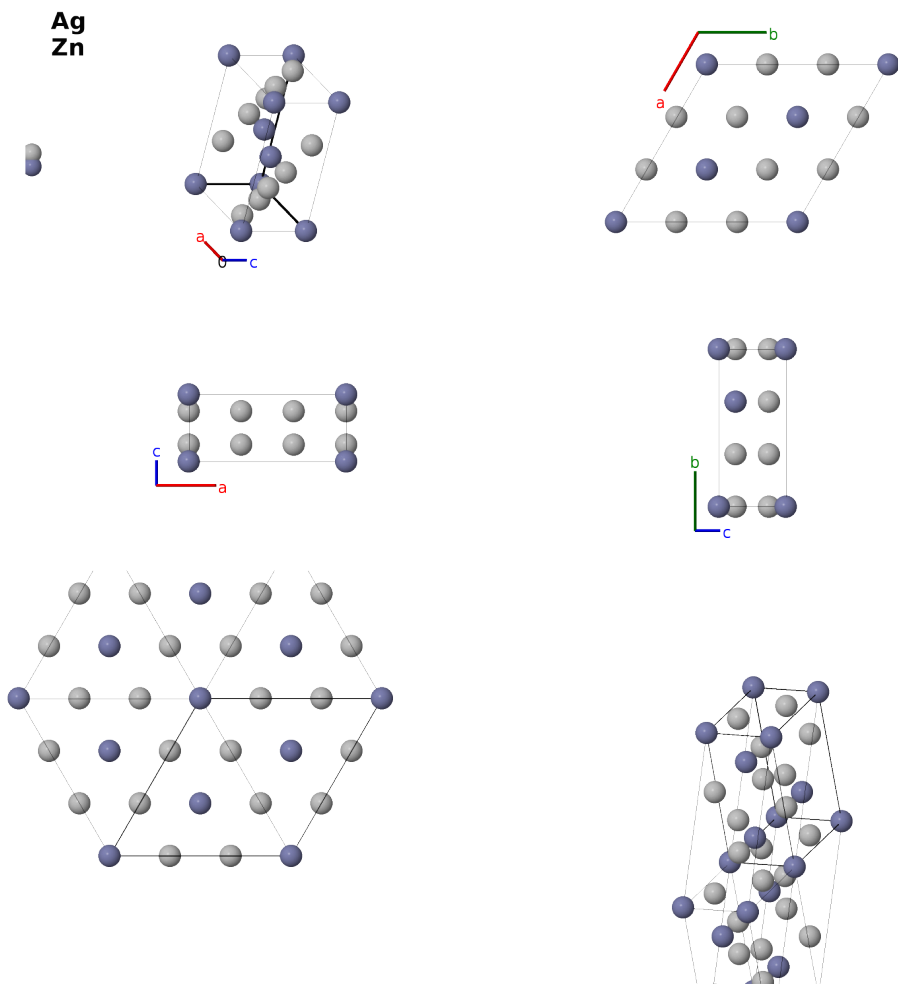
This structure previously used the label(s) **A2B_hP9_147_g_ad**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B_hP9_147_g_ad-001



Prototype	AgZn
AFLOW prototype label	A2B_hP9_147_g_ad-001
<i>Strukturbericht</i> designation	B_b
Pearson symbol	hP9
Space group number	147

Space group symbol $P\bar{3}$

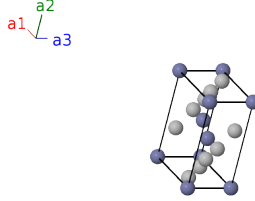
AFLOW prototype command `aflow --proto=A2B_hP9_147_g_ad-001`
`--params=a, c/a, z2, x3, y3, z3`

Other compounds with this structure

Ag₁₀CdZn₉, Ag₅₀MgZn₄₉

- When $z_2 = 0$, $x_3 = 1/3$, $y_3 = 0$, and $z_3 = 1/2$ this structure becomes the hexagonal omega ($C32$) structure.
- This is an alloy phase. The (1a) and (2d) sites are pure Zn, but the (6g) site is a mixture of Ag and Zn, so we designate it as “M.” If the system is stoichiometric then $M = (\text{Ag}_{0.75}\text{Zn}_{0.25})$. The CIF for this structure labels the M site as “Ag.”
- γ -AgZn (B_b) and PtBi₂ have the same AFLOW label, A2B_hP9_147_g_ad. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Trigonal (Hexagonal) primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	Zn I
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2d)	Zn II
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2d)	Zn II
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6g)	Ag I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6g)	Ag I
$\mathbf{B}_6$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6g)	Ag I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6g)	Ag I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6g)	Ag I
$\mathbf{B}_9$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6g)	Ag I

References

- [1] G. Bergman and R. W. Jaros, *On the Crystal Structure of the ζ Phase in the Silver-Zinc System and the Mechanism of the $\beta - \zeta$ Transformation*, Acta Cryst. **8**, 232–235 (1955), doi:10.1107/S0365110X55000765.

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