γ-AgZn (B_b) Structure: A2B_hP9_147_g_ad-001

This structure originally had the label `A2B_hP9_147_g_ad`. Calls to that address will be redirected here.

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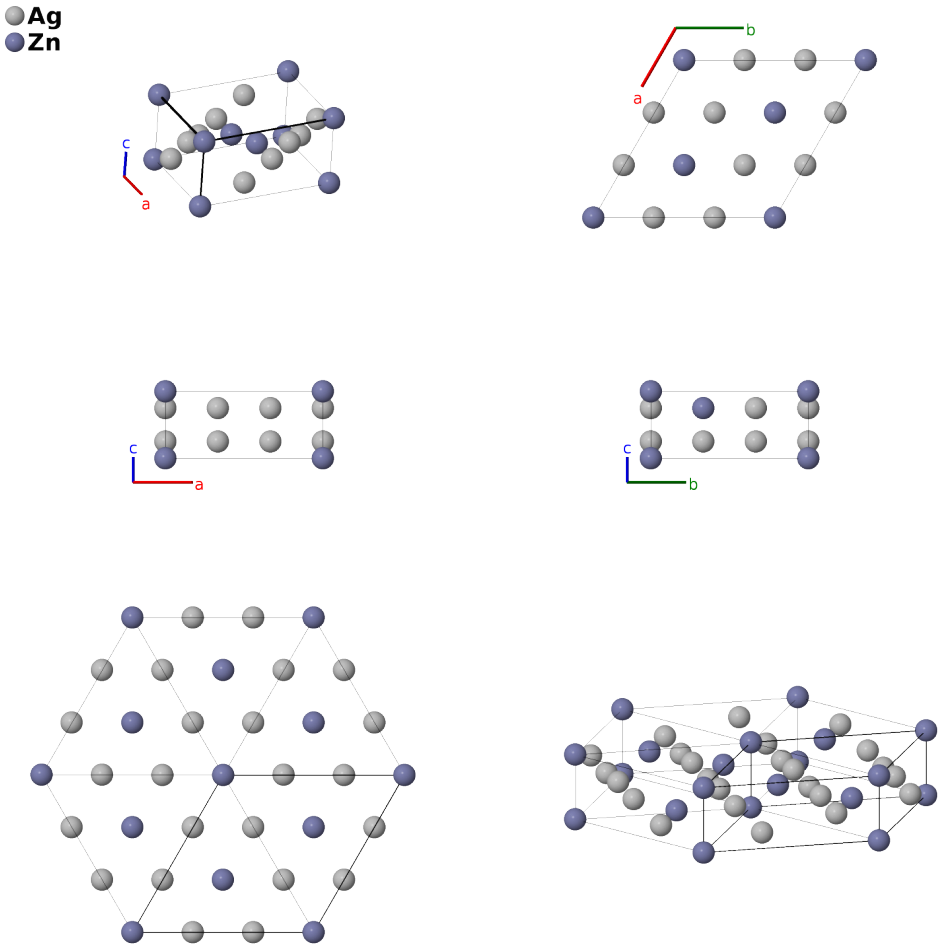
https://aflow.org/p/RQCB

https://aflow.org/p/A2B_hP9_147_g_ad-001



Prototype	AgZn
AFLOW prototype label	A2B_hP9_147_g_ad-001
***Strukturbericht* designation**	B_b
ICSD	none
Pearson symbol	hP9
Space group number	147
Space group symbol	$P\overline{3}$

AFLOW prototype command `aflow --proto=A2B_hP9_147_g_ad-001 --params=`$a, c/a, z_2, x_3, y_3, z_3$

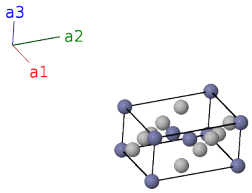
Other compounds with this structure

$Ag_{10}CdZn_9$, $Ag_{50}MgZn_{49}$

- 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 = $(Ag_{0.75}Zn_{0.25})$. The CIF for this structure labels the M site as "Ag."
- γ-AgZn (B_b) and $PtBi_2$ 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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.