α-MgAgSb Structure: ABC_tI48_120_abe_i_i-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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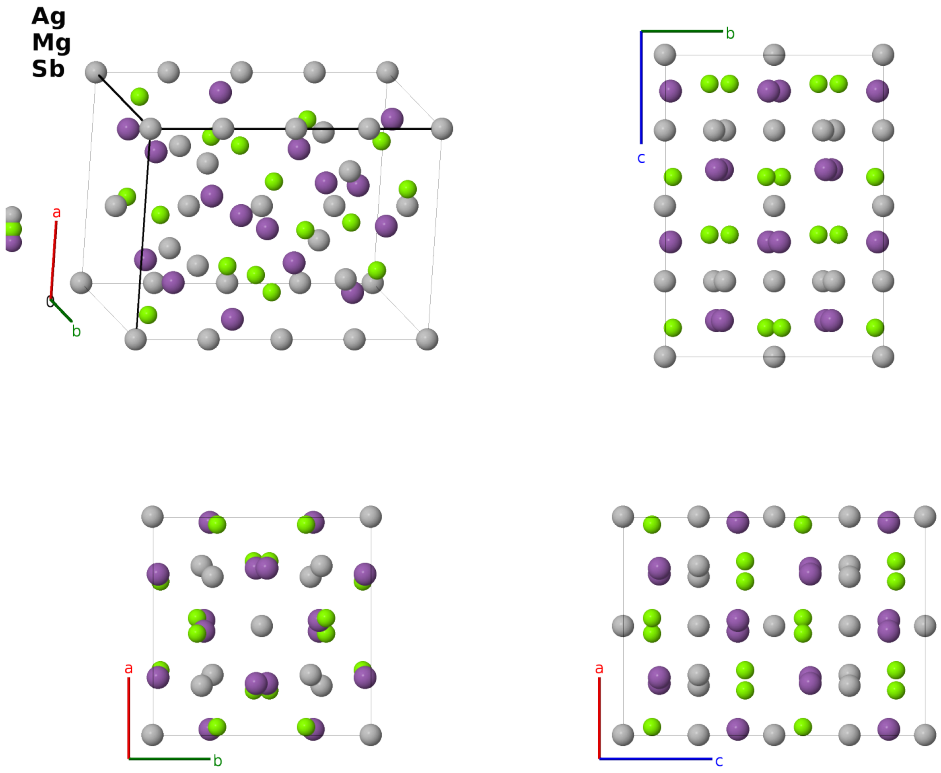
https://aflow.org/prototype-encyclopedia/ZUB8

https://aflow.org/prototype-encyclopedia/ABC_tI48_120_abe_i_i-001

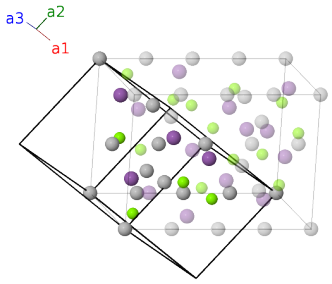


Prototype	AgMgSb
AFLOW prototype label	ABC_tI48_120_abe_i_i-001
ICSD	187151
CCDC	1696271
Pearson symbol	tI48
Space group number	120
Space group symbol	$I\bar{4}c2$
AFLOW prototype command	`aflow --proto=ABC_tI48_120_abe_i_i-001 --params=`$a, c/a, x_3, x_4, y_4, z_4, x_5, y_5, z_5$

- MgAgSb is found in three forms (Kirkham, 2012; Mi, 2017):
  - α-MgAgSb (this phase), the tetragonal ground state phase.
  - β-MgAgSb takes on the matlockite ($E0_1$ structure, which can be considered as a ternary form of Cu_2Sb ($C38$).
  - γ-MgAgSb is in the cubic half-Heusler ($C1_b$) structure.
- The range of stability of these structures is rather uncertain. The α-phase exists below 300°C, the β-phase is observed in the range 300-395°C, and γ-MgAgSb is found at all temperatures above 27°C.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Ag I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Ag I
$\mathbf{B_3}$	=	0	=	0	(4b)	Ag II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Ag II
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Ag III
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - 2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Ag III
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Ag III
$\mathbf{B_8}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Ag III
$\mathbf{B_9}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{10}}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{11}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{12}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{13}}$	=	$\left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{14}}$	=	$\left(y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{15}}$	=	$\left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Mg I

$\mathbf{B_{16}}$	=	$-\left(x_4+z_4-\frac{1}{2}\right)\mathbf{a}_1-\left(y_4+z_4-\frac{1}{2}\right)\mathbf{a}_2-(x_4+y_4)\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16i)	Mg I
$\mathbf{B_{17}}$	=	$(y_5+z_5)\mathbf{a}_1+(x_5+z_5)\mathbf{a}_2+(x_5+y_5)\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{18}}$	=	$-(y_5-z_5)\mathbf{a}_1-(x_5-z_5)\mathbf{a}_2-(x_5+y_5)\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{19}}$	=	$-(x_5+z_5)\mathbf{a}_1+(y_5-z_5)\mathbf{a}_2-(x_5-y_5)\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{20}}$	=	$(x_5-z_5)\mathbf{a}_1-(y_5+z_5)\mathbf{a}_2+(x_5-y_5)\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{21}}$	=	$\left(-y_5+z_5+\frac{1}{2}\right)\mathbf{a}_1+\left(x_5+z_5+\frac{1}{2}\right)\mathbf{a}_2+(x_5-y_5)\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{22}}$	=	$\left(y_5+z_5+\frac{1}{2}\right)\mathbf{a}_1+\left(-x_5+z_5+\frac{1}{2}\right)\mathbf{a}_2-(x_5-y_5)\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{23}}$	=	$\left(x_5-z_5+\frac{1}{2}\right)\mathbf{a}_1+\left(y_5-z_5+\frac{1}{2}\right)\mathbf{a}_2+(x_5+y_5)\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16i)	Sb I
$\mathbf{B_{24}}$	=	$-\left(x_5+z_5-\frac{1}{2}\right)\mathbf{a}_1-\left(y_5+z_5-\frac{1}{2}\right)\mathbf{a}_2-(x_5+y_5)\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16i)	Sb I

References

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First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).