Ag$_7$Ca$_2$ Structure:
A7B2_oC36_63_cgh_f-001

https://aflow.org/p/PMU3

https://aflow.org/p/A7B2_oC36_63_cgh_f-001
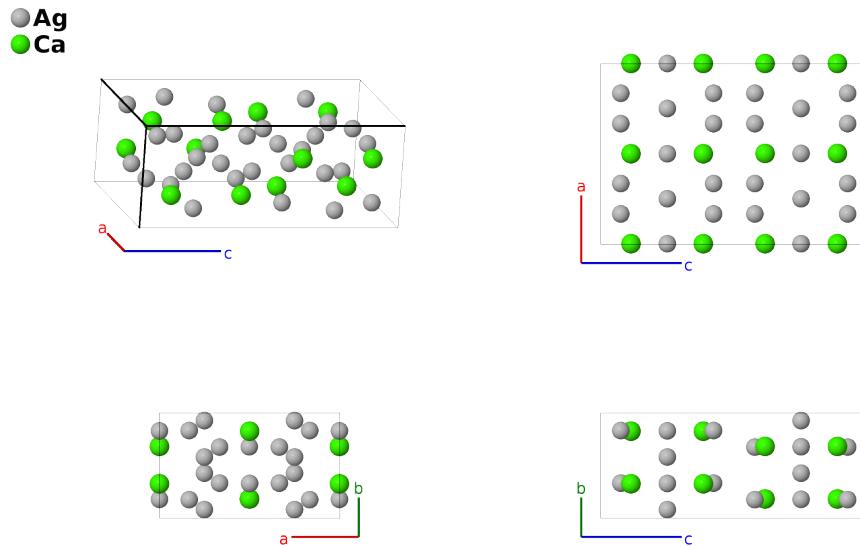
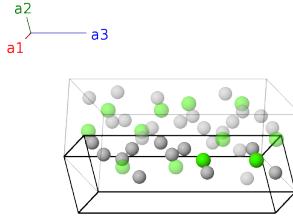|	
Prototype	Ag$_7$Ca$_2$
AFLOW prototype label	A7B2_oC36_63_cgh_f-001
ICSD	55510
Pearson symbol	oC36
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	aflow --proto=A7B2_oC36_63_cgh_f-001
	--params=$a, b/a, c/a, y_1, y_2, z_2, x_3, y_3, x_4, y_4, z_4$

Other compounds with this structure

Ag$_7$Yb$_2$

- (Pearson, 1967) and (Villars, 1991) put this in the "provisional" space group $P6_322$ #182. (Snyder, 1995).

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	$=$	$by_1\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_2}$	$=$	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	$=$	$-by_1\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_3}$	$=$	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	$=$	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8f)	Ca I
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Ca I
$\mathbf{B_5}$	$=$	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$by_2\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Ca I
$\mathbf{B_6}$	$=$	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	$=$	$-by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8f)	Ca I
$\mathbf{B_7}$	$=$	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Ag II
$\mathbf{B_8}$	$=$	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Ag II
$\mathbf{B_9}$	$=$	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Ag II
$\mathbf{B_{10}}$	$=$	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Ag II
$\mathbf{B_{11}}$	$=$	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{12}}$	$=$	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{13}}$	$=$	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{14}}$	$=$	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{15}}$	$=$	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{16}}$	$=$	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{17}}$	$=$	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(16h)	Ag III
$\mathbf{B_{18}}$	$=$	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16h)	Ag III

References

[1] G. J. Snyder and A. Simon, *Crystal structure of Ag_7Ca_2 – a new intermetallic structure type*, J. Alloys Compd. **223**, 65–69 (1995), doi:10.1016/0925-8388(94)01485-X.

[2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York,

Toronto, Sydney, Paris, Braunschweig, 1967).

[3] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.