$Ag_5Pb_2O_6$ Structure: A5B6C2_hP13_157_2ac_2c_b-001

This structure previously used the label(s) `A5B6C2_hP13_157_2ac_2c_b`. Calls to these addresses will be redirected here.

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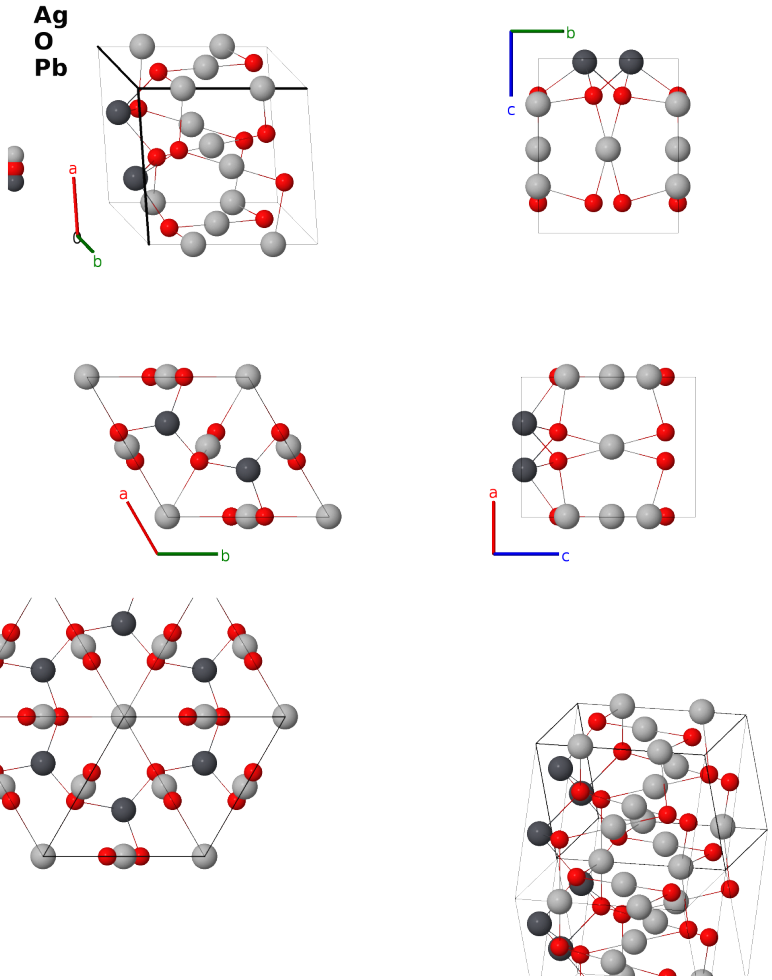
https://aflow.org/prototype-encyclopedia/1YM0

https://aflow.org/prototype-encyclopedia/A5B6C2_hP13_157_2ac_2c_b-001



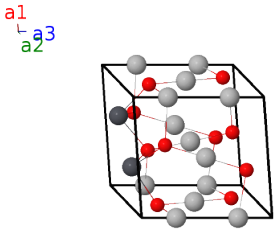
Prototype	$Ag_5O_6Pb_2$
AFLOW prototype label	A5B6C2_hP13_157_2ac_2c_b-001
ICSD	24038
CCDC	1600094
Pearson symbol	hP13

Space group number	157
Space group symbol	$P31m$
AFLOW prototype command	`aflow --proto=A5B6C2_hP13_157_2ac_2c_b-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, z_6$

- The original reference (Byström, 1950) lists this structure as $Ag_5Pb_2O_6$, while (Villars, 1985) lists it as Ag_2PbO_3. (Byström, 1950) provides three Wyckoff positions for Ag: (1a), (1a), and (3c), while (Villars, 1985) only provides two: (1a) and (3c), giving rise to the stoichiometry discrepancy. While both descriptions yield space group $P31m$ #157, we use the structure and coordinates provided by the original reference (Byström, 1950).

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Ag I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	Ag II
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	Pb I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	Pb I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(3c)	Ag III
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(3c)	Ag III
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(3c)	Ag III
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3c)	O II
$\mathbf{B_{12}}$	=	$x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3c)	O II
$\mathbf{B_{13}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(3c)	O II

References

[1] A. Byström and L. Evers, *The Crystal Structures of Ag_2PbO_2 and $Ag5Pb_2O_6$*, Acta Chem. Scand. **4**, 613–627 (1950), doi:10.3891/acta.chem.scand.04-0613.

Found in

[1] P. Villars and L. D. Calvert, eds., *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, vol. 1 (American Society of Metals, Materials Park, Ohio, 1985).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043