Ag_2O_3 Structure: A2B3_oF40_43_b_ab-001

This structure originally had the label `A2B3_oF40_43_b_ab`. Calls to that address will be redirected here.

Cite this page as: 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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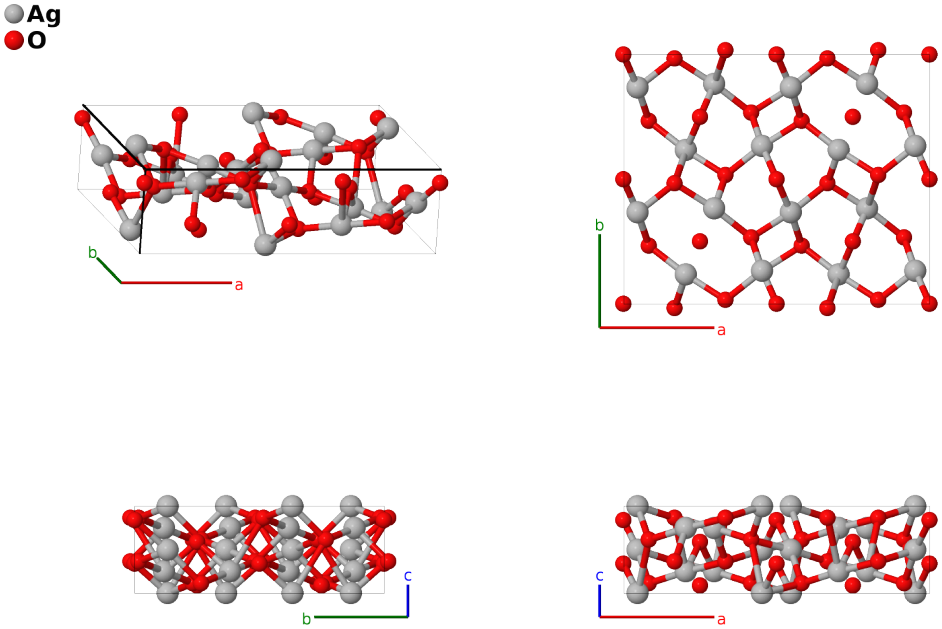
https://aflow.org/p/X02L

https://aflow.org/p/A2B3_oF40_43_b_ab-001

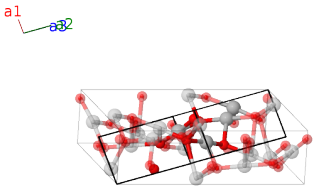


Prototype	Ag_2O_3
AFLOW prototype label	A2B3_oF40_43_b_ab-001
ICSD	59193
Pearson symbol	oF40
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=A2B3_oF40_43_b_ab-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- This structure is a distortion of the $D5_5$ Ag_2O_3 structure (A2B3_cP10_224_b_d), although (Standke, 1986) does not seem to be aware of the earlier work. This is most likely closer to the correct structure for Ag_2O_3 than the $D5_5$ structure is.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 - \left(z_1-\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_3}$	=	$(-x_2+y_2+z_2)\,\mathbf{a}_1 + (x_2-y_2+z_2)\,\mathbf{a}_2 + (x_2+y_2-z_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Ag I
$\mathbf{B_4}$	=	$(x_2-y_2+z_2)\,\mathbf{a}_1 + (-x_2+y_2+z_2)\,\mathbf{a}_2 - (x_2+y_2+z_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Ag I
$\mathbf{B_5}$	=	$-\left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_2-y_2-z_2+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_2-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Ag I
$\mathbf{B_6}$	=	$\left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_2-y_2+z_2-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_2+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Ag I
$\mathbf{B_7}$	=	$(-x_3+y_3+z_3)\,\mathbf{a}_1 + (x_3-y_3+z_3)\,\mathbf{a}_2 + (x_3+y_3-z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_8}$	=	$(x_3-y_3+z_3)\,\mathbf{a}_1 + (-x_3+y_3+z_3)\,\mathbf{a}_2 - (x_3+y_3+z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_9}$	=	$-\left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_3-y_3-z_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_{10}}$	=	$\left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_3-y_3+z_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	O II

References

[1] B. Standke and M. Jansen, *Darstellung und Kristallstruktur von Ag_2O_3*, Z. Anorganische und Allgemeine Chemie **535**, 39–46 (1986), doi:10.1002/zaac.1986535040.