Al_2PbO_4 Structure: A2B4C_oC28_40_c_abc_b-001

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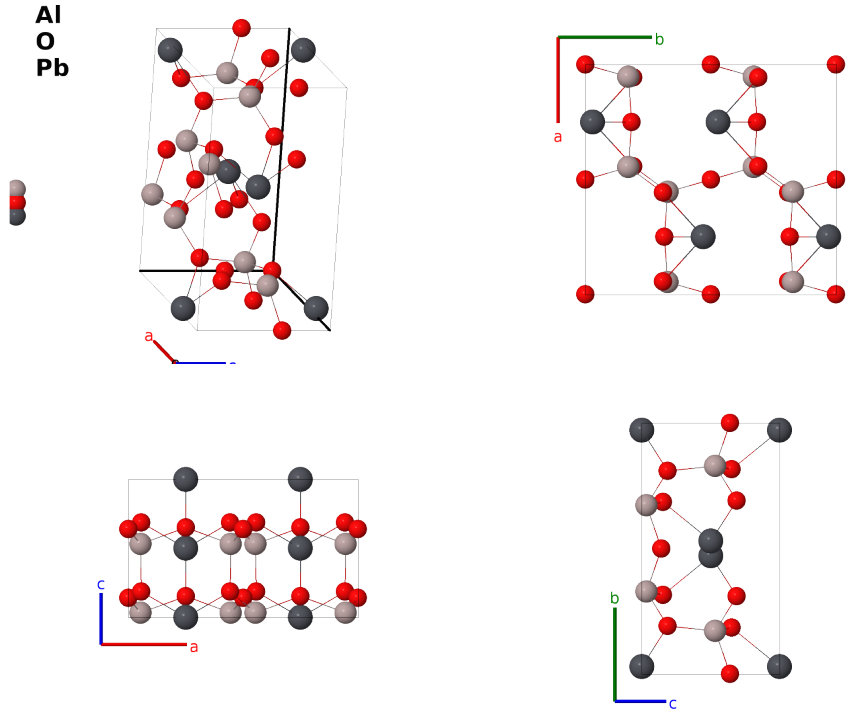
https://aflow.org/prototype-encyclopedia/N67X

https://aflow.org/prototype-encyclopedia/A2B4C_oC28_40_c_abc_b-001



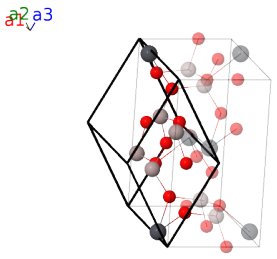
Prototype	Al_2O_4Pb
AFLOW prototype label	A2B4C_oC28_40_c_abc_b-001
ICSD	80128
CCDC	1640354
Pearson symbol	oC28
Space group number	40
Space group symbol	$Ama2$
AFLOW prototype command	`aflow --proto=A2B4C_oC28_40_c_abc_b-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Other compounds with this structure
Ga_2PbO_4

- (Plötz, 1982) originally placed this structure in the triclinic space group $P1$ #1. (Marsh, 1995) determined that their data fit in space group $Ama2$ #40, and we present their analysis here.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + (y_2 - z_2)\,\mathbf{a}_2 + (y_2 + z_2)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 - (y_2 + z_2)\,\mathbf{a}_2 - (y_2 - z_2)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Pb I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Pb I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B_9}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B_{10}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{13}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{14}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III

References

[1] R. E. Marsh and I. Bernal, *More Space-Group Changes*, Acta Crystallogr. Sect. B **51**, 300–307 (1995), doi:10.1107/S0108768194011857.

[2] K.-B. Plötz and H. Müller-Buschbaum, *Zur Kristallchemie der Oxoplumbate(II). III. Synthese und Aufbau von $PbAl_2O_4$ und $PbGa_2O_4$*, Z. Anorganische und Allgemeine Chemie **488**, 38–44 (1982), doi:10.1002/zaac.19824880104.

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