Minium-T (Pb_3O_4) Structure: A4B3_tP28_135_gh_dh-002

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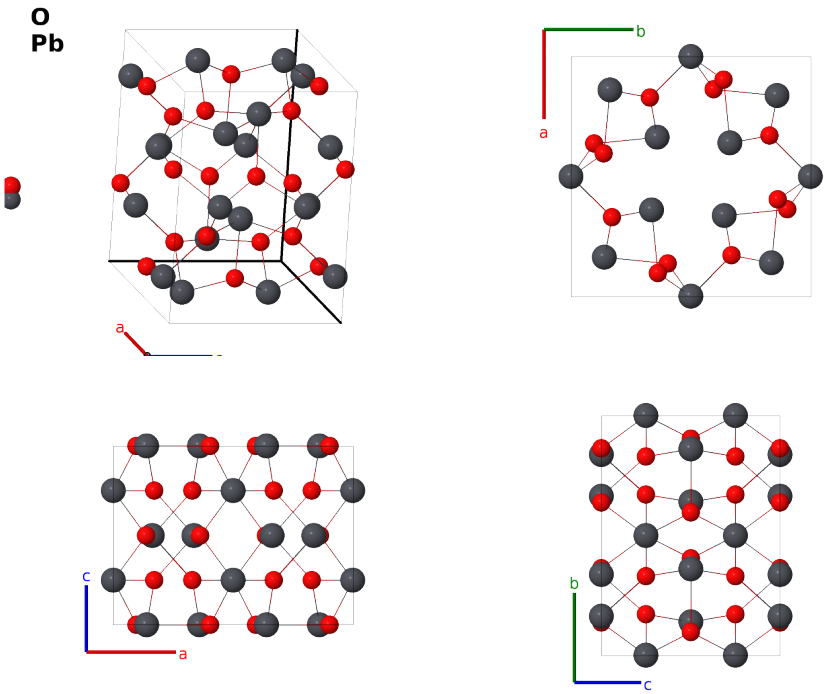
https://aflow.org/prototype-encyclopedia/68YC

https://aflow.org/prototype-encyclopedia/A4B3_tP28_135_gh_dh-002



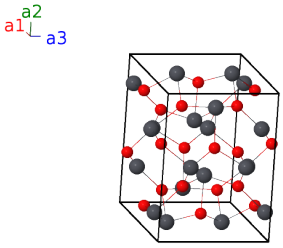
Prototype	O_4Pb_3
AFLOW prototype label	A4B3_tP28_135_gh_dh-002
Mineral name	minium
ICSD	4106
CCDC	1592812
Pearson symbol	tP28
Space group number	135
Space group symbol	$P4_2/mbc$
AFLOW prototype command	`aflow --proto=A4B3_tP28_135_gh_dh-002 --params=`$a, c/a, x_2, x_3, y_3, x_4, y_4$

- Pb_3O_4 has been observed in several structures (Wriedt, 1988; Dinnebier, 2003):

  - Below 170K (Wriedt, 1988) it is in the orthorhombic Minium-R structure. (Gavarri, 1978) tracks this structure up to 240K.
  - Above 170K it is in the tetragonal Minium-T structure (this structure).
  - At ambient temperature the Minium-T structure transforms into what is apparently the Minium-R structure at a pressure between 0.11 and 0.3 GPa. (Dinnebier, 2003) call this *Phase II*.
  - If the pressure is increased, between 5.54 and 6.6 GPa the structure transforms into orthorhombic Phase III structure.
- The first determination of this structure was made by (Gross, 1943), who assigned it to space group $P\bar{4}b2$ #117 (ICSD 29094, AFLOW label A4B3_tP28_135_gh_dh-001), but that structure is practically indistinguishable from the current structure.
- We assign tenary compounds related to this structure to prototype $ZnSb_2O_4$.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Pb I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Pb I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Pb I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{11}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{15}}$	=	$-y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{16}}$	=	$y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{17}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{18}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	O II

$\mathbf{B_{19}}$	=	$\left(y_3+\frac{1}{2}\right)\mathbf{a}_1+\left(x_3+\frac{1}{2}\right)\mathbf{a}_2+\frac{1}{2}\mathbf{a}_3$	=	$a\left(y_3+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{y}}+\frac{1}{2}c\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{20}}$	=	$-\left(y_3-\frac{1}{2}\right)\mathbf{a}_1-\left(x_3-\frac{1}{2}\right)\mathbf{a}_2+\frac{1}{2}\mathbf{a}_3$	=	$-a\left(y_3-\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{y}}+\frac{1}{2}c\hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B_{21}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}$	(8h)	Pb II
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}$	(8h)	Pb II
$\mathbf{B_{23}}$	=	$-y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\frac{1}{2}\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+\frac{1}{2}c\hat{\mathbf{z}}$	(8h)	Pb II
$\mathbf{B_{24}}$	=	$y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\frac{1}{2}\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+\frac{1}{2}c\hat{\mathbf{z}}$	(8h)	Pb II
$\mathbf{B_{25}}$	=	$-\left(x_4-\frac{1}{2}\right)\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\mathbf{a}_2$	=	$-a\left(x_4-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}}$	(8h)	Pb II
$\mathbf{B_{26}}$	=	$\left(x_4+\frac{1}{2}\right)\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\mathbf{a}_2$	=	$a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\hat{\mathbf{y}}$	(8h)	Pb II
$\mathbf{B_{27}}$	=	$\left(y_4+\frac{1}{2}\right)\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\mathbf{a}_2+\frac{1}{2}\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{y}}+\frac{1}{2}c\hat{\mathbf{z}}$	(8h)	Pb II
$\mathbf{B_{28}}$	=	$-\left(y_4-\frac{1}{2}\right)\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\mathbf{a}_2+\frac{1}{2}\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\hat{\mathbf{y}}+\frac{1}{2}c\hat{\mathbf{z}}$	(8h)	Pb II

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