

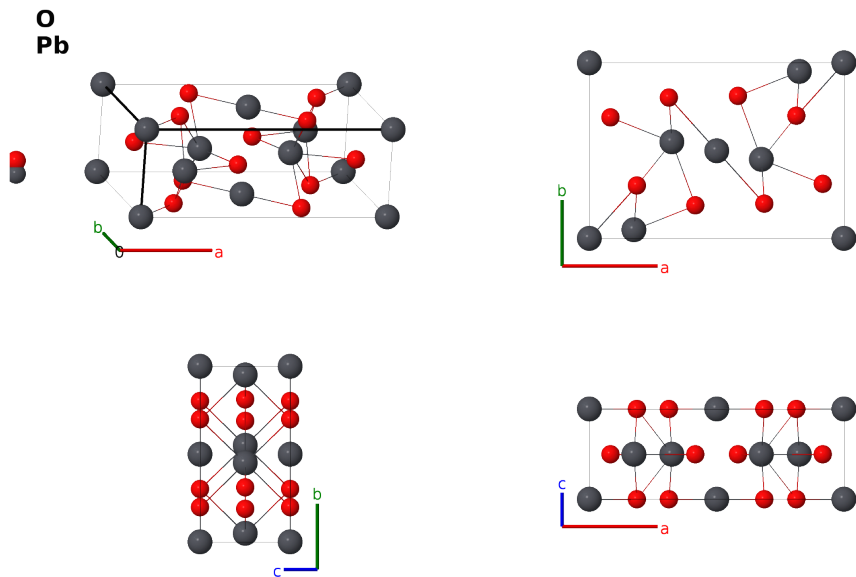
Possible Phase III Pb_3O_4 Structure: A4B3_oP14_55_gh_ah-001

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<https://aflow.org/prototype-encyclopedia/FVBJ>

https://aflow.org/prototype-encyclopedia/A4B3_oP14_55_gh_ah-001



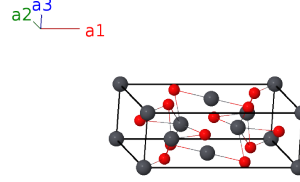
Prototype	O_4Pb_3
AFLOW prototype label	A4B3_oP14_55_gh_ah-001
ICSD	97282
CCDC	1656611
Pearson symbol	oP14
Space group number	55
Space group symbol	$Pbam$
AFLOW prototype command	<code>aflow --proto=A4B3_oP14_55_gh_ah-001</code> <code>--params=a, b/a, c/a, x2, y2, x3, y3, x4, y4</code>

- 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.

- 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 (this structure).
- We use the data taken at 13.3GPa and 295K. (Dinnebier, 2003) give the coordinates of the Pb I atom as (1/2 1/2 0). This is a (4e) Wyckoff position and makes the stoichiometry of the structure Pb_4O_4 . The ICSD entry corrects this to (0 1/2 0), the (2c) site. We use this, however AFLOW shifts the origin, moving the (2c) atoms to the (2a) site. Unfortunately, the resulting configuration of the lead atoms does not match that shown in Figure 5(c) of the paper. We have no resolution of this, so we have marked the structure as possible.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Pb I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2a)	Pb I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_5$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_6$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_7$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_8$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_9$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{10}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{11}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb II
$\mathbf{B}_{12}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb II
$\mathbf{B}_{13}$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb II
$\mathbf{B}_{14}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb II

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