

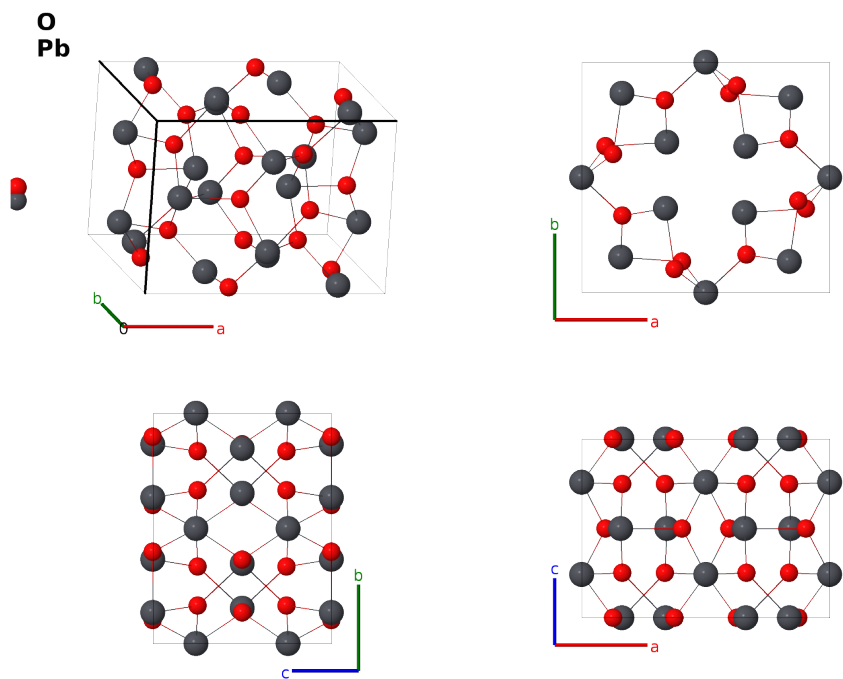
Minium-R (Pb_3O_4) Structure: A4B3_oP28_55_ghi_egh-001

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

https://aflow.org/prototype-encyclopedia/A4B3_oP28_55_ghi_egh-001



Prototype	O_4Pb_3
AFLOW prototype label	A4B3_oP28_55_ghi_egh-001
ICSD	4107
CCDC	1592813
Pearson symbol	oP28
Space group number	55
Space group symbol	$Pbam$
AFLOW prototype command	<code>aflow --proto=A4B3_oP28_55_ghi_egh-001</code> <code>--params=a, b/a, c/a, z1, x2, y2, x3, y3, x4, y4, x5, y5, x6, y6, z6</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 (this 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.

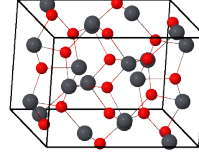
Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$

$\mathbf{a}_3$
 $\mathbf{a}_2$
 $\mathbf{a}_1$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_3$	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}}$	(4g)	Pb II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}}$	(4g)	Pb II
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Pb II
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Pb II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb III
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb III
$\mathbf{B}_{19}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb III
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pb III
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8i)	O III
$\mathbf{B}_{22}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8i)	O III

$$\begin{aligned}
\mathbf{B}_{23} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 = -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8i) & \text{O III} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 = a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8i) & \text{O III} \\
\mathbf{B}_{25} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8i) & \text{O III} \\
\mathbf{B}_{26} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8i) & \text{O III} \\
\mathbf{B}_{27} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 = a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8i) & \text{O III} \\
\mathbf{B}_{28} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 = -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8i) & \text{O III}
\end{aligned}$$

References

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Found in

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