

Pb(NO₃)₂ (*G*2₁) Structure: A2B6C_cP36_205_c_d_a-001

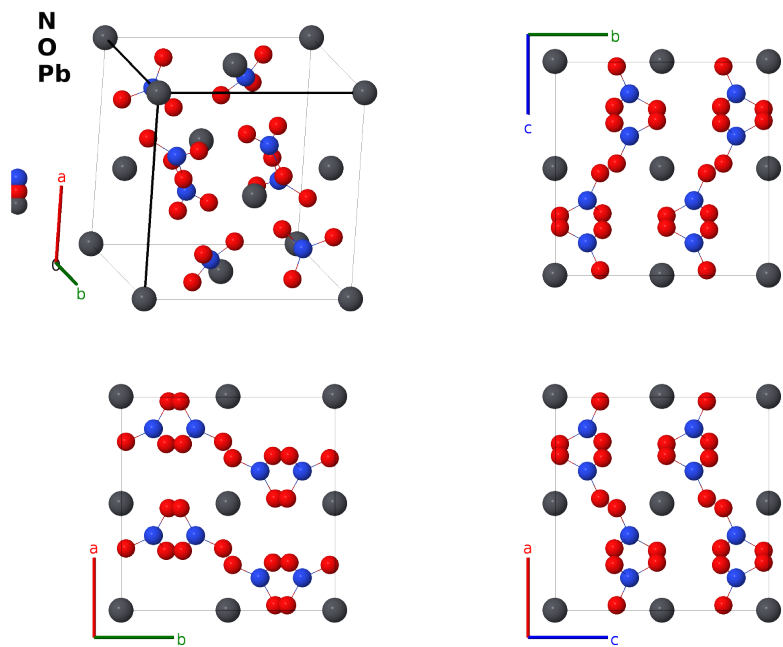
This structure previously used the label(s) **A2B6C_cP36_205_c_d.a**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B6C_cP36_205_c_d_a-001



Prototype	N ₂ O ₆ Pb
AFLOW prototype label	A2B6C_cP36_205_c_d_a-001
<i>Strukturbericht</i> designation	<i>G</i> 2 ₁
ICSD	62698
CCDC	1625908
Pearson symbol	cP36
Space group number	205
Space group symbol	<i>P</i> $\bar{a}$ 3
AFLOW prototype command	<code>aflow --proto=A2B6C_cP36_205_c_d_a-001</code> <code>--params=<i>a</i>, <i>x</i>₂, <i>x</i>₃, <i>y</i>₃, <i>z</i>₃</code>

Other compounds with this structure

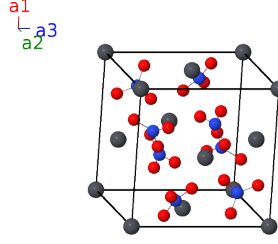
Ba(NO₃)₂, Sr(NO₃)₂

Simple Cubic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Pb I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	Pb I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	Pb I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	Pb I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	N I
$\mathbf{B}_6$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	N I
$\mathbf{B}_7$	$=$	$-x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	N I
$\mathbf{B}_8$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	N I
$\mathbf{B}_9$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	N I
$\mathbf{B}_{10}$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	N I
$\mathbf{B}_{11}$	$=$	$x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	N I
$\mathbf{B}_{12}$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	N I
$\mathbf{B}_{13}$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	O I
$\mathbf{B}_{14}$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	O I
$\mathbf{B}_{15}$	$=$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	O I
$\mathbf{B}_{16}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	O I
$\mathbf{B}_{17}$	$=$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	O I
$\mathbf{B}_{18}$	$=$	$(z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	O I
$\mathbf{B}_{19}$	$=$	$-(z_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	O I
$\mathbf{B}_{20}$	$=$	$-z_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	O I
$\mathbf{B}_{21}$	$=$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	O I

$$\begin{aligned}
\mathbf{B}_{22} &= \begin{matrix} -y_3 \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_3 \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{23} &= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 - x_3 \mathbf{a}_3 = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{24} &= \begin{matrix} -(y_3 - \frac{1}{2}) \mathbf{a}_1 - z_3 \mathbf{a}_2 + \\ (x_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{25} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{26} &= (x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{27} &= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 = ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{28} &= \begin{matrix} -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ z_3 \mathbf{a}_3 \end{matrix} = -a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{29} &= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3 = -az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{30} &= \begin{matrix} -(z_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \\ y_3 \mathbf{a}_3 \end{matrix} = -a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{31} &= (z_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3 = a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{32} &= z_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3 = az_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{33} &= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{34} &= y_3 \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{35} &= \begin{matrix} -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ x_3 \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{36} &= (y_3 + \frac{1}{2}) \mathbf{a}_1 + z_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3 = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I}
\end{aligned}$$

References

- [1] H. Nowotny and G. Heger, *Structure Refinement of Lead Nitrate*, Acta Crystallogr. Sect. C **42**, 133–135 (1986), doi:10.1107/S0108270186097032.

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