β-Na_2PtO_3 Structure: A2B3C_oF96_70_2e_fh_e-001

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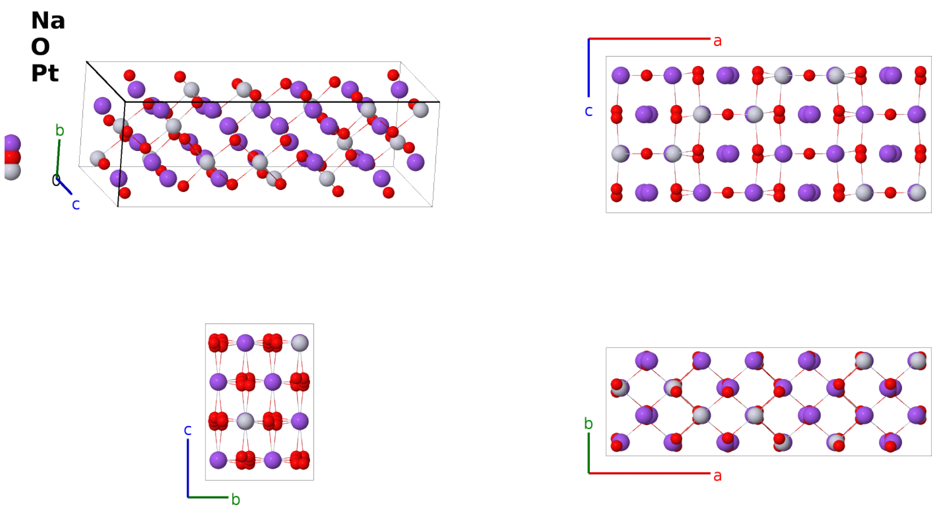
https://aflow.org/prototype-encyclopedia/7WUP

https://aflow.org/prototype-encyclopedia/A2B3C_oF96_70_2e_fh_e-001



Prototype	Na_2O_3Pt
AFLOW prototype label	A2B3C_oF96_70_2e_fh_e-001
ICSD	25020
CCDC	1601011
Pearson symbol	oF96
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=A2B3C_oF96_70_2e_fh_e-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, y_4, x_5, y_5, z_5$

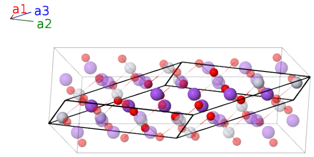
Other compounds with this structure

β-Li_2IrO_3, β-Na_2PrO_3

- Na_2PtO_3 can also be found in the α-Na_2PtO_3 phase, which has the Na_2PrO_3 structure.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$ =	$-\left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + \frac{1}{8}b\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16e)	Na I
$\mathbf{B_2}$ =	$x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + \frac{1}{8}b\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16e)	Na I
$\mathbf{B_3}$ =	$\left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + \frac{3}{8}b\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16e)	Na I
$\mathbf{B_4}$ =	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{3}{8}b\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16e)	Na I
$\mathbf{B_5}$ =	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + \frac{1}{8}b\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16e)	Na II
$\mathbf{B_6}$ =	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + \frac{1}{8}b\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16e)	Na II
$\mathbf{B_7}$ =	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + \frac{3}{8}b\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16e)	Na II
$\mathbf{B_8}$ =	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{3}{8}b\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16e)	Na II
$\mathbf{B_9}$ =	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + \frac{1}{8}b\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16e)	Pt I
$\mathbf{B_{10}}$ =	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + \frac{1}{8}b\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16e)	Pt I
$\mathbf{B_{11}}$ =	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{3}{8}b\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16e)	Pt I
$\mathbf{B_{12}}$ =	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{3}{8}b\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16e)	Pt I
$\mathbf{B_{13}}$ =	$y_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16f)	O I
$\mathbf{B_{14}}$ =	$-\left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16f)	O I
$\mathbf{B_{15}}$ =	$-y_4\,\mathbf{a}_1 + \left(y_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16f)	O I
$\mathbf{B_{16}}$ =	$\left(y_4 + \frac{3}{4}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(y_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} + b\left(y_4 + \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16f)	O I
$\mathbf{B_{17}}$ =	$\left(-x_5 + y_5 + z_5\right)\,\mathbf{a}_1 + \left(x_5 - y_5 + z_5\right)\,\mathbf{a}_2 + \left(x_5 + y_5 - z_5\right)\,\mathbf{a}_3$	=	$ax_5\,\mathbf{\hat{x}} + by_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(32h)	O II
$\mathbf{B_{18}}$ =	$\left(x_5 - y_5 + z_5\right)\,\mathbf{a}_1 + \left(-x_5 + y_5 + z_5\right)\,\mathbf{a}_2 - \left(x_5 + y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\mathbf{\hat{x}} - b\left(y_5 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(32h)	O II
$\mathbf{B_{19}}$ =	$\left(x_5 + y_5 - z_5\right)\,\mathbf{a}_1 - \left(x_5 + y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_5 + y_5 + z_5\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + by_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32h)	O II
$\mathbf{B_{20}}$ =	$-\left(x_5 + y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 + y_5 - z_5\right)\,\mathbf{a}_2 + \left(x_5 - y_5 + z_5\right)\,\mathbf{a}_3$	=	$ax_5\,\mathbf{\hat{x}} - b\left(y_5 - \frac{1}{4}\right)\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(32h)	O II

$\mathbf{B_{21}}$	$=$	$(x_5 - y_5 - z_5)\,\mathbf{a}_1 - (x_5 - y_5 + z_5)\,\mathbf{a}_2 - (x_5 + y_5 - z_5)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{22}}$	$=$	$-(x_5 - y_5 + z_5)\,\mathbf{a}_1 + (x_5 - y_5 - z_5)\,\mathbf{a}_2 + \left(x_5 + y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{23}}$	$=$	$-(x_5 + y_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_5 - y_5 - z_5)\,\mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{24}}$	$=$	$\left(x_5 + y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_5 + y_5 - z_5)\,\mathbf{a}_2 - (x_5 - y_5 + z_5)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	O II

References

[1] W. Urland and R. Hoppe, *Zur Kenntnis der Oxoplatinate Na_2PtO_2, Na_2PtO_3, "K_2PtO_3" und "Rb_2PtO_3"*, Z. Anorganische und Allgemeine Chemie **392**, 23–36 (1972), doi:10.1002/zaac.19723920104.

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