β-Na_2PtO_3 Structure: A2B3C_oF96_70_2e_fh_e-001

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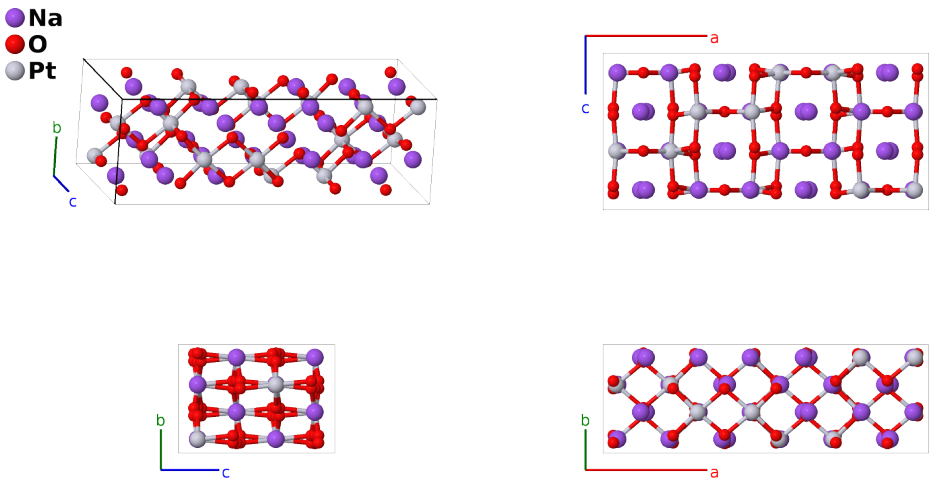
https://aflow.org/p/7WUP

https://aflow.org/p/A2B3C_oF96_70_2e_fh_e-001



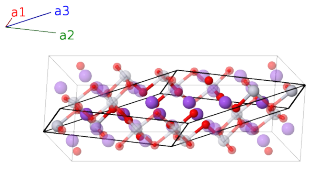
Prototype	Na_2O_3Pt
AFLOW prototype label	A2B3C_oF96_70_2e_fh_e-001
ICSD	25020
Pearson symbol	oF96
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=A2B3C_oF96_70_2e_fh_e-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, y_4, x_5, y_5, z_5$

Other compounds with this structure
β-Li_2IrO_3

- Na_2PtO_3 can also be found in the α-Na_2PtO_3 phase, which has the Li_2SnO_3 structure.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-\left(x_1-\frac{1}{4}\right)\,\mathbf{a}_1+x_1\,\mathbf{a}_2+x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1-\left(x_1-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_1-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_3}$	=	$\left(x_1+\frac{3}{4}\right)\,\mathbf{a}_1-x_1\,\mathbf{a}_2-x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1+\left(x_1+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_1+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1+\frac{3}{4}\right)\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_5}$	=	$-\left(x_2-\frac{1}{4}\right)\,\mathbf{a}_1+x_2\,\mathbf{a}_2+x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Na II
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1-\left(x_2-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_2-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Na II
$\mathbf{B_7}$	=	$\left(x_2+\frac{3}{4}\right)\,\mathbf{a}_1-x_2\,\mathbf{a}_2-x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Na II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1+\left(x_2+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_2+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{3}{4}\right)\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Na II
$\mathbf{B_9}$	=	$-\left(x_3-\frac{1}{4}\right)\,\mathbf{a}_1+x_3\,\mathbf{a}_2+x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1-\left(x_3-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_3-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B_{11}}$	=	$\left(x_3+\frac{3}{4}\right)\,\mathbf{a}_1-x_3\,\mathbf{a}_2-x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1+\left(x_3+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_3+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{3}{4}\right)\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a}_1-\left(y_4-\frac{1}{4}\right)\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_{14}}$	=	$-\left(y_4-\frac{1}{4}\right)\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(y_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}}-b\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_{15}}$	=	$-y_4\,\mathbf{a}_1+\left(y_4+\frac{3}{4}\right)\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_{16}}$	=	$\left(y_4+\frac{3}{4}\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(y_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}+b\left(y_4+\frac{3}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_{17}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1+(x_5-y_5+z_5)\,\mathbf{a}_2+(x_5+y_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{18}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1+(-x_5+y_5+z_5)\,\mathbf{a}_2-\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}-b\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{19}}$	=	$(x_5+y_5-z_5)\,\mathbf{a}_1-\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+(-x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{20}}$	=	$-\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+(x_5+y_5-z_5)\,\mathbf{a}_2+(x_5-y_5+z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-b\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	O II
$\mathbf{B_{21}}$	=	$(x_5-y_5-z_5)\,\mathbf{a}_1-(x_5-y_5+z_5)\,\mathbf{a}_2-(x_5+y_5-z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(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.