

NaPt₃O₄ Structure:

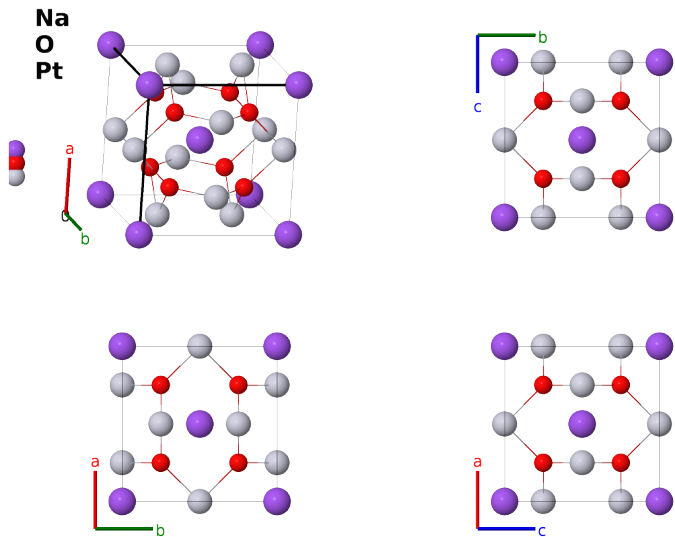
AB4C3_cP16_223_a_e_c-001

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<https://aflow.org/prototype-encyclopedia/R1MG>

https://aflow.org/prototype-encyclopedia/AB4C3_cP16_223_a_e_c-001



Prototype	NaO ₄ Pt ₃
AFLOW prototype label	AB4C3_cP16_223_a_e_c-001
ICSD	27052
CCDC	1602399
Pearson symbol	cP16
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<pre>aflow --proto=AB4C3_cP16_223_a_e_c-001 --params=a</pre>

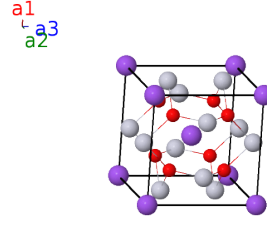
Other compounds with this structure

(Sr_xLi_{1-x})Pd₃O₄, Ag₃PdO₄, CaPd₃O₄, CdPd₃O₄, CdPt₃O₄, EuPd₃O₄, LiPt₃O₄, NaPd₃O₄, NaPt₃O₄, NiPt₃O₄, SrPd₃O₄

- The ICSD entry is from (Waser, 1950) and is identical to the information published in (Waser, 1951).

Simple Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Na I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a) Na I
$\mathbf{B}_3$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c) Pt I
$\mathbf{B}_4$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c) Pt I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(6c) Pt I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(6c) Pt I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6c) Pt I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6c) Pt I
$\mathbf{B}_9$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{10}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{11}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{12}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{13}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{14}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{15}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{16}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e) O I

References

- [1] J. Waser and J. E. D. McClanahan, *The Crystal Structure of NaPt₃O₄*, J. Chem. Phys. **19**, 413–416 (1951), doi:10.1063/1.1748239.
- [2] J. Waser and J. E. D. McClanahan, *The Structure of NaPt₃O₄*, Experientia **6**, 379–380 (1950).

First cited in

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