

Pt₃O₄ Structure:

A4B3_cI14_229_c_b-001

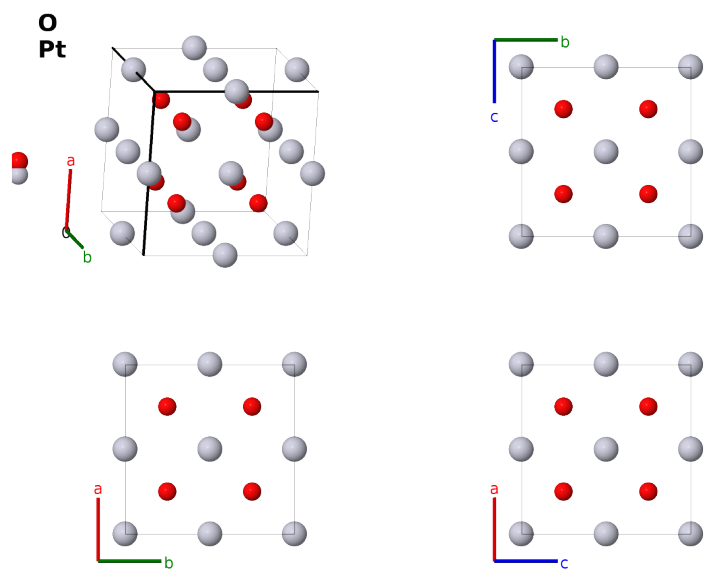
This structure previously used the label(s) **A4B3_cI14_229_c_b**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A4B3_cI14_229_c_b-001



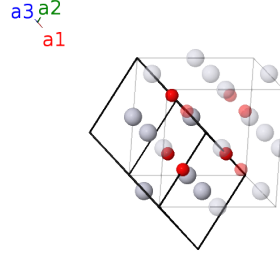
Prototype	O ₄ Pt ₃
AFLOW prototype label	A4B3_cI14_229_c_b-001
ICSD	27836
CCDC	1603014
Pearson symbol	cI14
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A4B3_cI14_229_c_b-001 --params=a</code>

- This is a simple defect superstructure of the CsCl (*B2*) structure. One atom has been removed from a $2 \times 2 \times 2$ supercell of CsCl.
- (Muller, 1968) argue that the correct Pt₃O₄ structure is NaPt₃O₄ with the sodium sites vacant.

- We use $a = 6.226\text{\AA}$ (Galloni, 1941), but the ICSD entry sets $a = 6.238\text{\AA}$.

Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(6b)	Pt I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(6b)	Pt I
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(6b)	Pt I
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	O I

References

- [1] E. E. Galloni and A. E. R. Jr., *The Crystalline Structure of Pt_3O_4* , J. Chem. Phys. **9**, 875–877 (1941), doi:10.1063/1.1750860.
- [2] O. Muller and R. Roy, *Formation and stability of the platinum and rhodium oxides at high oxygen pressures and the structures of Pt_3O_4 , β - PtO_2 and RhO_2* , J. Less-Common Met. **16**, 129–146 (1968), doi:10.1016/0022-5088(68)90070-2.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017