Pt_3O_4 Structure: A4B3_cI14_229_c_b-001

This structure originally had the label `A4B3_cI14_229_c_b`. Calls to that address will be redirected here.

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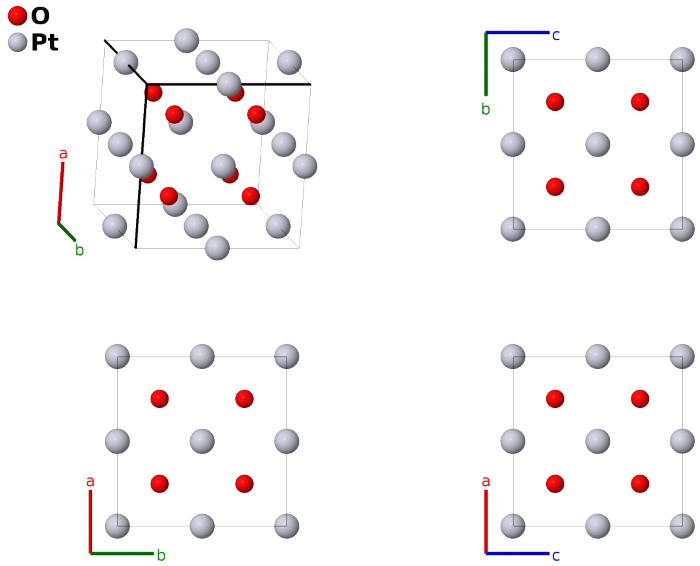
https://aflow.org/p/BYND

https://aflow.org/p/A4B3_cI14_229_c_b-001

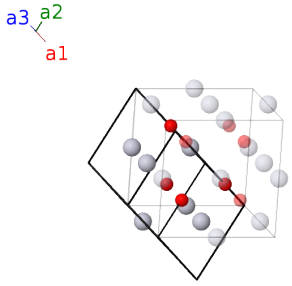


Prototype	O_4Pt_3
AFLOW prototype label	A4B3_cI14_229_c_b-001
ICSD	27836
Pearson symbol	cI14
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A4B3_cI14_229_c_b-001 --params=`a

- 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 Pt_3O_4 structure is $NaPt_3O_4$ with the sodium sites vacant.
- We use a = 6.226Å (Galloni, 1941), but the ICSD entry sets a = 6.238Å.

Body-centered Cubic primitive vectors

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



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.