

α -PbO Structure:

AB_oC8_67_a_g-002

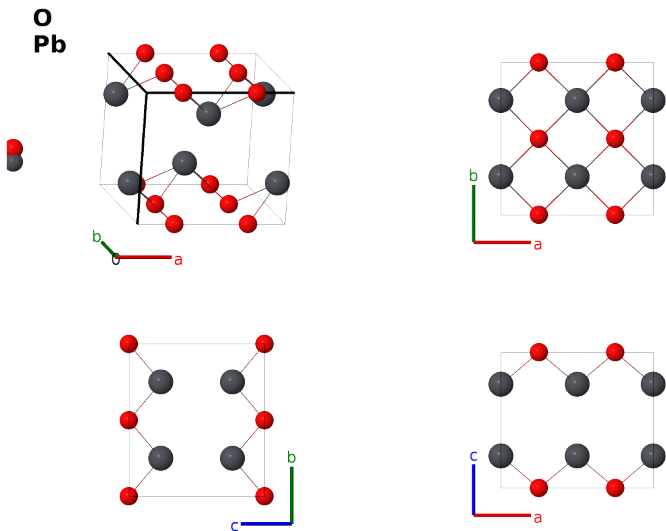
This structure previously used the label(s) **AB_oC8_67_a_g.PbO**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB_oC8.67_a_g-002



Prototype	OPb
AFLOW prototype label	AB_oC8_67_a_g-002
ICSD	62846
CCDC	1626027
Pearson symbol	oC8
Space group number	67
Space group symbol	$Cmme$
AFLOW prototype command	<code>aflow --proto=AB_oC8_67_a_g-002</code> <code>--params=a, b/a, c/a, z₂</code>

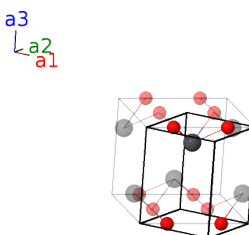
Other compounds with this structure

SnO, α -FeSe

- This is the orthorhombic low temperature form reported by (Boher, 1985), with data taken at 2K. They claim a transformation to the tetragonal ($B10$) PbO phase at about 77K.

- There is very little difference between the structures. Indeed, with the standard tolerance setting AFLOW (and VASP) agree that both structures are tetragonal. We can only resolve the difference by calling VASP with a tighter tolerance:
- `afLOW --proto=AB_oC8_67_a_g --tolerance=0.001 --params=a,c/a,z2` .
- α -FeSe and α -PbO have the same AFLOW prototype label, AB_oC8_67_a_g. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}}$	(4a)	O I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2$	$=$	$\frac{3}{4}a\hat{\mathbf{x}}$	(4a)	O I
$\mathbf{B}_3$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{4}b\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4g)	Pb I
$\mathbf{B}_4$	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4g)	Pb I

References

- [1] P. Boher, P. Garnier, J. R. Gavarri, and A. W. Hewat, *Monoxyde quadratique PbO α (I): Description de la transition structurale ferroélastique*, J. Solid State Chem. **57**, 343–350 (1985), doi:10.1016/0022-4596(85)90197-5.
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- [3] D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:10.1107/S2053273318003066.
- [4] A. L. Speck, *Single-crystal structure validation with the program PLATON*, Appl. Crystallogr. **36**, 7–13 (2003), doi:10.1107/S0021889802022112.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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