α-PbO Structure: AB_oC8_67_a_g-002

This structure originally had the label `AB_oC8_67_a_g.PbO`. Calls to that address will be redirected here.

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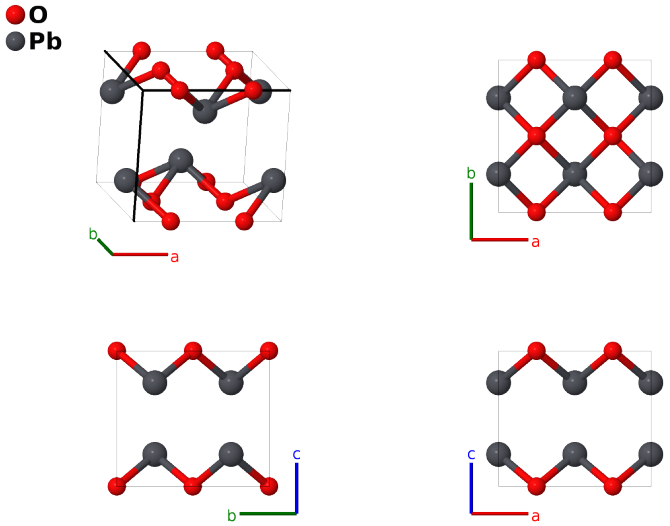
https://aflow.org/p/TSNN

https://aflow.org/p/AB_oC8_67_a_g-002



Prototype	OPb
AFLOW prototype label	AB_oC8_67_a_g-002
ICSD	62846
Pearson symbol	oC8
Space group number	67
Space group symbol	$Cmme$
AFLOW prototype command	`aflow --proto=AB_oC8_67_a_g-002 --params=`$a, b/a, c/a, z_2$

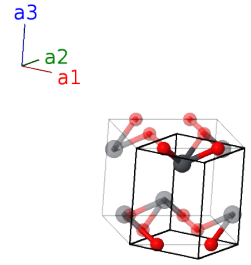
Other compounds with this structure
SnO, α-FeSe

- 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,z_2 .

- 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

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



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 PbOα(I): Description de la transition structurale ferroe'lastique*, J. Solid State Chem. **57**, 343–350 (1985), doi:10.1016/0022-4596(85)90197-5.

[2] H. T. Stokes and D. M. Hatch, FINDSYM*: program for identifying the space-group symmetry of a crystal*, J. Appl. Crystallogr. **38**, 237–238 (2005), doi:10.1107/S0021889804031528.

[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

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