α-PbO_2 Structure: A2B_oP12_60_d_c-003

This structure originally had the label `A2B_oP12_60_d_c`. Calls to that address will be redirected here.

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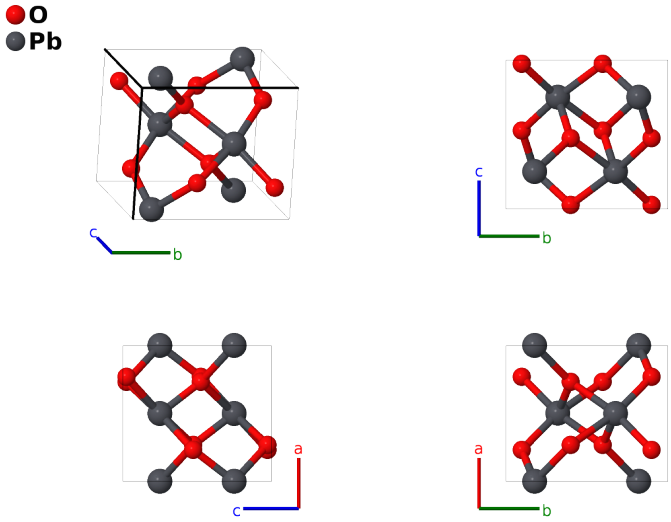
https://aflow.org/p/9BKR

https://aflow.org/p/A2B_oP12_60_d_c-003

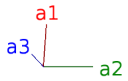


Prototype	O_2Pb
AFLOW prototype label	A2B_oP12_60_d_c-003
ICSD	32691
Pearson symbol	oP12
Space group number	60
Space group symbol	*Pbcn*
AFLOW prototype command	`aflow --proto=A2B_oP12_60_d_c-003 --params=`$a, b/a, c/a, y_1, x_2, y_2, z_2$

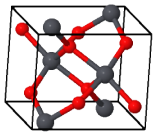
Other compounds with this structure
(Ti, Zr)O_2 (srilankite)

- (Hill, 1982) states the Pb site is only 49% occupied, so stoichiometrically this compound is closer to PbO_4. On the other hand, the ICSD entry gives lists 98% occupation, which is in better agreement with the claimed stoichiometry.
- This structure has the same AFLOW label as ζ-Fe_2N, but in that case the nitrogen site is fully occupied. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Pb I
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Pb I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Pb I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	O I

References

[1] R. J. Hill, *The Crystal Structures of Lead Oxides from the Positive Plate of the Lead/Acid Battery*, Mater. Res. Bull. **17**, 769–784 (1982), doi:10.1016/0025-5408(82)90028-9.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OK, 1991), vol. IV, chap. , p. 4745.