Litharge (tetragonal PbO, $B10$) Structure: AB_tP4_129_a_c-001

This structure previously used the label(s) `AB_tP4_129_a_c`. Calls to these addresses will be redirected here.

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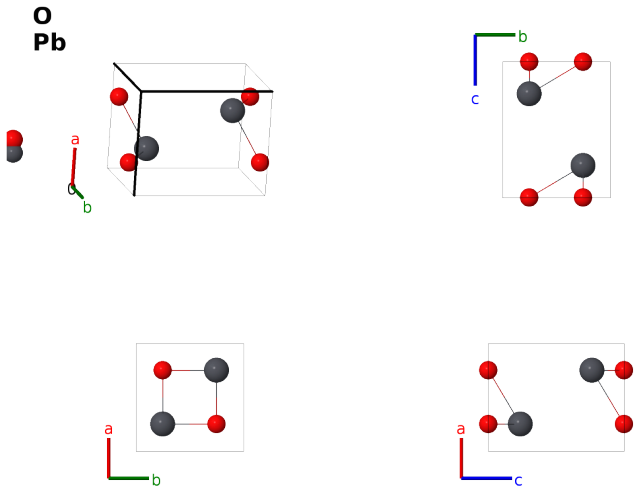
https://aflow.org/prototype-encyclopedia/CWTN

https://aflow.org/prototype-encyclopedia/AB_tP4_129_a_c-001



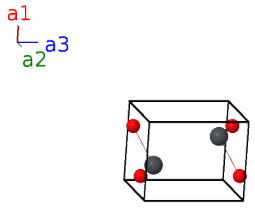
Prototype	OPb
AFLOW prototype label	AB_tP4_129_a_c-001
***Strukturbericht* designation**	$B10$
Mineral name	litharge
ICSD	62840
CCDC	1626021
Pearson symbol	tP4
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=AB_tP4_129_a_c-001 --params=`$a, c/a, z_2$

Other compounds with this structure
BiIn, FeS (mackinawite), FeSe, SnO, TlF-I

- This is the tetragonal room temperature form reported by (Boher, 1985), with data taken at 77.6K. They claim a transformation to the orthorhombic α-PbO phase below 77K. See the discuss of the problems with this transition on the α-PbO page.
- This structure is the binary version of the A_d (β-Np) structure.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Pb I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2c)	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.

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.

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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