α-$BaPbO_3$ Perovskite Structure: AB3C_mC20_12_i_ghi_e-001

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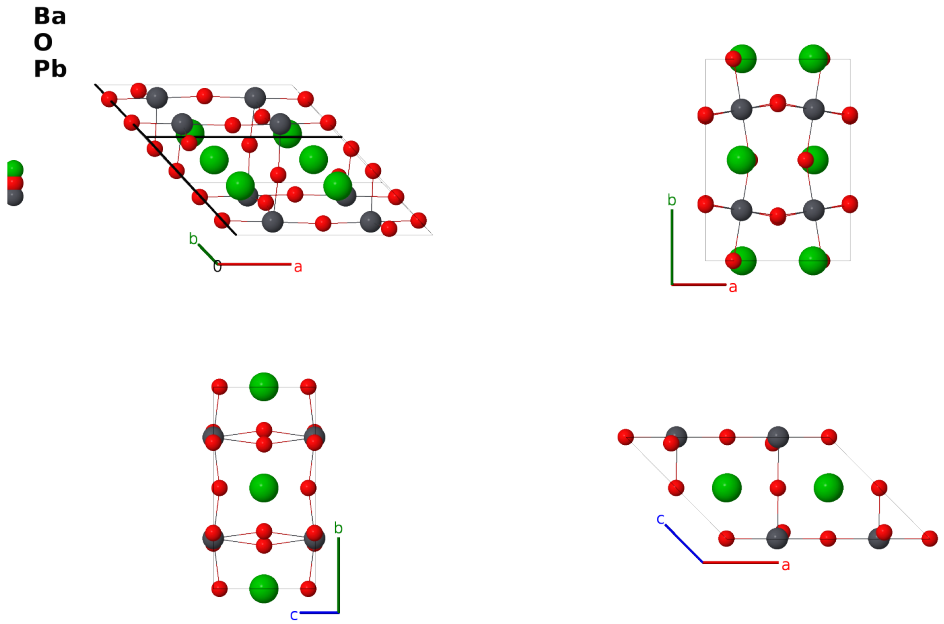
https://aflow.org/prototype-encyclopedia/729H

https://aflow.org/prototype-encyclopedia/AB3C_mC20_12_i_ghi_e-001



Prototype	BaO_3Pb
AFLOW prototype label	AB3C_mC20_12_i_ghi_e-001
ICSD	94313
CCDC	1653754
Pearson symbol	mC20
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB3C_mC20_12_i_ghi_e-001 --params=`$a, b/a, c/a, \beta, y_2, y_3, x_4, z_4, x_5, z_5$

Other compounds with this structure

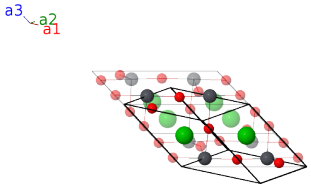
$Al(Pr_{1-x}La_x)O_3$, $Ba(Ce_{1-x}Nd_x)O_3$, $Ba(Ce_{1-x}Y_x)O_3$, $Ba(Pb_{1-x}Bi_x)O_3$, $LaTa(O, N)_3$, $SrTa(O, N)_3$

- As with most perovskites, $BaPbO_3$ has a number of phase transitions. The temperature-driven transitions are summarized in (Fu, 1995), (Moussa, 2001), and (Hestor, 2002). We will follow our usual convention and label the phases by Greek letters, increasing with temperature.

  - The low temperature structure is monoclinic α-$BaPbO_3$ (this structure).
  - At some point above 26 K (Ritter, 1989) we find orthorhombic β-$BaPbO_3$.
  - At 548 K it transforms into the tetragonal γ-$BaPbO_3$ in the γ-$SrZrO_3$ structure.
  - Finally, above 723-725 K δ-$BaPbO_3$ is in the cubic perovskite ($E2_1$) structure.
- The oxygen atoms may be replaced by nitrogen in some systems.
- We use the data taken by (Moussa, 2001) at 15 K.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4e)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}}$	(4e)	Pb I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$by_2\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-by_2\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ba I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ba I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III

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Found in

[1] *AFLOW Database*, https://aflow.org. $BaPbO_3$, ICSD entry 94313.

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