β-$BaPbO_3$ Perovskite Structure: AB3C_oI20_74_e_eg_a-001

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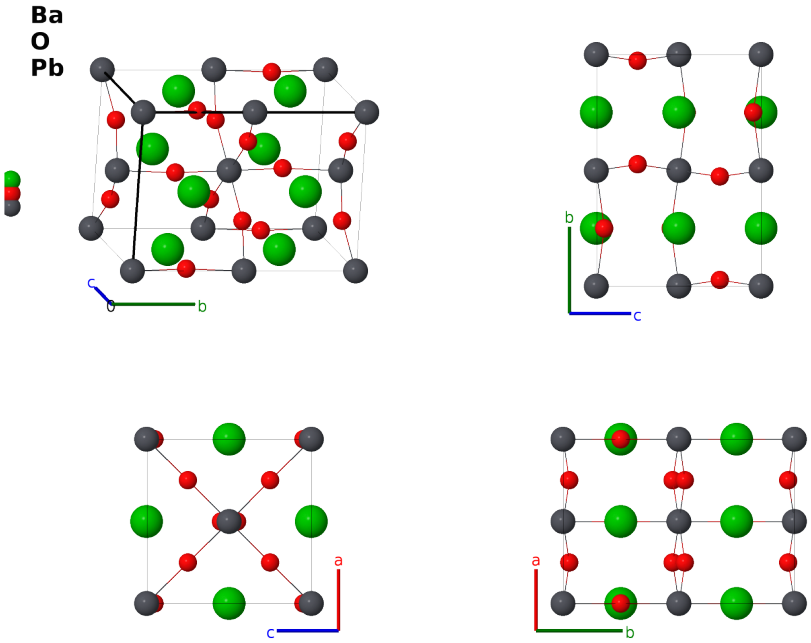
https://aflow.org/prototype-encyclopedia/Z961

https://aflow.org/prototype-encyclopedia/AB3C_oI20_74_e_eg_a-001



Prototype	BaO_3Pb
AFLOW prototype label	AB3C_oI20_74_e_eg_a-001
ICSD	78681
CCDC	1638954
Pearson symbol	oI20
Space group number	74
Space group symbol	*Imma*
AFLOW prototype command	`aflow --proto=AB3C_oI20_74_e_eg_a-001 --params=`$a, b/a, c/a, z_2, z_3, y_4$

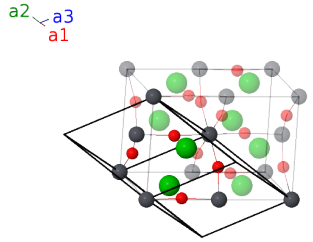
Other compounds with this structure

$AlCeO_3$, $BaCeO_3$, $BaPrO_3$, $BaTbO_3$, $BaThO_3$, $EuNbO_3$, $PuAlO_3$, $SrMoO_3$, $SrSnO_3$, $SrTcO_3$, $SrZrO_3$, $Ba(Ce_{1-x}In_x)O_3$, $Ba(Ce_{1-x}Zr_x)O_3$, $Ba(Pb_{1-x}Bi_x)O_3$, $Ba(Pb_{1-x}Tl_x)O_3$, $Ba(Sb_{1-x}Tl_x)O_3$, $(Ba_{1-x}K_x)BiO_3$, $(Bi_{1-x}La_x)FeO_3$, $(La_{1-x}Ba_x)MnO_3$, $(Na_{1-x}Pr_x)TiO_3$, $(Nd_{1-x}Sr_x)MnO_3$, $(Pr_{1-x}Ba_x)MnO_3$, $(Sr_{1-x}Ba_x)SnO_3$

- 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-$BaPbO_3$.
  - At some point above 26 K (Ritter, 1989) we find orthorhombic β-$BaPbO_3$ (this structure).
  - 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.
- All of the metallic sites may be alloyed, we have only listed a small number of possibilities. The oxygen sites may be partially filled, or partially replaced by nitrogen or fluorine.
- (Fu, 1995) gave the structural information in the *Ibmm* setting of space group #74. We used AFLOW to transform this to the standard *Imma* setting. This requires change of the axes so that $(xyz) \to (yzx)$.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	Pb I
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_4}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_5}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	=	$\left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_8}$	=	$-\left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_9}$	=	$-\left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{10}}$	=	$\left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O II

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