

BaPb₃ Structure:

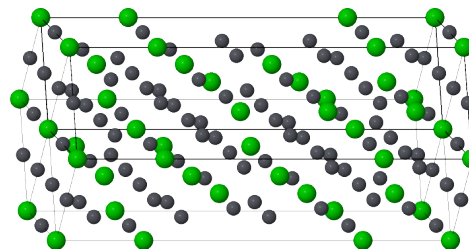
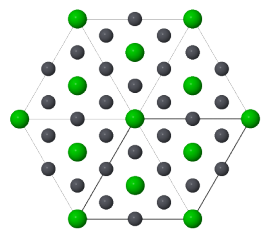
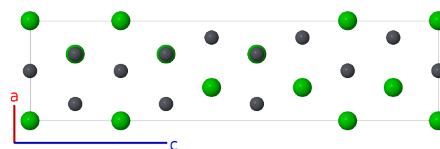
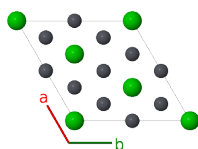
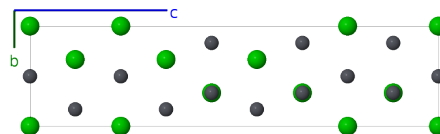
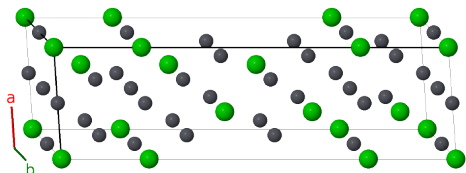
AB3_hR12_166_ac_ah-001

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<https://afLOW.org/p/NHXQ>

https://afLOW.org/p/AB3_hR12_166_ac_ah-001

● Ba
● Pb



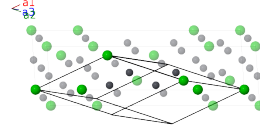
Prototype	BaPb ₃
AFLOW prototype label	AB3_hR12_166_ac_ah-001
ICSD	58665
Pearson symbol	hR12
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>afLOW --proto=AB3_hR12_166_ac_ah-001 --params=a, c/a, x₂, x₄, z₄</code>

Other compounds with this structure
GdAl₃, PuAl₃, TbAl₃, YAl₃

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(1a)	Ba I
\mathbf{B}_2	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Ba II
\mathbf{B}_3	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Ba II
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Pb I
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Pb I
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Pb I
\mathbf{B}_7	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Pb II
\mathbf{B}_8	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Pb II
\mathbf{B}_9	$x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Pb II
\mathbf{B}_{10}	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Pb II
\mathbf{B}_{11}	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Pb II
\mathbf{B}_{12}	$-x_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Pb II

References

- [1] D. E. Sands, D. H. Wood, and W. J. Ramsey, *The structures of Ba₅Pb₃, BaPb and BaPb₃*, Acta Cryst. **17**, 986–989 (1964), doi:10.1107/S0365110X64002547.

Found in

- [1] M. Langenmaier, M. Jehle, and C. Röhr, *Mixed Sr and Ba Tri-Stannides/Plumbides A^{II}(Sn_{1-x}Pb_x)₃*, Crystals **8**, 204 (2018), doi:10.3390/cryst8050204.