$BaPb_3$ Structure: AB3_hR12_166_ac_eh-001

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

https://aflow.org/prototype-encyclopedia/AB3_hR12_166_ac_eh-001

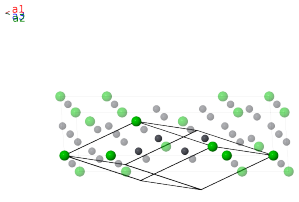
Prototype	$BaPb_3$
AFLOW prototype label	AB3_hR12_166_ac_eh-001
ICSD	58665
CCDC	1622670
Pearson symbol	hR12
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3_hR12_166_ac_eh-001 --params=`$a, c/a, x_2, x_4, z_4$

Other compounds with this structure
$GdAl_3$, $PuAl_3$, $TbAl_3$, YAl_3

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

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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 Ba_5Pb_3, BaPb and $BaPb_3$*, 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 $A^{II}(Sn_{1x}Pb_x)_3$*, Crystals **8**, 204 (2018), doi:10.3390/cryst8050204.

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Ba
Pb