BaPtSb Structure: ABC_hP3_187_b_c_e-001

This structure originally had the label `ABC_hP3_187_a_d_f`. Calls to that address will be redirected here.

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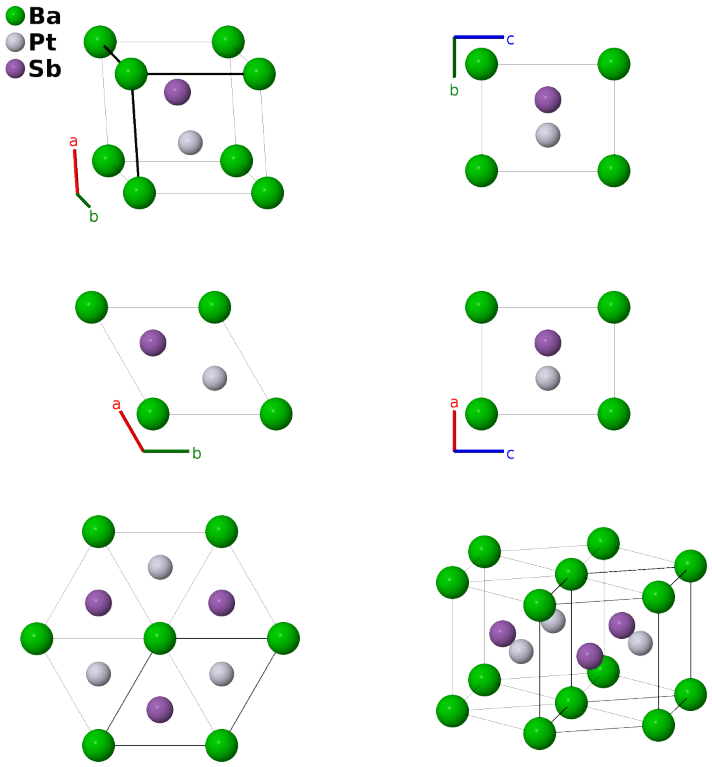
https://aflow.org/p/NKMF

https://aflow.org/p/ABC_hP3_187_b_c_e-001



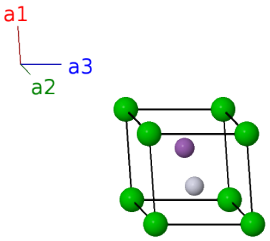
Prototype	BaPtSb
AFLOW prototype label	ABC_hP3_187_b_c_e-001
ICSD	59186
Pearson symbol	hP3
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=ABC_hP3_187_b_c_e-001 --params=`$a, c/a$

Other compounds with this structure

AsKZn, PtSbSr, DyPPt, GdPPt, KSbZn, LuPPt, PPtSm, PPtTb, PPtTm, PPtY, PPtYb, LiBaSi, KZnAs

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(1c)	Pt I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(1e)	Sb I

References

[1] G. Wenski and A. Mewis, *Trigonal-planar koordiniertes Platin: Darstellung und Struktur von SrPtAs (Sb), BaPtP (As, Sb), $SrPt_xP_{2-x}$, $SrPt_xAs_{0.90}$ und $BaPt_xAs_{0.90}$*, Z. Anorganische und Allgemeine Chemie **535**, 110–122 (1986), doi:10.1002/zaac.19865350413.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.