BaPtSb Structure: ABC_hP3_187_b_c_e-001

This structure previously used the label(s) `ABC_hP3_187_a_d_f`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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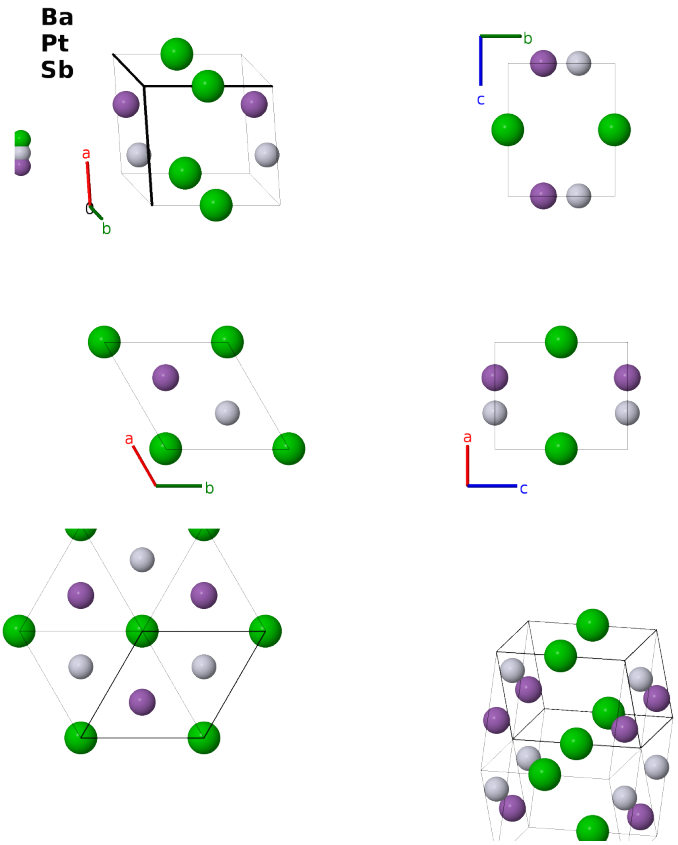
https://aflow.org/prototype-encyclopedia/NKMF

https://aflow.org/prototype-encyclopedia/ABC_hP3_187_b_c_e-001



Prototype	BaPtSb
AFLOW prototype label	ABC_hP3_187_b_c_e-001
ICSD	59186
CCDC	1623052
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=`$a, c/a$

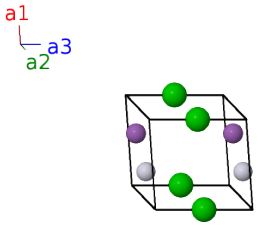
Other compounds with this structure

AlBaGe, AlBaLi, AlBaSi, AlCaSi, AlGeSi, AlGeSr, AlSiSr, AsBaPd, AsBaPt, AsCeNi, AsKZn, AsNiSm, AuSiTh, AuSiU, BaLiP, BaLiSi, BaPtSb, CuGeU, DyPPt, EuGeZn, GdPPt, HCeTe, HErTe, HHoSe, KSbZn, LiPSr, LuPPt, PPtSm, PPtTb, PPtTm, PPtY, PPtYb, PtSbSr

- If the atoms on the (1c) and (1e) sites are identical this becomes the hexagonal ω ($C32$) structure.
- The ICSD designates BaLiSb as the prototype for this structure.

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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017