

BaLiSi [1]; BaPtSb [2]; SrPtSb [2]; ThAuSi [4]; YbPtP [3]; YSeH [6]

Structural features: Infinite columns of base-linked LiBa₆ and SiBa₆ trigonal prisms share rectangular faces to form a dense 3D-framework. Substitution derivative of AlB₂. See Fig. IV.11.

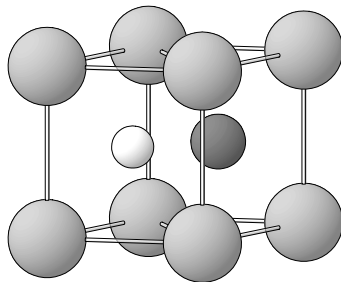


Fig. IV.11. **BaLiSi**

Arrangement of Ba₆ trigonal prisms (Ba atoms large) centered by Li (dark) and Si (light) atoms.

Axel H. et al. (1968) [1]

BaLiSi

$a = 0.438$, $c = 0.485$ nm, $c/a = 1.107$, $V = 0.0806$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	1e	-6m2	$\frac{2}{3}$	$\frac{1}{3}$	0		coplanar triangle Si ₃
Ba2	1d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper Li ₆ Si ₆ Ba ₈
Si3	1a	-6m2	0	0	0		coplanar triangle Li ₃

Transformation from published data: origin shift $\frac{2}{3} \frac{1}{3} \frac{1}{2}$

Experimental: single crystal, precession and Weissenberg photographs, X-rays, $R = 0.082$

Remarks: Identical to the phase called hexagonal BaSi₂ in [5]. Partial disorder Li/Si could not be excluded. In [1] the x -coordinate of the Si site is misprinted as $\frac{2}{2}$ instead of $\frac{2}{3}$.

References: [1] Axel H., Janzon K.H., Schäfer H., Weiss A. (1968), Z. Naturforsch. B 23, 108-109. [2] Wenski G., Mewis A. (1986), Z. Anorg. Allg. Chem. 535, 110-122. [3] Wenski G., Mewis A. (1986), Z. Kristallogr. 176, 125-134. [4] Albering J.H., Pöttgen R., Jeitschko W., Hoffman R., Chevalier B., Etourneau J. (1994), J. Alloys Compd. 206, 133-139. [5] Hladyshevsky E.I. (1959), Dopov. Akad. Nauk Ukr. RSR 1959, 294-297. [6] Schleid T., Meyer H. (1992), J. Alloys Compd. 189, 75-82.