Crystal structure of barium tristannide, BaSn₃

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Source of material: Single crystals of BaSn₃ were formed in the synthesis of ternary E13/E14 clathrates with Ba. Mixtures of the elements were loaded under Ar into Nb or Ta capsules. The sealed capsule was heated up to 1270 K (3 h), annealed at 970 K (2–3 d) and cooled down (see ref. 1).

The existence of the BaSn₃ phase is known for a long time but the structure was not determined (see ref. 2). BaSn₃ forms the *hP8* structure Ni₃Sn with Ba and Sn at the positions of Sn and Ni, respectively. Important interatomic distances: Ba–Sn = 3.663 Å (6x), 3.641 Å (6x); Sn–Sn = 3.058 Å (2x), 3.266 Å (4x), and Sn–Ba = 3.641 Å (2x), 3.663 Å (2x). Very recently the BaSn₃ structure was also determined by Fässler and Kronseder (see ref. 3), who knew our results. Both determinations are in agreement.

BaSn₃, hexagonal, *P6₃/mmc* (No. 194), *a* = 7.253(2) Å, *c* = 5.496(2) Å, *V* = 250.4 Å³, *Z* = 2, *R*(*F*) = 0.021, *R_w*(*F*) = 0.019.

Table 1. Parameters used for the X-ray data collection

Crystal:	silvery parallelepiped, size 0.3 x 0.2 x 0.1 mm
Wavelength:	Mo K _α radiation (0.71069 Å)
μ:	209.4 cm ⁻¹
Diffractometer:	SYNTEX P1
Scan mode:	ω
<i>T</i> _{measurement} :	293 K
2θ _{max} :	55°
<i>N</i> (<i>hkl</i>) _{unique} :	132
Criterion for <i>I</i> _o :	<i>I</i> _o > 3 σ(<i>I</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	8
Programs:	SHELXTL-plus, SHELXS-86, SHELX-76

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Ba	2c	1/3	2/3	1/4	0.0220(7)	0.0220(7)	0.0213(5)	0.022	0	0.0000(7)
Sn	6h	0.8594(1)	1.7188(1)	1/4	0.0263(5)	0.0180(4)	0.0175(4)	0.0180(4)	0	0

References

1. Kröner, R.: Zintl-Phasen der Alkalimetalle und des Bariums mit Clathratstruktur. Dissertation, Universität Stuttgart, 1989.
2. Ray, K. W.; Thompson, R. G.: *Metals Alloys* 1 (1930) 314.
3. Fässler, T. F.; Kronseder, C.: BaSn₃, ein Supraleiter im Grenzbereich zwischen Zintl-Phasen und intermetallischen Verbindungen: Realraum-analyse von Bandstrukturen. *Angew. Chem.* 109 (1997) 2800–2803.
4. Sheldrick, G. M.: Program Package SHELXTL-plus. Release 4.1. Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1990.
5. Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Large Structures. *Acta Crystallogr. A* 46 (1990) 467–473.
6. Sheldrick, G. M.: SHELXL-76, Programs for Crystal Structures Determination. Cambridge 1976.