

Ir₇Sn₄B₃*hP*28(176) *P*6₃/*m* – ih²cb**Sn₄Ir₇B₃** [1]

Structural features: BIr₆ trigonal prisms share edges to form NiAs-type columns parallel to [001] (six prism columns in the hexagonal cross-section); no B-B contact.

Klünter W., Jung W. (1996) [1]

B₃Ir₇Sn₄
 $a = 0.92663$, $c = 0.56319$ nm, $c/a = 0.608$, $V = 0.4188$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ir1	12 <i>i</i>	1	0.1253	0.3566	0.0013		non-colinear B ₂
B2	6 <i>h</i>	<i>m</i> ..	0.173	0.219	¹ / ₄		trigonal prism Ir ₆
Sn3	6 <i>h</i>	<i>m</i> ..	0.5025	0.0912	¹ / ₄		trigonal prism Ir ₆
Sn4	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		trigonal prism Ir ₆
Ir5	2 <i>b</i>	-3..	0	0	0		octahedron B ₆

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.045

References: [1] Klünter W., Jung W. (1996), Z. Anorg. Allg. Chem. 622, 670-674.