

ZrIrSn	<i>hP</i> 11	(189) <i>P</i> -62 <i>m</i> – hgfa
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**ZrIrSn** [1]

Structural features: Infinite columns of base-linked IrZr<sub>6</sub> trigonal prisms (split Ir site) share edges to form a 3D-framework; single columns of base-linked IrSn<sub>6</sub> trigonal prisms in channels parallel to [001]. Variant of ZrNiAl.

Zumdick M.F., Pöttgen R. (1999) [1]

IrSnZr

$a = 0.7321$ ,  $c = 0.3661$  nm,  $c/a = 0.500$ ,  $V = 0.1699$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ir1	4 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.4258	0.5	
Sn2	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.2704	0	$\frac{1}{2}$		
Zr3	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.6044	0	0		
Ir4	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism Sn <sub>6</sub> Zr <sub>3</sub>

Transformation from published data: -*x*, -*y*, -*z*

Experimental: single crystal, diffractometer, X-rays, R = 0.020

Remarks: Short interatomic distances for partly occupied site(s). Average structure; the superstructure was refined in space group (190) *P*-62*c* (new axes *a*, *b*, 2*c*).

References: [1] Zumdick M.F., Pöttgen R. (1999), Z. Kristallogr. 214, 90-97.