

IrSi_3	$hP8$	(186) $P6_3mc - cb$
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IrSi_3 [1]

Structural features: Kagomé-mesh Si layers in h stacking; Ir in voids between hexagons and triangles. Vacancy derivative of MgZn_2 (hexagonal Laves phase).

White J.G., Hockings E.F. (1971) [1]

IrSi_3

$a = 0.4351$, $c = 0.6622$ nm, $c/a = 1.522$, $V = 0.1086$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	$6c$	$.m.$	0.818	0.182	0.167		7-vertex polyhedron Si_4Ir_3
Ir2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0		9-vertex polyhedron Si_9

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.250

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.072$

Remarks: Preliminary data in [2]. Supersedes a report on IrSi_3 with Na_3As -type structure in [3]. The existence of hexagonal IrSi_3 could not be confirmed in [4] where an orthorhombic modification with related cell parameters was observed.

References: [1] White J.G., Hockings E.F. (1971), Inorg. Chem. 10, 1934-1935. [2] Bhan S., Schubert K. (1960), Z. Metallkd. 51, 327-339. [3] Finnie L.N. (1962), J. Less-Common Met. 4, 24-34. [4] Engström I., Zdansky E. (1982), Acta Chem. Scand. A 36, 857-858.