

Zr ₅ Ir ₃	<i>hP</i> 48	(178) $P6_122 - c^2b^2a^2$
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Zr₅Ir₃ [1]

Structural features: Deformation derivative of Mn₅Si₃ with twisted -Zr- chains.

Cenzual K., Parthé E. (1986) [1]

Ir₃Zr₅

$a = 0.79306$, $c = 1.7010$ nm, $c/a = 2.145$, $V = 0.9265$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zr1	12 <i>c</i>	1	0.2384	0.0062	0.3396		15-vertex Frank-Kasper Ir ₅ Zr ₁₀
Ir2	12 <i>c</i>	1	0.4137	0.0187	0.1444		tricapped trigonal prism Zr ₈ Ir
Zr3	6 <i>b</i>	..2	0.3710	0.7420	$\frac{1}{4}$		15-vertex Frank-Kasper Ir ₆ Zr ₉
Zr4	6 <i>b</i>	..2	0.6557	0.3114	$\frac{1}{4}$		15-vertex Frank-Kasper Ir ₆ Zr ₉
Zr5	6 <i>a</i>	.2.	0.2480	0	0		15-vertex Frank-Kasper Ir ₅ Zr ₁₀
Ir6	6 <i>a</i>	.2.	0.6111	0	0		pseudo Frank-Kasper Zr ₉ Ir ₂

Experimental: single crystal, diffractometer, X-rays, $wR = 0.046$, $T = 293$ K

References: [1] Cenzual K., Parthé E. (1986), Acta Crystallogr. C 42, 1101-1105.