

$\text{Zr}_3\text{Fe}_{1.2}\text{Se}_6$ $hP22$ (182) $P6_322$ – ifc**a****Fe_{0.41}ZrSe₂** [1]

Structural features: Close-packed Se layers in BBCC stacking; Zr in trigonal prismatic, Fe in octahedral voids (partial disorder). Infinite slabs of edge-linked ZrSe_6 trigonal prisms are interconnected via FeSe_6 octahedra to form a 3D-framework.

Gleizes A. et al. (1976) [1]

 $\text{Fe}_{1.19}\text{Se}_6\text{Zr}_3$ $a = 0.6011$, $c = 1.2787$ nm, $c/a = 2.127$, $V = 0.4001$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	12 <i>i</i>	1	0.3328	0.006	0.1302		square pyramid Fe_2Zr_3
Zr2	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.001		trigonal prism Se_6
Fe3	2 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.79	octahedron Se_6
Fe4	2 <i>b</i>	3.2	0	0	$\frac{1}{4}$	0.4	octahedron Se_6
Zr5	2 <i>a</i>	32.	0	0	0		trigonal prism Se_6

Transformation from published data: $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.051$, $T = 294$ K

References: [1] Gleizes A., Revelli J., Ibers J.A. (1976), J. Solid State Chem. 17, 363-372.