

$\text{Zr}_6\text{FeAl}_2\text{O}_{0.14}$ $hP11$ (189) $P\text{-}62m$ – gfdca**Zr₆FeAl₂O_x** [1]

Structural features: Filled-up derivative of $\beta_1\text{-K}_2\text{UF}_6$ antitype with O in trigonal bipyramidal (Zr_3Al_2) voids.

Yartys V.A. et al. (1999) [1]

 $\text{Al}_2\text{FeO}_{0.14}\text{Zr}_6$ $a = 0.7931$, $c = 0.33526$ nm, $c/a = 0.423$, $V = 0.1826$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	3g	$m2m$	0.2538	0	$\frac{1}{2}$		non-colinear Fe ₂
Zr2	3f	$m2m$	0.6049	0	0		non-colinear O ₂
Al3	2d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		colinear O ₂
O4	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0	0.07	colinear Al ₂
Fe5	1a	-62m	0	0	0		trigonal prism Zr ₆

Transformation from published data: $-x, -y, -z$ Experimental: powder, diffractometer, X-rays, $R_p = 0.065$

Remarks: Sample submitted to deuteration at rt and desorption at 973 K.

References: [1] Yartys V.A., Fjellvag H., Hauback B.C. (1999), J. Alloys Compd. 290, 157-163.