

$\text{Zr}_5\text{Al}_3\text{O}_{0.5}$ $hP52$ $(186) P6_3mc - dc^6ba$ **Zr₅Al₃O_{0.5}** [1]

Structural features: AlZr_8Zr monocapped square antiprisms (AlZr_6Zr_3 tricapped trigonal prisms) share atoms to form a 3D-framework with infinite columns of face-linked Zr_6 octahedra (in part centered by O) and infinite linear -Zr- chains. Filled-up derivative of Mn_5Si_3 with O in octahedral voids.

Larsson T. et al. (1993) [1]

 $\text{Al}_3\text{O}_{0.50}\text{Zr}_5$ $a = 1.41552$, $c = 0.56862$ nm, $c/a = 0.402$, $V = 0.9867$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	12 <i>d</i>	1	0.0168	0.337	0.0		14-vertex Frank-Kasper Al_6Zr_8
Al2	6 <i>c</i>	. <i>m</i> .	0.133	0.867	0.26		pseudo Frank-Kasper $\text{Zr}_9\text{Al}_2\text{O}_2$
Zr3	6 <i>c</i>	. <i>m</i> .	0.257	0.743	0.232		single atom O
Al4	6 <i>c</i>	. <i>m</i> .	0.469	0.531	0.25		pseudo Frank-Kasper Zr_9Al_2
Zr5	6 <i>c</i>	. <i>m</i> .	0.588	0.412	0.248		single atom O
Al6	6 <i>c</i>	. <i>m</i> .	0.799	0.201	0.204		icosahedron $\text{Zr}_9\text{Al}_2\text{O}$
Zr7	6 <i>c</i>	. <i>m</i> .	0.922	0.078	0.255		non-colinear O ₂
O8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0		octahedron Zr_6
O9	2 <i>a</i>	3 <i>m</i> .	0	0	0.0	0.5	octahedron Zr_6

Transformation from published data: - x , - y , - z ; origin shift 0 0 0.5Experimental: powder, diffractometer, neutrons, $R_B = 0.043$, $T = 293$ K

References: [1] Larsson T., Andersson Y., Rundqvist S., Tellgren R., Clark N.J., Wu E. (1993), Z. Phys. Chem. 179, 217-224.