

$\text{Zr}_4\text{Al}_3\text{H}_{2.68}$	$hP80$	$(182) P6_322 - i^4h^2g^2fe$
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**$\text{Zr}_4\text{Al}_3\text{H}_{2.68}$**  [1]

Structural features: Filled-up derivative of  $\text{Zr}_4\text{Al}_3$  with H in tetrahedral ( $\text{Zr}_4$ ) voids.

Riabov A.B. et al. (2003) [1]

$\text{Al}_3\text{D}_{2.68}\text{Zr}_4$

$a = 1.10017$ ,  $c = 1.11694$  nm,  $c/a = 1.015$ ,  $V = 1.1708$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	12i	1	0.007	0.249	0.259		pseudo Frank-Kasper $\text{Al}_4\text{Zr}_7\text{D}_2$
Zr2	12i	1	0.179	0.339	0.007		non-coplanar triangle $\text{D}_3$
D3	12i	1	0.366	0.511	0.001	0.883	tetrahedron $\text{Zr}_4$
Zr4	12i	1	0.4966	0.001	0.1256		non-coplanar triangle $\text{D}_3$
Al5	6h	..2	0.257	0.514	$\frac{1}{4}$		14-vertex Frank-Kasper $\text{Al}_4\text{Zr}_8\text{D}_2$
Al6	6h	..2	0.758	0.516	$\frac{1}{4}$		icosahedron $\text{Al}_4\text{Zr}_6\text{D}_2$
D7	6g	..2	0.144	0	0		tetrahedron $\text{Zr}_4$
D8	6g	..2	0.36	0	0	0.808	tetrahedron $\text{Zr}_4$
Zr9	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.019		non-coplanar triangle $\text{D}_3$
Zr10	4e	3..	0	0	0.1148		non-coplanar triangle $\text{D}_3$

Experimental: powder, diffractometer, neutrons,  $R_p = 0.059$ ,  $T = 293$  K

References: [1] Riabov A.B., Yartys V.A., Denys R.V., Hauback B.C. (2003), J. Alloys Compd. 356/357, 91-95.