$Zr_5Al_3O_{0.5}H_{2.67}$	*hP*102	(186) $P6_3mc$ – $d^3c^{10}b^2a$

$Zr_5Al_3O_{0.5}H_{2.67}$ [1]
Structural features: Filled-up derivative of Mn_5Si_3 with O in octahedral (Zr_6) voids, H in octahedral (Zr_6), trigonal bipyramidal (Zr_3Al_2), tetrahedral (Zr_3Al) and trigonal (Zr_3) voids.

Larsson T. et al. (1993) [1]
$Al_3D_{2.67}O_{0.50}Zr_5$
a = 1.4247, c = 0.57814 nm, c/a = 0.406, V = 1.0163 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	12*d*	1	0.0136	0.3405	0.0		non-colinear D_2
D2	12*d*	1	0.195	0.017	0.01	0.322	octahedron D_2Zr_3Al
D3	12*d*	1	0.472	0.157	0.499	0.573	non-coplanar triangle Zr_3
D4	6*c*	.*m*.	0.048	0.952	0.1	0.144	single atom O
D5	6*c*	.*m*.	0.048	0.952	0.4	0.144	single atom O
Al6	6*c*	.*m*.	0.1306	0.8694	0.255		non-colinear D_2
Zr7	6*c*	.*m*.	0.2551	0.7449	0.257		square pyramid D_5
D8	6*c*	.*m*.	0.395	0.605	0.42	0.147	single atom D
Al9	6*c*	.*m*.	0.4677	0.5323	0.251		single atom D
Zr10	6*c*	.*m*.	0.5908	0.4092	0.262		square pyramid D_5
D11	6*c*	.*m*.	0.73	0.27	0.09	0.147	single atom D
Al12	6*c*	.*m*.	0.8067	0.1933	0.199		non-coplanar triangle D_3
Zr13	6*c*	.*m*.	0.9183	0.0817	0.276		monocapped square prism D_9
O14	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0		pseudo Frank-Kasper Zr_6D_{14}
D15	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.5	0.628	octahedron D_6
M16	2*a*	3*m*.	0	0	0.0	0.773	octahedron D_6

M16 = 0.64O + 0.36D
Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.5
Experimental: powder, diffractometer, neutrons, R_B = 0.034, T = 293 K

Remarks: Short interatomic distances for partly occupied site(s).

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