$(Mg_{0.04}Zn_{0.96})_7(Ti_{0.33}Al_{0.67})_3FeAl_{12}O_{31}[OH]$	*hP*110	(186) $P6_3mc$ – $c^{12}b^{13}a^6$

$Zn_{14}(Al,Fe,Ti,Mg)_8Al_{24}O_{62}(OH)_2$ [1], zincohögbomite-16H
Structural features: Close-packed (O,OH) layers in hc_7 stacking; Al, (Al,Ti) and Fe in octahedral, (Zn,Mg,Al) in tetrahedral voids. Infinite slabs of edge-linked AlO_6 and $(Al,Ti)O_6$ octahedra share atoms with FeO_6 and additional AlO_6 octahedra and $(Zn,Mg,Al)O_4$ tetrahedra to form a 3D-framework with spinel-type slabs.

Armbruster T. et al. (1998) [1]
$Al_{14.38}FeHMg_{0.47}O_{32}Ti_{0.78}Zn_{6.37}$
$a = 0.5729$, $c = 3.7097$ nm, $c/a = 6.475$, $V = 1.0545$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*c*	.*m*.	0.1479	0.8521	0.323		tetrahedron Al_3Zn
M2	6*c*	.*m*.	0.166	0.834	0.47385		octahedron O_6
Al3	6*c*	.*m*.	0.1665	0.8335	0.22633		octahedron O_6
O4	6*c*	.*m*.	0.1867	0.8133	0.1304		tetrahedron Al_3Zn
O5	6*c*	.*m*.	0.4824	0.5176	0.197		tetrahedron Al_3Zn
Al6	6*c*	.*m*.	0.5001	0.4999	0.10049		octahedron O_6
O7	6*c*	.*m*.	0.5179	0.4821	0.3815		tetrahedron Al_2ZnFe
O8	6*c*	.*m*.	0.5197	0.4803	0.0056		tetrahedron Al_3Zn
O9	6*c*	.*m*.	0.8162	0.1838	0.0712		tetrahedron Al_3Zn
Al10	6*c*	.*m*.	0.8302	0.1698	0.35175		octahedron $O_5(OH)$
O11	6*c*	.*m*.	0.8342	0.1658	0.4464		non-coplanar triangle $FeAl_2$
O12	6*c*	.*m*.	0.8531	0.1469	0.2561		tetrahedron Al_3Zn
M13	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.02124		tetrahedron O_4
O14	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0748		tetrahedron Al_3Zn
Al15	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.1633		octahedron O_6
O16	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2533		tetrahedron $ZnAl_3$
M17	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.30524		tetrahedron O_4
M18	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.39702		tetrahedron O_4
O19	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.4489		tetrahedron Al_3Zn
Al20	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.538		octahedron O_6
O21	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.6274		tetrahedron $ZnAl_3$
M22	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.67918		tetrahedron O_4
M23	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.77269		tetrahedron O_4
O24	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.8258		tetrahedron Al_3Zn
Fe25	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.92195		octahedron O_6
O26	2*a*	3*m*.	0	0	0.0		tetrahedron Al_3Zn
M27	2*a*	3*m*.	0	0	0.05306		tetrahedron O_4
M28	2*a*	3*m*.	0	0	0.14746		tetrahedron O_4
O29	2*a*	3*m*.	0	0	0.2004		tetrahedron Al_3Zn
Al30	2*a*	3*m*.	0	0	0.2894		octahedron O_6
(OH)31	2*a*	3*m*.	0	0	0.3792		non-coplanar triangle Al_3

M2 = 0.74Al + 0.26Ti; M13 = 0.88Zn + 0.12Mg; M17 = 0.93Zn + 0.07Mg; M18 = 0.84Zn + 0.16Al; M22 = 0.91Zn + 0.09Mg; M23 = 0.95Zn + 0.05Mg; M27 = 0.91Zn + 0.09Mg; M28 = 0.95Zn + 0.05Mg
Transformation from published data: origin shift 0 0 0.37960
Experimental: single crystal, diffractometer, X-rays, R = 0.024

Remarks: Natural specimen from the Nezilovo area, Macedonia. Composition $Zn_{13.03}Mg_{0.49}(Fe^{3+})_{2.12}$_ $Ti_{1.15}Al_{29.21}O_{62}(OH)_2$ from electron microprobe analysis. Partial substitution Mg/Al on tetrahedral sites could not be quantified. When relevant, we changed the last digit of the atom coordinates to respect the

symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Armbruster T., Bermanec V., Zebec V., Oberhänsli R. (1998), Schweiz. Mineral. Petrogr. Mitt. 78, 469-477.