

$\text{Zn}_3\text{V}_2\text{O}_8[\text{H}_2\text{O}]_3$ $hP16$ (174) $P-6$ – lkihga **$\text{Zn}_3(\text{VO}_4)_2 \cdot 3\text{H}_2\text{O}$** [1]

Structural features: Infinite slabs of edge-linked ZnO_6 trigonal prisms are interconnected via units of two vertex-linked VO_4 tetrahedra to form a 3D-framework.

Hoyos D.A. et al. (2001) [1]

 $\text{H}_4\text{O}_{11}\text{V}_2\text{Zn}_3$ $a = 0.60788$, $c = 0.71827$ nm, $c/a = 1.182$, $V = 0.2299$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$6l$	1	0.11923	0.30737	0.3241		single atom V
Zn2	$3k$	$m..$	0.00323	0.50917	$\frac{1}{2}$		trigonal prism O_6
O3	$2i$	$3..$	$\frac{2}{3}$	$\frac{1}{3}$	0.3743		4-vertex polyhedron OZn_3
(OH_2)4	$2h$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.2		non-coplanar triangle O_3
V5	$2g$	$3..$	0	0	0.2542		tetrahedron O_4
O6	$1a$	$-6..$	0	0	0		colinear V_2

Transformation from published data: $-x, -y, -z$; origin shift $\frac{2}{3} \frac{1}{3} \frac{1}{2}$ Experimental: powder, diffractometer, X-rays, $R_p = 0.057$, $T = 293$ K

Remarks: Part of H not located. Refinement considering site (OH_2)4 in Wyckoff position $1b$ with occupancy 1.93(3); the authors state that the site is displaced into Wyckoff position $2h$ (published $2g$) to accommodate 2 H_2O per unit cell. We assigned an arbitrary value to the z -coordinate of (OH_2)4. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Ambiguous data: the chemical formula is written as $\text{Zn}_3(\text{VO}_4)_2 \cdot 3\text{H}_2\text{O}$, however, the structure does not contain VO_4 units.

References: [1] Hoyos D.A., Echavarria A., Saldarriaga C. (2001), J. Mater. Sci. 36, 5515-5518.