

$\text{Mn}_{6.87}[\text{V}_2\text{O}_7]_{0.2}[\text{VO}_4]_{3.6}[\text{OH}]_3$ *hP62*(186) *P6<sub>3</sub>mc* –  $d^2c^5b^3a$  **$\text{Mn}_{6.87}(\text{VO}_4)_{3.6}(\text{V}_2\text{O}_7)_{0.2}(\text{OH})_3$**  [1]

Structural features: Columns of edge- and face-linked  $\text{Mn}(\text{O}_4[\text{OH}]_2)$  octahedra are interconnected via common vertices,  $\text{V}_2\text{O}_7$  units (two vertex-linked tetrahedra) and  $\text{VO}_4$  tetrahedra (partial disorder) to form a 3D-framework; additional Mn in channels parallel to [001] ( $\text{MnO}_3$  trigonal units).

Zhang F. et al. (1999) [1]

 $\text{H}_3\text{Mn}_{6.87}\text{O}_{18.80}\text{V}_4$  $a = 1.32293$ ,  $c = 0.52547$  nm,  $c/a = 0.397$ ,  $V = 0.7964$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mn1	12 <i>d</i>	1	0.07902	0.42632	0.0137		octahedron $\text{O}_4(\text{OH})_2$
O2	12 <i>d</i>	1	0.3397	0.0726	0.1596		single atom V
O3	6 <i>c</i>	. <i>m</i> .	0.0801	0.9199	0.4417		non-colinear VMn
V4	6 <i>c</i>	. <i>m</i> .	0.15073	0.84927	0.4888		tetrahedron $\text{O}_4$
O5	6 <i>c</i>	. <i>m</i> .	0.1877	0.8123	0.2083		coplanar triangle VMn <sub>2</sub>
(OH)6	6 <i>c</i>	. <i>m</i> .	0.4738	0.5262	0.3009		non-coplanar square Mn <sub>4</sub>
O7	6 <i>c</i>	. <i>m</i> .	0.5998	0.4002	0.3721		non-colinear V <sub>2</sub>
V8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.036	0.199	trigonal bipyramid $\text{VO}_4$
O9	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.375	0.801	colinear V <sub>2</sub>
V10	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.7484	0.801	trigonal bipyramid $\text{VO}_4$
Mn11	2 <i>a</i>	3 <i>m</i> .	0	0	0.0	0.868	non-coplanar triangle $\text{O}_3$

Transformation from published data:  $-x, -y, -z$ Experimental: powder, diffractometer, X-rays,  $R_p = 0.085$ 

Remarks: General formula  $\text{Mn}^{2+}_6\text{Mn}^{3+}_{1-2z/3}(\text{OH})_3(\text{VO}_4)_3[(\text{VO}_4)_{1-2z}(\text{V}_2\text{O}_7)_z]$ . Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Zhang F., Zavalij P.Y., Whittingham M.S. (1999), J. Mater. Chem. 9, 3137-3140.