

$\text{K}(\text{Zn}_{0.83}\text{Mn}_{0.16})_3(\text{Mn}_{0.5}\text{Fe}_{0.5})_2\text{Si}_{12}\text{O}_{30}$
hP96

(184) *P6cc* – d^7cba
K(Zn,Mn)₃(Mn,Fe)₂Si₁₂O₃₀ [1], milarite-(Zn)

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with (Zn,Mn)O₄ tetrahedra and (Mn,Fe)O₆ octahedra to form a 3D-framework; K in the columns formed by superposed double 6-rings.

Pushcharovskii D.I. et al. (1972) [1]

 $\text{FeKMn}_{1.50}\text{O}_{30}\text{Si}_{12}\text{Zn}_{2.50}$
 $a = 1.052$, $c = 1.422$ nm, $c/a = 1.352$, $V = 1.3629$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.096	0.355	0.273		non-colinear Si ₂
Si2	12 <i>d</i>	1	0.103	0.346	0.389		tetrahedron O ₄
Si3	12 <i>d</i>	1	0.108	0.338	0.16		tetrahedron O ₄
O4	12 <i>d</i>	1	0.142	0.495	0.108		non-coplanar triangle SiZnFe
O5	12 <i>d</i>	1	0.146	0.49	0.44		single atom Si
O6	12 <i>d</i>	1	0.272	0.059	0.132		non-colinear Si ₂
O7	12 <i>d</i>	1	0.273	0.061	0.413		non-colinear Si ₂
M8	6 <i>c</i>	2..	$\frac{1}{2}$	0	0.023		tetrahedron O ₄
M9	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.035		octahedron O ₆
K10	2 <i>a</i>	6..	0	0	0.0		hexagonal prism O ₁₂

 $\text{M8} = 0.833\text{Zn} + 0.167\text{Mn}$; $\text{M9} = 0.5\text{Fe} + 0.5\text{Mn}$

Transformation from published data: origin shift 0 0 0.227

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.144$

Remarks: We assigned approximate values to the cation ratios of sites M8 and M9 based on the nominal composition.

References: [1] Pushcharovskii D.I., Baataryn T., Pobedinskaya E.A., Belov N.V. (1972), Sov. Phys. Crystallogr. 16, 628-630 (Kristallografiya 16, 721-724).