

$\text{H}_{1.04}\text{K}_{1.54}\text{Mg}_{1.93}\text{Si}_{1.89}\text{O}_7$  $hP26$  $(185) P6_3cm - c^2b^2a^3$  **$\text{K}_{1.54}\text{H}_{1.04}\text{Mg}_{1.93}\text{Si}_{1.89}\text{O}_7$**  [1], X phase

Structural features: Close-packed  $\text{K}_2\text{O}$  and  $\text{O}_3$  layers in  $hc_2$  stacking (partial vacancies ignored); Mg in octahedral, Si in tetrahedral voids. Infinite slabs of edge-linked  $\text{MgO}_6$  octahedra containing 6-rings share vertices with units of two vertex-linked  $\text{SiO}_4$  tetrahedra to form a 3D-framework (partial vacancies ignored); K in trigonal prismatic voids.

Yang H. et al. (2001) [1]

 $\text{K}_{1.54}\text{Mg}_{1.93}\text{O}_7\text{Si}_{1.89}$  $a = 0.50812$ ,  $c = 1.32112$  nm,  $c/a = 2.600$ ,  $V = 0.2954$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6c	.. $m$	0.3081	0	0.1578		single atom Si
O2	6c	.. $m$	0.6898	0	0.3402		single atom Si
K3	4b	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0016	0.77	anticuboctahedron $\text{O}_9\text{K}_3$
Mg4	4b	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2485	0.965	octahedron $\text{O}_6$
O5	2a	3.. $m$	0	0	0.0		colinear $\text{Si}_2$
Si6	2a	3.. $m$	0	0	0.1291	0.945	tetrahedron $\text{O}_4$
Si7	2a	3.. $m$	0	0	0.3736	0.945	tetrahedron $\text{O}_4$

Transformation from published data: origin shift 0 0 0.2056

Experimental: single crystal, diffractometer, X-rays, R = 0.037

Remarks: High-pressure phase. H not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Yang H., Konzett J., Prewitt C.T. (2001), Am. Mineral. 86, 1483-1488.