

$\text{K}_{0.5}\text{Mo}_{2.5}(\text{O}_{0.83}[\text{OH}]_{0.17})_3(\text{O}_{0.83}[\text{H}_2\text{O}]_{0.17})_6$ *hP26*(176) $P6_3/m - h^4b$ **KMo₅O₁₅OH·2H₂O** [1], HMB (hexagonal molybdenum bronze); Mo₃O₉·NH₃ [2]Structural features: Double infinite chains of edge-linked Mo[(O,OH₂)₂(O,OH)₃] octahedra (partial vacancies ignored) share vertices to form a 3D-framework; K in channels parallel to [001].

Krebs B., Paulat Boschen I. (1976) [1]

 $\text{H}_{2.51}\text{K}_{0.46}\text{Mo}_{2.42}\text{O}_9$ $a = 1.055$, $c = 0.3727$ nm, $c/a = 0.353$, $V = 0.3592$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>h</i>	<i>m</i> ..	0.0102	0.2738	¹ / ₄		single atom Mo
Mo2	6 <i>h</i>	<i>m</i> ..	0.10447	0.45998	¹ / ₄	0.808	octahedron O ₆
M3	6 <i>h</i>	<i>m</i> ..	0.2811	0.4981	¹ / ₄		single atom Mo
M4	6 <i>h</i>	<i>m</i> ..	0.5805	0.0797	¹ / ₄		non-coplanar triangle Mo ₃
K5	2 <i>b</i>	-3..	0	0	0	0.462	

M1 = 0.833O + 0.167OH₂; M3 = 0.833O + 0.167OH₂; M4 = 0.833O + 0.167OH

Experimental: single crystal, diffractometer, X-rays, wR = 0.031

Remarks: 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] Krebs B., Paulat Boschen I. (1976), Acta Crystallogr. B 32, 1697-1704. [2] Garin J.L., Blanc J.M. (1985), J. Solid State Chem. 58, 98-102.