

$\text{H}_{1.5}\text{Na}_{0.5}\text{Mo}_{2.67}\text{O}_9[\text{H}_2\text{O}]$ *hP*34(176) $P6_3/m - h^5e$ **NaH₃Mo_{5.33}O₁₈·2H₂O** [1], HMB (hexagonal molybdenum bronze); AgMo_{5.5}O_{17.5}H·1.1H₂O [2]

Structural features: Double infinite chains of edge-linked MoO₆ octahedra (partial vacancies ignored) share vertices to form a 3D-framework; Na (displaced from the axis) and H₂O in channels parallel to [001] (partial disorder).

McCarron E.M. III et al. (1987) [1]

 $\text{H}_{1.76}\text{Mo}_{2.66}\text{Na}_{0.46}\text{O}_{9.88}$ $a = 1.0595$, $c = 0.37224$ nm, $c/a = 0.351$, $V = 0.3619$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>h</i>	<i>m</i> ..	0.0109	0.2765	¹ / ₄		single atom Mo
Mo2	6 <i>h</i>	<i>m</i> ..	0.105	0.4616	¹ / ₄	0.888	octahedron O ₆
Na3	6 <i>h</i>	<i>m</i> ..	0.1181	0.1152	¹ / ₄	0.152	
O4	6 <i>h</i>	<i>m</i> ..	0.2801	0.4966	¹ / ₄		single atom Mo
O5	6 <i>h</i>	<i>m</i> ..	0.5798	0.0805	¹ / ₄		non-coplanar triangle Mo ₃
(OH ₂)6	4 <i>e</i>	3..	0	0	0.1421	0.441	

Experimental: single crystal, diffractometer, X-rays, R = 0.070

Remarks: General formula AH_{6x-1}Mo_{6-x}O₁₈, where A = Na·2H₂O. H not belonging to H₂O was not located. 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] McCarron E.M. III, Thomas D.M., Calabrese J.C. (1987), Inorg. Chem. 26, 370-373. [2] Guo J., Zavalij P., Whittingham M.S. (1995), J. Solid State Chem. 117, 323-332.