

$\text{Na}_{0.5}\text{Mo}_{2.68}\text{O}_{7.88}[\text{OH}]_{0.8}[\text{H}_2\text{O}]_{0.85}$ *hP30*(176)  $P6_3/m-h^5$ **NaH<sub>1.6</sub>Mo<sub>5.35</sub>O<sub>17.35</sub>•1.7H<sub>2</sub>O** [1], HMB (hexagonal molybdenum bronze)

Structural features: Double infinite chains of edge-linked MoO<sub>6</sub> octahedra (partial vacancies ignored) share vertices to form a 3D-framework; (Na,H<sub>2</sub>O) in channels parallel to [001] (displaced from the axis, partial disorder).

Guo J. et al. (1995) [1]

 $\text{H}_{1.54}\text{Mo}_{2.76}\text{O}_{9.53}$  $a = 1.06242$ ,  $c = 0.37261$  nm,  $c/a = 0.351$ ,  $V = 0.3642$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>h</i>	<i>m</i> ..	0.0101	0.2732	$\frac{1}{4}$	0.92	single atom Mo
(OH <sub>2</sub> )2	6 <i>h</i>	<i>m</i> ..	0.085	0.064	$\frac{1}{4}$	0.257	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
Mo3	6 <i>h</i>	<i>m</i> ..	0.104	0.4602	$\frac{1}{4}$	0.92	octahedron O <sub>6</sub>
O4	6 <i>h</i>	<i>m</i> ..	0.2836	0.504	$\frac{1}{4}$		single atom Mo
O5	6 <i>h</i>	<i>m</i> ..	0.5811	0.0796	$\frac{1}{4}$		non-coplanar triangle Mo <sub>3</sub>

Transformation from published data:  $y, x, -z$ Experimental: powder, diffractometer, X-rays,  $R_B = 0.040$ 

Remarks: Metastable phase. No attempt was made to distinguish Na and H<sub>2</sub>O in the refinement; OH not identified, part of H<sub>2</sub>O and/or Na 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] Guo J., Zavalij P., Whittingham M.S. (1995), J. Solid State Chem. 117, 323-332.