

$\text{Mo}_{2.65}\text{O}_{7.25}[\text{OH}]_{1.4}[\text{H}_2\text{O}]_{0.68}$ *hP28*(176) $P6_3/m - h^4ba$ **H_{2.8}Mo_{5.3}O_{17.3}·1.36H₂O** [1], HMB (hexagonal molybdenum bronze)Structural features: Double infinite chains of edge-linked MoO₆ octahedra (partial vacancies ignored) share vertices to form a 3D-framework; H₂O in channels parallel to [001] (partial disorder).

Guo J. et al. (1994) [1]

 $\text{H}_{1.36}\text{Mo}_{2.63}\text{O}_{9.31}$ $a = 1.0584$, $c = 0.37278$ nm, $c/a = 0.352$, $V = 0.3616$ 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> ..	0.0084	0.2756	$\frac{1}{4}$	0.875	single atom Mo
Mo2	6 <i>h</i>	<i>m</i> ..	0.1033	0.4583	$\frac{1}{4}$	0.875	octahedron O ₆
O3	6 <i>h</i>	<i>m</i> ..	0.2822	0.4947	$\frac{1}{4}$		single atom Mo
O4	6 <i>h</i>	<i>m</i> ..	0.5791	0.0848	$\frac{1}{4}$		non-coplanar triangle Mo ₃
(OH ₂)5	2 <i>b</i>	-3..	0	0	0	0.31	
(OH ₂)6	2 <i>a</i>	-6..	0	0	$\frac{1}{4}$	0.37	

Transformation from published data: $y, x, -z$ Experimental: powder, diffractometer, X-rays, $R_B = 0.039$

Remarks: 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. The same data are also reported in [2], where the composition is given as $\text{H}_{1.0}\text{Mo}_{5.35}\text{O}_{17.35}\text{H}_{1.6}\cdot 1.7\text{H}_2\text{O}$.

References: [1] Guo J., Zavalij P., Whittingham M.S. (1994), Eur. J. Solid State Inorg. Chem. 31, 833-842. [2] Guo J., Zavalij P., Whittingham M.S. (1995), J. Solid State Chem. 117, 323-332.