

[NH₄]_{0.5}Mo₃O₉

*hP*28

(176) *P*6₃/*m* – h⁴e

NH₄Mo₆O₁₈ [1], HMB (hexagonal molybdenum bronze)

Structural features: Double infinite chains of edge-linked MoO₆ octahedra share vertices to form a 3D-framework; NH₄ in channels parallel to [001] (partial disorder).

Jiang C.C. et al. (1999) [1]

H₂Mo₃N_{0.50}O₉

a = 1.0576, *c* = 0.3728 nm, *c/a* = 0.352, *V* = 0.3611 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> ..	0.0091	0.2743	¹ / ₄		single atom Mo
Mo2	6 <i>h</i>	<i>m</i> ..	0.1046	0.4593	¹ / ₄		octahedron O ₆
O3	6 <i>h</i>	<i>m</i> ..	0.2828	0.4989	¹ / ₄		single atom Mo
O4	6 <i>h</i>	<i>m</i> ..	0.5797	0.0792	¹ / ₄		non-colinear Mo ₂
(NH ₄)5	4 <i>e</i>	3..	0	0	0.105	0.25	

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, *R* = 0.034, *T* = 296 K

Remarks: We assigned an approximate value to the occupancy of site (NH₄)5 based on the nominal composition. 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] Jiang C.C., Liu G., Wei Y.G., Wang W., Zhang S.W. (1999), *Inorg. Chem. Commun.* 2, 258-260.