

Cs_{0.42}Mo₃O₉*hP26*(176) *P6₃/m – h⁴a***Cs_{0.14}MoO₃** [1], HMB (hexagonal molybdenum bronze)Structural features: Double infinite chains of edge-linked MoO₆ octahedra share vertices to form a 3D-framework; Cs in channels parallel to [001] (partial disorder).

Depero L.E. et al. (1993) [1]

Cs_{0.39}Mo₃O₉ $a = 1.062$, $c = 0.3722$ nm, $c/a = 0.350$, $V = 0.3635$ 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> ..	0.011	0.2771	¹ / ₄		single atom Mo
Mo2	6 <i>h</i>	<i>m</i> ..	0.10547	0.46067	¹ / ₄		octahedron O ₆
O3	6 <i>h</i>	<i>m</i> ..	0.2821	0.4996	¹ / ₄		single atom Mo
O4	6 <i>h</i>	<i>m</i> ..	0.5802	0.0789	¹ / ₄		non-coplanar triangle Mo ₃
Cs5	2 <i>a</i>	-6..	0	0	¹ / ₄	0.39	

Experimental: single crystal, diffractometer, X-rays, R = 0.047

Remarks: Short interatomic distances for partly occupied site(s). Similar models with Cs in Wyckoff position 2*b* were tested and rejected.

References: [1] Depero L.E., Zocchi M., Zocchi F., Demartin F. (1993), J. Solid State Chem. 104, 209-214.