

Mo₁₅Se₁₉*hP*68(176) *P*6₃/*m* – i⁴h²fe**Mo₁₅Se₁₉ α** [1]

Structural features: Mo₆Se₈ units (a Mo₆ octahedron surrounded by a Se₈ cube) and Mo₉Se₁₁ units (two fused Mo₆Se₈ units) in an α-Nd type (d.h.c.p.) arrangement. Mo₆ and Mo₉ clusters.

Davis B.D., Robinson W.R. (1990) [1]

Mo₁₅Se₁₉*a* = 0.9450, *c* = 1.9600 nm, *c/a* = 2.074, *V* = 1.5158 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mo1	12 <i>i</i>	1	0.0205	0.1731	0.0607		bicapped square prism Se ₅ Mo ₅
Mo2	12 <i>i</i>	1	0.3115	0.4928	0.1327		bicapped square prism Se ₅ Mo ₅
Se3	12 <i>i</i>	1	0.3300	0.2922	0.0473		4-vertex polyhedron Mo ₄
Se4	12 <i>i</i>	1	0.3757	0.0013	0.1441		4-vertex polyhedron Mo ₄
Mo5	6 <i>h</i>	<i>m</i> ..	0.1615	0.5111	¹ / ₄		bicapped square prism Se ₄ Mo ₆
Se6	6 <i>h</i>	<i>m</i> ..	0.3021	0.3379	¹ / ₄		4-vertex polyhedron Mo ₄
Se7	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0314		non-coplanar triangle Mo ₃
Se8	4 <i>e</i>	3..	0	0	0.1618		non-coplanar triangle Mo ₃

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

Experimental: single crystal, diffractometer, X-rays, R = 0.050, T = 296 K

References: [1] Davis B.D., Robinson W.R. (1990), J. Solid State Chem. 85, 332-336.