

Rb₂Mo₁₅In_{1.6}S₁₉*hP*78(176) $P6_3/m - i^4h^3fe$ **Rb₂In_{1.6}Mo₁₅S₁₉** [1]

Structural features: Mo₆S₈ units (a Mo₆ octahedron surrounded by a S₈ cube) and Mo₉S₁₁ units (two fused Mo₆S₈ units) in an α -Nd type (d.h.c.p.) arrangement; In (partial disorder) and Rb between the units. Mo₆ and Mo₉ clusters.

Salloum D. et al. (2004) [1]

In_{1.61}Mo₁₅Rb₂S₁₉ $a = 0.95597$, $c = 1.89349$ nm, $c/a = 1.981$, $V = 1.4986$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mo1	12 <i>i</i>	1	0.16764	0.01258	0.05738		tricapped trigonal prism S ₅ Mo ₄
S2	12 <i>i</i>	1	0.28375	0.31296	0.05141		4-vertex polyhedron Mo ₄
S3	12 <i>i</i>	1	0.38538	0.02224	0.1369		4-vertex polyhedron Mo ₄
Mo4	12 <i>i</i>	1	0.50084	0.31919	0.13184		tricapped trigonal prism S ₅ Mo ₄
In5	6 <i>h</i>	<i>m</i> ..	0.05547	0.22147	¹ / ₄	0.536	tricapped trigonal prism S ₆ MoIn ₂
S6	6 <i>h</i>	<i>m</i> ..	0.36132	0.31765	¹ / ₄		trigonal bipyramid Mo ₄ In
Mo7	6 <i>h</i>	<i>m</i> ..	0.5042	0.16184	¹ / ₄		pseudo Frank-Kasper S ₄ Mo ₆ In
Rb8	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.12705		7-vertex polyhedron S ₇
S9	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.53389		non-coplanar triangle Mo ₃
S10	4 <i>e</i>	3..	0	0	0.15819		trigonal prism Mo ₃ In ₃

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 293 K

References: [1] Salloum D., Gougeon P., Roisnel T., Potel M. (2004), J. Alloys Compd. 383, 57-62.