

Rb₅Mo₂₇Se₃₁*hP*126(176) *P*6₃/*m* – i⁸h²f³ea**Rb₅Mo₂₇Se₃₁** [1]

Structural features: Mo₁₂Se₁₄ units (a Mo₁₂ cluster formed by three face-sharing Mo₆ octahedra, one Se above each edge and the terminal faces) and Mo₁₅Se₁₇ units (a Mo₁₅ cluster formed by four Mo₆ octahedra, one Se above each edge and the terminal faces) in an α Nd-type (d.h.c.p.) arrangement.

Picard S. et al. (2001) [1]

Mo₂₇Rb₅Se₃₁*a* = 0.95208, *c* = 3.75113 nm, *c/a* = 3.940, *V* = 2.9447 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	12 <i>i</i>	1	0.00033	0.37507	0.13433		4-vertex polyhedron Mo ₄
Mo2	12 <i>i</i>	1	0.15373	0.17004	0.02926		10-vertex polyhedron Se ₄ Mo ₆
Mo3	12 <i>i</i>	1	0.17057	0.02231	0.09098		tricapped trigonal prism Se ₅ Mo ₄
Se4	12 <i>i</i>	1	0.29239	0.33446	0.08554		4-vertex polyhedron Mo ₄
Se5	12 <i>i</i>	1	0.32978	0.03282	0.03114		4-vertex polyhedron Mo ₄
Se6	12 <i>i</i>	1	0.33561	0.29845	0.18969		4-vertex polyhedron Mo ₄
Mo7	12 <i>i</i>	1	0.49557	0.31212	0.12957		tricapped trigonal prism Se ₅ Mo ₄
Mo8	12 <i>i</i>	1	0.51375	0.16352	0.19044		10-vertex polyhedron Se ₄ Mo ₆
Se9	6 <i>h</i>	<i>m</i> ..	0.00258	0.37164	¹ / ₄		4-vertex polyhedron Mo ₄
Mo10	6 <i>h</i>	<i>m</i> ..	0.49652	0.31483	¹ / ₄		10-vertex polyhedron Se ₄ Mo ₆
Rb11	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.02324		pseudo Frank-Kasper Se ₁₀ Mo ₃
Rb12	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.18715		icosahedron Se ₉ Mo ₃
Se13	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.57612		non-coplanar triangle Mo ₃
Se14	4 <i>e</i>	3..	0	0	0.1446		non-coplanar triangle Mo ₃
Rb15	2 <i>a</i>	-6..	0	0	¹ / ₄		14-vertex Frank-Kasper Se ₁₁ Mo ₃

Experimental: single crystal, diffractometer, X-rays, *R* = 0.047, *T* = 293 K

References: [1] Picard S., Gougeon P., Potel M. (2001), Acta Crystallogr. C 57, 663-664.