

**Rb<sub>3</sub>Mo<sub>15</sub>Se<sub>17</sub>** [1]; Cs<sub>3</sub>Mo<sub>15</sub>Se<sub>17</sub> [2]

Structural features: Mo<sub>15</sub>Se<sub>17</sub> units (a Mo<sub>15</sub> cluster formed by four face-sharing Mo<sub>6</sub> octahedra, one Se above each edge and the terminal faces) in a Mg-type (h.c.p.) arrangement are interconnected via additional Mo-Se contacts to form a 3D-framework. See Fig. IV.79.

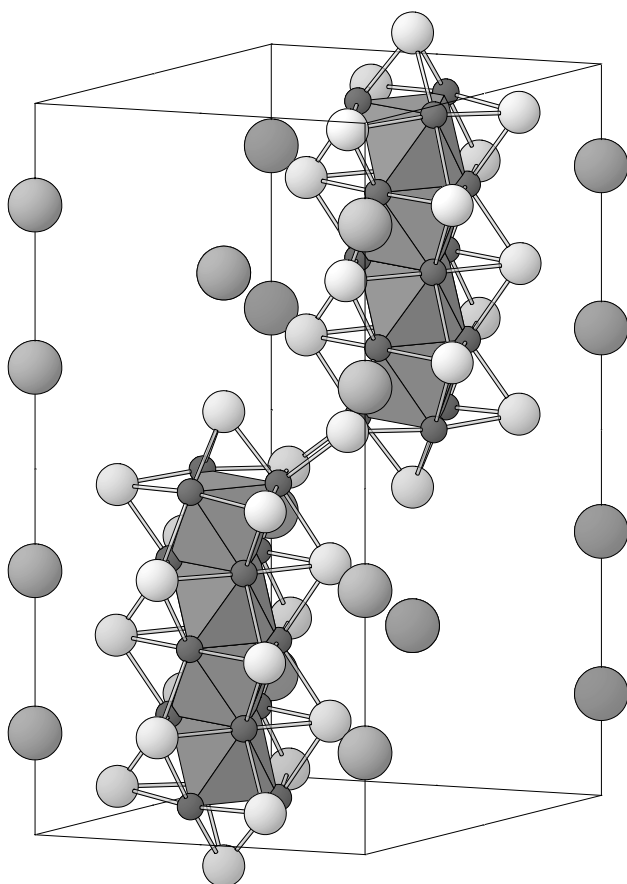


Fig. IV.79. **Rb<sub>3</sub>Mo<sub>15</sub>Se<sub>17</sub>**

Arrangement of Mo<sub>15</sub>Se<sub>17</sub> units (four Mo<sub>6</sub> octahedra, Mo atoms dark, Se atoms light) and Rb atoms (large).

Gougeon P. et al. (1989) [1]

Mo<sub>15</sub>Rb<sub>3</sub>Se<sub>17</sub>

$a = 0.94842$ ,  $c = 2.1006$  nm,  $c/a = 2.215$ ,  $V = 1.6363$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Se1	12i	1	0.3319	0.29061	0.04368		4-vertex polyhedron Mo <sub>4</sub>
Se2	12i	1	0.37042	0.00102	0.14243		4-vertex polyhedron Mo <sub>4</sub>
Mo3	12i	1	0.49605	0.31577	0.1438		bicapped square prism Se <sub>4</sub> Mo <sub>6</sub>
Mo4	12i	1	0.51704	0.16167	0.03502		tricapped trigonal prism Se <sub>5</sub> Mo <sub>4</sub>
Se5	6h	$m..$	0.3296	0.2942	$\frac{1}{4}$		4-vertex polyhedron Mo <sub>4</sub>
Mo6	6h	$m..$	0.5148	0.1623	$\frac{1}{4}$		bicapped square prism Se <sub>4</sub> Mo <sub>6</sub>
Se7	4f	3.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.06052		non-coplanar triangle Mo <sub>3</sub>
Rb8	4e	3.. $\frac{1}{3}$	0	0	0.13907		icosahedron Se <sub>9</sub> Mo <sub>3</sub>
Rb9	2c	-6.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		14-vertex Frank-Kasper Se <sub>11</sub> Mo <sub>3</sub>

Transformation from published data: origin shift  $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.021$ ,  $T = 295$  K

References: [1] Gougeon P., Potel M., Sergent M. (1989), *Acta Crystallogr. C* 45, 182-185. [2] Gougeon P., Potel M., Sergent M. (1989), *Acta Crystallogr. C* 45, 1413-1415.