

$K_{0.67}NbSe_2$	$hP8$	(187) $P-6m2 - h^2gfa$
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# $K_{0.67}NbSe_2$ [1]

Structural features: Directly superposed close-packed Se layers; Nb and K in trigonal prismatic voids.  $NbSe_6$  trigonal prisms share edges to form infinite slabs; K in trigonal prismatic voids between the slabs (stacking sequence BaB $\gamma$ BaB $\alpha$ ).

Omloo W.P.F.A.M., Jellinek F. (1970) [1]

$K_{0.67}NbSe_2$

$a = 0.348$ ,  $c = 1.704$  nm,  $c/a = 4.897$ ,  $V = 0.1787$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Se1	$2h$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.152		non-coplanar triangle Nb <sub>3</sub>
Se2	$2h$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.348		non-coplanar triangle Nb <sub>3</sub>
Nb3	$2g$	$3m.$	0	0	0.25		trigonal prism Se <sub>6</sub>
K4	$1f$	$-6m2$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$	0.667	anticuboctahedron Se <sub>6</sub> K <sub>6</sub>
K5	$1a$	$-6m2$	0	0	0	0.667	anticuboctahedron Se <sub>6</sub> K <sub>6</sub>

Transformation from published data:  $-x,-y,-z$ ; origin shift  $\frac{2}{3} \frac{1}{3} 0$

Experimental: powder, film, X-rays

Remarks: Structure type referred to as  $\eta-A_pMX_2$  type; in the isopointal so-called  $\zeta_2-A_pMX_2$  (or  $\xi_2-A_pMX_2$ ) type A and M are interchanged.

References: [1] Omloo W.P.F.A.M., Jellinek F. (1970), J. Less-Common Met. 20, 121-129.