$NbSe_2$	*hP*12	(187) *P*-6*m*2 – i^2hg^2da

$NbSe_2$ 4s(d) [1]
Structural features: Close-packed Se layers in AACACCAC stacking; Nb in trigonal prismatic and octahedral voids (stacking sequence AbA CbA CaC AbC). Layer structure with two kinds of sandwich consisting of three sublayers each: infinite slabs of edge-linked $NbSe_6$ trigonal prisms and infinite slabs of edge-linked $NbSe_6$ octahedra.

Kadijk F., Jellinek F. (1971) [1]
$NbSe_2$
$a = 0.348$, $c = 2.545$ nm, $c/a = 7.313$, $V = 0.2669$ nm^3, $Z = 4$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Se1	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.0625		non-coplanar triangle Nb_3
Se2	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.3125		non-coplanar triangle Nb_3
Nb3	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.25		octahedron Se_6
Se4	2*g*	3*m*.	0	0	0.1875		non-coplanar triangle Nb_3
Se5	2*g*	3*m*.	0	0	0.4375		non-coplanar triangle Nb_3
Nb6	1*d*	-6*m*2	$^1/_3$	$^2/_3$	$^1/_2$		trigonal prism Se_6
Nb7	1*a*	-6*m*2	0	0	0		trigonal prism Se_6

Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ $^1/_2$
Experimental: powder, film, X-rays, T = 1223 K

Remarks: Phase stable at 1183 < T < 1253 K. An alternative model in space group (156) *P*3*m*1 gave similar agreement.

References: [1] Kadijk F., Jellinek F. (1971), J. Less-Common Met. 23, 437-441.