$Nb_{1.1}Se_2$	*hP*8	(187) *P*-6*m*2 – ihgda

$Nb_{1.1}Se_2$ 2s(b) [1]
Structural features: Close-packed Se layers in BBCC stacking; Nb mainly in trigonal prismatic but also in octahedral voids. $NbSe_6$ trigonal prisms share edges to form infinite slabs; additional Nb in octahedral voids between the slabs (stacking sequence BaB α CbC α).

Huisman R. et al. (1967) [1]
$Nb_{1.10}Se_2$
$a = 0.3454$, $c = 1.258$ nm, $c/a = 3.642$, $V = 0.1300$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Se1	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.375		octahedron Nb_6
Se2	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.125		trigonal prism Nb_6
Nb3	2*g*	3*m*.	0	0	0.25	0.1	octahedron Se_6
Nb4	1*d*	-6*m*2	$^1/_3$	$^2/_3$	$^1/_2$		trigonal prism Se_6
Nb5	1*a*	-6*m*2	0	0	0		trigonal prism Se_6

Transformation from published data: *-x*,*-y*,*-z*
Experimental: powder, film, X-rays

Remarks: Homogeneity range Nb_xSe_2, $1.05 < x < 1.10$. We assigned an approximate value to the occupancy of site Nb3 based on the nominal composition.

References: [1] Huisman R., Kadijk F., Jellinek F. (1967), J. Less-Common Met. 12, 423-424.