

NbSe ₂	<i>hP</i> 12	(187) <i>P</i> -6 <i>m</i> 2 – <i>ih</i> ² <i>g</i> ² <i>f</i> <i>a</i>
-------------------	--------------	---

NbSe₂ 4s(a) [2]

Structural features: Close-packed Se layers in AABBCBB stacking; Nb in trigonal prismatic voids (stacking sequence AcA BaB CaC BaB). NbSe₆ trigonal prism share edges to form infinite slabs. Layer structure with sandwiches consisting of three sublayers (Se-Nb-Se).

Brown B.E., Beerntsen D.J. (1965) [1]

NbSe₂

a = 0.344, *c* = 2.524 nm, *c/a* = 7.337, *V* = 0.2587 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	2 <i>i</i>	3 <i>m</i> .	² / ₃	¹ / ₃	0.066		non-coplanar triangle Nb ₃
Se2	2 <i>h</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.185		non-coplanar triangle Nb ₃
Se3	2 <i>h</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.318		non-coplanar triangle Nb ₃
Nb4	2 <i>g</i>	3 <i>m</i> .	0	0	0.250		trigonal prism Se ₆
Se5	2 <i>g</i>	3 <i>m</i> .	0	0	0.432		non-coplanar triangle Nb ₃
Nb6	1 <i>f</i>	-6 <i>m</i> 2	² / ₃	¹ / ₃	¹ / ₂		trigonal prism Se ₆
Nb7	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		trigonal prism Se ₆

Transformation from published data: -*x*, -*y*, -*z*

Experimental: single crystal, precession and Weissenberg photographs, X-rays, *R* = 0.144

References: [1] Brown B.E., Beerntsen D.J. (1965), Acta Crystallogr. 18, 31-36. [2] Kaduk F., Huisman R., Jellinek F. (1964), Recl. Trav Chim. Pays-Bas 83, 768-775.