

$\text{Ti}_{0.35}\text{Nb}_3\text{Se}_4$	$hP16$	(176) $P6_3/m - h^2db$
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$\text{Ti}_{0.7}\text{Nb}_6\text{Se}_8$ [1]; $\text{K}_{0.52}\text{Ti}_6\text{Se}_8$ rt [2]

Structural features: Units of three face-linked NbSe_6 octahedra share edges to form a 3D-framework; Ti in channels of hexagonal cross-section parallel to [001] (partial disorder). Filled-up derivative of Nb_3Te_4 .

Boiler H., Klepp K. (1983) [1]

$\text{Nb}_3\text{Se}_4\text{Ti}_{0.35}$

$a = 1.0033$, $c = 0.3475$ nm, $c/a = 0.346$, $V = 0.3029$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Nb1	$6h$	$m..$	0.1078	0.487	$\frac{1}{4}$		8-vertex polyhedron Se_6Nb_2
Se2	$6h$	$m..$	0.2798	0.3399	$\frac{1}{4}$		4-vertex polyhedron Nb_4
Se3	$2d$	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		trigonal prism Nb_6
Ti4	$2b$	$-3..$	0	0	0	0.35	colinear Ti_2

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.055$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Boiler H., Klepp K. (1983), Mater. Res. Bull. 18, 437-442. [2] Bensch W., Koy J. (1992), Z. Kristallogr. 202, 298-299.