

Nb _{1.88} S ₃	<i>hP20</i>	(182) <i>P6₃22</i> – ifca
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Nb_{1.25}S₂ [1]

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic and octahedral voids. Infinite slabs of edge-linked NbS₆ trigonal prisms are interconnected via NbS₆ octahedra (partial disorder) to form a 3D-framework.

Huster J., Franzen H.F. (1985) [1]

Nb_{1.88}S₃

$a = 0.5785$, $c = 1.2229$ nm, $c/a = 2.114$, $V = 0.3544$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	12 <i>i</i>	1	0.333	0.003	0.1288		4-vertex polyhedron Nb ₄
Nb2	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5014		trigonal prism S ₆
Nb3	2 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.75	octahedron S ₆
Nb4	2 <i>a</i>	32.	0	0	0		trigonal prism S ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.048

Remarks: In the text of [1] the *a*-parameter is misprinted as 5.765 Å instead of 5.785 Å (given in table 1; checked on interatomic distances).

References: [1] Huster J., Franzen H.F. (1985), J. Less-Common Met. 113, 119-126.