$Nb_{0.92}S$	*hP*16	(186) $P6_3mc$ – c^2ba

$Nb_{1-x}S$ rt [1]; FeS ht [2]; MoN [3]
Structural features: Distorted close-packed S layers in h stacking; Nb in octahedral voids. Deformation derivative of NiAs with distortions towards the formation of Nb_3 triangular clusters.

Kadijk F., Jellinek F. (1969) [1]
$Nb_{0.92}S$
a = 0.6702, c = 0.6405 nm, c/a = 0.956, V = 0.2492 nm^3, Z = 8

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Nb1	6*c*	.*m*.	0.4785	0.5215	0.0		8-vertex polyhedron S_6Nb_2
S2	6*c*	.*m*.	0.8364	0.1636	0.25		trigonal prism Nb_6
S3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.25		trigonal prism Nb_6
Nb4	2*a*	3*m*.	0	0	0.0	0.68	octahedron S_6

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Phase stable at T < 1013-1053 K. Idealized z-coordinates. Additional reflections could be indexed with a 3-fold supercell (new axes 2a+b,-a+b,c). A structure proposal for MoN in space group (194) $P6_3/mmc$ ([4]; only Mo located) is superseded in [3]. A report on ht-FeS with orthorhombic FeAs-type structure [5] is superseded in [2]. In [1] the z-coordinate of former S(2) is misprinted as $^1/_4$ instead of $^3/_4$ (from the description of the structure).

References: [1] Kadijk F., Jellinek F. (1969), J. Less-Common Met. 19, 421-430. [2] Keller Besrest F., Collin G. (1990), J. Solid State Chem. 84, 194-210. [3] Bezinge A., Yvon K., Müller J., Lengauer V., Ettmayer P. (1987), Solid State Commun. 63, 141-145. [4] Schönberg N. (1954), Acta Chem. Scand. 8, 204-207. [5] King H.E. Jr., Prewitt C.T. (1982), Acta Crystallogr. B 38, 1877-1887.