Nb_4MnS_8	*hP*26	(176) $P6_3/m$ – ihfba

$MnNb_4S_8$ [1]
Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic (stacking sequence BaB CaC), Mn in octahedral voids. Infinite slabs of edge-linked NbS_6 trigonal prisms share faces with MnS_6 octahedra to form a 3D-framework (infinite linear -Mn-Nb- chains parallel to [001]).

Anzenhofer K., De Boer J.J. (1971) [1]
$Mn_{0.95}Nb_4S_8$
a = 0.6674, c = 1.2526 nm, c/a = 1.877, V = 0.4832 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12*i*	1	0.3387	0.1683	0.1261		4-vertex polyhedron Nb_3Mn
Nb2	6*h*	*m*..	0.0126	0.5067	$^1/_4$		trigonal prism S_6
S3	4*f*	3..	$^1/_3$	$^2/_3$	0.122		non-coplanar triangle Nb_3
Mn4	2*b*	-3..	0	0	0	0.948	octahedron S_6
Nb5	2*a*	-6..	0	0	$^1/_4$		trigonal prism S_6

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.045

Remarks: Space groups (182) $P6_322$ and (194) $P6_3/mmc$ were tested and rejected.

References: [1] Anzenhofer K., De Boer J.J. (1971), Recl. Trav. Chim. Pays-Bas 90, 56-64.