

NiS	<i>hP4</i>	(186) <i>P6₃mc</i> – ba
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NiS It [1]

Structural features: Close-packed S layers (slightly puckered) in h stacking; Ni occupies all octahedral voids. SNi₆ trigonal prisms share edges to form a 3D-framework. Deformation derivative of NiAs.

Trahan J. et al. (1970) [1]

NiS

$a = 0.34456$, $c = 0.5405$ nm, $c/a = 1.569$, $V = 0.0556$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.225		trigonal prism Ni ₆
Ni2	<i>2a</i>	<i>3m.</i>	0	0	0.0		8-vertex polyhedron S ₆ Ni ₂

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

Experimental: powder, diffractometer, X-rays, R = 0.049, T = 77 K

Remarks: Phase stable at T < 266 K. Space group (194) *P6₃/mmc* was tested and rejected (R = 0.052).

References: [1] Trahan J., Goodrich R.G., Watkins S.F. (1970), Phys. Rev. B: Solid State 2, 2859-2863.