

$W_{1.2}N$ $hP6$ $(186) P6_3mc - b^3$ **$W_{1.2}N$ [1]**

Structural features: Close-packed W layers in BBCC stacking with disordered vacancies in every second layer; N in trigonal prismatic voids (stacking sequence BcB CbC). Vacancy derivative of $2H-MoS_2$ antitype.

Khitrova V.I. (1964) [1]

NW_{1.20} $a = 0.289$, $c = 1.08$ nm, $c/a = 3.737$, $V = 0.0781$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
W1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0		non-coplanar triangle N ₃
W2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.25	0.2	non-coplanar triangle N ₃
N3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.625		trigonal prism W ₆

Transformation from published data ($P31c$): origin shift 0 0 0.12500Experimental: thin film, electron diffraction, $R = 0.269$

Remarks: Phase referred to as $\delta(IV)_H$. Idealized coordinates. The description in space group (159) $P31c$ in [1] does not take into consideration all symmetry elements of the proposed structure; correct space group is (194) $P6_3/mmc$ if the two W sites have the same occupancy. A structure proposal for a phase with the same name and cell parameters but different composition ($W_{0.6}N$) had earlier been published by the same author in [2]. In [1] the Hermann-Mauguin symbol for the space group is misprinted as $P3-1c$ instead of $P31c$, the z -coordinate of the N site as $\frac{1}{4}$ instead of $\frac{3}{4}$ and the chemical formula as $W_{2.2}N_2$ instead of $W_{2.4}N_2$ (from the description of the structure).

References: [1] Khitrova V.I. (1964), Sov. Phys. Crystallogr. 8, 701-703 (Kristallografiya 8, 873-876). [2] Khitrova V.I., Pinsker Z.G. (1962), Sov. Phys. Crystallogr. 6, 712-719 (Kristallografiya 6, 882-891).