

$W_{0.6}N$	$hP8$	(186) $P6_3mc - b^3a$
------------	-------	-----------------------

# $W_{0.6}N$ [1]

Structural features: Close-packed W layers in BBCC stacking with disordered vacancies in every second layer; N in trigonal prismatic voids (stacking sequence BacB CabC).

Khitrova V.I., Pinsker Z.G. (1962) [1]

$NW_{0.60}$

$a = 0.289$ ,  $c = 1.08$  nm,  $c/a = 3.737$ ,  $V = 0.0781$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
N1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0		tricapped trigonal prism $N_3W_6$
W2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.375		non-coplanar hexagon $N_6$
W3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.625	0.2	non-coplanar hexagon $N_6$
N4	$2a$	$3m.$	0	0	0.0		tricapped trigonal prism $N_3W_6$

Transformation from published data ( $P6_3$ ): origin shift 0 0 0.25

Experimental: thin film, electron diffraction

Remarks: Phase referred to as  $\delta(IV)_H$ . 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 ( $W_{1.2}N$ ) was later published by the same author in [2]. In [1] the  $z$ -coordinate of former W(II) is misprinted as 0.375 instead of 0.875 (from the drawing in fig. 6).

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