

WMnN ₂	<i>hP8</i>	(186) <i>P6₃mc</i> – b ² a ²
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MnWN₂ [1]

Structural features: Close-packed W and Mn layers in hc stacking; N in octahedral and tetrahedral voids in alternating interlayers.

Grins J. et al. (1995) [1]

MnN₂W

$a = 0.29213$, $c = 1.0957$ nm, $c/a = 3.751$, $V = 0.0810$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.2		octahedron W ₃ Mn ₃
W2	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.6		octahedron N ₆
N3	<i>2a</i>	<i>3m.</i>	0	0	0.0		tetrahedron W ₃ Mn
Mn4	<i>2a</i>	<i>3m.</i>	0	0	0.3		tetrahedron N ₄

Transformation from published data: origin shift 0 0 0.2

Experimental: powder, diffractometer, X-rays, R = 0.120

Remarks: A partly disordered model in space group (194) *P6₃/mmc* was tested and rejected.

References: [1] Grins J., Käll P.O., Svensson G. (1995), J. Mater. Chem. 5, 571-575.