

δ_H^{II} -NW₂ Structure: AB2_hP9_164_ad_c2d-001

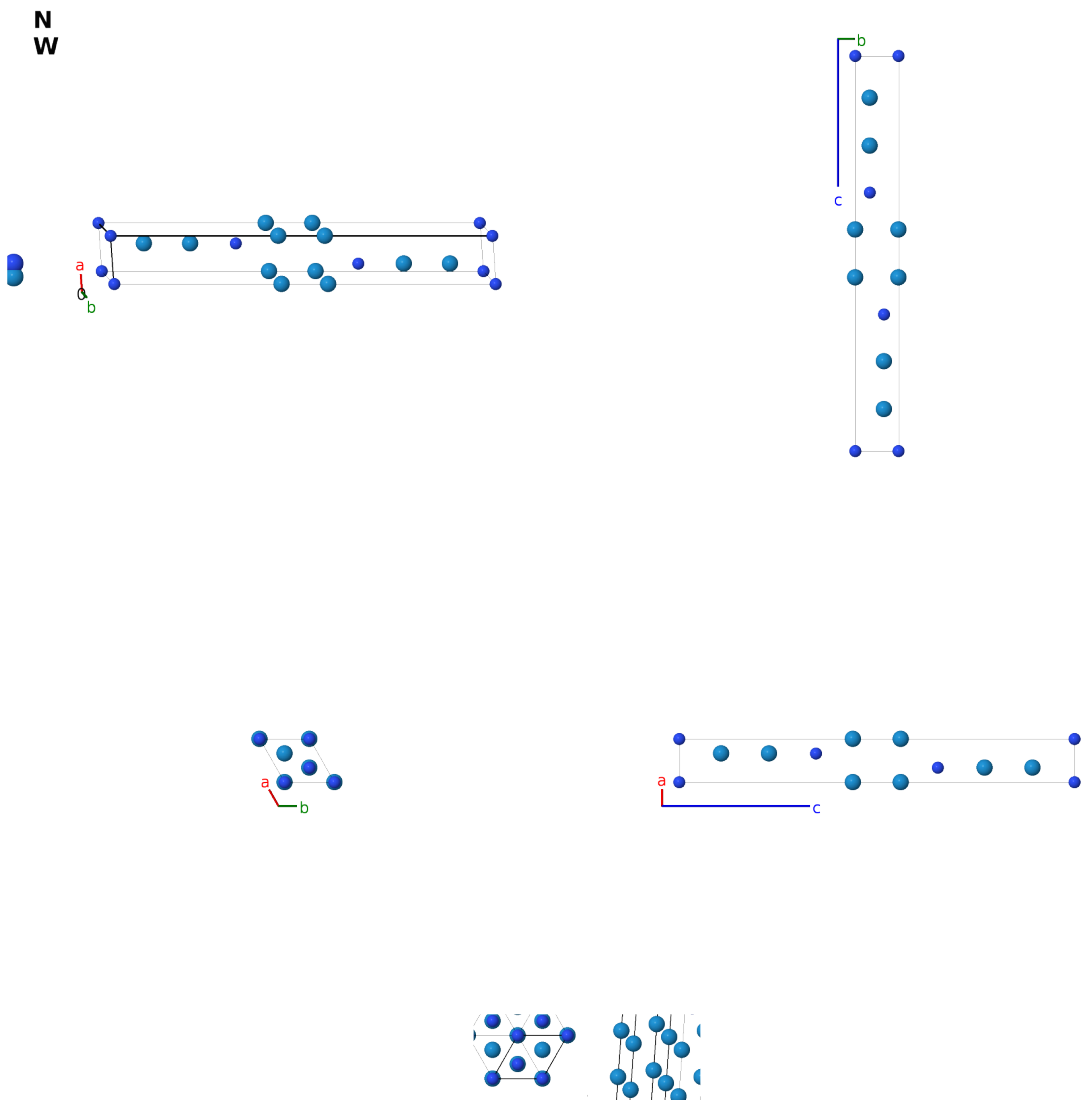
This structure previously used the label(s) **AB2_hP9_164_bd_c2d**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/Z07R>

https://aflow.org/prototype-encyclopedia/AB2_hP9_164_ad_c2d-001



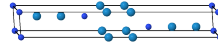
Prototype	NW ₂
AFLOW prototype label	AB2_hP9_164_ad_c2d-001
Pearson symbol	hP9

Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	<code>aflow --proto=AB2_hP9_164_ad_c2d-001</code> <code>--params=a, c/a, z₂, z₃, z₄, z₅</code>

- Khitrova and Pinkser put this structure in space group $P3$ #147, but the Wyckoff positions used are identical with space group $P3m1$ #164, so we assign this to the higher symmetry space group.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(1a)	N I
$\mathbf{B}_2$	$z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2c)	W I
$\mathbf{B}_3$	$-z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(2c)	W I
$\mathbf{B}_4$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2d)	N II
$\mathbf{B}_5$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2d)	N II
$\mathbf{B}_6$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2d)	W II
$\mathbf{B}_7$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2d)	W II
$\mathbf{B}_8$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2d)	W III
$\mathbf{B}_9$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(2d)	W III

References

- [1] V. I. Khitrova and Z. G. Pinkser, *Chemical Crystallography of Tungsten Nitrides and of Some Other Interstitial Phases*, Soviet Phys. Crystallogr. **6**, 712–719 (1962).

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