δ_H^{II}-NW_2 Structure: AB2_hP9_164_ad_c2d-001

This structure originally had the label `AB2_hP9_164_bd_c2d`. Calls to that address will be redirected here.

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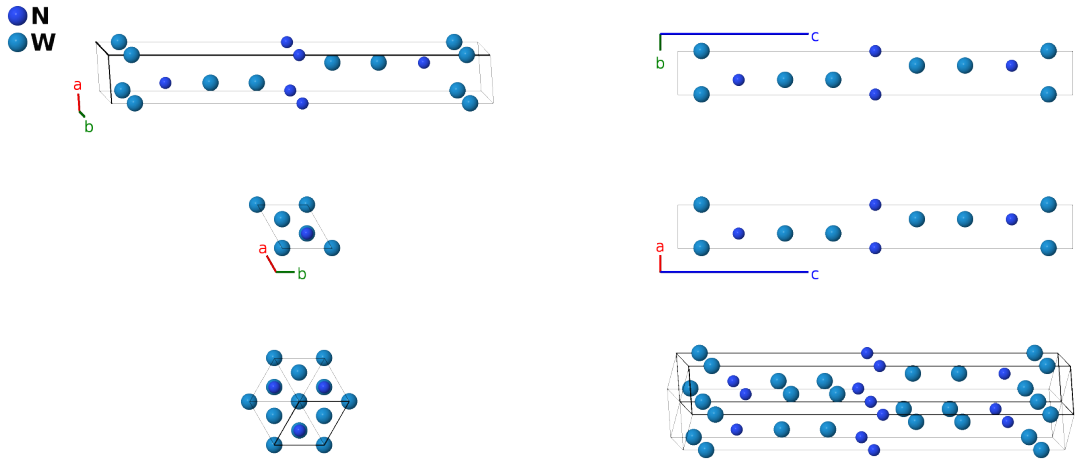
https://aflow.org/p/Z07R

https://aflow.org/p/AB2_hP9_164_ad_c2d-001

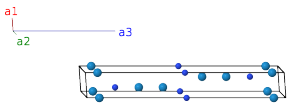


Prototype	NW_2
AFLOW prototype label	AB2_hP9_164_ad_c2d-001
ICSD	none
Pearson symbol	hP9
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=AB2_hP9_164_ad_c2d-001 --params=`$a, c/a, z_2, z_3, z_4, z_5$

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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).