ϵ-Hf_3N_2 Structure: AB_hR6_166_ac_bc-001

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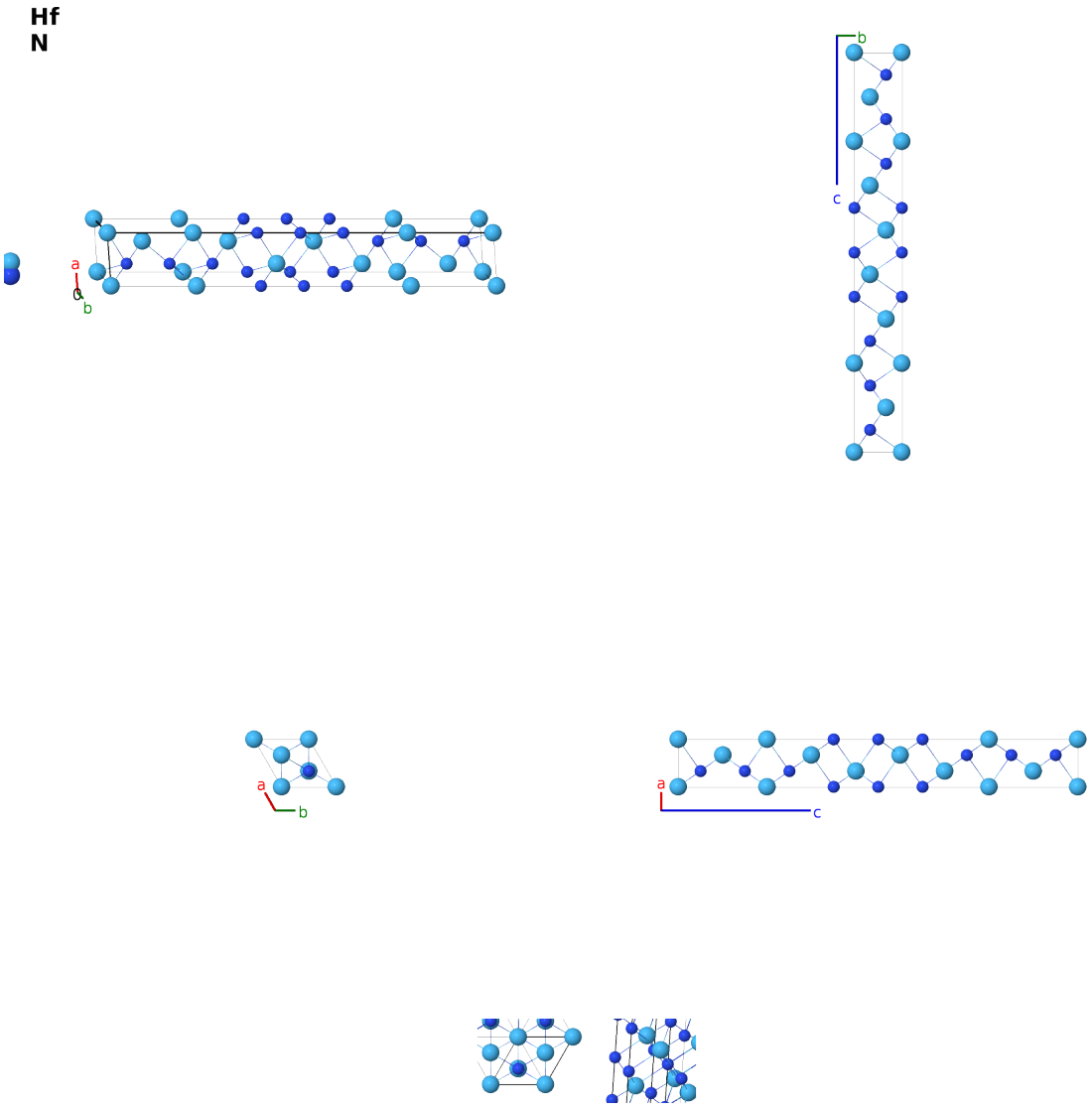
https://aflow.org/prototype-encyclopedia/LH0F

https://aflow.org/prototype-encyclopedia/AB_hR6_166_ac_bc-001



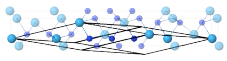
Prototype	Hf_3N_2
AFLOW prototype label	AB_hR6_166_ac_bc-001
ICSD	23572
CCDC	1599678

Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_hR6_166_ac_bc-001 --params=`$a, c/a, x_3, x_4$

- The Hf-N phase diagram has three known phases (Rudy, 1970; Villars, 2023):
  - HfN, stable up to the melting point of 3387°C, is in the NaCl ($B1$) structure.
  - ϵ-Hf_3N_2 is stable up to 1970°C.
  - ζ-Hf_4N_3 is stable in the range 1225-2300°C.
- Only 2/3 of the nitrogen sites are occupied, giving the observed stoichiometry.
- ϵ-Hf_3N_2 is also referred to as η-Hf_3N_2. We use the designation provide by (Rudy, 1970).
- Ta_2VC_2 is a ternary form of this structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Hf I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	N I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Hf II
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Hf II
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	N II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	N II

References

[1] E. Rudy, *The Crystal Structures of Hf_3N_2 and Hf_4N_3*, Metall. Trans. **1**, 1249–1252 (1970), doi:10.1007/BF02900238.

[2] P. Villars, ed., *PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database)* (Springer, Heidelberg, 2023), chap. Hf-N Binary Phase Diagram 0-100 at.% N c_0901275.

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