Re_3N Structure: AB3_hP4_187_a_bh-001

This structure originally had the label `AB3_hP4_187_e_fh`. Calls to that address will be redirected here.

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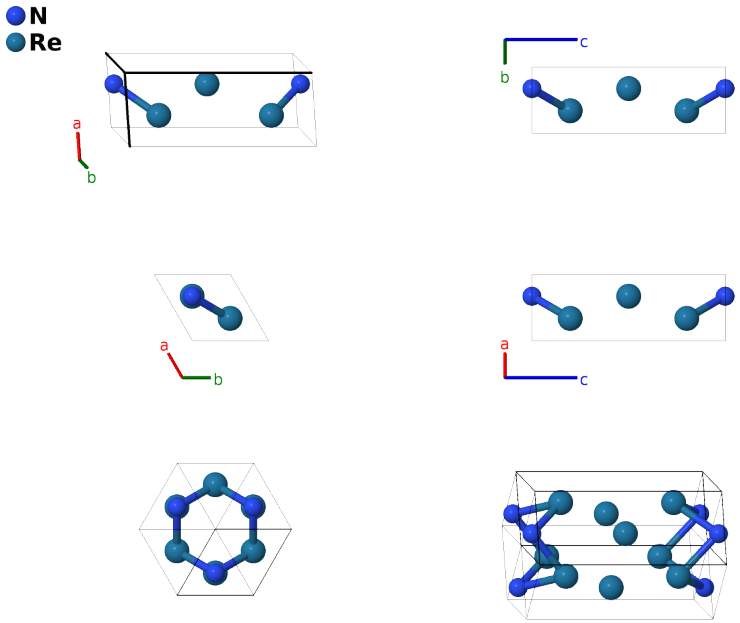
https://aflow.org/p/6BD5

https://aflow.org/p/AB3_hP4_187_a_bh-001

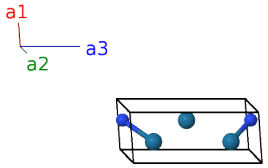


Prototype	NRe_3
AFLOW prototype label	AB3_hP4_187_a_bh-001
ICSD	169884
Pearson symbol	hP4
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=AB3_hP4_187_a_bh-001 --params=`$a, c/a, z_3$

- The reference presents both experimental findings and the results of density functional theory calculations. We obtain our data from the density functional theory calculations at equilibrium ($P = 0$), which are consistent with the lattice constants found experimentally.

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
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Re I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2h)	Re II
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2h)	Re II

References

[1] A. Friedrich, B. Winkler, L. Bayarjargal, W. Morgenroth, E. A. Juarez-Arellano, V. Milman, K. Refson, M. Kunz, and K. Chen, *Novel Rhenium Nitrides*, Phys. Rev. Lett. **105**, 085504 (2010), doi:10.1103/PhysRevLett.105.085504. August.