γ-N Structure: A_tP4_136_f-001

This structure previously used the label(s) `A_tP4_136_f`. Calls to these addresses will be redirected here.

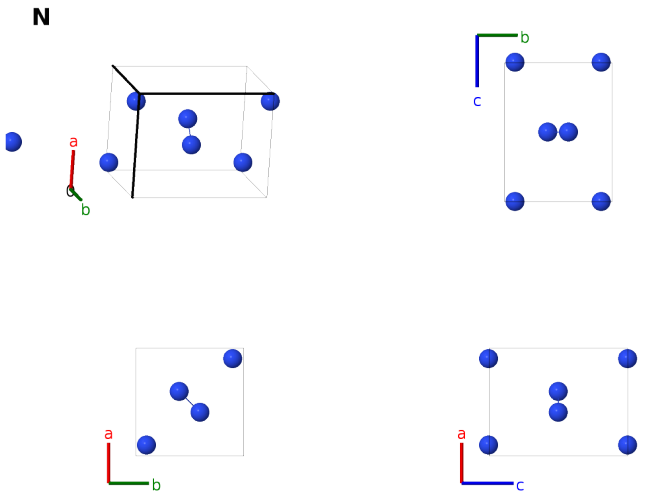
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/VJ5B

https://aflow.org/prototype-encyclopedia/A_tP4_136_f-001



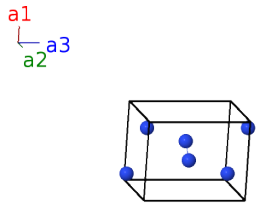
Prototype	N
AFLOW prototype label	A_tP4_136_f-001
ICSD	24891
CCDC	1600898
Pearson symbol	tP4
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	`aflow --proto=A_tP4_136_f-001 --params=`$a, c/a, x_1$

- Solid nitrogen is found in three forms (Mills, 1969; Donohue, 1974):
  - The ground state α-N structure, stable below 35.6K, found either in a centrosymmetric or a non-centrosymmetric cubic structure.
  - The hexagonal β-phase, which has freely rotating N_2 molecules and is stable up to the melting point, and
  - High-pressure γ-N, stable above 355 MPa.

- We use the data from (Mills, 1969) taken at 415 MPa and 20.5K.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(4f)	N I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}}$	(4f)	N I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	N I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	N I

References

[1] R. L. Mills and A. F. Schuch, *Crystal Structure of Gamma Nitrogen*, Phys. Rev. Lett. **23**, 1154–1156 (1969), doi:10.1103/PhysRevLett.23.1154.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017