α-N ($Pa\overline{3}$) Structure: A_cP8_205_c-001

This structure originally had the label `A_cP8_205_c`. Calls to that address will be redirected here.

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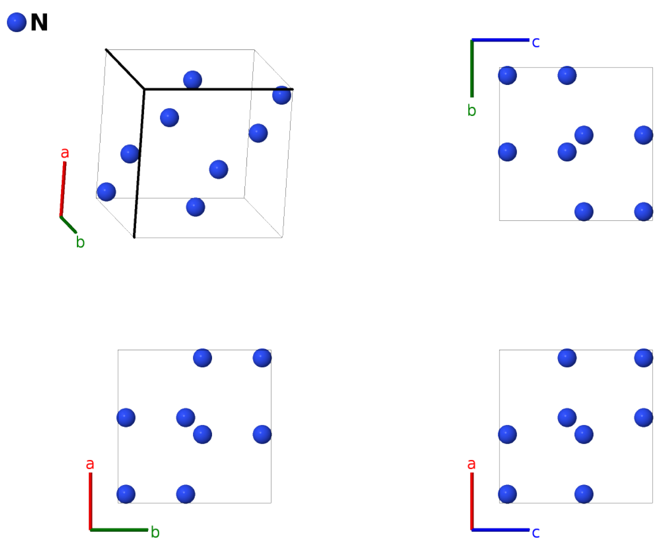
https://aflow.org/p/84Y3

https://aflow.org/p/A_cP8_205_c-001



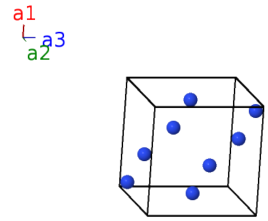
Prototype	N
AFLOW prototype label	A_cP8_205_c-001
ICSD	28179
Pearson symbol	cP8
Space group number	205
Space group symbol	$Pa\overline{3}$
AFLOW prototype command	`aflow --proto=A_cP8_205_c-001 --params=`a, x_1

- 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.
- There is considerable controversy about the crystal structure of α-N, as outlined in (Donohue, 1982, pp. 280-285). This page assumes the centrosymmetric $Pa\overline{3}$ #205 structure. The other possibility is the $P2_13$ #198 structure, where the N_2 dimers are offset from the inversion site. (Venables, 1974) makes a convincing case that the ground state is $Pa\overline{3}$, but we present both structures. Density Functional Theory calculations show no appreciable difference in energy between the Pa_3 and $P2_13$ structures. (Mehl, 2015)

- The ICSD entry for this structure is from (Venables, 1974).

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	N I

References

[1] T. H. Jordan, H. W. Smith, W. E. Streib, and W. N. Lipscomb, *Single-Crystal X-Ray Diffractions Studies of α-N_2 and β-N_2*, J. Chem. Phys. **41**, 756–759 (1964), doi:10.1063/1.1725956.

[2] 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.

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

[4] M. Ruhemann, *Röntgenographische Untersuchungen an festem Stickstoff und Sauerstoff*, Zeitschrift für Physik **76**, 368–385 (1932), doi:10.1007/BF01342540.

[5] J. A. Venables and C. A. English, *Electron diffraction and the structure of α-N_2*, Acta Crystallogr. Sect. B **30**, 929–935 (1974), doi:10.1107/S0567740874004067.

[6] M. J. Mehl, D. Finkenstadt, C. Dane, G. L. W. Hart, and S. Curtarolo, *Finding the stable structures of $N_{1-x}W_x$ with an* ab initio *high-throughput approach*, Phys. Rev. B **91**, 184110 (2015), doi:10.1103/PhysRevB.91.184110.

Found in

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