

Ammonia (NH₃, *D*0₁) Structure: A3B_cP16_198_b_a-001

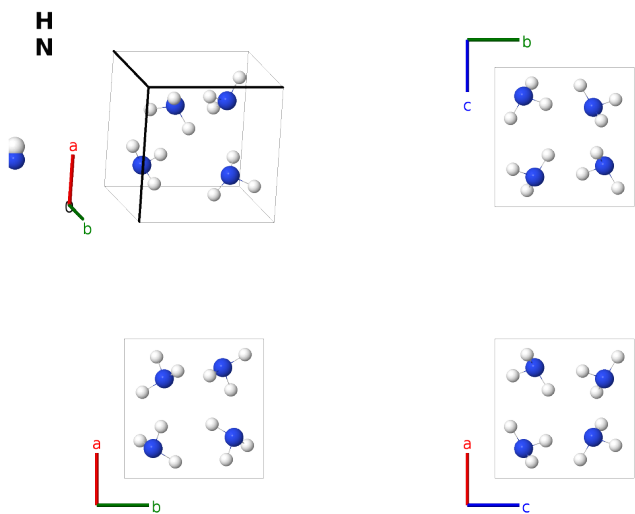
This structure previously used the label(s) **A3B_cP16_198_b_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/QTNQ>

https://aflow.org/prototype-encyclopedia/A3B_cP16_198_b_a-001



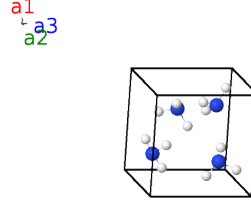
Prototype	H ₃ N
AFLOW prototype label	A3B_cP16_198_b_a-001
<i>Strukturbericht</i> designation	<i>D</i> 0 ₁
Mineral name	ammonia
ICSD	84461
CCDC	1644462
Pearson symbol	cP16
Space group number	198
Space group symbol	<i>P</i> 2 ₁ 3
AFLOW prototype command	<code>aflow --proto=A3B_cP16_198_b_a-001</code> <code>--params=<i>a</i>, <i>x</i>₁, <i>x</i>₂, <i>y</i>₂, <i>z</i>₂</code>

Other compounds with this structure
AsH₃, PH₃

- In the original *Strukturbericht* (Ewald, 1931) gave this structure the symbol *D1*. Following the revision of the type-*D* numbering beginning in volume II (Herman, 1937) this should be renamed *D0₁*. We previously used the *D1* designation, but now list this as *D0₁* for consistency with other *D*-type structures.

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_9$	$= z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{10}$	$= \left(z_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{11}$	$= -\left(z_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{12}$	$= -z_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-az_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{13}$	$= y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{14}$	$= -y_2 \mathbf{a}_1 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{15}$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(12b)	H I
$\mathbf{B}_{16}$	$= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 - z_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	H I

References

- [1] R. Boese, N. Niederprüm, D. Bläser, A. Maulitz, M. Y. Antipin, and P. R. Mallinson, *Single-Crystal Structure and Electron Density Distribution of Ammonia at 160 K on the Basis of X-ray Diffraction Data*, J. Phys. Chem. B **101**, 5794–5799 (1997), doi:10.1021/jp970580v.

- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
- [3] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

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