Ammonia (NH_3, $D0_1$) Structure: A3B_cP16_198_b_a-001

This structure originally had the label `A3B_cP16_198_b_a`. Calls to that address will be redirected here.

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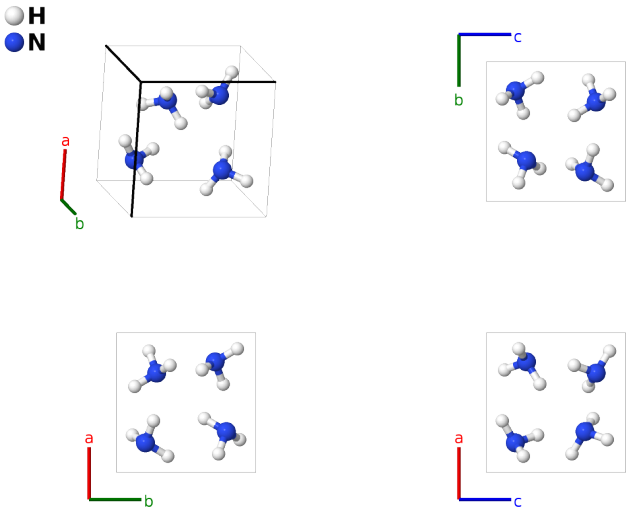
https://aflow.org/p/QTNQ

https://aflow.org/p/A3B_cP16_198_b_a-001



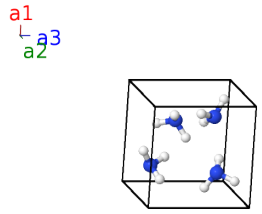
Prototype	H_3N
AFLOW prototype label	A3B_cP16_198_b_a-001
***Strukturbericht* designation**	$D0_1$
Mineral name	ammonia
ICSD	84461
Pearson symbol	cP16
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	`aflow --proto=A3B_cP16_198_b_a-001 --params=`a, x_1, x_2, y_2, z_2

Other compounds with this structure
AsH_3, PH_3

- 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 $D0_1$. We previously used the $D1$ designation, but now list this as $D0_1$ for consistency with other D-type structures.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(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).