NH_4HF_2 ($F5_8$) Structure: A2BC_oP16_53_eh_ab_g-001

This structure originally had the label `A2BC_oP16_53_eh_ab_g`. Calls to that address will be redirected here.

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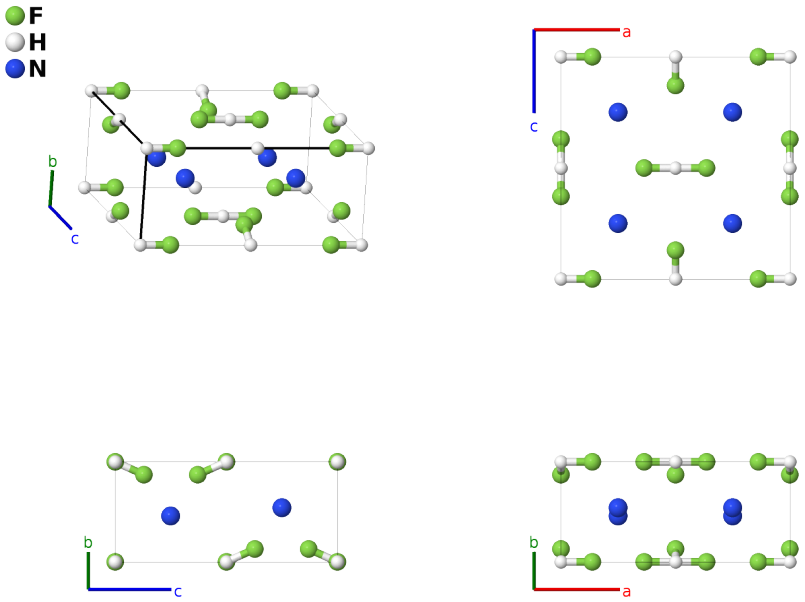
https://aflow.org/p/DCYY

https://aflow.org/p/A2BC_oP16_53_eh_ab_g-001



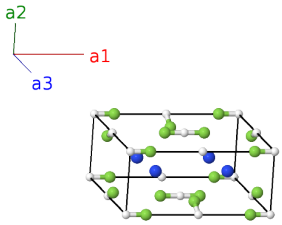
Prototype	F_2H_5N
AFLOW prototype label	A2BC_oP16_53_eh_ab_g-001
***Strukturbericht* designation**	$F5_8$
ICSD	28893
Pearson symbol	oP16
Space group number	53
Space group symbol	*Pmna*
AFLOW prototype command	`aflow --proto=A2BC_oP16_53_eh_ab_g-001 --params=`$a, b/a, c/a, x_3, y_4, y_5, z_5$

- This structure was first investigated by (Pauling, 1933) and assigned *Strukturbericht* designation $F5_8$ by (Gottfried, 1937). It was reinvestigated by (Rogers, 1940). Neither paper notes the positions of the hydrogen atoms, but under the assumption that the structure is similar to KHF_2 ($F5_2$), (Downs, 2003) puts some of them between pairs of fluorine atoms. The remaining hydrogen atoms are part of the NH_4 radical.

- The crystal structure was given in the *Pman* setting of space group #53. We used FINDSYM to change it to the standard *Pmna* structure.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	H I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	H II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	H II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1$	=	$ax_3\,\hat{\mathbf{x}}$	(4e)	F I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1$	=	$-ax_3\,\hat{\mathbf{x}}$	(4e)	F I
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B_{10}}$	=	$\frac{1}{4}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B_{12}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B_{13}}$	=	$y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4h)	F II
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	F II
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	F II
$\mathbf{B_{16}}$	=	$-y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4h)	F II

References

[1] M. T. Rogers and L. Helmholz, *A Redetermination of the Parameters in Ammonium Bifluoride*, J. Am. Chem. Soc. **62**, 1533–1536 (1940), doi:10.1021/ja01863a057.

[2] L. Pauling, *The Crystal Structure of Ammonium Hydrogen Fluoride, NH_4HF_2*, Z. Kristallogr. **85**, 380–391 (1933), doi:10.1524/zkri.1933.85.1.380.

[3] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).