

NH₄HF₂ (*F*5₈) Structure: A2BC_oP16_53_eh_ab_g-001

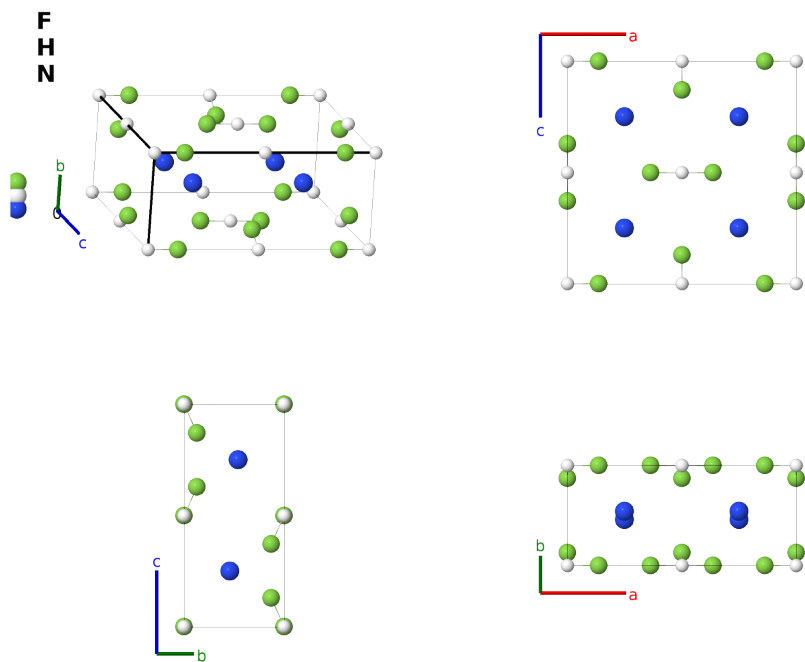
This structure previously used the label(s) **A2BC_oP16_53_eh_ab_g**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2BC_oP16_53_eh_ab_g-001



Prototype	F ₂ H ₅ N
AFLOW prototype label	A2BC_oP16_53_eh_ab_g-001
<i>Strukturbericht</i> designation	<i>F</i> 5 ₈
ICSD	28893
CCDC	1603927
Pearson symbol	oP16
Space group number	53
Space group symbol	<i>Pmna</i>
AFLOW prototype command	<code>aflow --proto=A2BC_oP16_53_eh_ab_g-001</code> <code>--params=a, b/a, c/a, x₃, y₄, y₅, z₅</code>

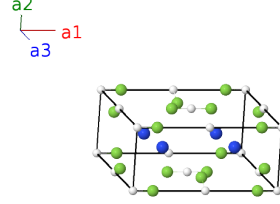
- This structure was first investigated by (Pauling, 1933) and assigned *Strukturbericht* designation $F5_8$ by (Gottfried, 1937). It was reinvestigated by (Rogers, 1940). Neither paper notes the positions of the hydrogen atoms, but under the assumption that the structure is similar to KHF_2 ($F5_2$), (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
$\mathbf{B}_5$	$x_3 \mathbf{a}_1$	$=$	$a x_3 \hat{\mathbf{x}}$	(4e)	F I
$\mathbf{B}_6$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B}_7$	$-x_3 \mathbf{a}_1$	$=$	$-a x_3 \hat{\mathbf{x}}$	(4e)	F I
$\mathbf{B}_8$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B}_9$	$\frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B}_{10}$	$\frac{1}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B}_{11}$	$\frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B}_{12}$	$\frac{3}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	NH I
$\mathbf{B}_{13}$	$y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4h)	F II
$\mathbf{B}_{14}$	$\frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	F II
$\mathbf{B}_{15}$	$\frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	F II
$\mathbf{B}_{16}$	$-y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-b y_5 \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(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).

First cited in

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.