

Author	Adrian, H.W.W.; Feil, D.
Title of Article	The structure of (N H <sub>4</sub> )F as determined by neutron and x-ray diffraction
Reference	Acta Crystallographica A (24,1968-38,1982) (1969) 25, p438-p443

N - H distances

Atom A	Ox	Wyck	Atom B	Ox	Wyck	Symmetry	Distance [Å]
N1	-3.00	2b	H1	+1.00	2b	x, y, z 555	0.962
N1	-3.00	2b	H2	+1.00	6c	x, y, z 555	0.871
			H2	+1.00	6c	x, x-y, z 555	0.871
			H2	+1.00	6c	-x+y, y, z 555	0.871

H - F distances

Atom A	Ox	Wyck	Atom B	Ox	Wyck	Symmetry	Distance [Å]
H1	+1.00	2b	F1	-1.00	2b	x, y, z 555	1.748
H2	+1.00	6c	F1	-1.00	2b	-x, -x+y, z+1/2 555	1.836

N - F distances

Atom A	Ox	Wyck	Atom B	Ox	Wyck	Symmetry	Distance [Å]
N1	-3.00	2b	F1	-1.00	2b	-x, -x+y, z+1/2 555	2.707
			F1	-1.00	2b	-x, -x+y, z+1/2 455	2.707
			F1	-1.00	2b	-x, -x+y, z+1/2 565	2.708
			F1	-1.00	2b	x, y, z 555	2.710

Struct. Formula	(N H <sub>4</sub> ) F
Space Group	P 63 m c (186)
Unit Cell	4.439(1) 4.439(1) 7.165(2) 90. 90. 120.
Cell Volume	122.27 Å <sup>3</sup>
Formula Units per Cell	2
Temperature	138 K
Pressure	atmospheric
PDF-numbers	01-073-1289 35-758
R-value	0.014

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Author	Calvert, L.D.; Whalley, E.
Title of Article	Structure of Ammonium Fluoride IV
Reference	Journal of Chemical Physics (1970) 53, p2151-p2155

N - F distances

Atom A	Ox	Wyck	Atom B	Ox	Wyck	Symmetry	Distance [Å]
N1	-3.00	4a	F1	-1.00	4b	$z, y+1/2, -x+1/2$ 545	2.885
			F1	-1.00	4b	$z+1/2, y, -x+1/2$ 455	2.885
			F1	-1.00	4b	$-z+1/2, -y+1/2, -x$ 555	2.885
			F1	-1.00	4b	$-z, y+1/2, x+1/2$ 444	2.885
			F1	-1.00	4b	$z+1/2, -y, x+1/2$ 444	2.885
			F1	-1.00	4b	$z+1/2, y+1/2, -x$ 444	2.885

Struct. Formula	(N H4) F
Space Group	F m $\bar{3}$ m (225)
Unit Cell	5.77(4) 5.77(4) 5.77(4) 90.90.90.
Cell Volume	192.10 Å <sup>3</sup>
Formula Units per Cell	4
Temperature	450 K
Pressure	40000 MPa
PDF-numbers	01-073-1216
R-value	No R value given in the paper