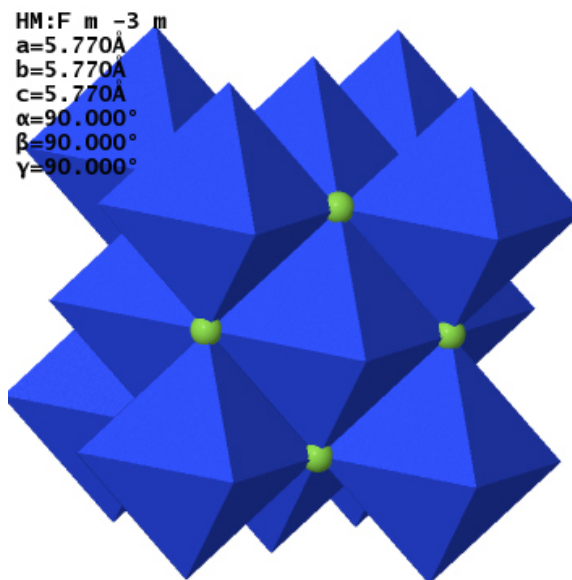


## Summary

Collection Code	23679
Struct Form	(N H4) F
Authors	Calvert, L.D.; Whalley, E.
Title of Article	Structure of Ammonium Fluoride IV.
Reference	Journal of Chemical Physics (1970) 53, p2151-p2155
Space Group	F m -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-Number	01-073-1216
R-Value	
Remark	
Warnings & Comments	Warnings / 1 Comments / 0

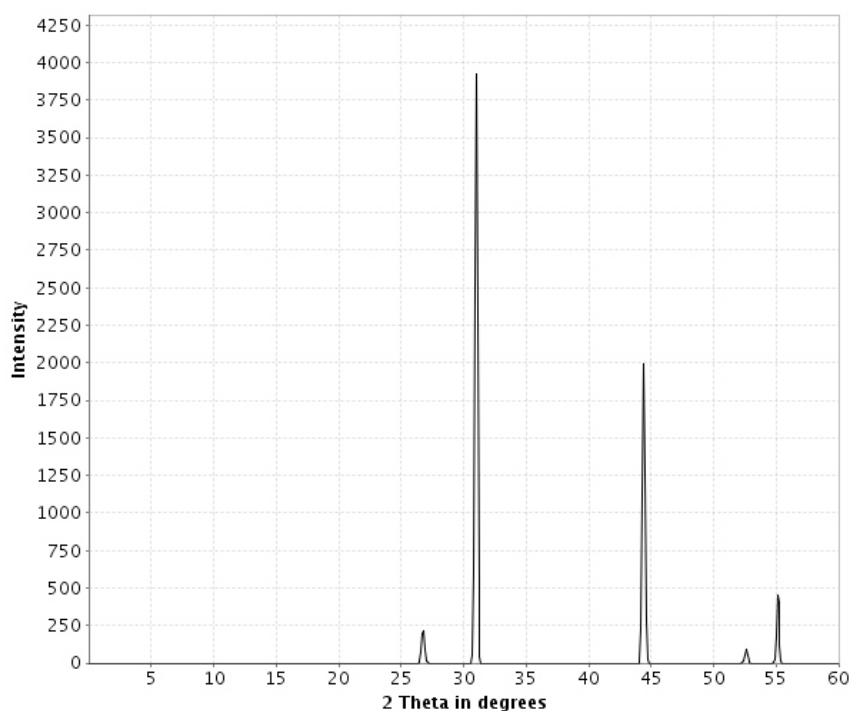
## Visualization

Published Crystal Structure



Ionic Radii [%] min: 80.0 max: 120.0

Powder Pattern



Radiation Type: X-Ray Diffractometer, Wave Length: 1.5418 Å

## Chemistry

Sum Form	H4 F1 N1
Struct Form	(N H4) F
Number of Formula Units	4
ANX Formula	XY
Cryst.Comp.	
AB Formula	AB
Chem.Comp.	
Chemical Name	Ammonium fluoride - IV
Mineral Name	
Mineral Group	

## Published Crystal Structure Data

Cell Parameters	a	5.77(4)
	b	5.77(4)
	c	5.77(4)
	$\alpha$	90.
	$\beta$	90.
	$\gamma$	90.
Volume		192.10
Space Group		F m -3 m
Formula Units per Cell		4
Crystal System		cubic
Laue Class		m-3m
Crystal Class		m-3m
Pearson Symbol		cF24
Wyckoff Sequence		b a
Calc Density		1.28
Meas Density		
Structure Type		NaCl
Axis Ratios	a/b	1.0000
	b/c	1.0000
	c/a	1.0000

Remark

EL	Lbl	OxState	WyckSymb	X	Y	Z	B	SOF	H
N	1	-3.00	4a	0	0	0	3.	1.	H4
F	1	-1.00	4b	0.5	0.5	0.5	3.		

## Standardized Crystal Structure Data

Cell Parameters	a	5.7700
	b	5.7700
	c	5.7700
	$\alpha$	90.000
	$\beta$	90.000
	$\gamma$	90.000
Volume		192.10
Space Group		F m $\bar{3}$ m
Formula Units per Cell		4
Crystal System		cubic
Laue Class		m-3m
Crystal Class		m-3m
Pearson Symbol		cF24
Wyckoff Sequence		b a
Calc Density		1.28
Structure Type		NaCl
Axis Ratios	a/b	1.0000
	b/c	1.0000
	c/a	1.0000
Transformation Method		Tidy
Transformation Info		Multiple transformations possible, first one selected
Remark		

EL	Lbl	OxState	WyckSymb	X	Y	Z	B	SOF
N	1	-3,00	4a	0.0000	0.0000	0.0000	3.0000	
F	1	-1,00	4b	0.5000	0.5000	0.5000	3.0000	

## Bibliography

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

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## Experimental Information

Temperature	450.00 K
Pressure	40000 MPa
Radiation Type	X-Ray
Sample Type	Powder
R-Value	
Additional Information	Rietveld refinement employed
Properties of Structure	

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## Warnings & Comments

Warnings	No R value given in the paper.
Comments	