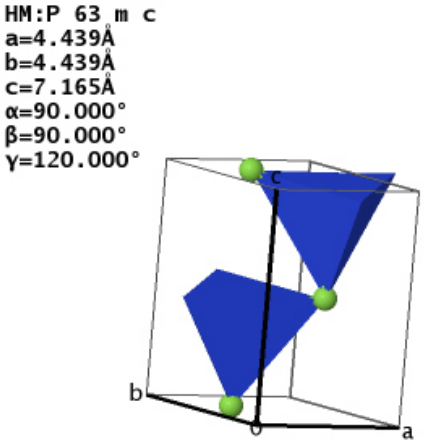
FIZ Karlsruhe ICSD

Summary

Collection Code	23765
Struct Form	(N H4) F
Authors	Adrian, H.W.W.; Feil, D.
Title of Article	The structure of (N H4) F as determined by neutron and x-ray diffraction
Reference	Acta Crystallographica A (24,1968-38,1982) (1969) 25, p438-p443
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 $Å^3$
Formula Units per Cell	2
Temperature	138 K
Pressure	atmospheric
PDF-Number	01-073-1289 35-758
R-Value	0.014
Remark	
Warnings & Comments	Warnings / 0 Comments / 0

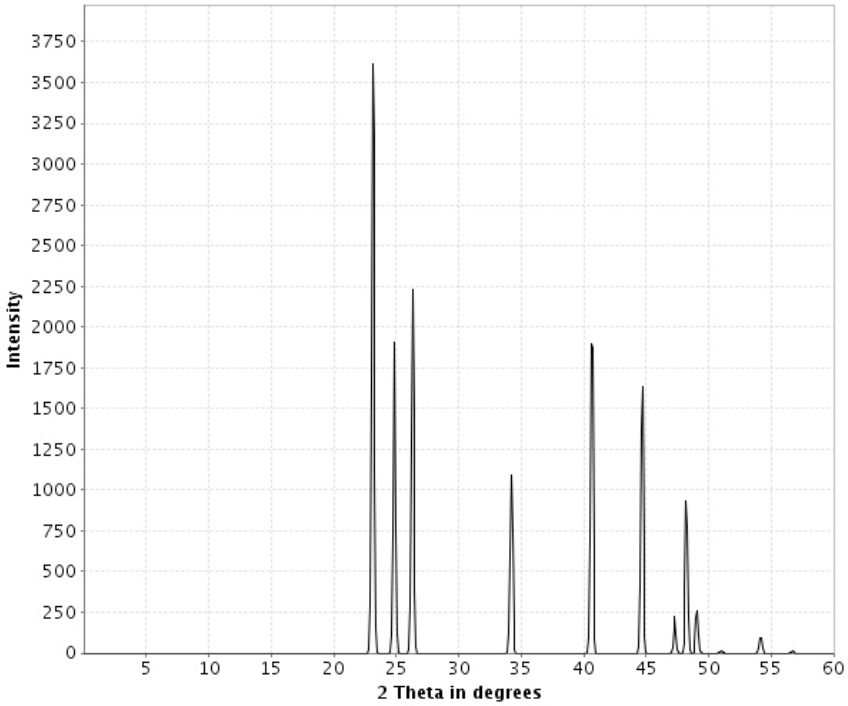
Visualization

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	2
ANX Formula Cryst.Comp.	XY
AB Formula Chem.Comp.	ABC4
Chemical Name	Ammonium fluoride
Mineral Name	
Mineral Group	

Published Crystal Structure Data

Cell Parameters	a	4.439(1)
	b	4.439(1)
	c	7.165(2)
	α	90.
	β	90.
	γ	120.
Volume		122.27
Space Group		P 63 m c
Formula Units per Cell		2
Crystal System		hexagonal
Laue Class		6/mmm
Crystal Class		6mm
Pearson Symbol		hP12
Wyckoff Sequence		b2
Calc Density		1.01
Meas Density		1.00
Structure Type		NH4F
Axis Ratios	a/b	1.0000
	b/c	0.6195
	c/a	1.6141
Remark		

EL	Lbl	OxState	WyckSymb	X	Y	Z	U	SOF	H
N	1	-3.00	2b	0.3333	0.6667	0.3782(3)	0.0129(4)	1.	H4
H	1	+1.00	2b	0.3333	0.6667	0.244(6)	0.018(5)		
H	2	+1.00	6c	0.441(3)	0.559(3)	0.416(2)	0.019(3)		
F	1	-1.00	2b	0.3333	0.6667	0			

EL	Lbl	U(1,1) [Å^2]	U(2,2) [Å^2]	U(3,3) [Å^2]	U(1,2) [Å^2]	U(1,3) [Å^2]	U(2,3) [Å^2]
N	1						
H	1						
H	2						
F	1	0.0122(5)	0.0122(5)	0.0133(6)	0.0061(3)	0	0

EL	Lbl	U(1,1) [Å^2]	U(2,2) [Å^2]	U(3,3) [Å^2]	U(1,2) [Å^2]	U(1,3) [Å^2]	U(2,3) [Å^2]

Standardized Crystal Structure Data

Cell Parameters	a	4.4390
	b	4.4390
	c	7.1650
	α	90.000
	β	90.000
	γ	120.000
Volume		122.27
Space Group		P 63 m c
Formula Units per Cell		2
Crystal System		hexagonal
Laue Class		6/mmm
Crystal Class		6mm
Pearson Symbol		hP12
Wyckoff Sequence		b2
Calc Density		1.01
Structure Type		NH4F
Axis Ratios	a/b	1.0000
	b/c	0.6195
	c/a	1.6141
Transformation Method		Tidy
Transformation Info		TRANS -x,-y,-z
Remark		

EL	Lbl	OxState	WyckSymb	X	Y	Z	U	SOF
N	1	-3,00	2b	0.3333	0.6667	0.1218	0.0129	
H	1	+1,00	2b	0.3333	0.6667	0.2560	0.0180	
H	2	+1,00	6c	0.4410	0.5590	0.0840	0.0190	
F	1	-1,00	2b	0.3333	0.6667	0.5000		

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Bibliography

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Experimental Information

Temperature	138.00 K
Pressure	0.101325 MPa (default)
Radiation Type	X-Ray
Sample Type	Single Crystal
R-Value	0.014
Additional Information	
Properties of Structure	

Warnings & Comments

Warnings	
Comments	