

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Jerome C. Birnbaum, Tyler O. Danby, Timothy J. Johnson, Molly Rose K. Kelly-Gorham, Rodica Lindenmaier, Tanya L. Myers

SAMPLE CONDITIONS & PHYSICAL PROPERTIES

Chemical name	Ammonium hydrogen difluoride
Chemical formula	H ₅ F ₂ N
Synonyms	Ammonium hydrogen fluoride; Ammonium bifluoride; Etching powder
CAS number	1341-49-7
Location of field sample	n/a
History of sample	n/a
Molecular Weight	57.04 g/mol
Melting Point	125 °C
Boiling Point	240 °C
Density (20° C)	1.5 g/cm ³
Hardness, Mohs scale	n/a
Crystallography:	
Cell dimension	a = Å b = Å c = Å
Crystal system	
H-M symbol (point gr)	
Space group	
H-M symbol (space gr)	
Crystal habit	
Color	White/Colorless
Diaphaneity	Translucent
Particle size	4036 ± 1017 µm
Particle size assessment	Optical microscopy
Supplier	Aldrich
Stated purity	99.999%
Date packed	05 August 2016 Weight: 1.225 grams
Synthesis method	n/a
Synthesis reference	n/a
Texture	Hard, wet, sticky crystals
Physical state	Solid
Surface roughness	n/a
Elemental composition	n/a
Isotopic composition	n/a
Moisture content	n/a
Temperature of sample	25 ± 2 °C
Substrate	n/a

INSTRUMENT PARAMETERS

IR Cube FT-IR manufactured by Bruker Optics

External diffuse reflectance accessory	A 562-G integrating sphere
Sphere diameter	75 mm
Angle to normal incidence	14.8°
Sphere opening diameter	19 mm (entrance port)
Spectral range	7,500 to 600 cm^{-1} saved; 7500 to 600 cm^{-1} reported
Beamsplitter	Ge on KBr
Detector (dia. Det. Port in sphere)	2×2 mm, 60° field of view MCT (550; 0.9); 1 cm
Apodization function	Blackman-Harris 3-term
Aperture	Open
Coadded scans	4096
Scanner speed	80 kHz
Switch gain on	512 points
Low pass filter	Open
Scan technique	double-sided, forward-backward
Non-linear correction	On
High and low folding limit	15800.54-0.00 cm^{-1}
Phase resolution	32.00
Phase correction mode	Mertz
Zerofilling	4×
Wavenumber accuracy	$\pm 0.4 \text{ cm}^{-1}$
Spectral resolution	4 cm^{-1}
Accuracy verification	11/17/2015
Wavelength vetted on:	ICL polystyrene standard #0009-7394-0025A, thin film
Reflectance:	$\pm 2\%$ using SRS reflectance standards 50-010-DH27B-4878

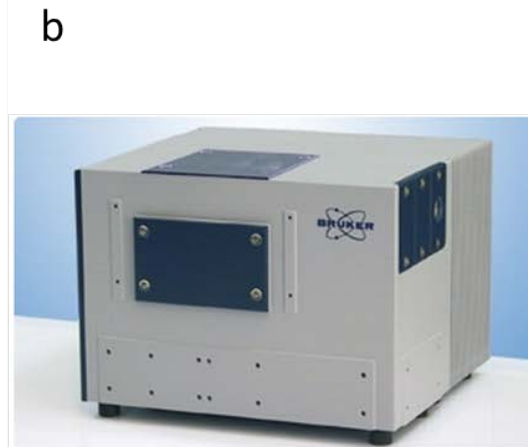
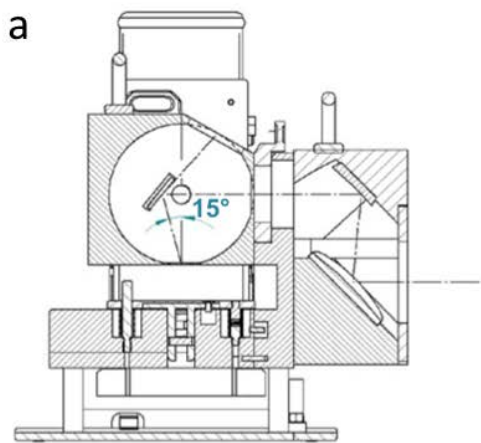


Figure 1: The Bruker 562-G integrating sphere (a) and IR Cube (b)

Photographs of sample Ammonium hydrogen difluoride



Figure 2: Ammonium hydrogen difluoride in Aldrich container.

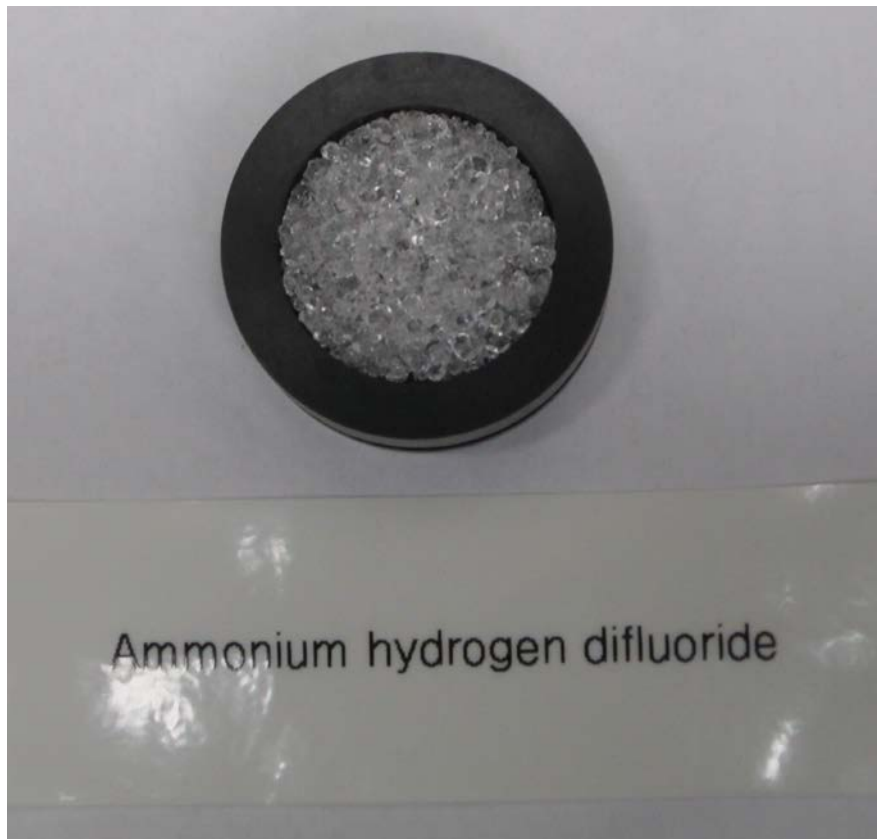


Figure 3: Ammonium hydrogen difluoride loaded in IR sample cup.

PARTICLE SIZE PREPARATION AND CHARACTERIZATION

Optical microscopy —

A Keyence VHX-1000 digital microscope with 16-bit resolution is used to provide photomicrographs of the various samples and particle sizes. Software included with the microscope differentiates the brightness and colors in the image and extracts the bright objects to produce a binary image. The software assumes all adjacent bright points are part of the same object then calculates the area for each of these objects. The area (A) is used to calculate the mean particle diameter (d) by assuming the particles are spherical and using the relationship $d = \sqrt{4A/\pi}$. Although the assumption of spherical particles is clearly not always valid, this procedure provides a reasonable estimate of the mean particle size. Only thirteen particles were examined under the microscope so a graph of the particle size distribution is not shown due to the limited number of particles used in the calculation.

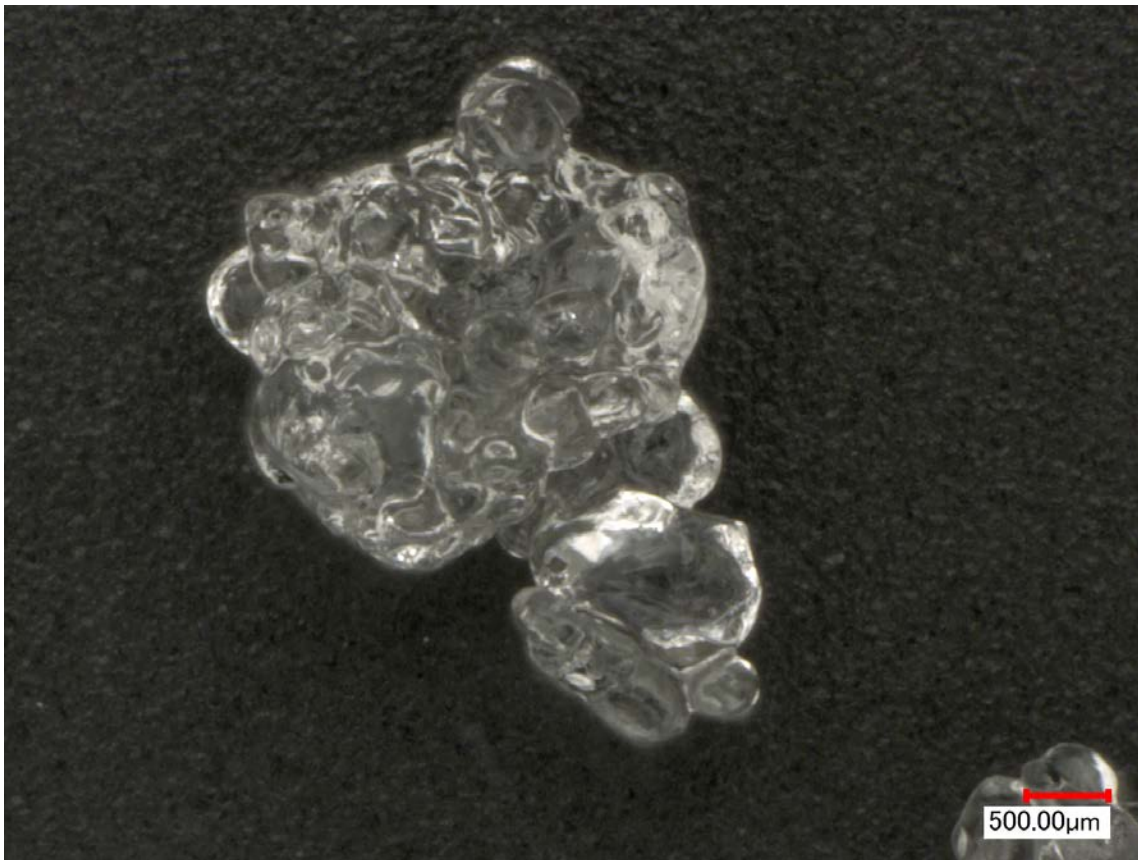


Figure 4: Photomicrograph of Ammonium hydrogen difluoride.

Only thirteen particles were examined under the microscope so a graph of the particle size distribution is not shown due to the limited number of particles used in the calculation.