

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	TNT
Chemical formula	$C_6H_2(NO_2)_3CH_3$ or $C_7H_5N_3O_6$
Synonyms	2,4,6-Trinitrotoluene; 2-Methyl-1,3,5-trinitrobenzene
CAS number	118-96-7
Location of field sample	n/a
History of sample	n/a
Molecular Weight	227.13 g/mole
Melting Point	80.8 °C
Boiling Point	240 °C (dec.)
Density (25 °C)	1.1 g/cm ³ (est.)
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	Yellow-orange
Diaphaneity	Opaque
Particle size	n/a
Particle size assessment	n/a
Supplier	Mil-Spec Industries (Lot #MS100M036-001)
Stated purity	99.5%
Date packed	23 February 2016 Weight: Approx. 1.4 grams
Synthesis method	n/a
Synthesis reference	n/a
Texture	Flakes and small nuggets of various sizes
Physical state	Solid
Surface roughness	n/a
Elemental composition	n/a
Isotopic composition	n/a
Moisture content	n/a
Temperature of sample	19 ± 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	6 mm
Coadded scans	2048
Scanner speed	40 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

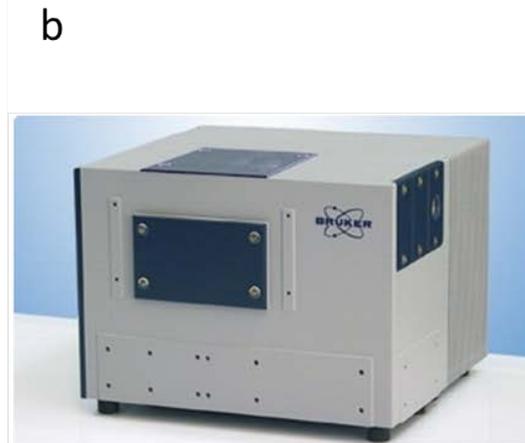
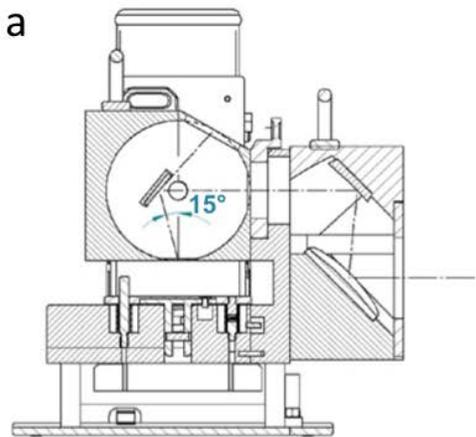


Figure 1: The Bruker 562-G integrating sphere (a) and IR Cube (b)

Photographs of sample TNT



Figure 2: TNT in IR sample cup with a volume of 1.25 cm³.