All data taken at Pacific Northwest National Laboratory (PNNL)

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**SAMPLE CONDITIONS & PHYSICAL PROPERTIES**

- **Chemical name:** 2,6-Dinitrotoluene
- **Chemical formula:** C₇H₆N₂O₄
- **Synonyms:** 2,6-DNT
- **CAS number:** 606-20-2
- **Location of field sample:** n/a
- **History of sample:** n/a
- **Molecular Weight:** 182.134 g/mole
- **Melting Point:** 56-61 °C
- **Boiling Point:** 285 °C
- **Density (25° C):** 1.32 g/cm³
- **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:** Off-white/pale yellow
- **Diaphaneity:** Sub-translucent to opaque
- **Particle size:** 157 ± 111 µm
- **Particle size assessment:** Optical microscopy
- **Supplier:** Aldrich
- **Stated purity:** 98%
- **Date packed:** 17 November 2015  
  **Weight:** 2.170 grams
- **Synthesis method:** n/a
- **Synthesis reference:** n/a
- **Texture:** Hard solid of irregularly shaped crystals
- **Physical state:** Crystalline solid
- **Surface roughness:** n/a
- **Elemental composition:** n/a
- **Isotopic composition:** n/a
- **Moisture content:** n/a
- **Temperature of sample:** 23 ± 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 ±0.4 cm⁻¹
Spectral resolution 4 cm⁻¹
Accuracy verification 11/17/2015

Wavelength vetted on: ICL polystyrene standard #0009-7394-0025A, thin film
Reflectance: ±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 2,6-Dinitrotoluene

Figure 2: 2,6-Dinitrotoluene in Aldrich container.

Figure 3: 2,6-Dinitrotoluene sample 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 \( d = (4 \times A / \pi)^{1/2} \). Although the assumption of spherical particles is clearly not always valid, this procedure provides a reasonable estimate of the mean particle size.

Figure 4: Photomicrograph of 2,6-Dinitrotoluene crystals.
Figure 5: Particle size distribution of 2,6-Dinitrotoluene crystals.