All data taken at Pacific Northwest National Laboratory (PNNL)

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**SAMPLE CONDITIONS & PHYSICAL PROPERTIES**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Chemical name</td>
<td>Naproxen sodium</td>
</tr>
<tr>
<td>Chemical formula</td>
<td>C_{14}H_{13}NaO_{3}</td>
</tr>
<tr>
<td>Synonyms</td>
<td>(S)-6-Methoxy-α-methyl-2-naphthaleneacetic acid sodium salt</td>
</tr>
<tr>
<td>CAS number</td>
<td>26159-34-2</td>
</tr>
<tr>
<td>Location of field sample</td>
<td>n/a</td>
</tr>
<tr>
<td>History of sample</td>
<td>n/a</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>252.24 g/mole</td>
</tr>
<tr>
<td>Melting Point</td>
<td>259-262 °C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>n/a</td>
</tr>
<tr>
<td>Density (25 °C)</td>
<td>n/a</td>
</tr>
<tr>
<td>Hardness, Mohs scale</td>
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</tr>
<tr>
<td>Crystallography:</td>
<td></td>
</tr>
<tr>
<td>Cell dimension</td>
<td>a = Å b = Å c = Å</td>
</tr>
<tr>
<td>Crystal system</td>
<td></td>
</tr>
<tr>
<td>H-M symbol (point gr)</td>
<td></td>
</tr>
<tr>
<td>Space group</td>
<td></td>
</tr>
<tr>
<td>H-M symbol (space gr)</td>
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</tr>
<tr>
<td>Crystal habit</td>
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</tr>
<tr>
<td>Color</td>
<td>White to off-white</td>
</tr>
<tr>
<td>Diaphaneity</td>
<td>Opaque</td>
</tr>
<tr>
<td>Particle size</td>
<td>17 ± 12 µm</td>
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<tr>
<td>Particle size assessment</td>
<td>Optical microscopy</td>
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<tr>
<td>Supplier</td>
<td>Alfa Aesar</td>
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<tr>
<td>Stated purity</td>
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</tr>
<tr>
<td>Date packed</td>
<td>9 November 2015</td>
</tr>
<tr>
<td>Synthesis method</td>
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<td>Synthesis reference</td>
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<tr>
<td>Texture</td>
<td>Powder with particles of different shapes</td>
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<tr>
<td>Physical state</td>
<td>Solid crystals</td>
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<td>Surface roughness</td>
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<tr>
<td>Elemental composition</td>
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<td>Isotopic composition</td>
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<tr>
<td>Moisture content</td>
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<tr>
<td>Temperature of sample</td>
<td>24 ± 2 °C</td>
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<tr>
<td>Substrate</td>
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</table>
**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 11/09/2015  
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 Naproxen sodium

Figure 2: Naproxen sodium in Alfa Aesar bottle.

Figure 3: Naproxen sodium 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 \( d = \left( \frac{4 \times A}{\pi} \right)^{1/2} \). 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 Naproxen sodium.
Figure 5: Particle size distribution of Naproxen sodium.