All data taken at Pacific Northwest National Laboratory (PNNL)

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SAMPLE CONDITIONS & PHYSICAL PROPERTIES

Chemical name Hydroxypropyl cellulose

Chemical formula $RO-(C_{12}H_{14}O_{10}R_6)_n$ -R in which R= H or $CH_2CH(OH)CH_3$

Synonyms n/a

CAS number 9004-64-2

Location of field sample n/a History of sample n/a

Molecular Weight ~ 80,000 g/mol (Avg.)

Melting Point n/a
Boiling Point n/a
Density (25 °C) 0.5 g/cm³
Hardness, Mohs scale n/a

Crystallography:

Cell dimension $a = \mathring{A} b = \mathring{A} c = \mathring{A}$

Crystal system

H-M symbol (point gr)

Space group

H-M symbol (space gr)

Crystal habit

Color White

Diaphaneity Sub-translucent to opaque Particle size $10 - 600 \mu m \text{ (mean } 84 \mu m)$

Particle size assessment Optical microscopy

Supplier Aldrich

Stated purity < 5 wt. % impurities

Date packed 16 March 2016 Weight: 0.999 grams

Synthesis method n/a Synthesis reference n/a

Texture Needle-like crystals of various sizes

 $\begin{array}{lll} \mbox{Physical state} & \mbox{Solid} \\ \mbox{Surface roughness} & \mbox{n/a} \\ \mbox{Elemental composition} & \mbox{n/a} \\ \mbox{Isotopic composition} & \mbox{n/a} \\ \mbox{Moisture content} & \mbox{n/a} \\ \mbox{Temperature of sample} & 25 \pm 2 \ ^{\circ} \mbox{C} \\ \mbox{Substrate} & \mbox{n/a} \\ \end{array}$

RELEASE 5.0 - 03/2017

INSTRUMENT PARAMETERS

Tensor 37 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

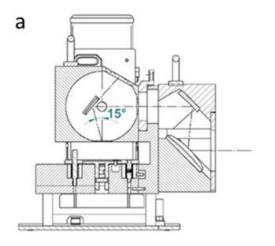
High and low folding limit 15800.54-0.00 cm⁻¹

Phase resolution 32.00Phase correction mode MertzZerofilling $4 \times$

Wavenumber accuracy $\pm 0.4 \text{ cm}^{-1}$ Spectral resolution 4 cm^{-1}

Accuracy verification 10/28/2015

Wavelength vetted on: ICL polystyrene standard #0009-7394-0025A, thin film Reflectance: ±2% using SRS reflectance standards 50-010-DH27B-4878



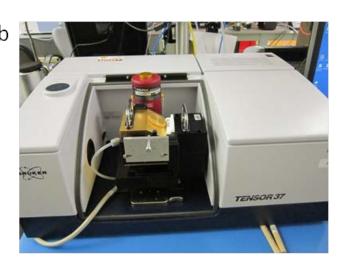


Figure 1: The Bruker 562-G integrating sphere (a) and Tensor 37 (b)

Photographs of sample Hydroxypropyl cellulose



Figure 2: Hydroxypropyl Cellulose in Aldrich container.

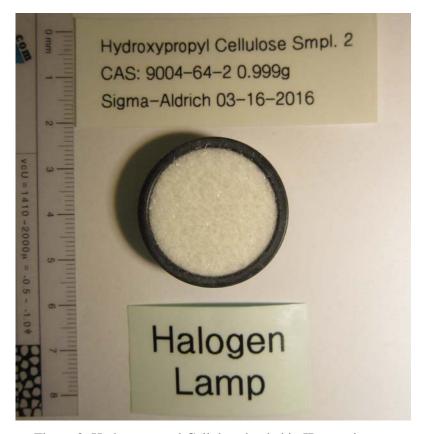


Figure 3: Hydroxypropyl Cellulose loaded in IR sample cup.

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 $d=(4*A/\pi)1/2$. Although the assumption of spherical particles is clearly not always valid, this procedure provides a reasonable estimate of the mean particle size.

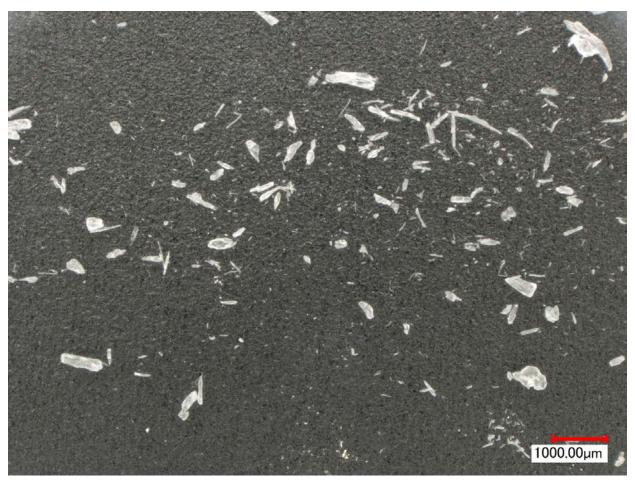


Figure 4: Photomicrograph of Hydroxypropyl Cellulose.

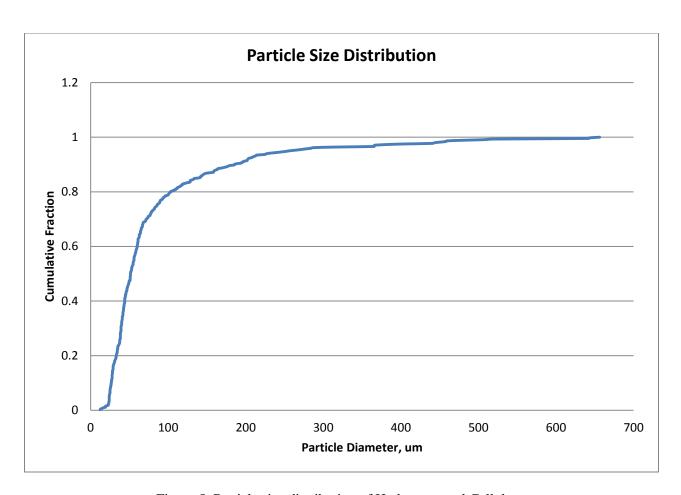


Figure 5: Particle size distribution of Hydroxypropyl Cellulose.