All data taken at Pacific Northwest National Laboratory (PNNL)

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SAMPLE CONDITIONS & PHYSICAL PROPERTIES

Chemical name	Sucrose
Chemical formula	$C_{12}H_{22}O_{11}$
Synonyms	Sugar; α-D-Glc-(1→2)-β-D-Fru; α-D-Glucopyranosyl β-D-fructofuranoside; β-D-Fructofuranosyl-α-D-glucopyranoside; D(+)-Saccharose
CAS number	57-50-1
Location of field sample	n/a
History of sample	n/a
Molecular Weight	342.30 g/mole
Melting Point	185-187 °C
Boiling Point	Decomposes
Density (25° C)	1.58 g/cm^3
Hardness, Mohs scale	n/a
Crystallography:	
Cell dimension	a = 10.89 Å b = 8.69 Å c = 7.77 Å
Crystal system	Monoclinic
H-M symbol (point gr)	2
Space group	4
H-M symbol (space gr)	$P2_1$
Crystal habit	Various
Color	White
Diaphaneity	Sub-translucent to opaque
Particle size	Bimodal distribution: 88 ± 62 µm and 1187 ± 147 µm
Particle size assessment	Optical microscopy
Supplier	Fluka
Stated purity	≥ 99.0%
Date packed	29 February 2016 Weight: 2.222 grams
Synthesis method	n/a
Synthesis reference	n/a
Texture	Crystalline
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

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	32.00
Phase correction mode	Mertz
Zerofilling	4×
Wavenumber accuracy	± 0.4 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

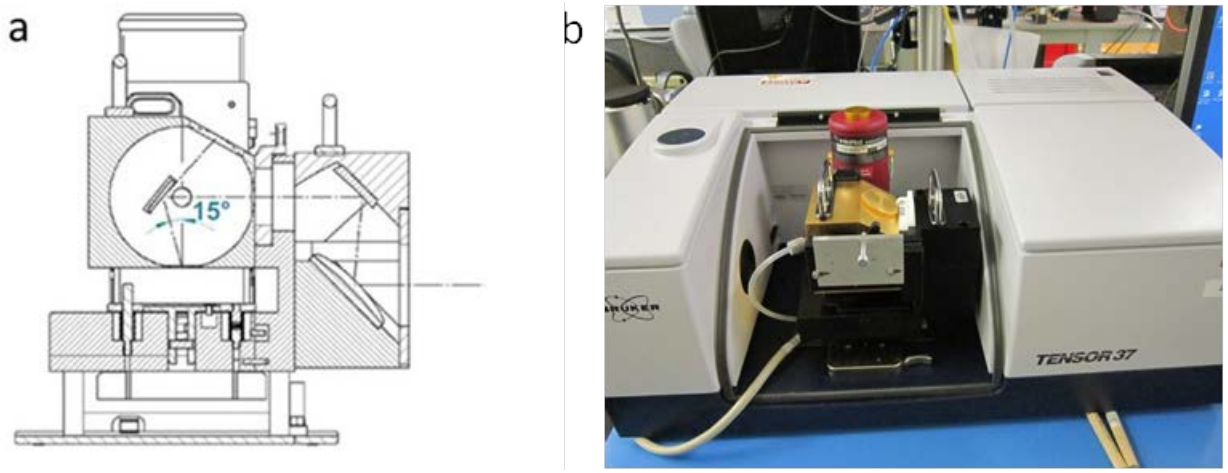

Figure 1: The Bruker 562-G integrating sphere (a) and Tensor 37 (b)

Photographs of sample Sucrose

Figure 2: Sucrose in Fluka container.

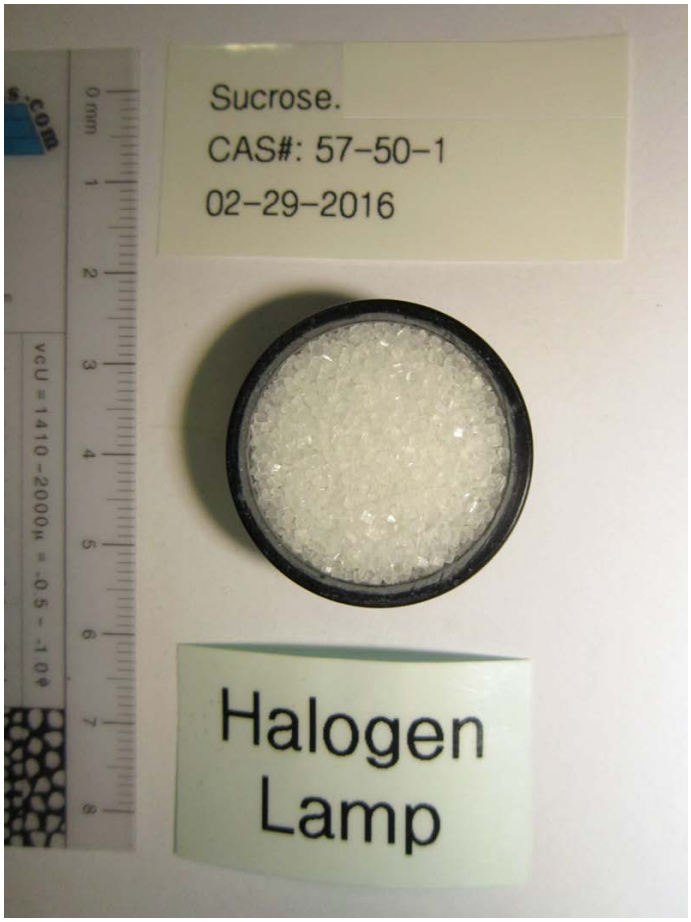

Figure 3: Sucrose sample loaded in IR sample cup.

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

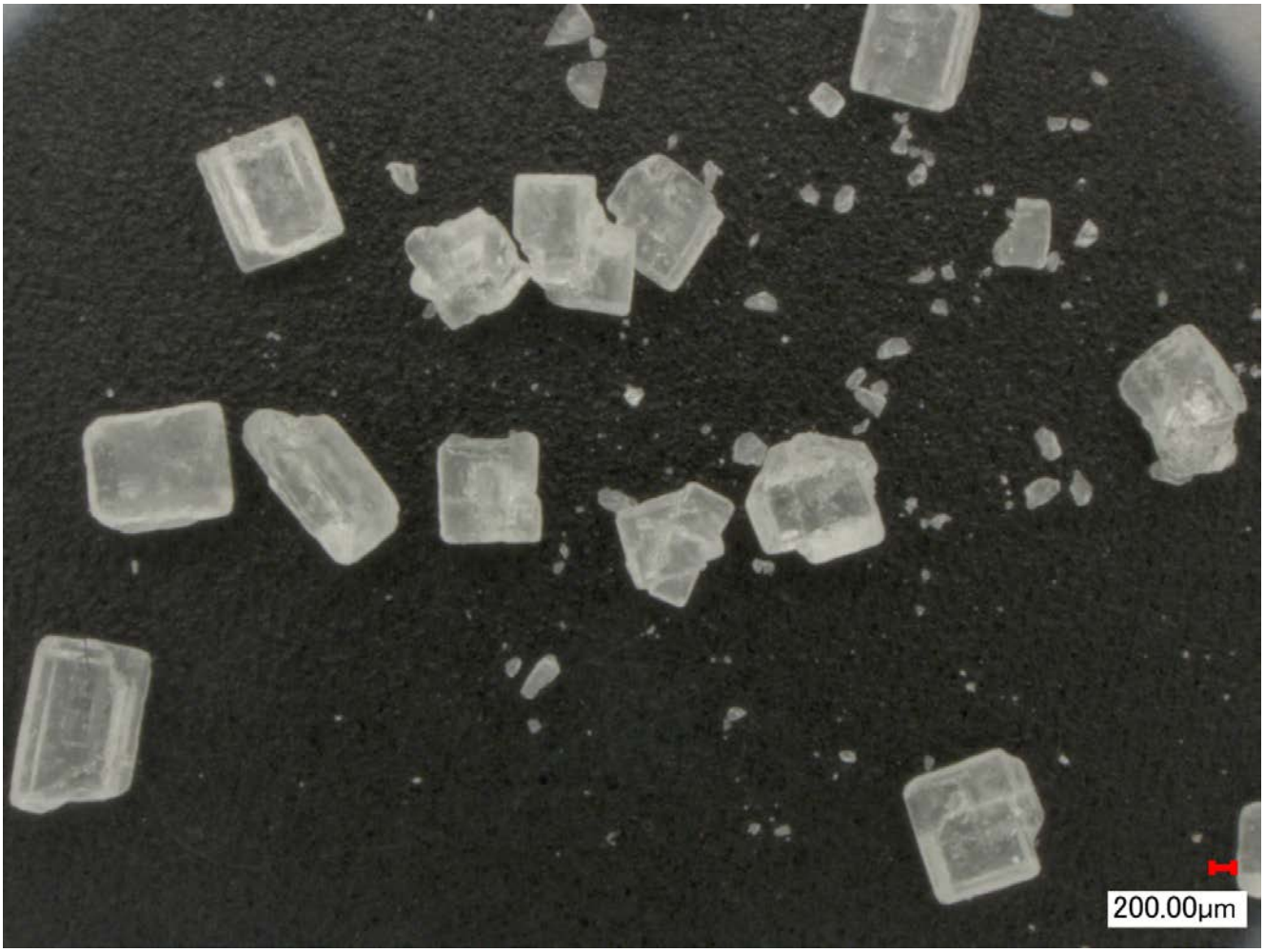

Figure 4: Photomicrograph of Sucrose.

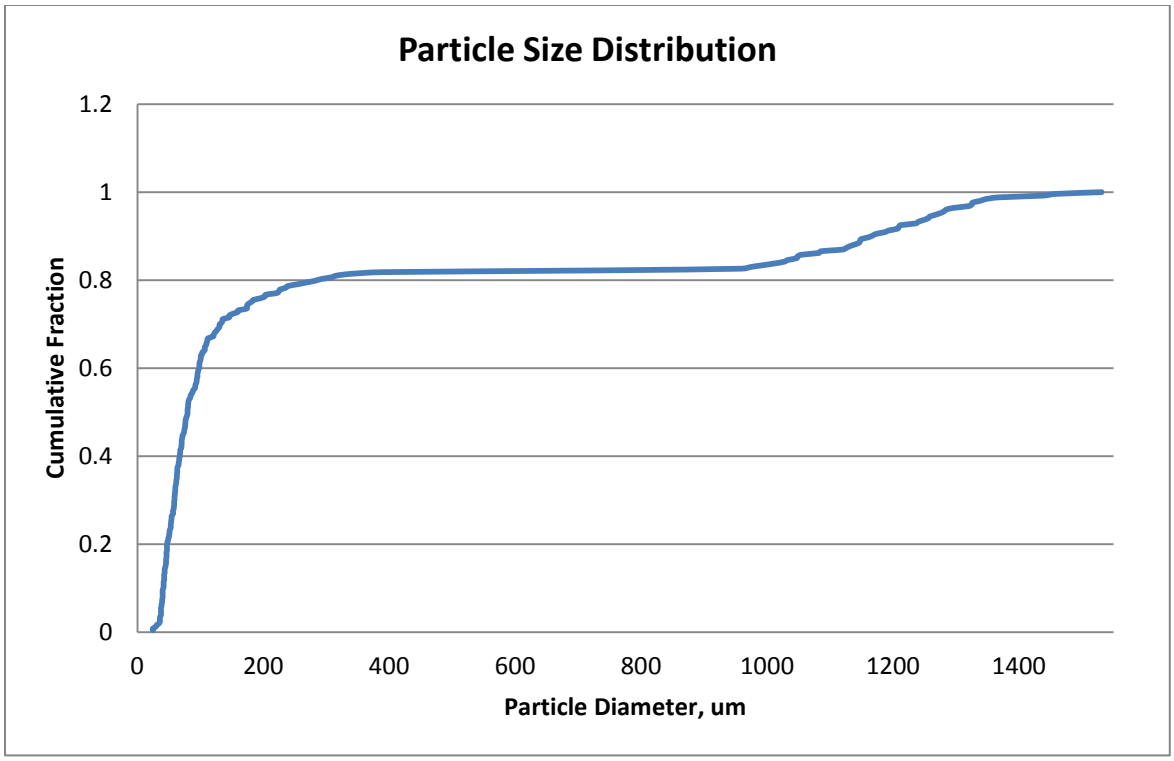

Figure 5: Particle size distribution of Sucrose.