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 Calcium hydroxide

Chemical formula Ca(OH)₂

Synonyms Slaked lime; Calcium dihydroxide

CAS number 1305-62-0

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

74.09 g/mole Molecular Weight **Melting Point** ≥ 450 °C **Boiling Point** n/a Density (25 °C) 2.24 g/cm³

n/a

Hardness, Mohs scale

Crystallography:

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

Crystal system

H-M symbol (point gr)

Space group

H-M symbol (space gr)

Crystal habit

Color White Diaphaneity Opaque Particle size $10 \pm 9 \,\mu m$

Optical microscopy Particle size assessment

Supplier Aldrich Stated purity 99.995%

Date packed 5 October 2016 Weight: 0.982 grams

Synthesis method n/a Synthesis reference n/a

Texture Fine powder

Physical state Solid Surface roughness n/a Elemental composition n/a Isotopic composition n/a Moisture content n/a 25 ± 2 °C Temperature of sample Substrate none

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

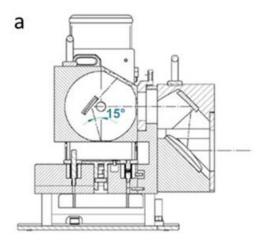
Non-linear correction Off

High and low folding limit 15802.38-0.00 cm⁻¹

Phase resolution 32.00 Phase correction mode Mertz Zerofilling $4\times$

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



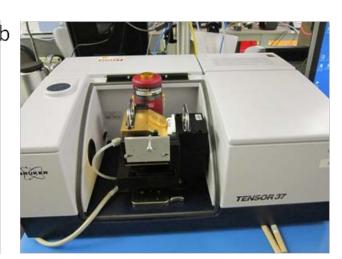


Figure 1: The Bruker 562-G integrating sphere (a) and Tensor 37 (b)

Photographs of sample Calcium hydroxide

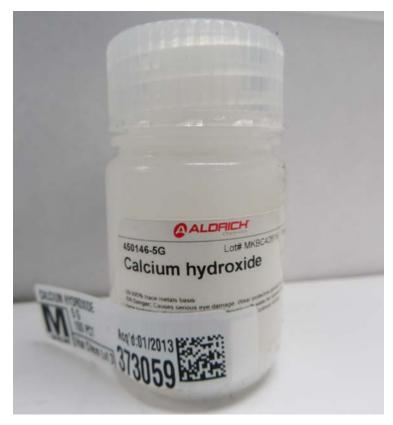


Figure 2: Calcium hydroxide in Aldrich container.



Figure 3: Calcium hydroxide 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.

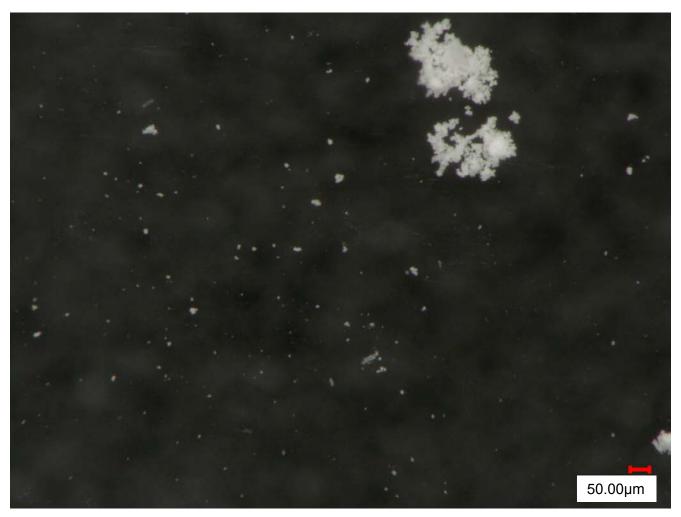


Figure 4: Photomicrograph of Calcium hydroxide.

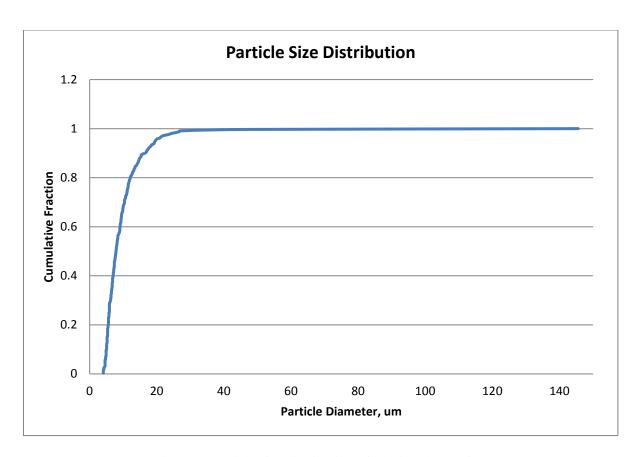


Figure 5: Particle size distribution of Calcium hydroxide.