

All data taken at Pacific Northwest National Laboratory (PNNL)

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### **SAMPLE CONDITIONS & PHYSICAL PROPERTIES**

Chemical name	Gypsum
Chemical formula	CaSO <sub>4</sub> •2(H <sub>2</sub> O)
Synonyms	Calcium sulfate dihydrate
CAS number	10101-41-4
Location of field sample	n/a
History of sample	n/a
Molecular Weight	172.17 g/mole
Melting Point	Dehydrates at 200-300 °C then melts at 1450 °C
Boiling Point	n/a
Density (20° C)	2.3 g/cm <sup>3</sup>
Hardness, Mohs scale	2
Crystallography:	
Cell dimension	a = 5.679 Å b = 15.202 Å c = 6.523 Å
Crystal system	Monoclinic-prismatic
H-M symbol (point gr)	(2/m)
Space group	15
H-M symbol (space gr)	A2/a
Crystal habit	Crystalline, massive, fibrous, tabular
Color	White and Gray
Diaphaneity	Opaque
Particle size	n/a
Particle size assessment	n/a
Supplier	Washington School Collection
Stated purity	n/a
Date packed	31 August 2016      Weight: 11.880 grams
Synthesis method	n/a
Synthesis reference	n/a
Texture	Cut and polished rock
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 $\text{cm}^{-1}$ saved; 7500 to 600 $\text{cm}^{-1}$ 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 $\text{cm}^{-1}$
Phase resolution	32.00
Phase correction mode	Mertz
Zerofilling	4×
Wavenumber accuracy	$\pm 0.4 \text{ cm}^{-1}$
Spectral resolution	4 $\text{cm}^{-1}$
Accuracy verification	10/28/2015
Wavelength vetted on:	ICL polystyrene standard #0009-7394-0025A, thin film
Reflectance:	$\pm 2\%$ using SRS reflectance standards 50-010-DH27B-4878



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

Photographs of sample Gypsum



Figure 2: Gypsum in Washington School Collection container.

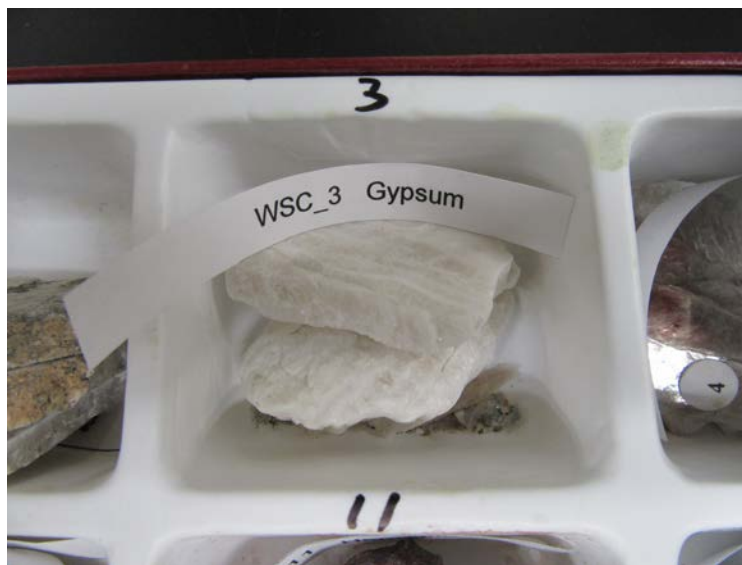


Figure 3: Gypsum in Washington School Collection container, close up.

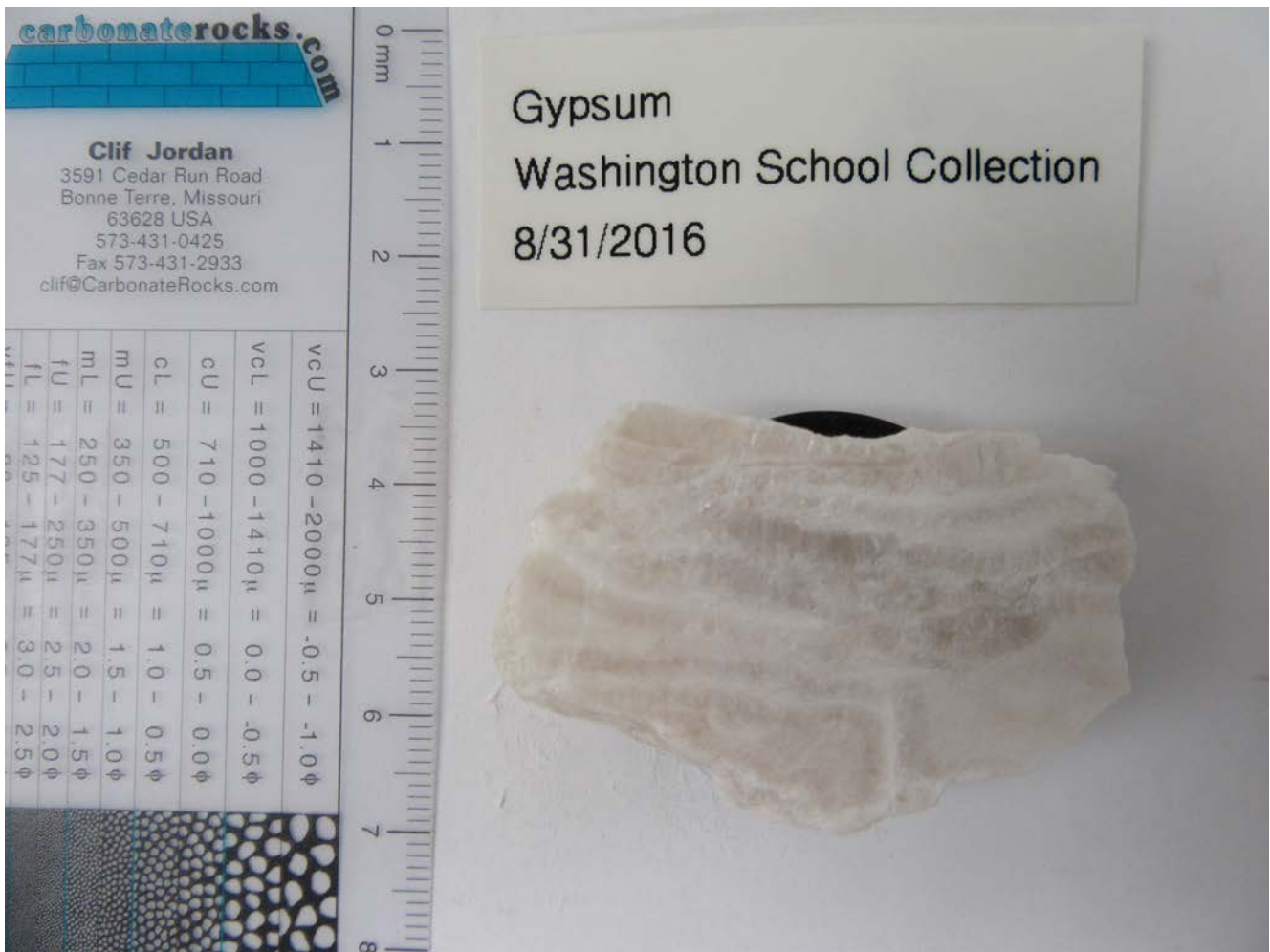


Figure 4: Gypsum loaded on IR sample cup.