

All data taken at Pacific Northwest National Laboratory (PNNL)

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SAMPLE CONDITIONS & PHYSICAL PROPERTIES

Chemical name	Pyrite
Chemical formula	FeS ₂
Synonyms	Iron pyrite; "Fools gold"; Iron sulfide
CAS number	1309-36-0
Location of field sample	n/a
History of sample	n/a
Molecular Weight	119.98 g/mol
Melting Point	n/a
Boiling Point	n/a
Density (20° C)	4.8 - 5 g/cm ³
Hardness, Mohs scale	6 - 6.5
Crystallography:	
Cell dimension	a = 5.417 Å b = Å c = Å
Crystal system	Isometric
H-M symbol (point gr)	Diploidal
Space group	Pa3
H-M symbol (space gr)	2/m3
Crystal habit	Typically cubic or pyritohedral, and combinations are common, resulting in striated faces. Often massive, granular, radiated, globular or stalactitic.
Color	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: 32.062 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 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	$\pm 0.4 \text{ cm}^{-1}$
Spectral resolution	4 cm^{-1}
Accuracy verification	10/28/2015
Wavelength vetted on:	ICL polystyrene standard #0009-7394-0025A, thin film
Reflectance:	$\pm 2\%$ using SRS reflectance standards 50-010-DH27B-4878

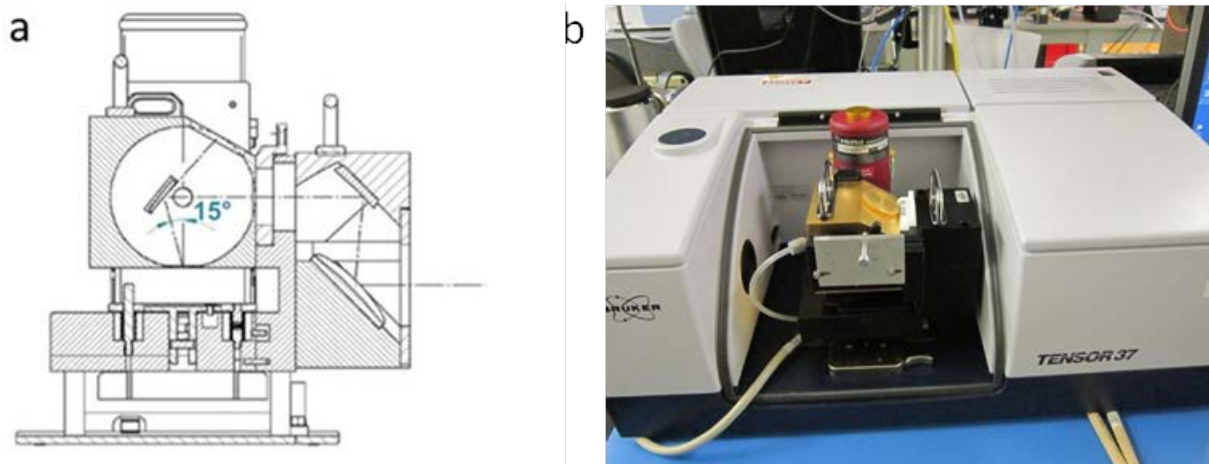


Figure 1: The Bruker 562-G integrating sphere (a) and Tensor 37 (b)

Photographs of sample Pyrite

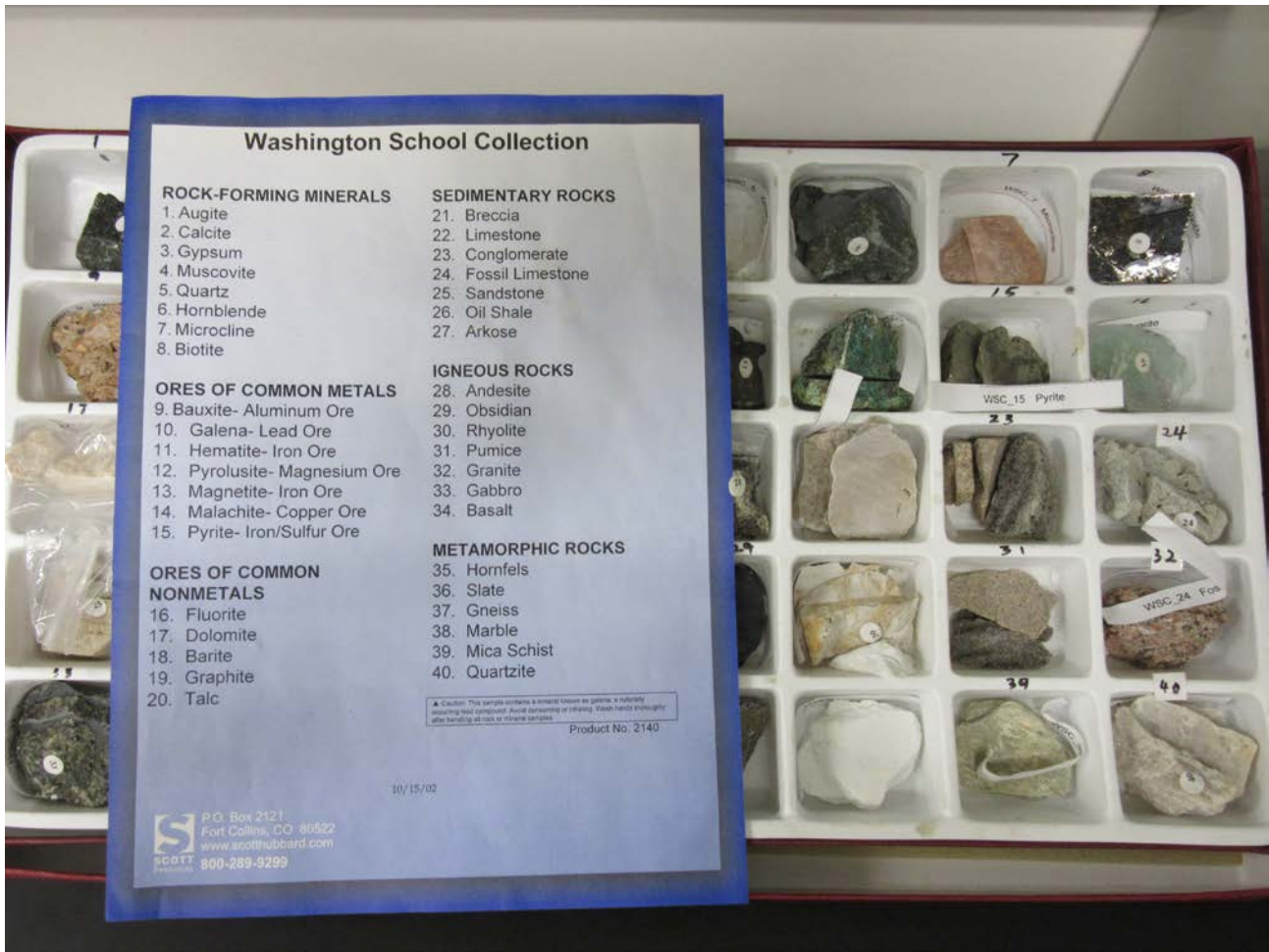


Figure 2: Pyrite in Washington School Collection container.



Figure 3: Pyrite in Washington School Collection box, close up.



Figure 4: Pyrite loaded on IR sample cup.