All data taken at Pacific Northwest National Laboratory (PNNL)

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## SAMPLE CONDITIONS & PHYSICAL PROPERTIES

Chemical name Chemical formula Synonyms CAS number Location of field sample History of sample Molecular Weight Melting Point Boiling Point Density (25° C)	Petroleum Jelly Mixture of saturated hydrod Vaseline 8009-03-8 n/a n/a Typical ranges 352-450 g/m 36-60 °C 302 °C 0.9 g/cm <sup>3</sup>	
Hardness, Mohs scale	n/a	
Crystallography:		
Cell dimension	$a = \overset{\circ}{A} b = \overset{\circ}{A} c = \overset{\circ}{A}$	
Crystal system		
H-M symbol (point gr)		
Space group		
H-M symbol (space gr)	)	
Crystal habit		
Color	Colorless/pale yellow	
Diaphaneity	Translucent	
Particle size	n/a	
Particle size assessment	n/a	
Supplier	Safeway	
Stated purity	100% pure white petroleum	jelly
Date packed	28 October 2015	Weight: 2.052 grams
Synthesis method	n/a	
Synthesis reference	n/a	
Texture	Oily gelatinous substance	
Physical state	Solid/gel	
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 <sup><math>-1</math></sup> saved; 7500 to 600 cm <sup><math>-1</math></sup> 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	

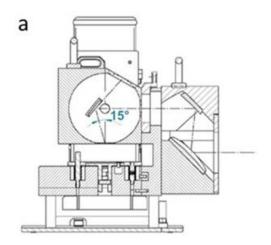




Figure 1: The Bruker 562-G integrating sphere (a) and Tensor 37 (b)

## Photographs of sample Petroleum Jelly



Figure 2: Petroleum Jelly in store container, front label.



Figure 3: Petroleum Jelly in store container, back label.



Figure 4: Petroleum Jelly loaded in IR sample cup.