

All data taken at Pacific Northwest National Laboratory (PNNL)

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SAMPLE CONDITIONS & PHYSICAL PROPERTIES

Chemical name	Benzalkonium chloride	
Chemical formula	$C_6H_5CH_2N(CH_3)_2RCl$ (R= C_8H_{17} to $C_{18}H_{37}$)	
Synonyms	Alkylbenzyltrimethylammonium chloride; Alkyldimethylbenzylammonium chloride	
CAS number	63449-41-2	
Location of field sample	n/a	
History of sample	n/a	
Molecular Weight	variable	
Melting Point	n/a	
Boiling Point	n/a	
Density (25 ° C)	0.98 g/cm ³	
Hardness, Mohs scale	n/a	
Crystallography:		
Cell dimension	a = Å b = Å c = Å	
Crystal system		
H-M symbol (point gr)		
Space group		
H-M symbol (space gr)		
Crystal habit		
Color	Clear	
Diaphaneity	Translucent	
Particle size	n/a	
Particle size assessment	n/a	
Supplier	Sigma-Aldrich	
Stated purity	≥ 95%	
Date packed	01 September 2016	Weight: 2.370 grams
Synthesis method	n/a	
Synthesis reference	n/a	
Texture	Viscous, gelatinous pseudo-solid w/ molasses-like or paste-like texture	
Physical state	Semi-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

IR Cube 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	Open
Coadded scans	4096
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	11/17/2015
Wavelength vetted on:	ICL polystyrene standard #0009-7394-0025A, thin film
Reflectance:	$\pm 2\%$ using SRS reflectance standards 50-010-DH27B-4878

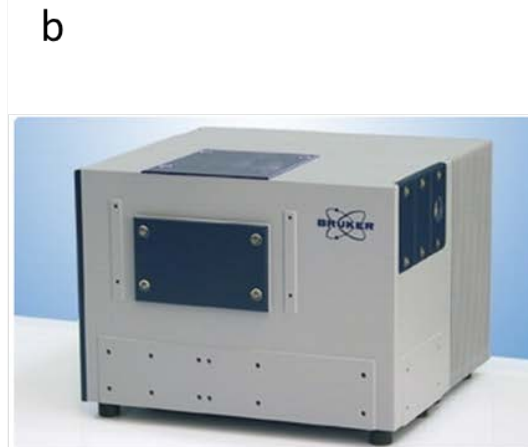
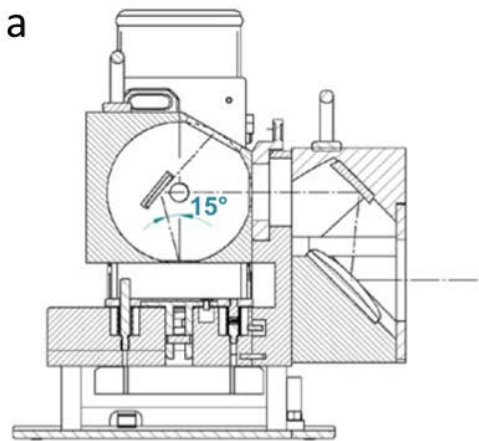


Figure 1: The Bruker 562-G integrating sphere (a) and IR Cube (b)

Photographs of sample Benzalkonium chloride



Figure 2: Benzalkonium chloride in Sigma-Aldrich container.



Figure 3: Benzalkonium chloride loaded in IR sample cup.