FTIR SPECTROSCOPY REFERENCE GUIDE

The Measure of Confidence

INTRODUCTION

Infrared spectroscopy is the study of the interactions between infrared electromagnetic energy and matter. The technique of infrared spectroscopy measures the vibrations of molecules, allowing for qualitative and quantitative measurements of samples. A Fourier transform infrared (FTIR) spectrometer is an ideal tool for the identification of unknown organic and inorganic samples whether they exist in the form of a gas, liquid or a solid.

ELECTROMAGNETIC SPECTRUM

Radiation in the infrared region is commonly referred to in terms of a unit called a wavenumber ($\bar{\nu}$), rather than wavelength (λ). Wavenumbers are expressed as reciprocal centimeters (cm^{-1}) and are the preferred unit as they are directly proportional to energy. A higher wavenumber corresponds to a higher energy.

Convert a wavenumber ($\bar{\nu}$) to a wavelength (λ) by using the following formula:

$$\bar{\nu}\ (cm^{-1}) = \frac{1}{\lambda\ (cm)}$$

Convert a wavenumber ($\bar{\nu}$) to Energy (E) by multiplying it by the speed of light (c, in centimeters per second) and Planck's constant (h):

$$E\ (J) = h\ (J.s) \times c\ (cm.s^{-1}) \times \bar{\nu}\ (cm^{-1})$$

A portion of the electromagnetic spectrum showing the relationship of the infrared region to other types of radiation *(not shown to scale)*. The relationship between energy, wavenumber, and wavelength is also highlighted.

COLLECTING AN FTIR SPECTRUM

There are three quick, simple steps involved in obtaining a spectrum of a sample:

STEP 1 Record a spectrum with no sample present. (Known as a 'background'.)

STEP 2 Insert the sample into the spectrometer.

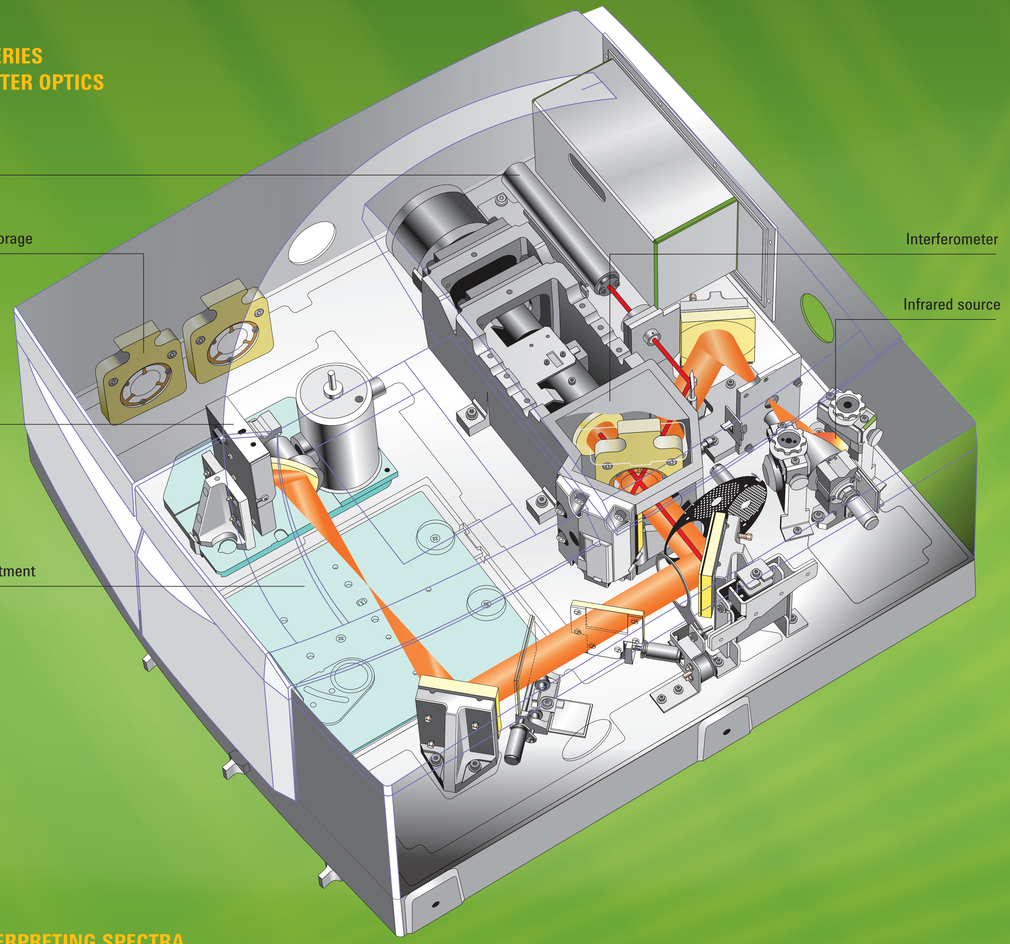
STEP 3 Record a second spectrum and interpret the data.

The key collection parameters are:
- The number of scans (background and sample)
- The scan range
- The spectral resolution.

In general increasing the number of scans that are co-added improves the signal-to-noise ratio of the spectrum and can assist in the analysis of weakly absorbing samples. The spectral resolution is user-defined and helps to distinguish closely spaced absorption peaks, and is expressed in wavenumbers.

The simplified correlation table on the right allows users to extract structural information from IR spectra. Computer-based search programs are also available for assisting in compound identification.

CARY 600 SERIES SPECTROMETER OPTICS



INTERPRETING SPECTRA

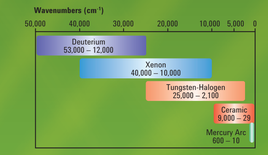
Bond	Type of Vibration		Wavenumber Range (cm^{-1})
C–H	Alkane	(stretch)	3000 – 2850
	$–CH_3$	(bend)	1450 & 1375
	$–CH_2–$	(bend)	1465
	Alkene	(stretch)	3100 – 3000
		(out-of-plane bend)	1000 – 650
	Aromatic	(stretch)	3150 – 3050
		(out-of-plane bend)	900 – 600
	Alkyne	(stretch)	~ 3300
	Aldehyde		2900 – 2700
C=C	Alkene		1680 – 1600
	Aromatic		1600 & 1475
C≡C	Alkyne		2250 – 2100
C=O	Aldehyde		1740 – 1720
	Ketone		1725 – 1705
	Carboxylic acid		1725 – 1700
	Ester		1750 – 1730
	Amide		1680 – 1630
	Anhydride		1810 & 1760

Bond	Type of Vibration	Wavenumber Range (cm^{-1})
C–O	Alcohols, esters, ethers, carboxylic acid, anhydrides	1300 – 1000
O–H	Alcohols, phenols	
	Free	3650 – 3600
	H-Bonded	3400 – 3200
	Carboxylic acids	3400 – 2400
N–H	Primary & secondary amines & amides	
	(stretch)	3500 – 3100
	(bend)	1640 – 1550
C–N	Amines	1350 – 1000
C=N	Imines & oximes	1690 – 1640
C≡N	Nitriles	2260 – 2240
N=O	Nitro ($R–NO_2$)	1550 & 1350
S–H	Mercaptans	2550
C–X	Halides	
	Fluoride	1400 – 1000
	Chloride	785 – 540
	Bromide, iodide	< 650

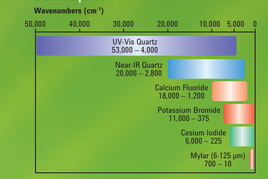
SPECTRAL RANGE COVERAGE

Spectral range coverage for common sources, beamsplitters, and detectors.
The combination of these components generate a spectrometer's working scan range.

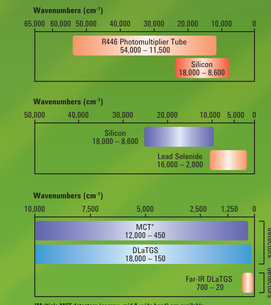
Sources



Beamsplitters



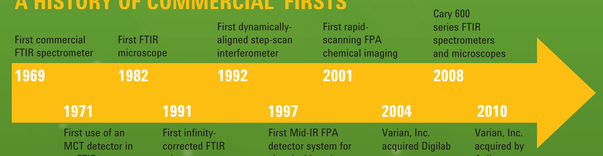
Detectors



THE COMPLETE SOLUTION

Several different accessories facilitate sample preparation and spectral acquisition, including:
- Attenuated Total Reflectance (ATR)
- Diffuse Reflectance
- Specular Reflectance
- Grazing Angle Reflectance
- Microscopy and Chemical Imaging
- ATR Chemical Imaging (Micro and Macro)
- Fiber Optic Probes
- PM-IRRAS
- Photoacoustic Spectroscopy
- TGA-FTIR
- GC-FTIR
- GPC-FTIR

A HISTORY OF COMMERCIAL 'FIRSTS'



Agilent Technologies