#### Spectros Associates Proudly Presents the Three Day Short Course

# **FTIR Analysis of Trace Evidence**

#### Instructor: Dr. Brian C. Smith

A comprehensive 3-day look at how to use an FTIR to obtain spectra of trace evidence, and how to interpret the spectra of these materials.

#### Day 1

#### I. The Basics of FTIR

## A. Introduction to Infrared Spectroscopy

- 1. The Properties of Light
- 2. What is an Infrared Spectrum?
- 3. Infrared Spectroscopy: Good and Bad Points

## **B.** The Advantages of FT-IR

- 1. Signal-to-Noise Ratio (SNR)
- 2. The Throughput Advantage
- 3. The Multiplex Advantage

## C. The Disadvantage of FTIR: Water and CO<sub>2</sub> Peaks

## **II. How an FT-IR Works**

## A. Interferometers & Interferograms

## **B.** How a Spectrum is Produced

- 1. The Fourier Transform
- 2. Background & Single Beam Spectra

## C. Optimizing Resolution & Minimizing Noise

## **D. FTIR Hardware**

- 1. Infrared Sources
- 2. Beamsplitters
- 3. Detectors
- 4. The He-Ne Laser

## E. Measuring Spectral & Instrument Quality

## **III. Spectral Manipulations: Handling Mixture Spectra**

## A. The Laws of Spectral Manipulation

- **B. Spectral Subtraction** 
  - 1. Theory
  - 2. Optimizing Subtraction Results
  - 3. Spotting Artifacts

## **C. Library Searching**

- 1. Background & Theory
- 2. The Search Process

- 3. Properly Interpreting Search Results
- 4. Subtract & Search Again: The Analysis of Mixtures

#### **IV. Infrared Microscopes**

## A. How an Infrared Microscope Works

#### **B.** Preparing Samples

- 1. Transmittance Analysis
- 2. Reflectance Analysis

## C. Forensic Applications

- 1. Powders
- 2. Paint Chips
- 3. Single Fibers
- **D.** Reflectance Sampling

#### V. Microscopic Attenuated Total Reflectance (ATR)

- A. Micro-accessory Design
- **B.** Variables Affecting Spectral Appearance
- **C.** Applications

## Day 2

## I. The Fundamentals of Infrared Interpretation

- A. Molecular Vibrations
- **B.** The Meaning of Peak Positions, Heights, and Widths

## **C. Different Types of Infrared Features**

## **D.** A Systematic Approach to Spectral Interpretation

- 1. Dealing with Mixtures
- 2. Performing Identities Properly
- 3. A Systematic 10-Step Approach to Infrared Interpretation

## II. Functional Group Analysis of Saturated Hydrocarbons

## A. Alkanes: C-H Stretching and Bending Vibrations

- 1. Straight Chain Alkanes
- 2. Estimating Hydrocarbon Chain Length
- 3. Branched Alkanes

#### III. Unsaturated Hydrocarbons

#### A. Alkenes:

- 1. Substitution Patterns
- 2. Distinguishing Cis/Trans Isomers
- 3. Natural & Synthetic Rubbers

## **B.** Aromatic Hydrocarbons

- 1. Mono-Substituted Benzene Rings
- 2. Distinguishing Ortho, Meta, and Para Isomers

#### IV. Molecules with C-O Bonds

#### A. Alcohols & Phenols

- 1. Differentiating Primary, Secondary, and Tertiary Alcohols
- 2. Phenols
- 3. Distinguishing Alcohols from Water

#### **B.** Ethers

- 1. Saturated & Branched Ethers
- 2. Aromatic Ethers
- 3. The Methoxy Group

## Day 3

V. The Carbonyl (C=O) Functional Group

- A. Ketones
- B. Aldehydes
- C. Carboxylic Acids
- **D.** Carboxylates (Soaps)
- E. Esters: The Rule of 3
- F. Organic Carbonates

## **VI. Organic Nitrogen Compounds**

## A. Amides

- 1. Structure, Nomenclature, and Bonding
- 2. Primary Amides
- 3. Secondary Amides
- 4. Proteins

#### B. Imides

## C. Amines

- 1. Distinguishing the Three Types of Amines
- 2. Methyl Groups Bonded to Nitrogen
- 3. Amine Salts

## **D.** Nitriles

## E. The Nitro Group

## VII. Introduction to the Infrared Spectra of Polymers

- A. Low and High Density Polyethylene
- **B.** Polypropylene
- C. Polystyrene
- **D.** Polyethylene Terephthalate (PET)
- **E.** Acrylates

## VIII. Spectra of Polymers with Complex Structures

- A. Polyurethanes
- **B.** Polycarbonates: Lexan
- C. Polyimides: Kapton D. Teflon

# IX. Inorganics

- A. Sulfates
- **B.** Silica
- C. Nitrates
- **D.** Inorganic Carbonates
- E. Phosphates