

Spectros Associates Proudly Presents the Three Day Short Course

Quantitative Infrared Gas Analysis

Instructor: Dr. Brian C. Smith

A 3-day discussion of how to properly measure and quantitate gas phase spectra obtained by extractive FTIR (Fourier Transform Infrared) instruments. The first day covers how an FTIR works, how to measure data quality, how to subtract out spectral interferants, and sample handling. On the second day, how and why molecules absorb infrared radiation and why gas phase spectra are unique is discussed. This section concludes with a detailed discussion of the spectra of gases relevant to you. On the third day, a detailed presentation of how to perform quantitative infrared gas analysis will be given, with an emphasis on the proper way to perform calibrations, what experimental variables to control to assure quality calibrations, and how to correctly measure calibration accuracy and robustness.

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 CO₂ Peaks

II. How an FTIR Works

A. Understanding the Interferometer

B. How Spectra are Calculated

C. Determining Resolution / Optimizing Spectral Quality

D. Gas Phase Resolution Considerations

E. Hardware: Sources, Detectors, & Beamsplitters

F. Measuring and Validating Data Quality

III. Manipulating Spectra to Gain More Information

- A. Spectral Subtraction: How to Remove Water Vapor
- B. Library Searching

IV. Gas Phase Sampling Techniques

- A. The 10 cm Gas Cell
- B. Long Path ("White") Gas Cells
- C. Grab & Flow Sampling

V. The Fundamentals of Infrared Interpretation

- A. The Properties of Light
- B. How Molecules Absorb Infrared Radiation
- C. The Meaning of Peak Positions, Heights, and Widths
- D. A Systematic Approach to Spectral Interpretation

Day 2**I. Rovibrational Spectra of Gas Phase Molecules**

- A. Molecular Rotations and Vibrations
- B. Examples of Gas Phase Spectra
 - 1. Linear Molecules - CO, CO₂
 - 2. Symmetric Molecules - Benzene
 - 3. Asymmetric Molecules - H₂O

II. Analysis of Atmospheric Gases

- A. Dealing with Water Vapor
- B. Carbon Dioxide, Carbon Monoxide, and Ozone
- C. Nitrogen Oxides (Nox)
- D. Sulfur Oxides (Sox)
- E. Halogen Halides: H-Cl, H-Br, H-F

III. Analysis of Hydrocarbons

- A. Aliphatic Hydrocarbons
 - 1. Alkanes
 - 2. The Spectra of Methane and Ethane
 - 3. Alkenes: The Spectrum of Ethylene
- B. Aromatic Hydrocarbons
 - 1. The Spectra of Benzene and Toluene
 - 2. Distinguishing Ortho, Meta, and Para Benzene Ring Isomers

IX. Functional Groups Containing the C-O Bond**A. Alcohols & Phenols**

1. The Spectra of Methanol and Ethanol
2. Phenols

B. Ethers

1. Ethyl Ether
2. Methyl t-Butyl Ether (MTBE)

X. The Carbonyl (C=O) Functional Group**A. Ketones & Aldehydes****B. The Spectra of Acetone and Formaldehyde****C. Esters: Ethyl Acetate****XI. Molecules Containing Nitrogen****A. Ammonia****B. Amines: Triethylamine****XII. Carbon/Halogen Compounds****A. Distinguishing Between the Halogens****B. The Spectra of Chloroform and Trichloroethylene****C. Freons****Day 3****I. Introduction to Infrared Quantitative Analysis****A. Terms and Definitions****B. Derivation of Beer's Law****C. Variables Affecting Calibrations**

1. Temperature & Pressure
2. Concentration & Composition

II. Single Analyte Quantitative Analysis**A. Calibration and Prediction with Beer's Law**

1. Introduction to Linear Regression
2. Measuring Calibration Accuracy and Robustness

B. Standard Methods**C. Measuring Absorbances Properly****D. Avoiding Experimental Errors**

1. Concentration & Spectroscopic Errors
2. 15 Common Experimental Pitfalls to Avoid
3. Instrumental Deviations from Beer's Law

III. Determining Multiple Analytes I**A. The Method of Independent Determination**

B. Simultaneous Determination of Multiple Analytes

1. The Additivity of Beer's Law

2. Intro. to Matrix Algebra

3. The Matrix Form of Beer's Law

C. The Classical Least Squares Method (K Matrix)

IX. Putting it All Together

A. Implementing and Maintaining Calibrations

B. Limitations of Quantitative Analysis

Wrap-up. Time for individual consultations and questions.