

Spectros Associates Proudly Presents the One Day Short Course

Infrared Spectral Interpretation III

Instructor: Dr. Brian C. Smith

An examination of the spectra of molecules with complex spectra and many functional groups. The course begins with an emphasis on commonly found cyclic structures such as cycloalkanes, polycyclic aromatic hydrocarbons, and heterocyclic rings. Then, the structures and spectra of sugars and carbohydrates are discussed. The spectra of molecules containing silicon, sulfur, halogens, and inorganics rounds out the survey of functional groups. The course concludes with a discussion of spectral interpretation aids. A full theoretical development of library searching and spectral subtraction are given. Attendees interpret many unknown spectra in class with the help of the instructor to enhance learning. A special 100 page "Interpretation III" training manual has been developed especially for this course.

I. Cyclic Alkanes

A. CH₂ in Cyclic Structures

B. Cyclohexyl Rings

1. Conformations

2. Spectra

C. Cyclopentane Rings

II. Highly Substituted Benzene Rings

A. Trisubstituted Rings

B. Tetrasubstituted Rings

C. The Summation Bands

III. Polycyclic Aromatic Hydrocarbons

A. Naphthalenes

B. Anthracenes and Phenanthrenes

IV. Heterocyclic Aromatic Rings

A. Pyridines

B. Pyrrole

V. Sugars and Carbohydrates

- A. Glucose and Other Sugars**
- B. Oligosaccharides**
- C. Cellulose**

VI. Amine Salts

- A. Structures**
- B. Distinguishing Primary, Secondary, and Tertiary Amine Salts**

VII. Organic Sulfur, Silicon, and Halogen Compounds

- A. Organic Sulfur Compounds**
 - 1. Thiols (Mercaptans)**
 - 2. Sulfoxides and Sulfites**
 - 3. Sulfones, Sulfonates, and Organic Sulfates**
- B. Siloxanes (Silicones)**
- C. Halogen/Carbon Bonds**

VIII. Inorganics

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

IX. Interpretation Aids

- A. Spectral Subtraction**
 - 1. Theory**
 - 2. Optimizing Results**
 - 3. Spotting Subtraction Artifacts**
- B. Spectral Library Searching**
 - 1. Search Algorithms**
 - 2. The Search Process**
 - 3. Interpreting Search Results**
 - 4. Analyzing Mixtures**

Wrap-up. Time for individual consultations and questions.