

Spectros Associates Proudly Presents the One Day Short Course

Quantitative Spectroscopic Analysis

Instructor: Dr. Brian C. Smith

This 1-day course is for anyone using spectroscopic absorbance measurements to determine concentrations of molecules in unknown samples. Users of infrared, near infrared, and UV/Vis instruments will find this course valuable. The course begins with an overview of how matter absorbs electromagnetic radiation, and the theory behind Beer's Law. After discussing simple single component quantitative analysis, we will cover practical, real world problems encountered in quant. work and how to avoid them. We will then tackle the difficult problem of multiple interfering analytes in complex mixtures. See how the mathematical power of factor analysis can pierce through these problems. The mathematics of factor analysis algorithms are discussed in words. Then, a process to follow to obtain accurate, robust calibrations is presented. Lastly, the practical aspects of implementing and supporting a calibration, and the fundamental limits of quantitative analysis are explored. Many example spectra and calibrations are used to illustrate important points. Material for this course is drawn from the 200 page hardcover textbook "Quantitative Spectroscopy: Theory and Practice" written by Dr. Smith and published by Academic Press.

I. The Absorption of Light By Matter

- A. Terms and Definitions**
- B. The Properties of Light**
- C. Derivation of Beer's Law**
- D. 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**

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**

- IV. Determining Multiple Analytes II: Factor Analysis**
 - A. Advantages & Disadvantages of Factor Analysis**
 - B. Factor Analysis Algorithms**
 - 1. Principal Components (PCR)
 - 2. Partial Least Squares (PLS)
 - 3. Which Algorithm Should You Use?
 - C. Training Set Design**
 - D. Spectral Pre-Processing**
 - 1. Mean Centering
 - 2. Spectral Derivatives
 - 3. Subtraction, Baseline Correction, and Smoothing
 - E. Cross Validation: Testing Model Quality**
 - 1. Spotting Concentration Outliers
 - 2. Spotting Spectral Outliers
 - F. Calibration: Choosing the Right Number of Factors**
 - 1. Reconstructed Spectra
 - 2. Factor Loadings
 - 3. The PRESS Plot
 - G. Validation: Checking a Model's Predictive Accuracy**
 - H. Prediction**
- V. Putting it All Together**
 - A. Implementing and Maintaining Calibrations**
 - B. Limitations of Quantitative Analysis**