B.S. Senior Year – Fall Semester Lab

CEM 495 Molecular Spectroscopy

Description: Experiments in magnetic resonance, optical, and vibrational spectroscopies.

Credit: 2 Credits (1 hour lecture and 4 hours laboratory per week)

Prerequisite: CEM 483 and CEM 395

Recommended Background: One year of physical chemistry

Students write a formal laboratory report for all but the first experiment; an informal report is submitted for the UV-Visible Spectroscopy experiment. Propagation of error used to determine the error in all calculations.

1. **UV-Visible Spectroscopy**

   (Spectroscopy basics: Examination of spectrophotometers (Spec 20, Beckman double beam, and AA); generation of spectral response curve; quantitative spectrophotometry; investigation of the effects of slit width and grating blaze density on monochromator resolution using Oriel components)

Condensed Phase Spectroscopies

2. **Molecular Fluorescence Spectroscopy**

   (Collection and comparison of absorption spectra with fluorescence excitation and emission spectra; investigation of secondary absorption and collisional quenching effects; measurement of fluorescence lifetimes using pulsed nitrogen laser; construction of a fluorescence spectrometer using Oriel components)

3. **Infrared and Raman Spectroscopy**

   (Collection of IR and Raman spectra; comparison of spectra, selection rules and spectrometers; semi-empirical AM-1 and *ab initio* calculations of vibrational frequencies using SPARTAN; construction of a Raman spectrometer using Oriel components and a Verdi diode laser)

Gas Phase Spectroscopies

4. **Rotational-Vibrational Absorption Spectroscopy**

   (FTIR spectra HCl/DCl, HBr/DBr; use of quantum mechanical theory and curve fitting to determine molecular parameters including bond lengths, fundmental vibrational frequencies, and bond force constants)

5. **Vibrational-Electronic Absorption & Emission Spectroscopy**

   (Collection of vibronic absorption and emission spectra of iodine using spectrometers build from Oriel components and a Verdi laser (emission); application of quantum mechanics to determine parameters associated with the ground and first excited electronic state potential energy wells (including dissociation energies, harmonic vibrational frequency, and anharmonicity factors); comparison of the parameters for the two states)