

**Colorado State University  
Department of Chemistry**

**CHEM 431  
Instrumental Analysis Laboratory**

**Notes for  
Infrared Spectroscopy - Transmission versus  
Attenuated Total Reflectance Modes**

The following is a set of short notes to outline the experiment in question and to provide helpful guidance to those executing the experiment.

- A.** Traditionally, Infrared (IR) spectroscopy has been performed using the **transmission mode** where the electromagnetic energy or light is passed through the sample and is selectively attenuated by absorption of the sample itself. A number of interesting opportunities and constraints are presented to the experimentalist by this method including quantification of species and handling of various sample phases, that is, solid, liquid and gas. Consider these dimensions and be prepared to expound on them in your final laboratory report. It is very appropriate to use reference works to help you organize, develop and align your thoughts.
- B.** More recently, a different observation mode, **attenuated total reflectance (ATR)**, has been developed and put into use in many situations. In this mode the sample is placed in contact with an IR transparent material, often a crystal, with a refractive index in a particular range and the IR light is passed through the crystal in such a fashion that it reflects off of the sample-contacted surface before being analyzed. Consider how the IR light can interact with the sample on the other side of the interface created by the crystal and the sample - in other words, how ATR works at all.
- C.** Compare transmission and ATR methods using pure liquid acetone and solutions of water in acetone and some other (solid) samples.
- D.** Measure the molar extinction of acetone (at all wavelengths, don't be cheap) using transmission mode. Then by measuring the absorbance in ATR mode. Determine the "path length" in ATR mode.
- E.** Measure the molar extinction of water in acetone solution by creating a good, old calibration curve.
- F.** Collect a few spectra of some solid halogenated (brominated and chlorinated) methanes (just like in Fundamental Experimental Physical Chemistry) using ATR. How does this spectroscopy compare to the (corresponding chlorinated) solution measurements?