Colorado State University

CHEM 372
Physical Chemistry Laboratory

Notes for
Vibrational Spectra of Halogenated Methanes and Normal 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. Absorption spectra can be interpreted to yield fundamental information about the molecules giving rise to them. The work in this experiment examines some aspects of this state of affairs in detail. Specifically, the infrared (IR) absorption spectra of some simple halogenated hydrocarbons are collected and analyzed to yield insight into the fundamental mathematical and physical principles of the arrangement of atoms in the molecules that give rise to specific details of the spectra.

B. Absorption features in IR spectra are a direct result of molecular (or molecular-fragment) dipole vectors that are modulated by changes in the molecular configuration or structure. Example changes in structure or configuration include vibrations that result in bond stretching or in "bending" (the bond between two atoms is not bent but the angle formed of three atoms changes).

C. Group Theory is a field of mathematics that can be used to understand the many modes of motion that can occur within a molecule - based solely on the arrangement of the atoms and their linkages (bonds). It can be used to analyze and predict many aspects of IR spectra from first principles.

D. Chlorinated methanes (dichloromethane, trichloromethane and tetrachloromethane) provide a convenient series of homologous molecules that permits evaluation of the principles of group theory relevant to IR spectra.

E. Corresponding brominated and iodinated methanes can also be used to illustrate important features of this process of analysis and synthesis of IR spectra.

F. Obtain high quality IR spectra (use "absorbance" mode not "percent transmittance") of as many halogenated methanes that are available in the laboratory. Some are liquid at laboratory temperatures (use no more than one mL of each and do not contaminate the stock containers) and pressures and can be studied using the salt-plate (NaCl) sample containment. Others are solids (use no more than 100 mg of each and do not contaminate the stock containers) and must be dissolved in a suitable (choose wisely!) solvent to record spectra of them.

G. Transfer ASCII-format (text) files from the IR spectrophotometer and analyze them in a single experiment of Igor Pro.

H. Assign the absorption signals. Identify absorption patterns associated with the various halogen substitution patterns. Identify the effects of halogen substitution on the position of the various absorption patterns. Recall the results of the earlier experiment you performed on the Quantum Computation of the Vibrational Spectroscopy of Diatomic Molecules. Explain how the patterns and the substituents yield the carbon-halogen spectra.