IR Infrared Spectroscopy of HCl

Objective
The objective of this experiment is to determine from the IR spectrum of HCl the following: v_o the vibrational frequency, B_o the rotation constant, I the moment of inertia, and r the bond length.

References
Refer to pages in lecture textbook on "vibration of diatomic molecules."

Operating Instructions for FT-IR Spectrometer

Materials
HCl (aq) either concentrated or 10N (less than 0.5mL)

Hazard: concentrated HCl is corrosive. Avoid skin contact. If HCl contacts your skin, wash it off immediately with water, and notify the professor.

Equipment and Supplies
Fourier Transform Infrared Spectrophotometer (FT-IR)
NaCl salt plate windows
Gas cell
Cell holder with long arm.

Instructions
Set up the gas cell in the following manner. Without touching the faces of the salt plate, place one salt plate in one of the plastic end caps of the gas cell. Slip the end cap/salt plate onto one end of the glass gas cell. Repeat the process on the other end of the cell.

Place a rubber septum in one of the two side arms of the gas cell. Use the cell holder that has a long side arm to hold the assembled cell in the FT-IR beam path. Obtain a background spectrum on the empty cell.

Remove the cell from the holder and perform the next few steps in the hood. Use a disposable pipet to add about 8 drops of concentrated HCl to the inside of the cell. Place a septum over the open side arm and wait a few minutes while some of the HCl goes into the vapor phase. As you move the cell about, you want to keep the cell level so the hydrochloric acid does not flow to the ends of the cell and touch the salt plates.

Carefully return the cell to the holder and obtain the IR spectrum. If you do not obtain the desired spectrum (look in the 2600 to 3100 cm^{-1} region) try waiting a few minutes to let more HCl go into the vapor phase.

When finished, return the normal holder to the instrument and disassemble the gas cell. Rinse the glass part in distilled water and acetone make sure glass parts are dry. Wipe off the NaCl windows gently with a perfectly dry kimwipe and return the NaCl windows to the dessicator. Return all parts to the drawer.

Calculations method I

Compare your IR spectrum to HCl(g) spectrum in lecture textbook. Notice, textbook figure may have frequency increasing to the right, but IR spectrometers print spectra with frequency increasing to the left.

Label each peak with a peak label **n**, as shown below. Calculate the frequency (in cm^{-1}) of each peak in your HCl spectrum, v(**n**). Prepare a table of **n** and v(**n**) values. Plot v(**n**) as a function of **n**. You should obtain a straight line which follows the equation

$$v(\mathbf{n}) = v_o + 2\, B_o\, \mathbf{n}$$

where v_o is the vibrational frequency and B_o is the rotation constant. Perform a linear regression to obtain values for v_o and B_o, both in cm^{-1} units.

Use textbook equations to calculate I, the moment of inertia for HCl. Use the appropriate equation to calculate the bond length r (in pm) for HCl.

Compare your values for v_o, B_o, and r to literature values.

Alternate Calculations method II

Calculate the frequency of each peak in the HCl spectrum. Finally, calculate B_e, a_e, n_o, I_e, and r_e following the method indicated below. A comparison of r_e to the accepted value will suggest if you need to recheck your analysis. Redo your analysis if your results are not within 10% of the accepted value.

Analysis is based on the following equation

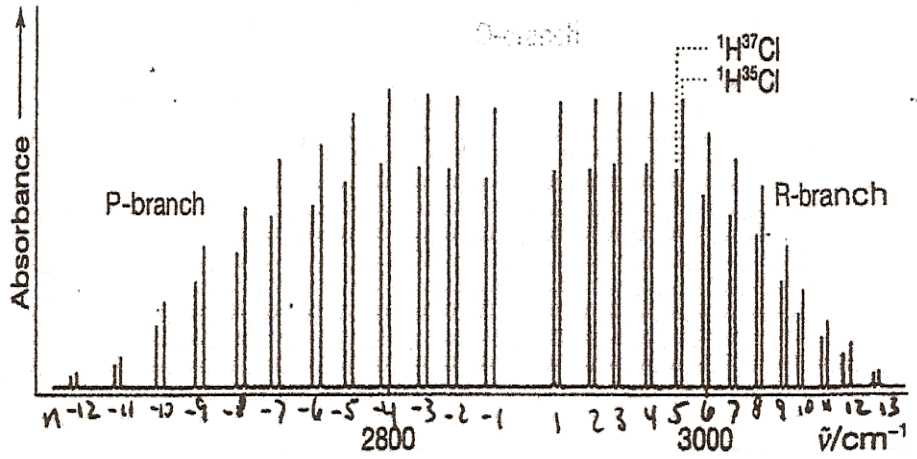
$$v = v_o + (2B_e - 2\, a_e)\, m - a_e\, m^2$$

where v is the wavenumber or reciprocal of the frequency, ñ Show that the above equation gives the result below when finding the difference of two adjacent spectral lines.

$$\Delta v\,(m) = v\,(m + 1) - v\,(m) = (2B_e - 3\, a_e) - 2\, a_e\, m$$

Using the above equation plot Δv versus m where slope = $-2a_e$ and the intercept = $(2B_e - 3a_e)$ and use these results to find B_e, a_e, n_o, I_e, and r_e.

Compare results of two methods above and compare to literature.


Absorbance
P-branch
R-branch
$^1H^{37}Cl$
$^1H^{35}Cl$
n -12 -11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 1 2 3 4 5 6 7 8 9 10 11 12 13
2800
3000
$\tilde{\nu}/cm^{-1}$