I. Introduction

Infrared spectroscopy is used to probe the structure, dynamics and concentrations of chemical compounds. An infrared spectrum comes from transitions that arise from the vibration of molecules caused by the periodic change in their dipole moments. In gaseous samples, one may also observe the changes in the rotational energy. One thereby sees as well the rotational fine structure. The energies between successive rotational levels are about 1000 times less than between vibrational levels, with the result that a band spectrum is observed.

In this experiment, the vibration-rotation spectra of hydrogen chloride and deuterium chloride are analyzed by assigning spectral lines to differences in energies of properly identified levels. It is carried out by matching a series of observed line positions with a series of expected level positions until all of the observed lines are accounted for in terms of the proposed level scheme. When the analysis is complete so that the observed spectrum can be predicted as the expected transitions among the levels described by a few simple equations, one is left with a set of vibrational and rotational parameters, which are the molecular constants.

II. Theory

The simplest model of a vibrating diatomic molecule is a harmonic oscillator, for which the potential energy depends quadratically on the change in internuclear distance.

![Diagram of Harmonic Oscillator Model](image)

Fig. 1. Harmonic oscillator model for a diatomic molecule. A change $\Delta r$ from the equilibrium internuclear distance $r_e$ occurs as the molecule vibrates.
The allowed energy levels of a harmonic oscillator, as calculated from quantum mechanics and expressed as term values $G(\nu)$ are:

$$G(\nu) = (\nu + \frac{1}{2}) \cdot \nu_e$$

where $\nu$ is the vibrational quantum number having integral values 0, 1, 2, and $\nu_e$ is the oscillator's vibrational wavenumber. Term values express energy in wavenumbers.

In practice, the vibrations of a diatomic molecule are not exactly those of a harmonic oscillator and so, for precise work, we need to include an anharmonicity constant $x_e$:

$$G(\nu) = \frac{1}{2} \cdot \nu_e \cdot (\nu + \frac{1}{2}) - x_e \cdot \nu_e \cdot (\nu + \frac{1}{2})^2$$

The vibrational wavenumber $\nu_e$ is determined by the masses of the atoms and the force constant of the bond according to the expression:

$$\frac{1}{2} \cdot \nu_e = \frac{\frac{\hbar}{2\pi c} \left( \frac{k}{\mu} \right)^{1/2}}{c} = \frac{\nu_{osc}}{c}$$

where $\mu$ is the reduced mass:

$$\mu = \frac{M_1 \cdot M_2}{M_1 + M_2}$$

We are going to examine the spectrum arising from the fundamental frequency $\nu_{osc}$, but other weak bands, called overtone bands could also be observed such as the first overtone (second harmonic) at about $2 \cdot \nu_{osc}$, the second overtone (third harmonic) at around $3 \cdot \nu_{osc}$, and so on. These observed overtones have frequencies less than $2 \cdot \nu_{osc}$, $3 \cdot \nu_{osc}$ because of the anharmonicity.

A diatomic molecule also rotates in space and the easiest way of describing this motion is to regard it as a dumbell or rigid rotor. The rotational energies of a rigid rotor $V$ are:

$$F(J) = B \cdot J \cdot (J+1)$$

where the rotational constant $B$ is given by:

$$B = \frac{\hbar}{8\pi^2 c \cdot I}$$

Here, $J$ is the rotational quantum number and $I$ is the moment of inertia of the molecule:

$$I = \mu \cdot r^2$$

In practice, centrifugal distortion slightly reduces the rotational energies:

$$F(J) = B \cdot J \cdot (J+1) - D \cdot J^2 \cdot (J+1)^2$$
where D is the centrifugal stretching constant.

The moment of inertia of a molecule increases at higher vibrational energies, so that the value of B in the ground vibrational state, \( B_0 \), is different from that in the first excited state, \( B_1 \). In general:

\[
B_v = B_c - \alpha e (v + \frac{1}{2})
\]

(9)

where \( B_c \) is the value at \( r = r_e \), the equilibrium separation, and \( \alpha e \) the vibration-rotation interaction constant.

Since diatomic molecules vibrate and rotate at the same time, we describe such coupled motion assuming additivity in their energies:

\[
T(\nu,J) = G(\nu) + F(J)
\]

(10)

The vibrational spectrum of HCl consists of a single fundamental band, accompanied by an increase (R branch) or decrease (P branch) in the rotational quantum number according to the selection rule

\[
\Delta J = \pm 1
\]

(11)

The transition would then be from various \( \nu'' \) levels of the vibrational ground state (\( \nu'' = 0 \)) to \( \nu' \) levels the first excited vibrational state (\( \nu' = 1 \)). That is,

\[
\Delta T = T(\nu,J)_{\text{final}} - T(\nu,J)_{\text{initial}}
\]

\[
= T(1, J+1) - T(0, J) \quad \text{for the R branch}
\]

\[
= T(1, J-1) - T(0, J) \quad \text{for the P branch}
\]

The wavenumbers of the rotation-vibration transitions are then given by:

\[
\nu_R(J) = \nu_0 + (B_0 + B_1)(J+1) - (B_0 - B_1)(J+1)^2 - 4D(J+1)^3
\]

(12)

\[
\nu_P(J) = \nu_0 - (B_0 + B_1)J - (B_0 - B_1)J^2 - 4DJ^3
\]

(13)

where

\[
\nu_0 = \nu_e - 2x_e \nu_e
\]

(14)

In these expressions, \( J \) is the rotational quantum number in the lower vibrational state, \( \nu_0 \) is the band origin, and \( B_0 \) and \( B_1 \) are the values of B in the ground and first excited vibrational states, respectively. These series of lines given in Eqs. 12 and 13 are indicated in the energy level diagram below and give rise to a spectrum as in Fig. 3.
Fig. 2. Rotational energy levels for the ground vibrational state ($v'' = 0$) and the first excited state ($v' = 1$) in a diatomic molecule. The vertical arrows indicate allowed transitions in the R and P branches; numbers in parentheses index the value $J''$ of the lower state.
We use the above expressions to determine the spectroscopic and molecular constants for HCl.

When an isotopic substitution is made in a diatomic molecule, the equilibrium bond length $r_e$ and the force constant $k$ are unchanged, since they depend only on the behavior of the bonding electrons. However, the reduced mass does change and this will affect the vibration and rotation of the molecule. For H$^{35}$Cl and D$^{35}$Cl, this results in a shift in the vibrational frequency according to:

$$\frac{V_{0,H^{35}Cl}}{V_{0,D^{35}Cl}} \approx \left( \frac{\mu_{D^{35}Cl}}{\mu_{H^{35}Cl}} \right)^{1/2}$$

(15)

Since HCl gas is a mixture of H$^{35}$Cl and H$^{37}$Cl molecules, an isotope effect due to the $^{35}$Cl and $^{37}$Cl should be present. However, the ratio of the reduced masses is only 1.0015. This results to a very small frequency shift and consequently, the above spectrum (Fig. 3) shows a superposition of the D$^{35}$Cl and the D$^{37}$Cl spectra. The same is observed for HCl.

III. FOURIER TRANSFORM INFRARED SPECTROSCOPY

A form of infrared spectroscopy that is most widely used today is Fourier Transform infrared spectroscopy. It differs from the conventional form of spectral acquisition by using a polychromatic source of light to irradiate the sample and manipulating the response with a mathematical process called Fourier transformation. One finds in an FTIR spectrometer an
interferometer that makes this method of acquisition possible. Shown in Fig. 4 is an idealized Michelson interferometer.

![Fig. 4. Schematic of a basic Michelson interferometer. S = source, M₁ = fixed mirror, M₂ = moving mirror, x = displacement, D = detector, and B = beam splitter.](image)

The infrared light coming from the source S is directed to a beam splitter B which allows part of the light to pass through while the rest of the light is reflected back. The reflected part of the beam travels to the fixed mirror M₁, is reflected there and hits the beam splitter again. The same happens to the light that passed through the beam splitter. It hits the reflecting mirror M₂. However, this mirror is moving back and forth by a r distance x. When the beams coming from M₁ and M₂ recombine at the beam splitter, they have a difference in path length so that they interfere. The beam leaving the interferometer goes through the sample and finally reaches the detector. The signal that emerges from the sample is called an interferogram and is given by:

\[ S(x) = K \cdot \Phi \cdot \cos(4\pi x \cdot \nu) \]  \hspace{1cm} (16)

where K = a constant that includes detector response and geometrical factors,
- x = mirror displacement,
- \( \nu \) = wavenumber of the signal
Since the radiation coming from the sample is made up of polychromatic light and since the molecule absorbs and transmits light at different frequencies, the signal is the integral over all frequencies:

\[ S(x) = \int_{-\infty}^{\infty} \Phi_\nu \cdot \cos(4\pi x \cdot \nu) \cdot \nu \]  \hspace{1cm} (17)

or by doing a Fourier transform, the spectrum is obtained:

\[ \Phi_\nu = \int_{-\infty}^{\infty} S(x) \cdot \cos(4\pi x \cdot \nu) \cdot \nu \]  \hspace{1cm} (18)

This method of spectroscopy provides various advantages: (1) wave number accuracy; (2) a throughput advantage so that more light reaches the sample; and (3) all the frequencies coming from the light source hit the detector simultaneously resulting in an acquisition of a broad range of frequencies in a single measurement.
IV. EXPERIMENTAL PROCEDURE

A. Apparatus

The following equipment is required for this experiment:

3L bulb of HCl
3L bulb of DCl
Genesis II Fourier Transform Spectrometer
Gas cell with NaCl windows
Liquid nitrogen trap (coldfinger) with ball/socket connections and isolating valves
2L liquid nitrogen (from Chemistry-SES stockroom) and dewar
1000 torr Baratron pressure gauge
Vacuum line (see Fig. 6) and mechanical pump with hose connections

B. Sample Cell Preparation

A few points must be kept in mind while operating the vacuum line for this experiment. HCl and DCl are extremely corrosive gases, which, if allowed to escape from the bulb or vacuum line, would attack the skin, eyes, nose, throat, etc. of any person near the leak. For this reason, the bulbs must be handled and attached with care. To decrease the risk of extensive leakage in the event of a mistake, the teaching assistant has prepared two bulbs of HCl and DCl at moderate pressure.

Incorrect operation of the valves may result in escape of gaseous HCl or DCl. Valve handles are marked with blue to indicate the position of the opening in the valve stem. Before performing any operation on the vacuum line, verify that all valves are in their proper settings. Also, when turning valves, grasp the outer body of the valve with one hand while turning with the other hand. This minimizes the strain placed on the connecting glass tubing.

Safety goggles must be worn at all times!

1. Go over to the Chemistry Stockroom in 4320 SES (same floor as Chemistry Department Main Office) and fill up the large dewar with liquid nitrogen.
2. Look at Fig. 6 for the diagram of the vacuum line: the lettering below refers to various points on this diagram. Verify that all vacuum line valves are in the closed position. The bulb and IR cell should not yet be attached.

![Diagram of vacuum line](image)

*Fig. 6. Vacuum line for sample cell preparation.*

3. Fit the cold trap between the hose that leads to the mechanical pump and valve C. Attach the spring clips across the two joints but do not tighten them.

4. Place the empty dewar under the cold trap, raising it until it covers most of the trap. Clamp the dewar.

5. Tighten the spring clips across the joints of the trap.

6. Fill the dewar with liquid nitrogen until the trap is completely immersed in liquid nitrogen.

7. Turn on the mechanical pump. Make sure that valve G, to which the Baratron is attached, is open. The Baratron reads in torr (1 unit = 1 torr = 1mm Hg, where 1 atm =760 mm Hg).

8. Turn ON the exhaust line (Note: Exhaust line should be ON when ever mechanical pump is ON)
9. Then open valves A, B, and C and observe the pressure readings as the gas line evacuates. The Baratron may display negative values.

10. Remove the IR cell from the dessicator.

11. Fit the inlet ball of the IR cell into the socket under valve D, and place a spring clip across the joint. You may need to use a clamp to support the cell. The valves on the IR cell should be closed.

*Note: Do not allow the NaCl windows of the IR cell to come into contact with any g moisture. Placing fingers on the window surfaces will cause damage.*

12. Open valve D to evacuate the region between D and H. Then proceed to open valve H to evacuate the cell. The second IR cell valve should always be closed. If you suspect a leak, isolate the gas line by closing valve C and observe any pressure changes.

(l) If you are going to record the spectrum of the empty cell, close the valves H and D, then remove the cell and proceed to the directions attached entitled:

**Instrument Operation for the Genesis II FTIR - I. Loading the Software**

Follow these through **Running a Background Scan**. Or else (2) if you are going to ~ till the cell with gas (HCl or DCl), proceed to step 13.

13. Get the HCl bulb from the TA (valve I closed) and fit its inlet ball into the socket under valve E. Attach a spring clip across the joint but do not tighten holding screw. Support the bulb with the metal ring. Now, tighten the holding screw of the clip. Evacuate the region between valves E and I by opening E and leaving I closed.

14. To fill the cell, first close valves A and C. Then carefully open valve I SLOWLY to admit about 125 Torr of gas into the IR cell. Do not exceed 175—torr. Record the pressure of the gas in the cell and close valve H.

15. Slowly open valve C. Once the pressure has stabilized, open value A to the mechanical pump to fully evacuate the line.
16. Verify that valve I is closed. Then close valves E and D. The bulb and the IR cell may be removed at this time by first removing the supporting rings and then removing the clips. Gently free the ball and socket connections.

17. You are now ready to acquire an IR spectrum of HCl. See directions attached entitled Instrument Operations for the Genesis II FTIR - III. Running a Scan

*Do not use a background spectrum from a previous day or lab section.*

18. After measuring the spectrum of the gas, attach the IR cell to the vacuum line by fitting the inlet ball of the IR cell into the socket under valve D, and placing a spring clip across the joint. The valves on the IR cell should remain closed.

19. Close valve A, keeping valves B, C open. Evacuate the cell by opening valves D and H. The Baratron gauge should show a quick increase then a decrease in pressure. When the pressure stabilizes, open valve A to evacuate the line completely.

20. After evacuating the cell, close valves D and H and remove the cell from the gas line.

21. Take the IR cell to the hood and open both valves of the IR cell and return the cell to the dessicator.

22. When you are finished using the gas line, you must remove the cold trap and allow it to release the trapped HCl or DCl into a hood. To do this, close valve C first. Then close valves B and A. Turn off the mechanical pump. Carefully remove the liquid nitrogen dewar. Remove the clips near valves A and B, and then carefully remove the sealed trap from the gas line and bring to the hood. Valves A and B should be opened when the trap is in under the hood and the valve openings are pointed away from you. Leave the trap under the hood.

23. Turn OFF the exhaust line.
V. CALCULATIONS

1. With the H$^{35}$Cl and D$^{35}$Cl spectra, index the lines with the appropriate J values. Do not work on H$^{37}$Cl and D$^{37}$Cl. See Fig. 3.

2. For both H$^{35}$Cl and D$^{35}$Cl, do the following:
   (a) Make a table of J values and the experimental corresponding frequencies from the R and P branches.
   (b) Plot $\frac{1}{2}[ν_R(J) + ν_P(J + 1)]$ against (J+1)$^2$ and draw the best straight line through the points. This is function $f = f[(J+1)^2]$. Use Excel or any other program that you can use to calculate a linear regression.
   (c) Compute the function $f = f[(J+1)^2]$ using Eqs. 12 and 13 to determine what the slope and the intercept represent.
   (d) Plot $\frac{ν_R(J) - ν_P(J + 1)}{J + 1}$ against (J+1)$^2$ and draw the best straight line through the points. This is function $g = g[(J+1)^2]$. Use Excel or any other program that you can use to calculate a linear regression.
   (e) Do the same as in (c) for $g = g[(J+1)^2]$.
   (f) Calculate $I_e$, the moment of inertia and $r_e$, the internuclear distance.
   (g) Tabulate the values of $ν_0$, $B_e$, $B_0$, $B_1$, $α_e$, $D$, $I_e$ and $r_e$.

3. Compute the ratio $\frac{ν_{0,H^{35}Cl}}{ν_{0,D^{35}Cl}}$.

4. Using the results from the simulation and following the diagrams in Figs. 2 and 3, draw simulated IR spectra of HCl and DCl indicating their line positions as predicted by the Diatomic Molecular Simulation program.
VI. DISCUSSION

1. What assumptions are being made in the vibrational analysis and, consequently, in the calculation of molecular constants?

2. Compare the molecular constants calculated with literature data from [2].

3. Give some possible reasons for the difference between the calculated ratio $\frac{v_{0, H^{35} Cl}}{v_{0, D^{35} Cl}}$ and the predicted value given by Eq. 15.

VII. REFERENCES

Instrument Operation for the Genesis II FTIR

I. Loading the Software.

The IR software that is used for this experiment is WinFIRST. To start the program, double click on the 'WinFIRST' icon on the windows desktop. Before any scans can be completed, the 343 file must be initiated. To do this, go to the tool bar, which is located on the top of the screen, and click on TOOLS. Then choose CONTROL PANEL. Once this is done, another screen entitled 'Control Panel' should appear. Click on LOAD METHODS. If this does not appear on the 'Control Panel' 'screen then click on OPTIONS. You should see the LOAD METHODS button. Next, a 'Load Scan Method' screen should appear. Scroll up or down to locate the chem343.ini file. Highlight this file. Then click OK. The 'Control Panel' screen should appear again. The appropriate software is loaded and you are now able to start this experiment.

II. Running a Background Scan

A background scan allows the user to easily subtract out the contributions of the sample holder, solvent, instrument, and atmosphere inside the instrument from the spectra. For every run, different solvent, or different technique of acquiring a spectrum, you must first acquire a background spectrum. The same background, however, may be used for many spectra. A new background should be acquired after ~60 minutes has elapsed, to account for any change in the instrument over time.

To open the sample compartment slide the door open to the right and insert the empty IR cell by sliding it along the grooves of the holder. (The background sample will typically be an empty cell or it may only be air.) Close the sample compartment. You want to minimize the amount of time the compartment remains open to reduce the purge time.

Allow the instrument to purge for live minutes before you run a background. ALWAYS allow sufficient and consistent purge time between opening and closing the IR panels (it has been experimentally determined that if the small panel is open for ~5 seconds then ~3 minutes for the purge time is required and if the large slide panel is open for ~5 seconds then ~7 minutes of purge time is required). The more consistent you are on purging the better your spectra will look.
On the 'Control Panel' screen, make sure that you select Background and then click the green SCAN button. A window will appear that will say “Please prepare for a background scan”. Click OK. The spectrometer will take 16 scans and produce a spectrum that is an average of them. Check the background spectrum. If it is acceptable then you can proceed to acquire a sample spectrum. To determine if your background is acceptable, consider what the background consists of and how it contributes to the spectrum. You do not need to save the background spectrum.

III. Running a Sample Scan

Once your sample is prepared and ready to be scanned, slide the lid open, place your sample in the sample holder, and close the sample compartment cover. The spectrometer needs to be purged for ~5 minutes after closing the cover. For the best results, be conscientious about how long you purge for each sample or background scan. After 5 minutes, locate the 'Control Panel’ screen. If the 'Control Panel’ window is not open, click on TOOLS, and then click on CONTROL PANEL to open the dialog box. Select Sample and then click on the green SCAN button. Another screen will appear that says "Please prepare for a sample scan". Click OK. 16 scans of your sample will be acquired and the spectrometer will average them and subtract the current background spectrum from the result.

Once the spectrum appears on the screen, check if it is acceptable. If acceptable, you can remove the cell from the sample holder and begin to prepare the next sample that needs to be scanned. To print:

a) First save the spectrum so you can return to this point if necessary
b) Zoom into the region of interest in the spectrum by holding the left mouse button and drawing a box around the relevant region and then releasing it. You can unzoom by clicking anywhere on the spectrum. (2900 cm⁻¹ for HCl; 2100 cm⁻¹ K for DCl)
c) If necessary, adjust the baseline, which is described below
d) Pick peaks, which is also described below
e) Print the spectrum

IV. Saving Your Data

To save the spectrum, click on the following in this order:
File (on the tool bar at the top of the screen)
Save Sample As
Click on c:\
Data
Chem343
Appropriate semester and year
Then give this file a name and click OK

Once you save your first spectrum to this directory be sure to remain there so all of your data stays together and can be easily found.

V. Labeling Peaks

Once your spectrum appears on the screen, you might want to adjust the baseline of the spectrum if it is poor. To perform this operation, click on MATH on the tool bar, at the top of the screen and then choose BASELINE. A red window will appear that is entitled 'Choose a New Baseline'. With the right mouse button, click on the baseline of the farthest left part of your spectrum at a point that you would want the new baseline to fall. Click the 'Ok' button in the 'Choose a New Baseline' window.

To label the peaks, click on TOOLS on the toolbar and then choose 'Annotator'. A window should appear entitled 'Notate'. To label a peak, click on the Hrst button on the top row of the spectrum that you want to label, being careful to click on the center peak that you are interested in choosing. The software will label that peak with the wavelength. To label additional peaks, again click on the first button on the top row of the 'Notate' window. Then choose a peak that you want labeled. Continue this process until you have enough peaks labeled. To know if you have enough peaks labeled, check the reference spectra in the science library before you run a scan. This will help you to compare your spectrum to the reference spectrum. You will also need to hand in a copy of the reference spectra with your report. Once you have labeled all of the peaks you will want to print your spectrum as described below.

VI. Printing Data

To print a spectrum, click on FILE, PLOT, and then PLOT again. Once the spectrum has been printed, click on DONE. Then close the WinFIRST program.
Vibrational and Rotational Motion of HCl and DCl

Diatom Molecular Simulation Program

I. Background

The Diatomic program illustrates the translational, rotational, and vibrational motions of diatomic molecules from the perspectives of classical, quantum, and statistical mechanics. For this lab you will perform three simulations on each of HCl and DCl after completing the HCl/DCl infrared experiment. These simulations will give a better idea of the fundamental physical principles upon which rotational and vibrational spectroscopy are based.

1. Classical motion. While you will not collect data from this section you should observe those aspects of motion which are independent and those which are concerted in the rotation and vibration of the molecules.
2. Quantum vibrational motion. You will obtain printouts of the first 20 vibrational energy levels for the 1) Morse, 2) harmonic, and 3) Lennard-Jones potentials. Be sure to record the numerical values for the energy levels.
3. Quantum rotational motion. You will obtain printouts of the first 10 rotational energy levels for the vibrational states \( \nu = 0 \) and \( \nu = 1 \). Again, be sure to record the numerical values for the energy levels.

II. Simulations

Double click on the 'Diatomic' icon then click on START.

Classical motion. Click on CLASSICAL at the top of the page and choose HCl from the drop down menu in the upper left corner. Click on FORWARD to start the simulation. Select Vibration and Rotation to observe these motions separately and together. (You must stop and reset the motion after changing any conditions.)

The classical equations of motion are unable to duplicate the effects of quantum mechanics and a classical simulation cannot give ro-vibrational spectra such as you have obtained for HCl and DCl.

Quantum vibrational motion. Click on QUANTUM at the top of the page, and then select the 'Vibration' tab. In the Levels box, you must right click and select Double Entries in order to get more than 16 levels. Highlight the first 20 levels (by scrolling while holding down
the mouse button or using the control key). Before printing your simulation you must go to printer set up and make sure the printer is set on its highest resolution. (If you do not, the energy levels will be too faint to read). Print the plot and record the numerical values for the energy levels. Then change the potential (by clicking on EDIT POTENTIAL ENERGY and selecting the potential you want) and repeat the simulations for 1) Morse, 2) harmonic, and 3) Lennard-Jones potentials.

**Quantum rotational motion.** Select the 'Rotation' tab. Choose v = 0 and the first 10 J states. Print the plot and record the numerical values for the energy levels. Do the same for v = 1.

**Instructions for DCl Simulation**

You will need to modify the HCl parameters for DCl. Select HCl from the drop down menu. Click on INSPECTOR and select Atoms and Bond. Change Atom 1 label from H to D then click on ADD MOLECULE TO LIST. Close 'Inspector' window. Select DCl from the drop down menu and click on INSPECTOR. Select Molecule Data. A spread sheet will open listing parameters for various molecules. Go to DCl and replace the following column entries with the DCl parameters that you looked up in the references listed in the lab write-up. Be sure to employ the appropriate units and enter all significant figures.

- **Mass, m**  g mol⁻¹  atomic mass of deuterium atom
- **Radius, r**  pm  covalent radius of deuterium atom
- **Spin, J**  nuclear spin of deuterium atom
- **Bond Energy**  kJ mol⁻¹  bond energy of DCl molecule
- **ωₑ**  cm⁻¹  νₑ in lab write-up
- **ωₑxₑ**  cm⁻¹  xₑνₑ in lab write-up
- **Bₑ, αₑ**  cm⁻¹
- **Dₑ**  cm⁻¹  Dₑ in references

Click on SAVE TO FILE and replace the existing tile 'diatomic.ddf' with the edited file, keeping the same name. Close the 'Inspector' window, go to the drop down menu, select DCl, click on INSPECTOR, and check that the edited parameters were properly saved. You can now proceed with the DCl simulations. After completing them, click on Molecule Data in the
’Inspector’ window, go to DCI data, highlight each column entry individually, and delete the entries in all the columns. Save the file and replace the existing ’diatomic.ddf’ with the file with the DCI data deleted. Close the program and reopen to check that DCI is deleted from the drop down menu.

III. Calculations

**Vibrational motion.** For each potential calculate the band origin. For the Morse I and harmonic potentials, estimate \( r_e \) for \( \nu = 0, 5, 10, \) and 15 and compare these values.

**Rotational motion.** You will use these values to produce your simulated IR spectra.