Physics 338 Advanced Physics Laboratory

Absorption Spectroscopy of Molecular Iodine

First "Draft" - graphs and results	**Tuesday, October 22, 2024 11:00 am**
Second Draft Full Report	**Tuesday, October 29, 2024 11:00 am**
Peer Review Report	**Friday, November 1, 2024 12:00 noon**
Final Report	**Friday, November 8, 2024 5:00 pm**

Safety

UV: The quartz halogen lamp used in this experiment gives off a significant amount of ultraviolet (UV) light. So can the mercury pen lamp used to calibrate the spectrometer. UV light can be hazardous, particularly to the eyes. It is important to wear UV goggles when working with the light. After everything is set up, you should cover the lamp to shield everyone else from the UV light, and then you may remove the goggles.

Heat/fire: The lamps can get quite hot. The iodine vapor cell is also wrapped in heating tape, which can get hot. Be careful touching hot things. When you cover the lamps with boxes to shield the UV light, make sure the cardboard is not touching "hot spots" to avoid fire risk. It's likely you will set up at least one "long run" of 1-8 hours, in which case you will leave the lamp and heater on and unattended. Please be sure to come back ASAP and turn them off. This does not completely eliminate a fire risk, but it does minimize it.

Mercury: Mercury is highly toxic. The mercury in the mercury lamp is safely enclosed by quartz. However, if the lamp were to somehow break (very unlikely), you should not attempt to clean it up yourself. Please put a note out to alert your fellow students to the problem, and contact me so we can sort it out together.

1 Introduction

Spectroscopy is a powerful and precise tool for probing the structure of atoms and molecules. In atoms, the emission and absorption of optical radiation is associated with a change in an atom's electronic state. In molecules, electronic transitions are still possible, but transitions involving changes in vibrational and/or rotational states are also possible.

In this experiment, you will use absorption spectroscopy to study some of the transitions involving electronic and vibrational states in molecular iodine I_2. In absorption spectroscopy, white light is shone through a vapor and then into a spectrometer. Wavelengths that correspond to a transition will be preferentially absorbed, and will show up as a dip in the measured intensity.

A reasonable model of a diatomic model such as iodine is to consider it as two atoms connected by a spring. The potential arises from the rather complex coulombic interac-

tion between the two atomic charge distributions. For small displacements around the equilibrium separation, the potential can be approximated as an harmonic oscillator. The molecule is also free to rotate about its center of mass, so rotational states must be considered as well.

It is helpful to think of a molecule's energy structure in terms of three internal *degrees of freedom*: electronic, vibrational, and rotational. The time scales of these three types of motion are quite different; electrons move much faster than the relatively heavy nuclei, and a molecule vibrates much faster than it rotates. These mismatches in time-scales allow the total energy to be separated into three terms

$$E = E_{el} + E_{vib} + E_{rot}$$

where the couplings among the electronic energy E_{el}, the vibrational energy E_{vib}, and the rotational energy E_{rot}, are weak and can be ignored to first order. (The separation of the electronic motion from the nuclear motion is known as the Born-Oppenheimer approximation.[1].)

The energies for electronic excitation of a molecule are typically on the same order as those in an atom—several electron-Volts, corresponding to transitions in the visible to ultraviolet portion of the electromagnetic spectrum. The characteristic energies of the vibrational degree of freedom are typically a factor of 100 smaller and are generally in the near- to mid-infrared region of the electromagnetic spectrum, with wavelengths from $1.0\,\mu$m to $20\,\mu$m. Rotational energies are yet another factor of 100 smaller, falling into the far-infrared to microwave region, with wavelengths beyond $30\,\mu$m.

In this experiment, we will study a series of transitions involving both electronic and vibrational states. (The energies involved due to changes in the rotational states are too small to be resolved with our spectrometer.) This experiment is based on one described by George and Krishnamurthy[2].

2 Theory

2.1 Vibrational Energy

As suggested above, we can think of a diatomic molecule as two masses attached by a spring. For any particular electronic state, the spring constant is nearly fixed. As long as the vibrational amplitude does not get too large, the energy levels associated with the vibrational motion are accurately described by the quantum mechanical harmonic oscillator

$$E_{vib} = hf\left(v + \frac{1}{2}\right), \tag{1}$$

where v is the vibrational quantum number, and f is the frequency associated with the vibrational motion. (The notation is unfortunate here—the letter "vee" for the vibrational quantum number v is typographically similar to the Greek letter ν often used for the frequency.)

This two-body problem (with masses m_1 and m_2 on either end of a spring of spring constant k) can be reduced to a single-body central-force problem by using

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$$

where μ is the reduced mass

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}.$$

Thus measurements of the vibrational spectrum can yield information about the inter-atomic potential.

2.2   Wave Numbers and Notation

Spectroscopy is an extraordinarily precise science. Precision measurements of wavelengths laid the foundation for quantum mechanics, and continue to provide precision tests of theory. For a recent example, see the article on "Diatomic Molecules: A window onto fundamental physics" in the December 2015 issue of *Physics Today*[9]. Accordingly, it is conventional to present results in terms of directly-measured wavelengths (and wavenumbers) rather than in terms of energy, since conversion to energy units historically involved multiplication by constants that introduce their own uncertainties.[1]

In addition, the spectra of atoms and molecules can be extremely complex; any notation able to capture that complexity is likely to be itself rather complex. Historically, that notation has evolved within its own community, so some of the terms may be unfamiliar to newcomers. For this experiment, we will follow the notation as outlined in Ref. [6].

Since the energy of a photon $\epsilon = hc/\lambda$ depends inversely on the wavelength, it is useful to define a *wavenumber*, $\tilde{\nu}$, defined by

$$\tilde{\nu} = \frac{1}{\lambda}$$

For visible light, it is conventional to express the wavelength λ in nanometers. The wavenumber is commonly expressed in cm^{-1}. So, for example, the mercury green line

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[1]With the 2018 redefinition of the fundamental SI units, both Planck's constant and the speed of light are now defined quantities. See https://www.nist.gov/si-redefinition. Still, unconverted wavenumbers still offer the most precise and stable comparisons with the published literature.

with wavelength $\lambda = 546.074\,\text{nm}$ corresponds to a wavenumber

$$\tilde{\nu} = \frac{1}{546.1\,\text{nm}} = 1.8313 \times 10^{-3}\,\text{nm}^{-1} = 18313\,\text{cm}^{-1}\ .$$

The energy relation in Eq. 1 can be expressed in terms of wavenumbers by dividing both sides by hc.

$$\frac{E_{vib}}{hc} = G(v) = \omega_e \left(v + \frac{1}{2} \right), \tag{2}$$

where ω_e is known as the vibration wavenumber. Again, the notation is unfortunate. The ω_e here has units of reciprocal length, and is commonly expressed in cm^{-1}. The vibrational term $G(v)$ also has units of reciprocal length, but plays the role of an energy, and is often called the vibrational energy.

As is the case for nearly any oscillator, if you carefully analyze the energy structure of a diatomic molecule, you will find deviations from the ideal harmonic behavior, especially for higher vibrational levels. Recall that when analyzing the harmonic oscillator, we began by assuming that the restoring force varies linearly with displacement (and hence that the potential varies quadratically). Deviations from harmonic behavior arise from a breakdown of this linear assumption. In a molecular spectrum, evidence for this *anharmonicity* of the potential energy function is seen in the spacing of adjacent energy levels. The harmonic oscillator analysis predicts equal spacing, but molecular spectra typically show spacings that decrease with vibrational number v.

The potential energy that governs molecular vibration is, therefore, not simply a parabola. Figure 1 compares a harmonic potential (i.e., a quadratic) to a model potential[5] for diatomic iodine. In the region near the equilibrium position, r_e, the harmonic oscillator potential is an excellent approximation to the molecular curve. The real potential, however, differs substantially from a parabola when r differs significantly from r_e. To better approximate the molecular potential at large separations, higher-order correction terms can be added to the harmonic solution. For example, the vibrational energy formula (Eq. 2) can be modified by adding a second-order correction term as

$$G(v) = \omega_e \left(v + \frac{1}{2} \right) - \omega_e x_e \left(v + \frac{1}{2} \right)^2 \tag{3}$$

where $\omega_e x_e$ is a single term.[6] Again, ω_e and $\omega_e x_e$ are measured in inverse centimeters. This notation may look unusual, but it is traditional. (A cubic correction term, $\omega_e y_e \left(v + \frac{1}{2} \right)^3$ is also often included, and does make a difference with sufficiently high resolution data.[8].)

The vibrational states of the nuclei become unbound above a certain point. This corresponds to the molecule breaking apart, called dissociation. The dissociation energy, D_e,
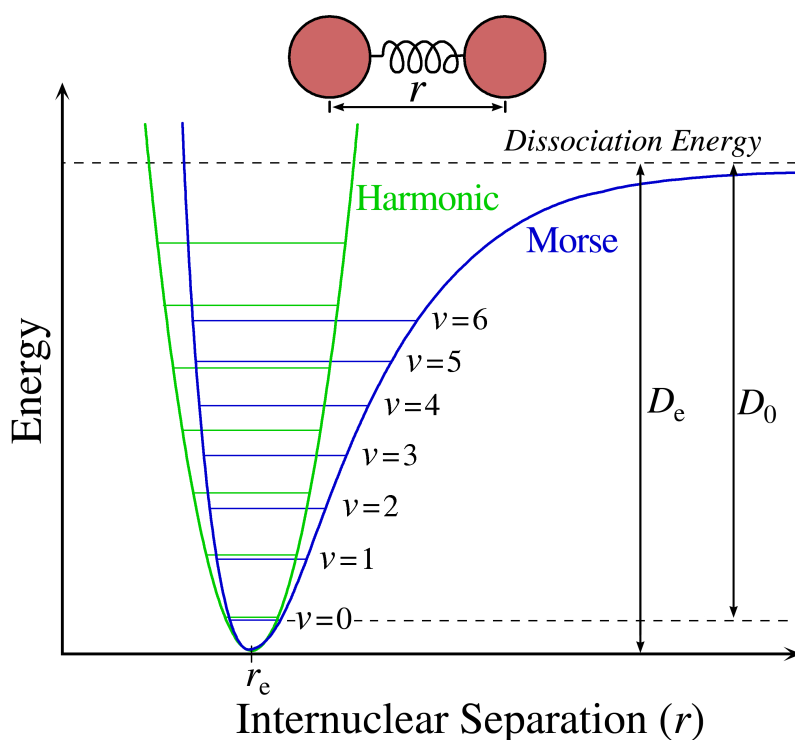
Figure 1: Potential energy of a harmonic oscillator and a Morse potential [5] for the I$_2$ ground state. (Image by Somoza[10].)

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of a molecule is an important physical parameter, which, it turns out, can be determined spectroscopically from $G(v)$. Specifically, if $G(v)$ is given by Eq. 3, then the dissociation energy can be found by measuring ω_e and $\omega_e x_e$:

$$D_e = \frac{\omega_e^2}{4\,\omega_e x_e} - \frac{\omega_e}{2} + \frac{\omega_e x_e}{4} \,, \tag{4}$$

where D_e is measured in wavenumbers. (This is actually labeled D_0 in Fig. 1. The difference is whether or not you include the ground state energy.)

Derivation of this result should be part of your report.

3   Electronic Transitions

Figure 2 shows the potential energy curves of two different electronic states of molecular iodine: the ground state (typically labeled as the X-state) and the second optically-active
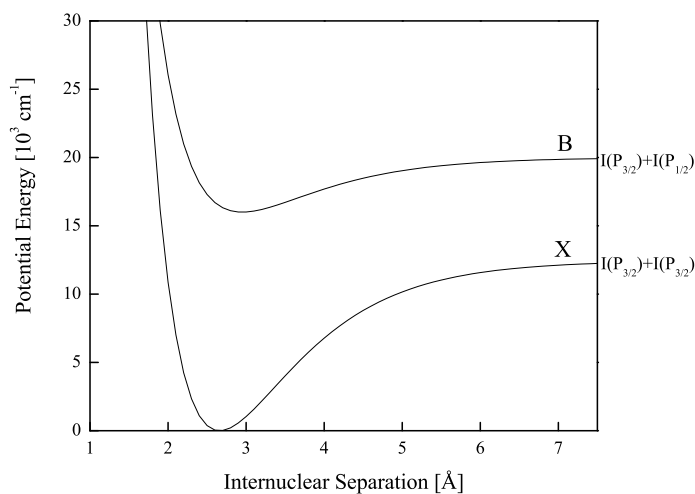
Figure 2: Potential energy curve for the ground X-state and the electronically excited B-state of I_2. Notice the different equilibrium position of the nuclei for these two electronic states.

excited state (typically labeled as the B-state). In general, the vibrational constants, ω_e and $\omega_e x_e$, are different for the two states because the different electronic configurations produce differently shaped potential curves. Conventional spectroscopic notation dictates that the upper electronic state's parameters are labeled with single primes, ω_e' and $\omega_e x_e'$, and the ground state's parameters are labeled with double primes, ω_e'' and $\omega_e x_e''$. The electronic energy of the ground state is defined to be zero, and the electronic energy of the excited state is labeled as T'. The total energy of a vibrational level in an excited electronic state therefore is $E(v') = E_{el} + E_{vib}$. Dividing by hc and expressing everything in wavenumbers yields

$$\frac{E(v')}{hc} = T' + G(v') = T' + \omega_e'\left(v' + \frac{1}{2}\right) - \omega_e x_e'\left(v' + \frac{1}{2}\right)^2. \qquad (5)$$

A transition between two different electronic states of a diatomic molecule usually involves a simultaneous change in vibrational motion. The wavenumber of a photon absorbed when a molecule undergoes an electronic transition from vibrational state v'' in the ground state to state v' in the B-state is

$$\tilde{\nu}(v', v'') = \frac{1}{hc}(E(v') - E(v''))$$
$$= T + \omega_e'\left(v' + \frac{1}{2}\right) - \omega_e x_e'\left(v' + \frac{1}{2}\right)^2 - \omega_e''\left(v'' + \frac{1}{2}\right) + \omega_e x_e''\left(v'' + \frac{1}{2}\right)^2. \qquad (6)$$

November 5, 2024

Since there are no explicit restrictions on the change of the vibrational quantum numbers during an electronic transition, the resulting spectrum is quite complex.[2] Consider an ensemble of diatomic molecules in the lowest vibrational state ($v'' = 0$) of the ground electronic state. When exposed to a continuum light source, these molecules can absorb radiation and make transitions to a wide range of v'-levels in an electronically excited state. An analysis of the resulting absorption spectrum can yield the vibrational constants of the excited electronic state. If, on the other hand, the ensemble is initially in a distribution of vibrational levels of the ground electronic state, then an analysis of the spectrum can also yield the vibrational constants of the ground electronic state.

We will perform an absorption experiment and carry out the analysis to determine the properties of the ground state (X-state) and an excited state (B-state) of molecular iodine, I_2. We will measure the optical absorption spectrum of iodine vapor in a 10 cm long cell held slightly above room temperature. Near room temperature, most iodine molecules are found in the lowest vibrational state of the ground electronic state. When illuminated by white light, the molecules will absorb photons with energies corresponding to the differences between the $v'' = 0$ vibrational level of the ground electronic state and various vibrational levels of the electronically excited state. These transition energies are given by Eq. 7 with $v'' = 0$:

$$\tilde{\nu}(v', 0) = T' + \omega_e' \left(v' + \frac{1}{2} \right) - \omega_e x_e' \left(v' + \frac{1}{2} \right)^2 - \frac{1}{2} \omega_e'' + \frac{1}{4} \omega_e x_e''. \tag{7}$$

As a result of these absorptions, the intensity of the light passing through the iodine vapor cell will be suppressed at wavelengths given by

$$\lambda = \frac{1}{\tilde{\nu}(v', 0)}. \tag{8}$$

Equations 8 and 9 suggest that the resulting spectrum of a continuum light source should contain a simple progression of absorption features, with each feature corresponding to a particular value of v'. If the sample is heated, additional transitions corresponding to $v'' > 0$ in Eq. 7 will be observed as well. Compare Figs. 3 and 4.

The continuum light source in this experiment is called a quartz halogen lamp—a lamp with a tungsten filament but with the normal glass replace by quartz and the bulb filled with low-pressure halogen gas. The quartz is used because it transmits ultraviolet light much better than normal glass and because it can withstand higher temperatures. The halogen gas extends the lifetime of the tungsten filament and lets the filament run at higher temperatures, producing higher intensities at shorter wavelengths.

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[2]For details on how vibrational states influence transition probabilities, see the discussion of the Franck-
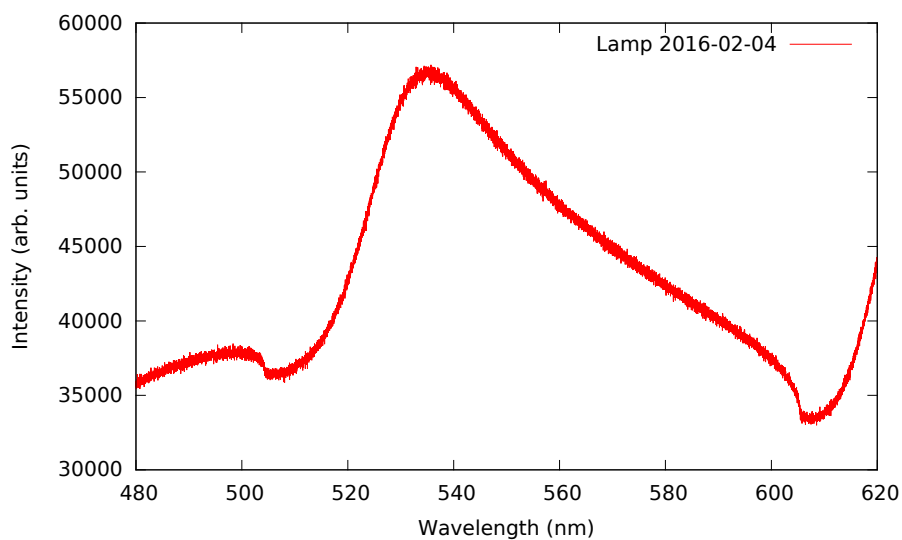
Figure 3: Spectrum of the quartz halogen lamp without any absorption cell

Since the lamp emits considerable light in the ultraviolet, you must be careful to use protective goggles when the lamp is on. While acquiring data, you should enclose it with a box.
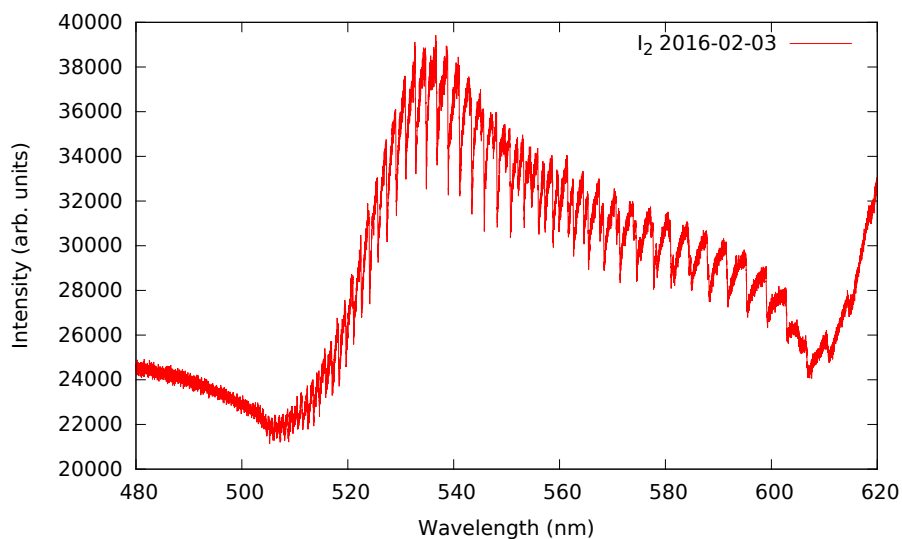

Figure 4: Absorption spectrum for I_2.

Condon Principle in Chapter 5 of Ref. [3], or the Franck-Condon Wikipedia article[11].

4 Procedure

Data acquisition for this experiment is very similar to that used in the Optical Spectroscopy experiment in Phys 215 lab. (A copy of the *Getting Started* guide is in the room with the spectrometer, and also is available from the course website.)

There are two stages to data collection. The first is a calibration using a mercury lamp, which is set up on the side ("Lateral") entrance to the spectrometer.

1. Turn on the mercury pen lamp and cover it with a box.

2. Perform a rough scan over a large wavelength range in order to identify intense peaks in the mercury spectrum.

3. Compare these peaks to known peaks in the Hg spectrum (e.g. NIST database).

4. Perform detailed, "zoomed-in" scans for each intense peak which can be correlated to a known intense Hg line.

5. Use the position of your measured peaks vs. the known peaks to create an equation to convert your measured wavelengths to "corrected wavelengths". Typically, a linear relation is sufficient. This is a typical way to calibrate a spectrometer.

The output of a quartz halogen lamp passes through an iodine vapor cell and is focused onto the front ("Axial") entrance slit of the SPEX 1250M spectrometer.

1. Put on UV safety goggles.

2. The quartz halogen lamp is mounted in a "cage". The lamp's output is collimated with a lens such that it passes through the vapor cell and in to the spectrometer's entrance slit. Set the voltage for the lamp to 5.0 V. (The maximum is 6.0 V, but 5.0 V should work well.) Be careful—the bulb will get hot. Remember not to look at the bulb without the UV safety goggles.

3. The absorption features are weak at room temperature. The melting point of iodine is 114°C, so it is possible to increase the vapor pressure, and thus the absorption signal, by gently heating the I_2 cell. Use the heating tape to to gently heat the iodine cell. **Treat the iodine cell with care as it is fragile and expensive.** Set the power supply to 24.0 V. Use the temperature probe to record the temperature of the cell. Record the voltage and temperature in your notebook. If the temperature is over 50°, turn down the power supply. It will take a while to reach equilibrium, so come back and check the temperature later.

4. Gently place the light-shield box over the lamp, being careful not to disturb the alignment.

5. Set up for a quick trial scan. Set the input slit to height $0.2\,\mathrm{cm}$, width about $10\,\mu\mathrm{m}$, and the output slit to about $10\,\mu\mathrm{m}$. Set the photomultiplier voltage to $850\,\mathrm{V}$ and the integration time to $0.1\,\mathrm{s}$. Record the spectrum from 490 nm to 550 nm. Since you are just trying to see if everything is working, use a large step size, say a 1 nm increment. You should see that absorption features begin to appear at wavelengths longer than about 500 nm, as in Fig. 4.

6. Make any necessary adjustments until you get a good quality spectrum. Time spent getting a good clean signal here will be time well spent, so don't rush this part. Try a few high resolution (0.005 nm step size) scans over a couple of small regions to see how well it works. Give careful thought to the integration time too–you want to get good quality data, but you also want to finish in a reasonable amount of time. (An integration time of $0.1\,\mathrm{s}$ seems to work well. Shortening that time does not significantly speed up the acquisition—the spectrometer spends more time stepping between readings than actually taking the readings.)

7. For a successful analysis of the ground and excited states, the wavelengths of all of the vibrational transitions from 500 nm to 600 nm must be measured. High resolution is required to sort out the closely spaced transitions. Record the iodine spectrum from about 490 nm to 610 nm at a small wavelength interval, say $0.005\,\mathrm{nm}$ per step. (There is not much value in a smaller step size with this apparatus.) A full scan will take about 3 hours. A scan with $0.01\,\mathrm{nm}$ step size works about as well, and completes in about 90 minutes.

8. Save you work. Switch to the `Data` tab under the graph. By default, the `SynerJY` program stores data in a hard-to-find folder. Instead, either make a folder on the Desktop, or use the `Spectrometer User` folder on the Desktop. You should also export your data as an `ASCII` file (either `.TXT` or `.CSV` format can work. (`.DAT` also just gives a plain text file with two columns, but the "DAT" suffix might confuse some programs. *Mathematica* can handle any of these `ASCII` suffixes just fine.) Save your data to a USB flash drive as well. Contact your instructor if you need assistance.

   Open your saved file in a program such as `EXCEL` to verify it saved correctly.

9. Try to interpret the qualitative features of the spectrum in terms of the expected progression of absorption energies predicted by Eq. 7. You are not taking any measurements yet, just checking whether the data are sufficient to proceed. (Within the `SynerJY` program, you can use the Zoom icon to zoom in on different parts of the spectrum.)

   From about 545 nm to 500 nm the spectrum is relatively uncomplicated; the absorption features in this region are known to originate from the $v'' = 0$ vibrational level of the ground electronic state. Features corresponding to transitions from $v'' = 0$ into higher v' are observed as you move towards shorter wavelengths. The wave-

length separation between adjacent features decreases towards shorter wavelength, until eventually the features blend into one another at about 500 nm. The intensity of the features also decreases dramatically near 500 nm as you progress towards the dissociation limit.

For wavelengths longer than about 545 nm, the spectrum becomes more complicated due to the appearance of transitions originating from the $v'' = 1$ and $v'' = 2$ levels. Near room temperature most, but not all, of the iodine molecules are in the $v'' = 0$ level. However, the non-zero population of vibrationally excited molecules lead to extra transitions in the spectrum. The number of molecules in these states are relatively small, and the absorption features originating from these levels are weak in intensity. The $v'' = 1$ progression is observed in the 590–545 nm wavelength range, and the $v'' = 2$ progression is observed in the 600–570 nm region.

Once you are satisfied with your data, move on to the analysis.

5   Analysis

It will be simplest to convert your absorption data to wavenumbers before beginning detailed calculations. You may do all of your analysis within SynerJY, but you will probably find it more convenient to use a tool such as Excel or Mathematica (or both).

Convert your raw absorption values to vacuum wavelengths[3] and then convert to wavenumbers in cm^{-1}.

5.1   Determining the Excited State (B) Molecular Constants

5.2   The $v'' = 0$ Transitions.

Your first need to find the wavenumbers for all the absorption features corresponding to the $v'' = 0$ transitions. These are most readily identified in the wavelength range $500 - 550\,\text{nm}$, which corresponds to the wavenumber range $18,000 - 20,000\,\text{cm}^{-1}$. Use whatever plotting software you find convenient. You can make a convenient plot in *Mathematica* with the following command:

```
ListPlot[Tooltip[wns], PlotRange -> {{18000, 20000}, Automatic},
        ImageSize -> 700]
```

The Tooltip command labels each data point so that the coordinates appear when you hover over the graph with the mouse. The PlotRange option zooms in on the region of interest. Adjust it as needed.

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[3]The relationship between the wavelength in vacuum and the wavelength is air is $\lambda_{vacuum} = \lambda_{air} \cdot n_{air}$ where $n_{air} \approx 1.00028$.

1. Each absorption dip corresponds to a transition from $v'' = 0$ to a different excited v' level. Make a table with two columns, v' and the corresponding wavenumber $\tilde{\nu}(v', 0)$. It is not possible to unambiguously determine the upper state vibrational numbering v' from these absorption measurements. Although it is not strictly necessary to determine them for this part, it will be helpful for later on. In the literature, Williamson lists the $v'' = 0$ to $v' = 25$ transition to have a wavelength of 545.96 nm, or a wavenumber of $18316\,\mathrm{cm}^{-1}$[8]. Use this value to number your progression of transitions. (Note: Williamson reports a list of both vibrational and rotational states in their Supporting Information. Note that the $18316\,\mathrm{cm}^{-1}$ cited here represents an average over the rotational states, which range from $18307 - 18321\,\mathrm{cm}^{-1}$.

   This part can be tricky, so you may have to come back and revise your assignments later. The pattern of lines is fairly regular, with lines getting closer as the wavenumber gets larger. You may find it helpful to compute the differences between adjacent wavenumbers, and also to plot $\tilde{\nu}(v', 0)$ *vs.* v' as you go along.

   Keep adding as many points as you can reliably identify that fit the curve.

2. Plot $\tilde{\nu}(v', 0)$ *vs.* v'. The data should form a smooth curve. If there are any points that appear out of line, go back and re-check your measurements and tabulations.

3. Fit Eq. 8 to your data and determine ω_e', $\omega_e x_e'$, and the corresponding uncertainties. (Note that you can also determine the sum of the three constants, $T' + \frac{1}{2}\omega_e'' + \frac{1}{4}\omega_e x_e''$, but you can't determine them individually.)

5.3   Determining the Ground State (X) Molecular Constants

To perform the analysis for the $v'' = 1$ and $v'' = 2$ series, you need to identify a number of the remaining features and assign the appropriate v' numbers. One convenient way to organize the data is in a "Deslandes" table[6]. In this table, the columns correspond to different v'' values, and rows correspond to v' values. The elements in the $v'' = 0$ column were already determined in Section 5.1.

v'	v''		
	0	1	2
$\dots$	$\dots$	$\dots$	$\dots$
15	$\tilde{\nu}(15, 0)$	$\tilde{\nu}(15, 1)$	$\tilde{\nu}(15, 2)$
16	$\tilde{\nu}(16, 0)$	$\tilde{\nu}(16, 1)$	$\tilde{\nu}(16, 2)$
17	$\tilde{\nu}(17, 0)$	$\tilde{\nu}(17, 1)$	$\tilde{\nu}(17, 2)$
18	$\tilde{\nu}(18, 0)$	$\tilde{\nu}(18, 1)$	$\tilde{\nu}(18, 2)$
$\dots$	$\dots$	$\dots$	$\dots$

As discussed above, the $v'' = 1$ progression is observed in the 545–590 nm wavelength

range, which corresponds to a wavenumber range of $17,000 - 18,400\,\mathrm{cm}^{-1}$. Similarly, the $v'' = 2$ progression is observed in the 570–600 nm wavelength range, which corresponds to a wavenumber range of $16,500 - 17,500\,\mathrm{cm}^{-1}$.

1. You may find it easier to pick out the $v'' = 2$ features first, since they don't overlap as much with other features, particularly in the small wavenumber range.

   Don't worry about the v' numbering just yet—make an arbitrary guess. You will probably find it helpful to make a plot of $\tilde{\nu}(v', 2)$ *vs.* v' as you go along, and add that to plot you made above (also, see Fig. 5 below). The data should form a smooth curve.

2. Similarly, add the $v'' = 1$ features to your table. Again, plot $\tilde{\nu}(v', 1)$ *vs.* v' as you go along.

3. To determine the appropriate v' numbering, consider pairs of transition that start at the same v' value and end at different v'' values. For example, consider the columns for $v'' = 0$ and $v'' = 1$. The differences between adjacent entries should be the same for every v'. That is $\tilde{\nu}(v', 1) - \tilde{\nu}(v', 0)$ should be constant. Add a column to your table to compute the difference, and move the data in the $v'' = 1$, column up or down until the differences are approximately constant. (If you use `Excel`, this can be a little tricky. As you move columns up or down, `Excel` tries to adjust the formulae appropriately; this may not always do exactly what you want, so be sure to check any calculated columns frequently to make sure they remain correct.)

4. Finally, repeat this analysis for $v'' = 2$ to assign the appropriate v' values.

5.4   Fitting Data

There are a variety of methods in the literature to approach determining the ground state parameters. However, the most direct is to do a multi-parameter fit for all of your data to Eq. 7. You can easily do this in *Mathematica* with `NonlinearModelFit`. `Excel` can also do this with the `LINEST` function[7]. Consult with your instructor if you need help on this step.

One useful way to present your results is to enhance the plot you made above to include all three sets of wavenumbers. That is, on the same graph, plot $\tilde{\nu}(v', 0)$ *vs.* v', $\tilde{\nu}(v', 1)$ *vs.* v', and $\tilde{\nu}(v', 2)$ *vs.* v'. The data should form a smooth non-intersecting curves. If they do not, go back and re-consider your assignments of v' and v''. On the same graph, include the results of your fit to Eq. 7. Your result should look something like Fig. 5.
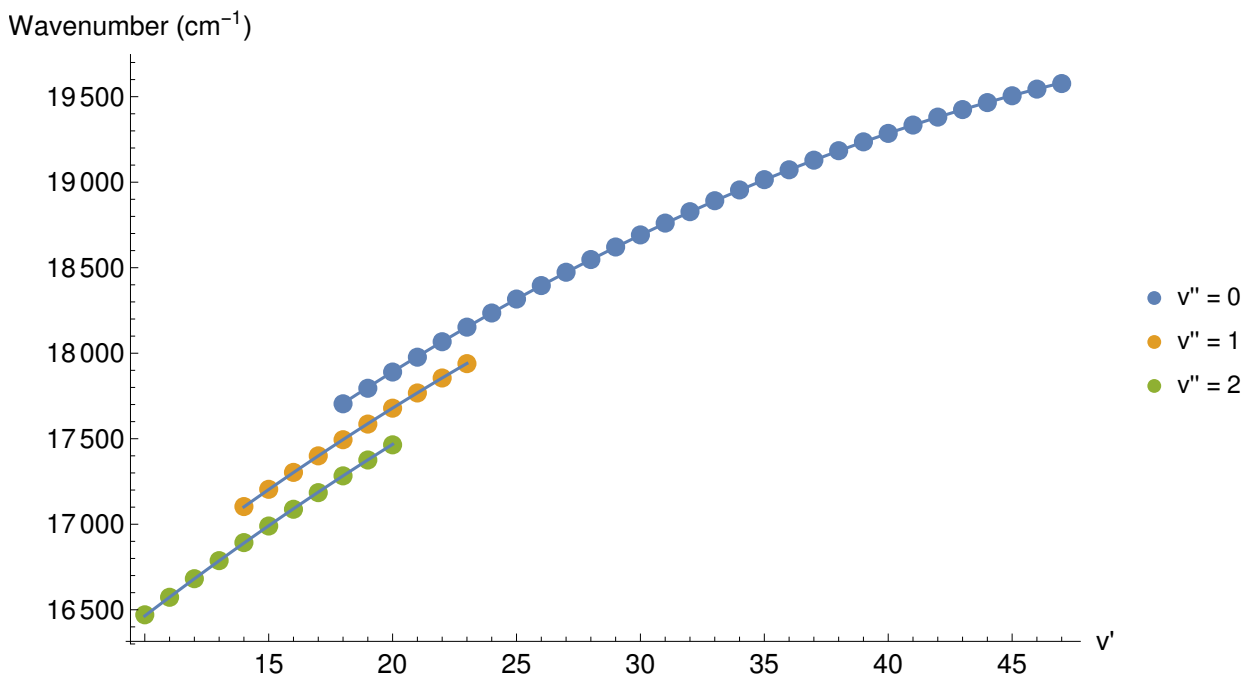
Figure 5: Data and fits for all three series: $v'' = 0$, $v'' = 1$, and $v'' = 2$.

5.5　Results

Report your final results for T, ω_e', $\omega_e x_e'$, ω_e'', $\omega_e x_e''$, and the dissociation energy D_e. Compare them to the literature values [2]. Discuss your results.

References

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