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1 Introduction

The purpose of this experiment is to gain an understanding of molecular spectroscopy. Using spectra, information about molecular constants of the I_2 molecule shall be gained. By taking both an emission and an absorption spectrum, important constants of the first excited iodine state should be calculated and relevant transitions identified.

2 Theory

If not specified otherwise, the information in this section is taken from the staatsexamen [1].

2.1 Molecular Term Symbols

To identify a molecular state, so-called molecular term symbols are used. These are written in the following form:

$$^{2S+1}\Lambda^{(+/-)}_{\Omega(g/u)} \tag{1}$$

For this form,

- S describes the total spin quantum number of the molecule, and 2S + 1 is the multiplicity, which equals the amount of the magnetic spin quantum numbers.
- Λ is the projection of the orbital angular momentum onto the molecular axis. To denote $\Lambda = 1, 2, 3, \ldots$, the symbols $\Sigma, \Pi, \Delta, \ldots$ are used.
- (+/-) indicates the sign change of the wave function when mirrored along a plane perpendicular to the molecular axis.
- Ω is the projection of the total angular momentum of the molecule onto the molecular axis.
- (g/u) denotes the behavior of the wave function when mirrored at the center of symmetry. If the sign of the wave function does not change, g (gerade) is used, otherwise u (ungerade) is used.

This notation does not include the electronic state of the molecule. To do so, letters are often added in front of the term symbol. When doing so, The electronic ground state is represented by X while excited states are labeled A, B, C, \ldots in their energetic order.

2.2 Electronic Transitions

Selection rules are used to determine whether electronic transitions between molecular states are possible. The relevant selection rules in this experiment are:

$$\bullet \ g \ \leftrightarrow \ u, \, g \ \nleftrightarrow \ g, \, u \ \nleftrightarrow \ u$$

- $\Delta\Omega = 0, \pm 1$
- $\Delta\Lambda = 0, \pm 1$
- $\Delta S = 0$

While some of these selection rules are universal, the last two cases are only valid for one of Hound's coupling cases.

In this experiment, the transition of interest is

$$X^1 \Sigma_{0q}^+ \leftrightarrow B^3 \Pi_{0u}^+$$
 (2)

This transition does not fulfill the last selection rule, however, due to the strong spin-orbit interaction of the iodine molecule, the corresponding coupling case the last selection rule is valid for does not apply.

The electronic transition is accompanied by a system of vibrational transitions to be observed in this experiment. In addition, it should be possible to observe various rotational transitions. However, the energy of peaks caused by rotational transitions can not be resolved with the setup of this experiment.

2.3 Born-Oppenheimer Approximation

The Born-Oppenheimer approximation considers the movement of the electrons and the nuclei as separate. The wave function of the molecule Ψ_{mol} can then be written as a product of the individual wave functions Ψ_{el} of the electrons and Ψ_{vib} and the nuclei,

$$\Psi_{\rm mol}(r_i, R_j) = \Psi_{\rm vib}(R_j) \cdot \Psi_{\rm el}(r_i, R_j), \qquad (3)$$

where r_i and R_j refer to the coordinates of the electrons and the nuclei, respectively.

It is based on the fact that nuclei, compared to electrons, have a very high mass and move slowly. Therefore, the relative position of nuclei can be taken as approximately constant during electronic transitions and a separation of the different degrees of freedom can be applied.

2.4 Franck-Condon Principle

The Franc-Condon principle is also based on the assumption that the relative position of nuclei is considered constant during an electronic transition. It states that the probability of an electronic transition depends on the overlap of the potential curves of the ground state and excited state. The probability can be determined with the Franck-Condon factor

$$FC(\nu_i, \nu_k) = \left| \int \Psi_{\text{vib}}(\nu_i) \Psi_{\text{vib}}(\nu_k) dR \right|^2, \tag{4}$$

where Ψ_{vib} refers to the normalized vibration wave function and ν_i and ν_k are the vibration quantum numbers for the ground and excited state. For a harmonic approximation, the Franck-Condon factors can be computed analytically. A visualization of the Franck-Condon principle can be found in fig. 1.



Figure 1: Visualization of the Franck-Condon principle for a transition between the ground and first excited state. As the distance of the nuclei is assumed constant, the only possible transitions are those represented by straight lines up or down. Also, the transitions are most likely between wave function maxima.

2.5 Morse Potential

The vibration wave function of the molecule depends on the molecule's potential energy. As the potential is quite complex, approximations are needed. One possible approximation is a harmonic potential, which provides a good representation of the actual potential close to the equilibrium position, but strongly deviates from the potential for large distances of the nuclei. Another possible approximation is the Morse potential

$$V(R) = D_e \cdot \left[1 - e^{-a(R - R_e)}\right]^2.$$
 (5)

In this equation, R describes the distance between the nuclei, R_e describes the equilibrium distance for which the potential is minimal, D_e is the well depth and a is a constant describing the width of the potential well. The Morse potential is a good approximation for large distances R up to distances around the equilibrium point R_e , and large R, but deviates from the real potential for small R.

Using the Morse potential, the Schrödinger equation can be solved analytically. The energy eigenvalues of the vibration states are given by

$$E_{\rm vib}(\nu) = hc\omega_e \left(\nu + \frac{1}{2}\right) - hc\omega_e x_e \left(\nu + \frac{1}{2}\right)^2.$$
 (6)

Often, the energy is given in terms of G = E/hc, leading to

$$G_{\rm vib}(\nu) = \omega_e \left(\nu + \frac{1}{2}\right) - \omega_e x_e \left(\nu + \frac{1}{2}\right)^2.$$
(7)

The vibrational constants are given by

$$\omega_e = a \sqrt{\frac{\hbar D_e}{\pi c \mu}} \tag{8}$$

$$\omega_e x_e = \frac{\hbar a^2}{4\pi\mu c},\tag{9}$$

where μ corresponds to the reduced mass of the molecule.

The well depth, which is equal to the electronic energy, can be calculated using eqs. (8) and (9) with

$$D_e = \frac{\omega_e^2}{4\omega_e x_e} \,. \tag{10}$$

2.6 Birge-Sponer Plot

To calculate the vibrational constants ω'_e and $\omega'_e x'_e$ for the first excited state, a Birge-Sponer plot can be used. For this, the energy difference between neighboring energy levels

$$\Delta G\left(\nu' + \frac{1}{2}\right) = G(\nu' + 1) - G(\nu')$$

= $\omega'_e - \omega'_e x'_e (2 + 2\nu')$
= $\omega'_e - \omega'_e x'_e \left[1 + 2\left(\nu' + \frac{1}{2}\right)\right]$
= $-2\omega'_e x'_e \left(\nu' + \frac{1}{2}\right) + (\omega'_e - \omega'_e x'_e)$ (11)

is calculated.

Then, the energy difference ΔG is plotted against $\nu' + 1/2$. The *x*-axis intercept of the Birge-Sponer plot corresponds to ν'_{diss} , which is the highest vibration quantum number for which the molecule is still bound. The electronic energy D_0 , measured from the vibrational ground state can then be calculated using

$$D_0 = \sum_{\nu=0}^{\nu_{\rm diss}} \Delta G\left(\nu + \frac{1}{2}\right).$$
 (12)

To calculate the total electronic energy D_e , the energy of the ground state G(0) has to be taken into account. The electronic energy is then given by

$$D_e = G(0) + D_0 = \frac{1}{2}\omega_e - \frac{1}{4}\omega_e x_e + \sum_{\nu=0}^{\nu_{\text{diss}}} \Delta G\left(\nu + \frac{1}{2}\right).$$
(13)

3 Setup of the Experiment

In the following, the setup used in this experiment will be described. The experiment consists of three slightly different setups. First, the absorption spectrum is measured using a CCD spectrometer. Next, the emission spectrum of a mercury lamp is recorded with a monochromator and an amplifier unit. In the last part of the experiment, the emission of the iodine molecule is measured in the same way.



Figure 2: The setup used for the absorption spectrum measurement. The focal length of lens 1 is $f_1 = 1000 \text{ mm}$, the focal length of lens 2 is $f_2 = 70 \text{ mm}$.

To measure the absorption spectrum of the iodine molecule, white light emitted by a halogen lamp is used. It is first collimated using a lens with a focal length of $f_1 = 100$ mm. Then, a mirror reflects the light through the iodine tube. Behind the tube, another mirror is used to aim the light at the spectrometer. Another lens with a focal length of $f_2 = 70$ mm is then used to focus the light onto the entrance of the spectrometer. The setup is visible in fig. 2.



Figure 3: Setup for the calibration measurement of the absorption spectrum of the mercury lamp. The focal length of lens 1 is $f_1 = 1000 \text{ mm}$, the focal length of lens 2 is $f_2 = 70 \text{ mm}$.

For the next part of the experiment, the halogen lamp is replaced by a mercury vapor lamp. The second mirror is removed and the second lens is positioned at its place. Now, the beam exiting the iodine tube is aimed toward the monochromator. The second lens is used to focus the light onto the entrance of the monochromator. The setup is depicted in fig. 3.



Figure 4: Setup for the measurement of the absorption spectrum of the iodine molecule. The focal length of lens 2 is $f_2 = 70$ mm. The laser used is a Helium-neon laser and emits light at a wavelength of 632.8 nm.

For the last part of the experiment, the mercury vapor lamp is removed. The Helium-Neon laser is positioned perpendicular to the iodine tube. Using a mirror on top of the tube, the beam is directed into the tube. Inside the iodine tube, another mirror redirects the beam towards the monochromator. Once again, the second lens is used to focus the light onto the entrance slit of the monochromator. The setup is depicted in fig. 4.

As the emission peak of the laser occurs at a wavelength, for which no peaks from the iodine spectrum are expected, the iodine tube does not have to be removed for the measurement of the laser spectrum.

To be able to record the emission spectrum of the iodine itself, the laser beam provides the necessary energy to excite it. After a while, the iodine molecule relaxes into the ground state, emitting light at frequencies from which the transitions can be calculated.

4 Execution of the Experiment

In this section, the execution of the experiment is described step by step.

Measurement of the Absorption Spectrum

The setup for this part of the experiment can be found in fig. 2.

First, the halogen lamp was fastened on the optical axis. The first lens was positioned right behind the halogen lamp. The height and position perpendicular to the optical axis of the lens were adjusted, until the light emitted by the halogen lamp was centered on the lens. It was not possible to do this with high precision, as there was no screen to check the height of the beam along the optical axis and the height of the filament in the halogen lamp was unknown. Next, the first mirror was moved perpendicular to the incoming light beam until the beam was centered on the mirror. The inclination and rotation of the mirror were adjusted to maximize the light shining onto the entrance of the iodine tube. Then, the second mirror was adjusted. It was moved along the optical axis until the reflected light was aligned with the entrance of the CCD spectrometer. Then, the second lens was positioned in front of the spectrometer. The distance to the spectrometer was approximately set to the focal length $f_2 = 70$ mm. The height and the position perpendicular to the beam of the lens were adjusted to aim the beam onto the spectrometer entrance. Therefore, also the inclination and rotation of the second mirror were slightly changed to maximize the light shining on the lens. Now, the position of the first lens along the optical axis and the angles of both mirrors were carefully readjusted until a clear image of the filament was visible directly in front of the second lens. To do so, the angles of the mirrors were changed until the image was centered, the position of the first lens along the optical axis was varied to get a clear picture. The position of the first lens perpendicular to the beam was adjusted to ensure an image without distortion. This was verified by holding a sheet of paper in front of the second lens. A final image of the filament can be seen in fig. 19.

Calibration with the Mercury Lamp

The setup for this part of the experiment can be found in fig. 3.

First, the halogen lamp and the second mirror were replaced by the mercury lamp and the second lens, respectively. The height of the lens and position perpendicular to the beam were adjusted to center the light, and the position along the beam was adjusted until the light was focused on the entrance of the monochromator. The first lens and mirror were not moved. Instead, the mercury lamp was moved along the optical axis until the image of the mercury lamp in front of the second lens was clear. A slit width of the monochromator of 51 µm was found to be the best. Then, a test measurement was started. The discriminator range was set to have the peaks as high as possible without cutting them off. The selected setting was 3 M. Next, the time constant and the uncertainty were adjusted to minimize both. In the end, the time constant was 0.01 s, the uncertainty was 0.4 %. The discriminator level was set to 0, as a lot of noise was observed for higher levels. The settings were checked by doing measurements with high scan rates. Finally, the spectrum was recorded with a scan rate of 2 Å s^{-1} for wavelengths from 4000 Å to 6000 Å. The range of scanned wavelengths was determined using the scale attached to the monochromator.

Spectrum of the Laser

The setup for this part of the experiment can be found in fig. 4.

The mercury lamp was removed and the laser turned on. The position of the second lens and the discriminator range were adjusted to maximize the signal. The range was set to 1 M. The slit width was set to 57 µm, at which the signal-to-noise ration was optimized. This was verified by measuring the laser peak back and forth, using a high scan rate. As a lot of noise could be observed for high discriminator levels, it was once again set to 0. The uncertainty was set to 0.2%, the time constant to $0.1 \,\mathrm{s}$. The laser spectrum was recorded with a scan rate of $2 \,\mathrm{\AA\,s^{-1}}$ for wavelengths from 6260 Å to 6380 Å.

Emission Spectrum of Iodine

The setup for this part of the experiment can be found in fig. 4.

As the signal from the iodine spectrum is very weak compared to the laser, the range had to be scaled down. The range, time constant, uncertainty, discriminator level, and slit width were readjusted as described above. The slit width was set to 432 µm, the discriminator level to 0, the range was set to 10 000, the uncertainty to the smallest possible value of 0.2%, which results to a time constant of 1 s. It is of note that the time constant was very large. However, as a scan rate was set to a mere 1 Å s^{-1} , the rather large time constant is justifiable.

5 Data Analysis

5.1 Absorption Spectrum

In the first part of the experiment, the absorption spectrum of the iodine molecule is examined. Using the CCD-spectrometer as described in section 3, the spectrum of the halogen lamp after passing through the iodine tube was recorded. Due to the excitation of the iodine molecules, discrete absorption peaks are expected in the spectrum at a wavelength of around 545.8 nm [1]. The recorded spectrum can be seen in fig. 5.



Figure 5: Full absorption spectrum of the iodine molecule excited with a halogen lamp. The spectrum was taken using the setup section 3. The minimum at the wavelength $\lambda = 545.8$ nm is expected to originate from the transition $\nu'' = 0 \leftrightarrow \nu' = 25$ [1] and is therefore indicated. The relevant transitions with $\nu'' = 0$ seem to occur in a spectral range of approximately 504 nm to 559 nm.

The expected transitions from the electronic ground state $X^1\Sigma_{0g}^+$ to the first excited state $B^3\Pi_{0u}^+$ can be seen in a spectral range of approximately 504 nm to 559 nm. The minima at wavelengths above 559 nm probably originate from other transitions with $\nu'' > 0$ and are not taken into account here. As quoted in [1], the absorption peak at $\lambda = 545.8$ nm originates from the transition between the vibrational states $\nu'' = 0$ and $\nu' = 25$. The other absorption minima can be assigned to the transitions below and above, according to the Franck-Condon principle.

5.1.1 Identification of the Absorption Minima

A close-up view of the relevant wavelength interval can be seen in fig. 6.



Figure 6: Relevant part of the absorption spectrum of the iodine molecule excited with a halogen lamp. The spectrum was taken using the setup in section 3. The positions of the absorption minima and their uncertainties were estimated by hand, taking the width of the peak profile into account. The numbers indicate the initial vibrational state ν' of the transition.

To create a Birge-Sponer plot, The positions of the absorption minima and their uncertainties were estimated by hand, taking the width of the peak profile into account. The vibrational states ν' could be enumerated according to the Franck-Condon principle, starting from $\nu' = 25$ for $\lambda = 545.8$ nm [1]. It can be seen that starting from $\lambda \approx 545$ nm additional peaks occur between the absorption peaks for $\nu'' = 0$. As the intensities of peaks originating from rotational transitions are probably too low to be measured, it is likely that these occur due to other transitions with $\nu'' > 0$.

5.1.2 Birge-Sponer Plot

To derive the vibrational constants ω'_e and $\omega'_e x'_e$, a Birge-Sponer plot is used. As described in section 2.6, a linear relation between the term difference ΔG and $\nu' + 1/2$ is expected. ΔG can be calculated from the difference in wave number

$$\Delta G = G(\nu'+1) - G(\nu') = \frac{1}{\lambda_{\nu'+1}} - \frac{1}{\lambda_{\nu'}}$$

$$s_{\Delta G} = \sqrt{\left(\frac{s_{\lambda_{\nu'+1}}}{\lambda_{\nu'+1}^2}\right)^2 + \left(\frac{s_{\lambda_{\nu'}}}{\lambda_{\nu'}^2}\right)^2}.$$
(14)

The uncertainty has been calculated through gaussian error propagation. For the Birge-Sponer plot in fig. 7, ΔG is plotted against the corresponding value of $\nu' + 1/2$.



Figure 7: Birge-Sponer plot used to derive the vibrational constants ω'_e and $\omega'_e x'_e$. The term difference ΔG is plotted against the corresponding $\nu' + 1/2$ as a linear relation between these two values is expected in eq. (11). A linear fit and the 1- σ -confidence interval are displayed as well. The optimal fit parameters can be found in eq. (15).

To obtain the vibrational constants, a weighted linear regression was performed using spipy.optimize.curve_fit. The fit is also visible in fig. 7 together with a 1- σ -confidence-interval. The linear regression

$$\Delta G\left(\nu' + \frac{1}{2}\right) = \alpha \left(\nu' + \frac{1}{2}\right) + \beta \tag{15}$$

provides the following optimal values

$$\alpha = (-1.99 \pm 0.17) \,\mathrm{cm}^{-1} \tag{15a}$$

$$\beta = (130 \pm 7) \,\mathrm{cm}^{-1} \,. \tag{15b}$$

The reduced χ^2 -value was calculated to

$$\chi^2_{\nu} = 0.144$$

According to eq. (11), the vibrational constants can be calculated from slope and intercept using the following equations

$$\omega'_e x'_e = -\frac{\alpha}{2} \qquad \qquad s_{\omega'_e x'_e} = \frac{s_\alpha}{2} \tag{16}$$

$$\omega'_e = \beta - \frac{\alpha}{2} \qquad \qquad s_{\omega'_e} = \sqrt{s_\beta^2 - \left(\frac{s_\alpha}{2}\right)^2}, \qquad (17)$$

which leads to

$$\omega'_e x'_e = (0.99 \pm 0.09) \,\mathrm{cm}^{-1}$$

 $\omega'_e = (131 \pm 7) \,\mathrm{cm}^{-1}$.

The uncertainties have been calculated using gaussian error propagation.

5.1.3 Characterization of the Potential

To get a better understanding of the observed transitions, the internuclear potential is now examined. An approximated potential for the ground state and the first excited state can be seen in fig. 8. In the following, the naming from fig. 8 is applied.



Figure 8: Approximated Morse potential showing the relevant energy differences between the electronic ground state $X^1\Sigma_{0g}^+$ and the excited state $B^3\Pi_{0u}^+$. D_e describes the potential depth and E_{diss} the dissociation energy. $G(0) = D_e - D_0$ is the energy difference between the potential minimum and the vibrational ground state. The figure was taken from [1].

Determination of the Electronic Energy

First, the electronic energy D'_e , which corresponds to the potential depth of the first excited state, is calculated. Assuming a Morse potential, it can be approximated using

eq. (10), with an uncertainty as a result due to gaussian error propagation

$$D'_{e,m} = \frac{\omega'^{2}_{e}}{4\omega'_{e}x'_{e}} \qquad \qquad s_{D'_{e,m}} = \sqrt{\left(\frac{\omega'_{e} \cdot s_{\omega'_{e}}}{2\omega'_{e}x'_{e}}\right)^{2} + \left(\frac{\omega'^{2}_{e} \cdot s_{\omega'_{e}x'_{e}}}{4\left(\omega'_{e}x'_{e}\right)^{2}}\right)^{2'}}.$$
 (18)

This leads to an electronic energy of

 $D'_{e,\mathrm{m}} = (4300 \pm 590) \,\mathrm{cm}^{-1}$.

Using eq. (13), the electronic energy can also directly be derived from the observed absorption peaks. To do so, the vibrational state of dissociation ν'_{diss} needs to be found. Considering fig. 7, it can be seen that ν'_{diss} corresponds to the *x*-axis intercept of the Birge-Sponer plot. This can be obtained from the condition

$$\Delta G\left(\nu' + \frac{1}{2}\right) = \alpha \left(\nu'_{\text{diss}} + \frac{1}{2}\right) + \beta \stackrel{!}{=} 0,$$

which leads to

$$\nu_{\rm diss}' = -\frac{\beta}{\alpha} - \frac{1}{2} \qquad \qquad s_{\nu_{\rm diss}'} = \sqrt{\left(\frac{s_{\beta}}{\alpha}\right)^2 + \left(\frac{\beta \cdot s_{\alpha}}{\alpha^2}\right)^2}, \qquad (19)$$

with a propagated error. Using the optimal parameters, $\nu_{\rm diss}'$ can be calculated to be

$$\nu'_{\rm diss} = (65 \pm 7)$$
.

To calculate the electronic energy, the sum in eq. (13) can, in good approximation, be replaced by an integral over the linear regression in the Birge-Sponer plot for an interval of $\nu' \in [0, \nu'_{diss}]$. This is equivalent to the surface of the triangle formed by the linear fit and the *x*-axis for the given interval. This approximation leads to

$$D'_{e,b} = G'(0) + \sum_{\nu'=0}^{\nu_{\text{diss}'}} \Delta G' \left(\nu' + \frac{1}{2}\right) = \frac{\beta \cdot \nu'_{\text{diss}}}{2}$$

$$s_{D'_{e,b}} = \frac{1}{2} \sqrt{\left(\nu'_{\text{diss}} \cdot s_{\beta}\right)^{2} + \left(\beta \cdot s_{\nu'_{\text{diss}}}\right)^{2}},$$
 (20)

with an uncertainty due to gaussian error propagation. Using the values provided above, the electronic energy is given by

$$D'_{e,b} = (4198 \pm 480) \,\mathrm{cm}^{-1}$$

For further calculations, the average value for the electronic energy is taken using

This gives a final result of

$$D'_e = (4247 \pm 380) \,\mathrm{cm}^{-1}$$



Figure 9: Absorption spectrum of the iodine molecule with the estimated wavelength of dissociation The spectrum was taken using the setup section 3. The wavelength of dissociation was estimated as the wavelength where no absorption peaks are visible any more, as this strongly indicates the dissociation of the molecule.

Determination of the Dissociation Energy

Next, the dissociation energy E_{diss} is determined. It is the energy at which the bond energy between the two iodine atoms is surpassed and the molecule dissociates. Considering the measured spectrum in fig. 9, the dissociation energy can be derived from the wavelength where no absorption peaks can be observed anymore. It can be assumed that this wavelength provides the necessary energy to surpass the bond energy so that no absorption will be visible due to the dissociation of the molecule.

Using the measured intensities the wavelength of dissociation was estimated to be

$$\lambda_{
m diss} = (501.0 \pm 1.5) \,
m nm$$
 .

With the known conversion

$$E = \frac{1}{\lambda} \qquad \qquad s_E = \frac{s_\lambda}{\lambda^2}, \qquad (22)$$

the dissociation energy can be calculated to

$$E_{\rm diss} = (19\,960\pm60)\,{\rm cm}^{-1}$$
.

Determination of the Excitation Energy

With this information, now the excitation energy T_e can be calculated. It corresponds to

the energy difference between the two minima of the electronic ground state and the first excited state. As visible in fig. 8, it can be calculated using

$$E_{\text{diss}} = T_e - G''(0) + D'_e \approx T_e - G'(0) + D'_e = T_e + D'_0.$$
(23)

The approximation $G''(0) \approx G'(0)$ had to be made so that the energy-difference between the potential minimum and the vibrational ground state could be calculated using the vibrational constants from the Birge-Sponer plot. Gaussian error propagation was used to determine the uncertainty.

This leads to

$$G'(0) = (65 \pm 3) \,\mathrm{cm}^{-1}$$

Using the correlation from eq. (23), the excitation energy can be calculated using

$$T_e = E_{\rm diss} - D'_e + G'(0) \qquad \qquad s_{T_e} = \sqrt{s_{E_{\rm diss}}^2 + s_{D'_e}^2 + s_{G'(0)}^2} \,. \tag{25}$$

As a result, one gets

$$T_e = (15\,780 \pm 390)\,\mathrm{cm}^{-1}$$

Approximation of the Morse Potential

Finally, the Morse potential can be approximated. Considering eq. (5), the potential for the first excited electric state is given by

$$V(R) = D'_{e} \cdot \left[1 - e^{-a(R-R_{e})}\right]^{2} + T'_{e}.$$
(26)

The constant a controls the width of the well and can be calculated using

$$a = \sqrt{\frac{\pi c\mu}{D'_e \hbar} {\omega'_e}^2} = \sqrt{\frac{4\pi c\mu}{\hbar} \omega'_e x'_e} \qquad \qquad s_a = \sqrt{\frac{\pi c\mu}{\hbar}} \frac{s_{\omega'_e x'_e}}{\sqrt{\omega'_e x'_e}}.$$
 (27)

Here, it is important to use all constants in the cgs-Unit-System to get the correct results. The constants μ (the reduced mass of the iodine molecule) and R_e (the equilibrium distance between the nuclei) were taken from [1]. The values are

$$\mu = 1.053 \cdot 10^{-22} \text{ g}$$

 $R'_e = 29.79 \text{ nm}$

respectively. Using eq. (26), the approximated Morse potential was plotted in fig. 10 against the internuclear distance R.

To allow a comparison of the obtained potential, also a Morse potential based on literature values was plotted. The values

$$D_{e',\text{lit}} = 4391.0 \text{ cm}^{-1}$$
$$(\omega'_e x'_e)_{\text{lit}} = 0.7016 \text{ cm}^{-1}$$
$$T_{e',\text{lit}} = 15\,770.59 \text{ cm}^{-1}$$

were taken from [2].



Figure 10: Approximated Morse potential of the first excited state of the iodine molecule. The potential is given by eq. (26), the values were calculated in section 5.1.3. For better comparability, another Morse potential was plotted using literature values from [2].

5.2 Emission Spectrum

Now the emission spectrum of the excited iodine molecules can be examined. This was done with the setup pictured in figs. 3 and 4 in section 3.

5.2.1 Calibration

As the spectrum can only be recorded in intensity I against steps s with the provided software, a calibration from steps to the corresponding wavelengths λ is necessary. To do so, the spectrum of a mercury vapor lamp was taken in a spectral range of 4000 Å to 6000 Å, as five discrete peaks are expected there. The start and stop wavelength displayed by the the monochromator was noted and can be found in appendix A.1. The resulting spectrum can be seen in fig. 16 in appendix A. With the provided setup it was not possible to measure clear peaks. Additionally, a lot of noise could be observed, and changing the discriminator settings and the other parameters would not change it. The finally chosen settings can be taken from section 4. To use as clear a signal as possible for the analysis, the data was post-processed using a continuous average over 5 steps. The intensities Iused for analysis were calculated from the measured intensities I' using

$$I_i = \frac{1}{5} \sum_{n=i}^{i+4} I'_n \,. \tag{28}$$



Figure 11: Emission spectrum of the mercury vapor lamp used to calibrate the monochromator. The data has been post-processed using a continuous average over 5 values, as described in eq. (28). A figure with the raw output can be seen in fig. 16 in appendix A. The peak positions were estimated by hand with uncertainties due to the width of the peaks.

Despite the smoothing of the data, no sharp peaks could be observed, and unfortunately, the expected double peak appears as a single peak. However, it was possible to determine the maximum peak positions by hand, estimating major uncertainties. The maximum peak positions and the expected wavelengths can be found in table 1.

Steps s	λ [Å]
210 ± 90	4046.6
$1320\pm~60$	4358.3
$5500\pm~60$	5460.7
$6540\pm~60$	5769.6
$6660\pm~60$	5790.7

Table 1: Estimated peak positions in the mercury spectrum used for calibration. The corresponding wavelengths were taken from [1].

The estimated peak positions are plotted in fig. 12 against the expected wavelength difference λ , which can be calculated from the difference $\lambda = \lambda_{\text{lit}} - 4000 \text{ Å}$. The 4000 Å



Figure 12: Linear fit used for the calibration of the monochromator. The estimated peak positions and their uncertainties as well as the expected wavelengths can be seen in table 1. The weighted linear fit was performed using scipy.optimize.curve_fit and the results can be seen in eq. (29). eq. (30) and eq. (31) provide the conversion from wavelength to steps and the other way around.

have to be taken into account due to the initial offset as the measurement was started at 4000 Å with the monochromator. The literature values λ_{lit} were taken from [1].

To calibrate the monochromator, a weighted linear regression was performed using scipy.optimize.curve_fit because a linear correlation between the recorded steps and the provided wavelength is expected. The fit is visible in fig. 12 together with the $1-\sigma$ -confidence-interval. The model function

$$s(\lambda) = \alpha \cdot \lambda + \beta \tag{29}$$

was used together with the optimum fit parameters

$$\alpha = (3.71 \pm 0.04) \,\text{\AA}^{-1} \tag{29a}$$

$$\beta = 20 \pm 60 \,. \tag{29b}$$

Comparing the model function to the data leads to a reduced χ^2 -value of

$$\chi^2_{\nu} = 0.622$$

With this calibration, the conversion from wavelength into steps and the vice versa can be

calculated using

$$s(\lambda) = \alpha \cdot \lambda + \beta \qquad \qquad s_{s(\lambda)} = \sqrt{(\lambda s_{\alpha})^2 + (\alpha s_{\lambda})^2 + s_{\beta}^2} \qquad (30)$$

$$\lambda(s) = \frac{s - \beta}{\alpha} \qquad \qquad s_{\lambda(s)} = \sqrt{\left(\frac{s_s}{\alpha}\right)^2 + \left(\frac{s_\beta}{\alpha}\right)^2 + \left(\frac{s - \beta}{\alpha^2} \cdot s_\alpha\right)^2}, \qquad (31)$$

with the uncertainties due to gaussian error propagation. For the conversion, it is important to use only the wavelength difference because the recorded steps always start at 0 while the start wavelength changes from measurement to measurement. The used wavelengths can be found in appendix A.1. It is also important that this conversion depends on the used settings at the monochromator, which will be relevant for the excitation spectrum later.

5.2.2 Emission Spectrum of the HeNe Laser

Next, the emission spectrum of the HeNe laser was taken to compare it to the expected emission wavelength. Again a continuous average (see eq. (28)) was calculated for the intensities in order to minimize the visible noise. The final spectrum of the laser can be seen in fig. 13. The measured spectrum before post-processing can be found in fig. 18 in appendix A.



Figure 13: Emission spectrum of the HeNe laser used to excite the iodine. The data has been post-processed using a continuous average over 5 values as described in eq. (28). A figure with the raw output can be seen in fig. 17 in appendix A. The expected position of the maximum was calculated using eq. (30) and is also shown together with the propagated uncertainty.

As HeNe lasers are known for their high purity of the emitted spectrum, a very clear peak at 6330 Å [1] was expected. It can be seen that the measured spectrum does not satisfy this expectation, as no clear gaussian-like maximum can be seen. To compare the peak to the expected wavelength, $s(\lambda = 6300 \text{ Å})$ is also shown in fig. 13 together with the uncertainty, calculated using eq. (30). This wavelength corresponds quite well to the visible peak due to its high uncertainty.

5.2.3 Emission Spectrum of the Excited Iodine

After further calibration as described in section 3, the emission spectrum of the excited iodine could be taken. Again the continuous average (see eq. (28)) was taken to flatten some of the noise. The processed spectrum can be seen in fig. 14, the measured data in fig. 18 in appendix A.



Figure 14: Emission spectrum of the Iodine, excited using the HeNe laser. The data has been post-processed using a continuous average over 5 values, as described in eq. (28). A figure with the raw output can be seen in fig. 18 in appendix A. The peak positions and their uncertainties were estimated by hand, taking the width of the peaks into account. Both can be found in table 3 in appendix A together with the corresponding wavelengths and wave numbers.

To identify the transition induced by the laser, the maximum peak positions were estimated together with their uncertainties, taking into account the width of the peak profile. For the big peak occurring between 6000 Å and 8000 Å, no reliable maximum could be found but it can be expected that two maxima are overlapping in this area. Using eq. (31), the corresponding wavelengths and uncertainties could be calculated for each peak. As the mercury calibration spectrum was recorded at 2 Å s^{-1} but the emission spectrum of the iodine at 1 Å s^{-1} , the factor 2 has to be considered for the steps. The calculated values can

be found in table 3. It can be expected that all the transitions begin on the same initial state ν' and end on consecutive final states $\nu'' = [\nu''_0, \nu''_0 + 1, \dots, \nu''_0 + 8, \nu''_0 + 11, \nu''_0 + 12]$.

To find the corresponding transitions, the wave numbers were calculated using

The wave numbers are plotted in fig. 15 against the expected final states ν'' of the transitions.



Wave Numbers of the lodine Peaks

Figure 15: Wave numbers of the Iodine Peaks calculated using eqs. (31) and (32) for the most probable consecutive final states ν'' of the transitions. The literature wave numbers of the most probable transition with $\nu' = 5$ and $\nu''_0 = 4$ were calculated using eq. (33) and are also shown in the figure. The wave numbers as well as the theoretically predicted values can be found in table 3 in appendix A.

According to [1], the expected wave number for a transition $\nu' \rightarrow \nu''$ can be calculated using

$$k_{\text{theo}}(\nu',\nu'') = T'_e + G'(\nu') - G''(\nu'')$$

$$G(\nu) = \omega_e \left(\nu + \frac{1}{2}\right) - \omega_e x_e \left(\nu + \frac{1}{2}\right)^2.$$
(33)

The constants

$$T'_{e} = 15\,770.59\,\mathrm{cm}^{-1}$$
$$\omega'_{e} = 125.273\,\mathrm{cm}^{-1}$$
$$\omega'_{e}x'_{e} = 0.7016\,\mathrm{cm}^{-1}$$
$$\omega''_{e} = 214.518\,86\,\mathrm{cm}^{-1}$$
$$\omega''_{e}x''_{e} = 0.607\,38\,\mathrm{cm}^{-1}$$

were taken from [2] and [3]. To find the most probable transition, the literature wave numbers were calculated for 10 different initial states $\nu' = [0, \ldots, 9]$ to 10 different final states for the consecutive transitions $\nu''_0 = [0 \text{ to } 12, \ldots, 9 \text{ to } 21]$. For each of these 100 data sets, a χ^2 value was calculated to compare the estimated wave numbers with the calculated literature values. It could be found that the visible emissions most likely occur due to a transition from $\nu' = 5 \rightarrow \nu''_0 = 4$. Also possible is a transition from $\nu' = 7 \rightarrow \nu''_0 = 5$. The literature wave numbers for $\nu' = 5$ and $\nu''_0 = 4$ are also shown in fig. 15.

6 Summary and Discussion

Absorption Spectrum

In the first part of the experiment, the absorption spectrum of iodine was examined. The positions of the absorption minima with $\nu'' = 0$ and their uncertainties were estimated and assigned to the corresponding initial states. Using the 35 estimated minima, a Birge-Sponer plot (see fig. 7) could be created and a linear regression (eq. (15)) was performed. It is visible in fig. 7 that all the estimated values fit well to the linear model as this always lies within the 1- σ -interval of each value. Also the reduced χ^2 -value of $\chi_{\nu} = 0.144$ indicates a good accordance with the fit. This procedure allows to calculate the vibrational constants

$$\begin{split} \omega'_e x'_e &= (0.99 \pm 0.09) \, \mathrm{cm}^{-1} & \frac{s_{\omega'_e x'_e}}{\omega'_e x'_e} = 9 \,\% \\ \omega'_e &= (131 \pm 7) \, \mathrm{cm}^{-1} & \frac{s_{\omega'_e}}{\omega'_e} = 5 \,\% \,. \end{split}$$

The relative uncertainties are rather high, which results from the fact that the fit was performed as a weighted linear regression, considering the *y*-uncertainties. As they were estimated quite high due to the width of the peak profiles and minor fluctuations in the spectrum, this is not surprising. Comparing them with the literature-values from [2]

$$\begin{aligned} (\omega'_e x'_e)_{\text{lit}} &= 0.7016 \,\text{cm}^{-1} & t = 3.2 \\ (\omega'_e)_{\text{lit}} &= 125.273 \,\text{cm}^{-1} & t = 0.81 \end{aligned}$$

leads to surprisingly different results. The parameter ω'_e seems to correspond very well with the theory, as it lies within a 1- σ interval, the parameter $\omega'_e x'_e$ shows a discrepancy to the theory, as it lies only in a 4- σ interval within the theoretical value.

With these results, the potential between the two iodine atoms could be characterized and important constants and energy levels calculated. The electronic energy, the depth of the potential well, was estimated in two ways, using the Morse approximation and the vibrational constants from the Birge-Sponer plot. The final values were

$$\begin{aligned} D'_{e,\mathrm{m}} &= (4300 \pm 590) \,\mathrm{cm}^{-1} & \frac{s_{D'_{e,\mathrm{m}}}}{D'_{e,\mathrm{m}}} &= 14 \,\% \\ D'_{e,\mathrm{b}} &= (4198 \pm 480) \,\mathrm{cm}^{-1} & \frac{s_{D'_{e,\mathrm{b}}}}{D'_{e,\mathrm{b}}} &= 11 \,\% \\ D'_{e} &= (4247 \pm 380) \,\mathrm{cm}^{-1} & \frac{s_{D'_{e}}}{D'_{e}} &= 9 \,\% \,. \end{aligned}$$

It can be seen that both values lie very well within the 1- σ -interval of each other, leading to a *t*-value of t = 0.13. Comparing the mean value to the literature value $D_{e,\text{lit}} = 4391.0 \text{ cm}^{-1}$ [2] provides a *t*-value of 0.38. So despite the big relative uncertainties, it can be said that both methods are consistent and are compatible to the literature.

From further analysis of the measured data, the dissociation energy E_{diss} could be estimated to

$$E_{\rm diss} = (19\,960\pm60)\,{\rm cm}^{-1}$$
 $\frac{S_{E_{\rm diss}}}{E_{\rm diss}} = 0.3\,\%\,.$

The relative uncertainty is very small due to the fact that the uncertainty of the wavelength needed for the calculation could be estimated to a quite small value. Finally, with this result the excitation energy T_e could be calculated to

$$T_e = (15\,780 \pm 390) \,\mathrm{cm}^{-1}$$
 $\frac{s_{T_e}}{T_e} = 2.5\,\%$.

The relative uncertainty is quite low, though many previous results contribute to this value. This is mostly because of the very small relative uncertainty of the dissociation energy, which has a major effect on this result. Comparing the excitation energy with the literature value $T_{e,\text{lit}} = 15\,770.59\,\text{cm}^{-1}$ [2] shows a very good accordance between the result and the literature value with a *t*-value of only t = 0.024.

Using the previous results, an approximated Morse potential could be calculated and plotted for the internuclear distances around the equilibrium distance of both nuclei. For comparison, another Morse potential using literature values from [2] was plotted. It can be seen in fig. 10 that both estimated potentials show only small differences in the depth of the potential well and its width. However, it can be said that they are in good accordance.

Considering the relative uncertainties and the t-tests with the literature values its can be said that the experiment states a very good compliance with the literature data from [2]. The CCD-spectrometer seems very suitable for this type of measurement within the aspired uncertainty.

Emission Spectrum

In the second part of the experiment, the emission spectrum of iodine was examined after being excited by a HeNe laser. For this a monochromator was used and calibrated using the emission spectrum of a mercury vapor lamp. Unfortunately the peaks in fig. 11 were not as well visible as expected. Each one had a major plateau with a lot of noise so that post-progressing had to be applied. Furthermore, the double peak appeared as one single peak very similar to the others. Adjusting the provided settings did not end in a better result. To verify this, a single peak was scanned forwards and backwards again many times with always slight changes in one setting. In addition, adjusting the discriminator level did only lead to more noise on top of the peaks. To compensate this, the uncertainties for the peak positions were estimated higher. Regardless, the calibration could be performed quite well with a reduced χ^2 -value of $\chi^2_{\nu} = 0.622$.

Next, the laser spectrum itself was measured to see if the expected peak at $\lambda = 6330$ Å would appear sharp and at the correct wavelength. In fig. 13 can be seen that the wavelength roughly corresponds to the expected value but the sharp, gaussian-like peak that should be emitted from a HeNe laser is not visible. It has several maxima at different heights and as there is no reason to believe that the laser is not working properly, there is probably a problem with the monochromator leading to this mountainous shape.

Finally, the emission spectrum of the excited iodine could be measured. As before, high noise and partly unclear peaks were seen. Despite this, it was possible to get a good

signal by post-processing the data (see fig. 14) and to distinguish several emission peaks. Using the calibration, the corresponding wave numbers could be calculated (table 3). After comparing the data with several possible transitions it could be found that the laser most probably excites the iodine to $\nu' = 5$, which will then fall back in the states with $\nu'' = 4$ to 16. The probability of a transition from $\nu' = 7$ to $\nu''_0 = 5$ is also quite high and can not be rejected. As no literature values are available for these excitations, the values can not be compared. However, they both seem possible.

To get more reliable results, it is nessecary to change the setup. The monochromator, if working correctly, provides a clear view over the full emitted spectrum. However, as this was not the case, a clear measurement of the spectrum was not possible, and no reliable results could be generated.

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Positions of the Minima in the Absorption Spectrum of Iodine

ν'	$\lambda \; [\mathrm{nm}]$
55	504.15 ± 0.15
54	504.65 ± 0.16
53	505.35 ± 0.16
52	506.00 ± 0.16
51	506.70 ± 0.16
50	507.50 ± 0.16
49	508.20 ± 0.16
48	509.05 ± 0.16
47	510.10 ± 0.18
46	511.00 ± 0.18
45	511.95 ± 0.18
44	513.10 ± 0.18
43	514.15 ± 0.18
42	515.60 ± 0.18
41	516.70 ± 0.18
40	518.00 ± 0.18
39	519.30 ± 0.18
38	520.8 ± 0.2
37	522.30 ± 0.18
36	523.80 ± 0.18
35	525.4 ± 0.2
34	527.2 ± 0.2
33	528.8 ± 0.2
32	530.8 ± 0.2
31	532.6 ± 0.2
30	534.6 ± 0.2
29	536.6 ± 0.2
28	538.9 ± 0.4
27	541.0 ± 0.2
26	543.2 ± 0.2
25	545.8 ± 0.3
24	548.0 ± 0.2
23	550.5 ± 0.2
22	553.2 ± 0.3
21	556.0 ± 0.2
20	558.7 ± 0.2

Table 2: Estimated positions of the iodine absorption minima. The measured data can be seen in fig. 6. The position of the minima and their uncertainties were estimated by hand, taking the width of the beam profile into account. The initial state $\nu' = 25$ for $\lambda = 545.8$ nm was given in [1], the other states were enumerated using the Franck-Condon principle.

n	s	λ [Å]	$k [\text{\AA}^{-1}]$	$k_{\text{lit},1} [\text{\AA}^{-1}]$	$k_{\mathrm{lit},2} [\mathrm{\AA}^{-1}]$
0	640 ± 40	$6481 \pm \ 19$	15430 ± 50	15486	15510
1	1320 ± 90	$6570\pm~30$	15210 ± 70	15277	15302
2	1960 ± 90	$6660\pm~30$	15020 ± 70	15070	15096
3	2600 ± 80	$6750\pm~30$	14820 ± 60	14864	14892
4	3220 ± 80	$6830\pm~30$	14640 ± 60	14659	14688
5	3870 ± 90	$6920\pm~30$	14460 ± 60	14456	14486
6	$4620 \pm \ 110$	$7020\pm~30$	14250 ± 70	14253	14284
7	5280 ± 90	$7110\pm~30$	14070 ± 60	14052	14085
8	5880 ± 90	$7190\pm~30$	13910 ± 60	13852	13886
9	-	-	-	13653	13688
10	-	-	-	13456	13492
11	$8240 \pm \ 120$	$7510\pm~40$	13320 ± 70	13260	13297
12	$8840 \pm \ 100$	$7590 \pm \ 30$	13180 ± 60	13065	13103

Peak Positions in the Emission Spectrum of Iodine

Table 3: Peak positions in the emission spectrum of the excited iodine. The full emission spectrum can be seen in fig. 14. n enumerates the peaks, as it is expected that they originate from transitions with consecutive final states. s is the estimated maximum peak position in steps, with the uncertainty due to the width of the peak profile. The peaks for n = 9 and n = 10 could not be distinguished and could not be taken into account, finding the most probable transition. The corresponding wavelengths λ were calculated using the results of the linear regression in fig. 12 and eq. (31). The wave numbers k can be obtained using eq. (32), the theoretical values were calculated using eq. (33) with the literature values from [2, 3]. $k_{\text{lit},1}$ corresponds to the most probable transition $\nu' = 5 \rightarrow \nu''_0 = 4$, $k_{\text{lit},2}$ to another possible transition with $\nu' = 7 \rightarrow \nu''_0 = 5$. The values can be seen in fig. 15.



Raw Emission Spectra

Figure 16: Emission spectrum of the mercury vapor lamp used to calibrate the monochromator. A figure with the processed output can be seen in fig. 11. The peak positions were estimated by hand with uncertainties due to the width of the peaks.



Figure 17: Emission spectrum of the HeNe laser used to excite the iodine. A figure with the processed output can be seen in fig. 13. The expected position of the maximum was calculated using eq. (30) and es also shown together with the propagated uncertainty.



Figure 18: Emission spectrum of the Iodine, excited using the HeNe laser. A figure with the processed output can be seen in fig. 14. The peak positions were estimated by hand with the uncertainties due to the width of the peaks and can be found in table 3 together with the corresponding wavelengths and wave numbers.

Image of the Filament



Figure 19: Final image of the filament of the halogen lamp, taken directly in front of the second lens. The positions and angles of the lens and both mirrors were set so that a sharp image with a minimum of distortion could be seen.

A.1 Lab Notes

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