

Experiment 6: Lab Report Template

Put Your Name Here

October 27, 2023

Abstract

A good abstract should include a clear statement of the experimental aim, some significant data points presented correctly, as well as a concise summary of trends and observations concerning your data. A great abstract will mention the specific methods used and the validity/level of error in the presented data.

When in doubt, please consult the laboratory report guidelines available on Learn.

1 Introduction

Vibrational Energy

The vibrational population can be transferred from ground state to a higher state by absorbing energies. The *fundamental absorption* described the transition from $v=0$ to $v=1$, and the energy usually in range of 500 cm^{-1} to 4000 cm^{-1} , which was within the infrared region.

The energy levels for a diatomic molecules in an anharmonic state could be expressed as shown in equation 1.

$$G(v) = (v + \frac{1}{2})\omega_e - (v + \frac{1}{2})^2\omega_e x_e \quad (1)$$

In first part of the equation 1 represented the energy of a harmonic oscillator, while the second part was the correction term for an anharmonic oscillator. The energy of anharmonic oscillator was lower than the energy of harmonic oscillator with a amount depend on the anharmonic constant $\omega_e x_e$. The frequency of the anharmonic oscillator was shown as ω_e . With the equation 1, the ground state energy could be shown as equation 2 with $v=0$, and so as the first excitation state ($v=1$) and the second excitation state ($v=2$).

$$G(0) = \frac{1}{2}\omega_e - \frac{1}{4}\omega_e x_e \quad (2a)$$

$$G(1) = \frac{3}{2}\omega_e - \frac{9}{4}\omega_e x_e \quad (2b)$$

$$G(2) = \frac{5}{2}(\omega_e - \frac{25}{4}\omega_e x_e) \quad (2c)$$

With equation 2, the energy of the fundamental absorption ($v=0$ to $v=1$) and the energy of the first overtone ($v=0$ to $v=2$) could be calculated as shown in equation 3.

$$G(0 \rightarrow 1) = G(1) - G(0) = \omega_e - 2\omega_e x_e \quad (3a)$$

$$G(0 \rightarrow 2) = G(2) - G(0) = 2(\omega_e - 3\omega_e x_e) \quad (3b)$$

Rotational Energy

The rotational energy could be described using equation 4 for a diatomic molecule.

$$F(J) = B_v(J + 1) \quad (4)$$

In this equation, J was the rotational quantum number, while B_v was the rotational constant, which was related to the moment of inertia I as shown in equation 5.

$$B_v = \frac{h}{8\pi^2 c I} \quad (5a)$$

$$I = \mu r^2 \quad (5b)$$

Transition Energy

Since the vibrational transition and the vibrational transition involved two very different frequencies. The energy for vibrational rotational transition could be expressed as equation 6, while the centrifugal distortion was ignored here.

$$S(v, J) = (v + \frac{1}{2})\omega_e - (v + \frac{1}{2})^2\omega_e x_e + B_v(J + 1) \quad (6)$$

The scale of the constant B would change with increasing vibrational state.

Rotational Selection Rules

1. P branch - A transition where $J=-1$
2. Q branch - A transition where $J=0$
3. R branch - A transition where $J=+1$

The Q branch usually would not appeared in the spectrum because it was forbidden (photon unit energy). However, it could appear in the spectrum when ...

2 Methodology

The 10 cm^3 gas cell was flushed with nitrogen and sealed with the Teflon lids. The background scan was performed with this cell using **FT-IR spectrometer** in the range 6000 cm^{-1} - 2000 cm^{-1} for **64 folds with resolution as 0.5**. Three drops of concentrated HCl was added into the cell, and the spectrum was recorded under the same conditions.

The background scan was performed again under the same conditions with a larger gas cell. Cigarette smoke was captured in the cell. The spectrum of cigarette smoke was recorded under the same conditions.

3 Results

The IR spectrum of HCl was recorded. The fundamental absorption was observed at 2880 cm^{-1} as shown in Figure 1, while the first overtone was observed at 5760 cm^{-1} as shown in Figure 2.

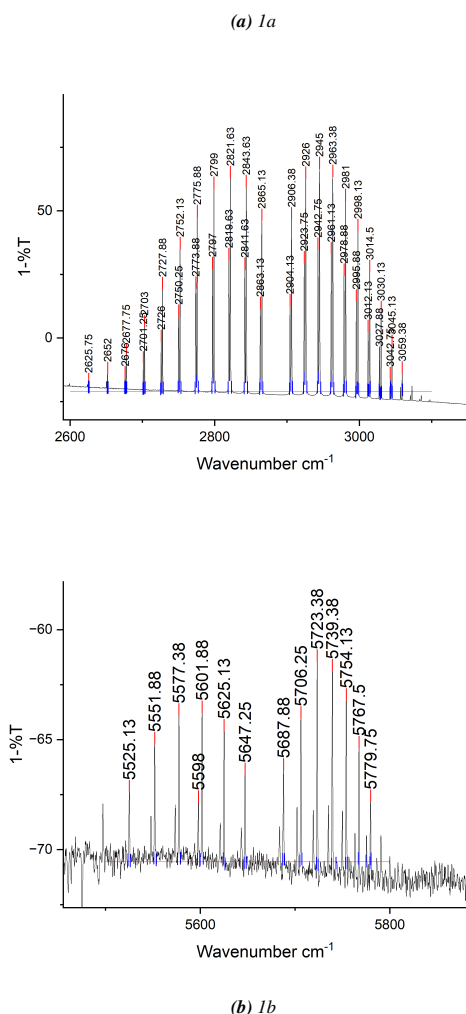


Figure 1: plots of....

The trends; identify the P, Q, R branches in the spectrum.

The wavenumber of the fundamental absorption for HCl^{35} and HCl^{37} were recorded separately in Table 1 and Table 2. The value of $R(J)-P(J)$ and $R(J)-P(J+2)$ were calculated to determine the rotational constant B_0 and B_1 for HCl^{35} and HCl^{37} respectively as shown in Table 1 and Table 2.

Table 1: The wavenumber of the fundamental absorption for HCl^{35} in *P* branch and *R* branch.

J	P (cm ⁻¹)	R (cm ⁻¹)	R(J)-P(J) (cm ⁻¹)	R(J)-P(J+2) (cm ⁻¹)
0	-	2906.38	-	62.75
1	2865.13	2926.00	60.87	104.37
2	2843.63	2945.00	101.37	146.00
3	2821.63	2963.38	141.75	187.50
4	2799.00	2981.00	182.00	228.87
5	2775.88	2998.13	222.25	270.25
6	2752.13	3014.50	262.37	311.50
7	2727.88	3030.13	302.25	352.38
8	2703.00	3045.13	342.13	-
9	2677.75	-	-	-

Table 2: The wavenumber of the fundamental absorption for HCl^{37} in P branch and R branch.

J	P (cm ⁻¹)	R (cm ⁻¹)	R(J)-P(J) (cm ⁻¹)	R(J)-P(J+2) (cm ⁻¹)
0	-	2904.13	-	62.50
1	2863.13	2923.75	60.62	104.12
2	2841.63	2942.75	101.12	145.75
3	2819.63	2961.13	141.50	187.25
4	2797.00	2978.88	181.88	228.63
5	2773.88	2995.88	222.00	269.88
6	2750.25	3012.13	261.88	310.88
7	2726.00	3027.88	301.88	351.88
8	2701.25	3042.75	341.50	-
9	2676.00	-	-	-

The rotational constant B_0 could be obtained by plotting the R(J)-P(J) against (J+1/2) based on [equation x](#) as shown in Figure 3(a) for HCl³⁵. The rotational constant B_1 could be obtained by plotting the R(J)-P(J+2) against (J+3/2) based on [equation x](#) as shown in Figure 3(b) for HCl³⁵.

The slope in Figure 3(a) was $41.3950 \pm \text{error}$, which was four times the rotational constant B_0 , which was calculated

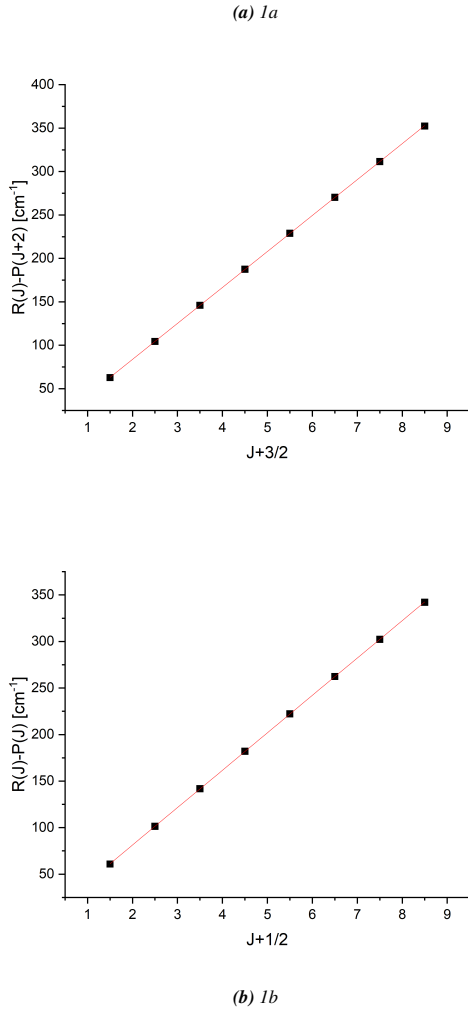


Figure 2: plots of....

as shown in equation x.

$$B_0 = \frac{41.3950}{4} = 10.3488 \text{ cm}^{-1} \quad (7)$$

The slope in Figure 3(b) was 40.1825 \pm error, which was four times the rotational constant B_1 , which was calculated as shown in equation x.

$$B_1 = \frac{40.1825}{4} = 10.0456 \text{ cm}^{-1} \quad (8)$$

The rotational constant B_e could be calculated based on B_0 and B_1 as shown in equation x based on equation x.

$$10.3488 = B_e - \alpha_e(0 + 1/2) \quad (9a)$$

$$10.0456 = B_e - \alpha_e(1 + 1/2) \quad (9b)$$

The value of B_e was determined by solving these two equations, which was 10.5003 cm^{-1} . The value of α_e was also obtained as 0.3029 cm^{-1} .

The bond length of HCl in different vibrational could be calculated using B_0 , B_1 , and B_e based on equation 5(a) and equation 5(b) respectively as shown in equation x.

$$\mu = \frac{m_H m_{^{35}\text{Cl}}}{m_H + m_{^{35}\text{Cl}}} = 1.6273 \times 10^{-25} \text{ kg} \quad (10a)$$

$$r_0 = \sqrt{\left(\frac{h}{8\pi^2 \mu B_0 c}\right)} \quad (10b)$$

$$r_1 = \sqrt{\left(\frac{h}{8\pi^2 \mu B_1 c}\right)} \quad (10c)$$

$$r_e = \sqrt{\left(\frac{h}{8\pi^2 \mu B_e c}\right)} \quad (10d)$$

The equilibrium oscillator frequency ω_e and the anharmonic constant x_e could be calculated based on the energy of the fundamental absorption and the first overtone as shown in equation 3. The frequency of the fundamental absorption was 2885.76 cm^{-1} , while the frequency of the first overtone was 5667.57 cm^{-1} . The value of ω_e and x_e were calculated as shown in equation x.

$$2885.76 = \omega_e - 2\omega_e x_e \quad (11a)$$

$$5667.57 = 2(\omega_e - 3\omega_e x_e) \quad (11b)$$

$$\omega_e = 2989.70 \text{ cm}^{-1} \quad (11c)$$

$$\omega_e x_e = 51.9725 \text{ cm}^{-1} \quad (11d)$$

$$x_e = 0.0017384 \quad (11e)$$

The zero point energy of HCl^{35} could be calculated using equation 2(a) with the value of ω_e and x_e as shown in equation x.

$$G(0) = \frac{1}{2}\omega_e - \frac{1}{4}\omega_e x_e = 1494.86 \text{ cm}^{-1} \quad (12)$$

The force constant of HCl^{35} bond could be calculated as shown in equation x and the reduced mass (μ) of HCl^{35} was calculated as 1.6273×10^{-25} .

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} = 2885.76 \text{ cm}^{-1} \quad (13a)$$

$$k = \mu \nu^2 (2\pi)^2 = 1.0001 \times 10^3 \text{ Nm}^{-1} \quad (13b)$$

The value of B_0 , B_1 , B_e , α_e , r_0 , r_1 , r_e , ω_e , x_e , $G(0)$, and k for HCl^{35} were summarized and for HCl^{37} were calculated using the same method as shown in Table 3. This value was compared with the literature value.

The IR spectrum of the cigarette was recorded as shown in Figure 3.

Table 3: The value of B_0 , B_1 , B_e , α_e , r_0 , r_1 , r_e , ω_e , x_e , $G(0)$, and k for HCl^{35} and HCl^{37} .

	HCl^{35}	HCl^{37}	Literature value
B_0 (cm^{-1})	10.3488		
B_1 (cm^{-1})	10.0456		
B_e (cm^{-1})	10.5003		
α_e (cm^{-1})	0.3029		
r_0 (pm)	127.9		
r_1 (pm)	128.9		
r_e (pm)	128.4		
ω_e (cm^{-1})	2989.70		
x_e	0.0017384		
$G(0)$ (cm^{-1})	1494.86		
k (Nm^{-1})	1.0001×10^3		

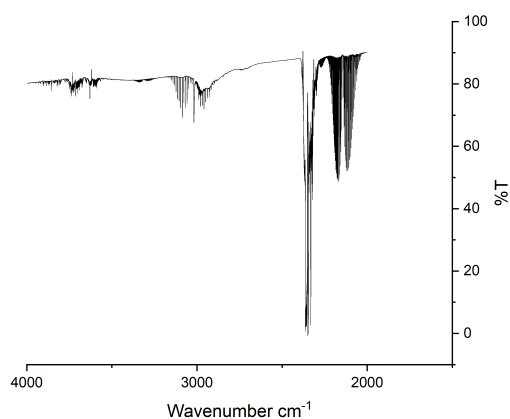


Figure 3: The IR spectrum of the cigarette.

4 Discussion

5 Investigation Question

this is a citation¹

References

- [1] P. C.-A. Dr Author, *Molecular Physics*, 2018, **5**, 255–268.