المملكة العربية السعودية
وزارة التعليم
جامعة الامام محمد بن سعود الإسلامية
كلية العلوم
قسم الفيزياء

Spectral Properties of a Conjugated Chalcone in Liquid State.

By

FAHAD MOHAMMED ALNAFEA

Supervisor

Dr. KHALID HASSAN IBNAOUF

February 2025

ACKNOWLEDGMENT

I begin by thanking Allah Almighty for His infinite blessings and guidance, without which this achievement would not have been possible. I am deeply grateful to my dear parents, whose unwavering support, prayers, and encouragement have been the foundation of my success. They have been, after Allah, the primary reason for enabling me to reach this significant milestone.

I would also like to extend my sincere appreciation to the Head of the Physics Department, for his continuous support, valuable guidance, and for fostering an academic environment that greatly contributed to the successful completion of this project.

Finally, I wish to express my heartfelt thanks to my supervisor, Dr. Khalid Hassan Ibnoauf, for his exceptional mentorship, generous support, and dedication of his time and expertise, which played an indispensable role in shaping this research. I am also immensely grateful to my family members and colleagues, whose moral support and encouragement were invaluable throughout this project.

ABSTRACT

In this project, the spectral properties of a conjugated chalcone were studied. The absorption and emission spectrum were recorded under varying concentrations, solvents, and temperatures. The results revealed that the absorption and emission properties were influenced by the dielectric constant of the solvent, the solvent's nature, and the temperature of the solution. Additionally, the optical band gap, extinction coefficients, and Stokes shift were calculated.

المستخلص

في هذا المشروع، تمت دراسة الخصائص الضوئية لأحد مركبات الشالكون التي تمت تصنيعها في الجامعة تحت تأثير ثلاثة عوامل مختلفة: المذيبات، التراكيز، ودرجة الحرارة. وأظهرت النتائج أن لكل عامل تأثيراً كبيراً على الخصائص الضوئية للمركب، وتمت مناقشة هذه التأثيرات وتبعاتها بشكل مفصل في الفصل الخامس من هذا العمل، وبالاعتماد على النتائج المستخلصة، تم حساب العديد من المتغيرات المهمة، مثل معامل الامتصاص، فجوة الطاقة البصرية، وإزاحة ستوكس. وقد تم تحليل هذه المتغيرات ومناقشتها بعمق لتوفير فهم أوسع لسلوك المركب تحت الظروف المختلفة. يبرز هذا البحث العلاقة الدقيقة بين هذه العوامل والخصائص الضوئية لمركب الشالكون، مما يقدم رؤى قيمة حول تطبيقاته المحتملة.

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CHAPTER ONE

1. Introduction

1.1. Chalcones

Chalcone is an organic compound that belongs to the flavonoid family. It consists of two aromatic rings connected by a ketone group (C=O) and a double bond (C=C) as illustrated in Figure (1.1) [1]. This relatively simple chemical structure forms the basis for a wide range of derivatives with diverse physical and chemical properties. Chalcone compounds hold significant importance due to their ability to interact with light, exhibiting unique optical properties such as absorption and emission in the ultraviolet-visible (UV-Vis) spectrum[1]. They also demonstrate distinctive biological activity, making them focus of research in medical applications. Chalcone compounds are used in the development of optical sensors, photonic materials, and organic dyes [1]. Some chalcone derivatives exhibit antioxidant, anticancer, antimicrobial, and anti-inflammatory activities, making them valuable in drug development. chalcone is used in the production of organic polymers, UV-resistant materials, and advanced coatings. The N,N dimethyl amino group attached to para-position in rig B in chalcones enhances its photophysical properties via intramolecular charge transfer (ICT) [1]. The photophysical properties of the chalcones have attracted much attention during the past decade due to their increasing application in electronic and optoelectronic devices.

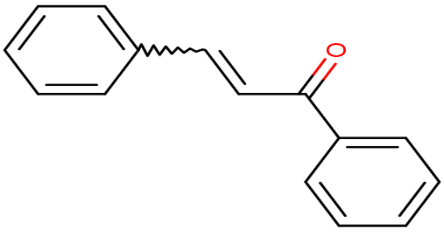

Fig 1.1 The molecular structure of the main core of the chalcones

1.2. Motivations

The primary motivation behind this project is the need to address knowledge gaps related to the optical behavior of chalcones under the influence of different environmental factors, such as solvent type, concentration, and temperature. While there are numerous studies on chalcones, a comprehensive understanding of these effects is still limited.

1.3. Objectives

- Study the effect of dissolving chalcone in different solvents to determine the most suitable solvent based on its absorption and emission behavior.
- Study the effect of changing the concentration of the compound in the chosen solvent on its optical properties.
- Study the effect of temperature changes on the absorption and emission behavior while keeping the solvent concentration constant.
- Calculate the main optical parameters based on the obtained results, such as band gap and Stokes' shift.
- Enhance future applications by gaining an accurate understanding of the behavior of chalcone in different environments.

CHAPTER TWO

2. Literature Review

2.1. Introduction

In scientific research, a literature review is a very important step that aims to analyze previous studies related to the project topic. Chalcone compounds have been widely studied in terms of their chemical structure, optical properties, and various applications. This section will summarize the main studies that focused on the effects of solvents, concentration, and temperature on the optical properties of chalcone compounds, in addition to the analytical methods used and the main results of these studies. Many studies have shown that the type of solvent greatly affects the optical absorption and emission behavior of chalcone compounds [1]. This effect is attributed to the interactions between solvent molecules and solute molecules, which leads to changing the chemical environment surrounding the compound. For example, this study confirmed that polar compounds exhibit significant changes in their absorption and emission spectrum when solvents with varying polarity are used. Research suggests that concentration plays a crucial role in determining the intensity of absorption and emission. As concentration increases, effects such as molecular aggregation may occur, which may reduce the intensity of emission due to intermolecular interactions [1]. Among the light emitting materials, organic compounds and their derivatives have fascinated many researchers owing to their unique optical homogeneity, easy to synthesis and design, costless, capability of light emission and the smoothness to govern their structure and fabrication management allow familiarizing controlled changes in development their properties. The interest in light-emitting organic materials as a new optical material has started two decades by the scientist. Many researchers have shown that changes in temperature can alter the absorption and emission spectra of chalcone compounds. This is due to thermodynamic changes, such as enhanced molecular interactions or transitions in electronic states. For example, a study observed a slight decrease in emission intensity with increasing temperature, which is attributed to increased molecular vibrations [1].

CHAPTER THREE

3. Theoretical Background

3.1. Molarity

Molarity (M) is defined as the number of moles of solute per liter of solution. It is a fundamental concept in solution chemistry, often expressed as[2]:

$$\boldsymbol{M = \frac{n}{V}} \qquad (\mathbf{3.1})$$

Where n represents the number of moles of the solute, and V is the volume of the solution in liters. Molarity provides a quantitative measure of the concentration of a solution, making it essential for stoichiometric calculations and understanding solution behavior in chemical and physical experiments.

To adjust or decrease the concentration of a solution, the dilution equation is commonly applied[2]:

$$\boldsymbol{C_1V_1 = C_2V_2} \qquad (\mathbf{3.2})$$

In this equation:

- C_1 represents the initial concentration of the solution.
- V_1 is the volume of the concentrated solution being used.
- C_2 is the final, desired concentration of the solution.
- V_2 corresponds to the final total volume of the diluted solution.

The equation reflects the principle of conservation of moles, where the total amount of solute remains constant before and after dilution. By adding a specific volume of solvent to the initial solution, the concentration decreases proportionally while maintaining the total solute content.

3.2. Lambert-Beer Law

The Lamber-Beer law describes the relationship between the absorption of light by a substance, the concentration of that substance, and the length of the optical path. The law states that absorbance is directly proportional to the concentration of the substance and the length of the optical path [3].

$$\boldsymbol{A = \varepsilon \cdot c \cdot l = \alpha \cdot l} \qquad (3.3)$$

$$\boldsymbol{I_t = I_o e^{-A}} \qquad (3.4)$$

- $A: Absorbance$
- $\varepsilon: Extinction\ coefficient\ (\frac{L}{mol \cdot cm})$
- $c: Concentration\ (M)$
- $l: Path\ lenggt\ (cm)$
- $I_t : Transmitted\ intensity$
- $I_o : incident\ intensity$
- $\alpha : absorption\ coefficient\ (cm^{-1})$

3.3. Stoke's shift.

Stokes' shift is the difference between the wavelength or energy of the absorbed light and the wavelength or energy of the emitted light in a fluorescent system. This difference occurs due to the loss of energy during the return of a molecule from an excited state to its ground state, where the excess energy is lost in the form of vibrations or non-radiative interactions before light is emitted[4].

$$\boldsymbol{\Delta\lambda = \lambda_{em} - \lambda_{abs}} \qquad (3.5)$$

- $\Delta\lambda$: Stoke shift
- λ_{em} : Wavelength ofemitted light
- λ_{abs} : Wavelength of absorbed light

3.4. Lippert-Mataga equation

The Lippert-Mataga equation describes the effect of solvent polarity on the Stokes shift, which is the difference between absorption and emission spectra of certain molecules. It relates the molecular dipole moment changes in ground and excited states to the solvent's polarity [5].

$$\bar{\nu}_a - \bar{\nu}_f = \frac{2}{hc}(\Delta\mu)^2(a)^{-3}\Delta f(\varepsilon, n) + const \qquad (3.6)$$

$$\Delta f = \left[\frac{\varepsilon - 1}{2\varepsilon + 1}\right] - \left[\frac{n^2 - 1}{2n^2 + 1}\right] \qquad (3.7)$$

- $\bar{\nu}_a$: *wave-numbers maxima in cm^{-1} for the absorption*
- $\bar{\nu}_f$: *wave-numbers maxima in cm^{-1} for the fluorescence*
- $\Delta\mu$: *Change in dipole between ground state and excited state*
- a : *Effective Radius*
- ε : *Dielectric constant of solvent*
- *n: Refractive Index*
- h : *blank constant*
- c : *Speed of light*
- Δf : *orientation polarisability*

3.5. Tauc equation

The Tauc Equation is used in materials science to determine the optical band gap of semiconductors by analyzing their absorption spectra. It relates the absorption coefficient to the photon energy [6].

$$(\alpha h\nu)^n = A(h\nu - E_g) \qquad (3.8)$$

- α : *Absorption coefficient of the material* (cm^{-1})
- $h\nu$: *Photon energy* (eV)
- A : *Material – dependent constant*
- E_g : *Band gap energy* (eV)
- n : *Depends on the type of electronic transition*
- $n = \frac{1}{2}$: *Direct allowed transition*
- $n = 2$: *Indirect allowed transition*

CHAPTER FOURE

4. Experimental Setup

4.1. Chalcone Synthesized

This chalcone was Synthesized via simple reaction between 4-dimethyl aminobenzaldahyde (0.01 mole) and 4-chloroacetophenpne (0.01 mole) in the presence of NaoH (1.0 gm) and alcohol ($CH3CH2OH$ 50ml). The mixture was placed in the glass vessel and left for steering at room temperature overnight, afterward the product recrystallized from ethanol and washed with distilled water in order to achieve pure final product as seen in Figure 4.1. The chalcone was characterized by FTIR, H1NMR and UV-Vis spectroscopy. Each molecule of this compound contains 24 hydrogen atoms, 22 carbon atoms, one nitrogen atom, one oxygen atom, and one chlorine atom, as illustrated in Figure (4.2).

Fig 4.1 The synthetized of the used chalcone

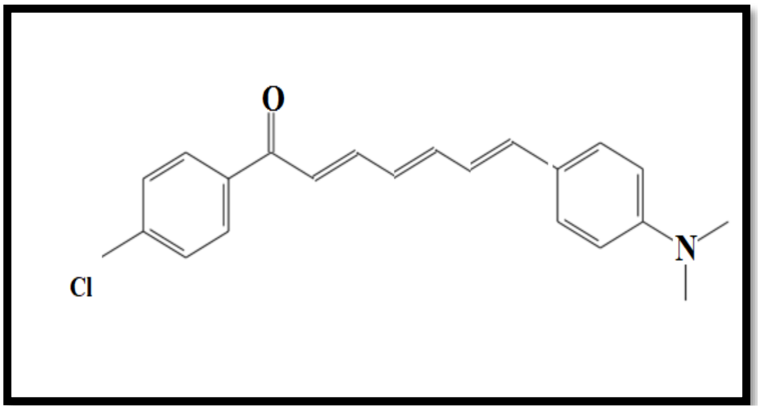

Fig 4.2 Molecular Structures of the used chalcone

The solutions shown in Figure (4.3) were prepared using a sensitive balance (German-made, Zurich model) depicted in Figure (4.4) to accurately measure the required weights. These weights were then dissolved in various organic solvents with differing polarities, as illustrated in Figure (4.5) and described in Table (4.1). The solvents, sourced from Fluka and Sigma Aldrich, were carefully selected to ensure proper solubility and consistency in the prepared solutions. Several concentrations of the chalcone compound were prepared by dissolving it in ethyl acetate solvent, as illustrated in Figure (4.6).

Fig 4.3 Chalcone in different solvents at a concentration of 0.05mM.

Fig (4.4) The sensitive Balance

Fig 4.5 The Solvents that used in the project

Fig 4.6 Chalcone in in Ethyl acetate for different concentrations

Table 4.1 The Used Solvents

Solvent	Dielectric constant
Glycerin (Gly)	42.5
Acetone (Act)	20.7
Ethyl acetate (EA)	6.02
Benzene (Benz)	2.27

4.2. Spectrophotometer

The Spectrophotometer (UV-1900I: Shimadzu), as illustrated in Figure (4.7), shows the absorbed intensity at varying photon energies absorbed by the molecule through a graph where the x-axis represents the wavelength, and the y-axis represents the absorbed intensity. The wavelength at which the absorption is at its maximum is referred to as the peak. The range of wavelengths emitted by the device is determined, and then two cuvettes specific to the device are used, featuring two opaque sides and two transparent sides, as shown in Figure (4.8). The transparent sides are aligned with the light source and the intensity measurement detector, while the opaque sides assist in improving the accuracy of the light intensity measurement. And they are placed in their designated positions within the device (see Figure (4.9)). The first cuvette contains only the solvent, and the second cuvette contains the solution, this setup helps determine the absorbance value of the compound itself without interference from the absorbance of the solvent. The device, in a precise scientific sense, studies the behavior of the molecule during its transition to the excited state, as indicated by the red arrow in Figure (4.13).

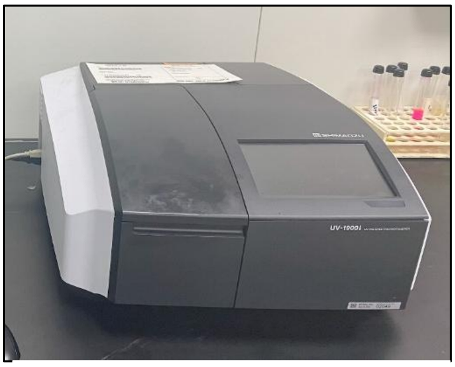

Fig 4.7 Spectrophotometer (UV-1900I: Shimadzu)

Fig 4.8 The quartz cuvette used for the absorption measurements

Fig 4.9 Double beam Spectrophotometer (inside view)

4.3. Spectrofluorometer

The Spectrofluorometer (RF-6000 – Shimadzu), as illustrated in Figure (4.10), shows the emitted intensity resulting from the return of excited molecules to the ground state at varying photon energies emitted by the molecule. This is represented through a graph where the x-axis corresponds to the wavelength and the y-axis represents the emitted intensity. The wavelength with the highest absorbance is first determined, and the solution is then placed in a cuvette specifically designed for the emission device, where all sides of the cuvette are transparent, as shown in Figure (4.11). Subsequently, the cuvette is placed in its designated position, as illustrated in Figure (4.12). The device, in a precise scientific sense, examines the behavior of the molecule during its transition from the excited state to the ground state, as indicated by the green arrow in Figure (4.13).

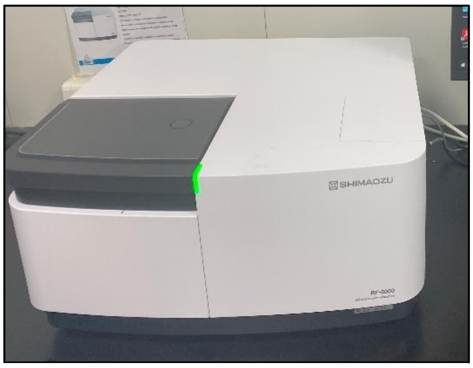

Fig 4.10 Spectrofluorometer (RF-6000 – Shimadzu)

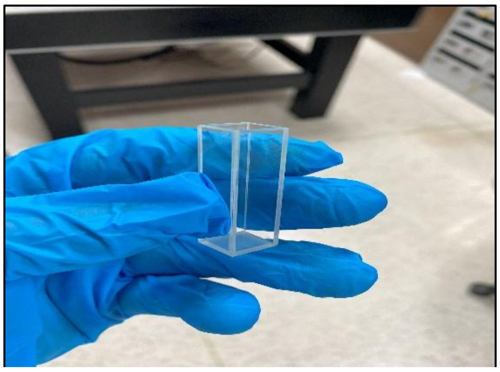

Fig 4.11 The quartz cuvette used (4 sides polished) for the emission measurements

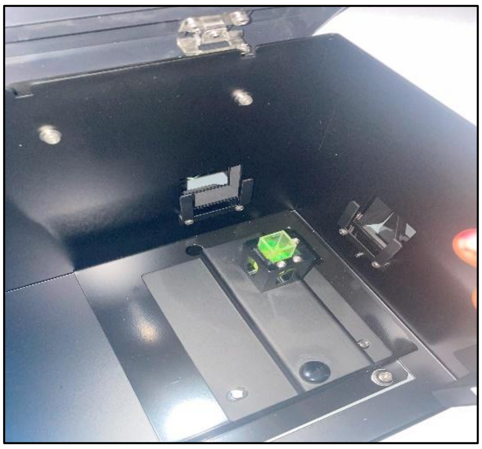

Fig 4.12 Spectrofluorometer (inside view)

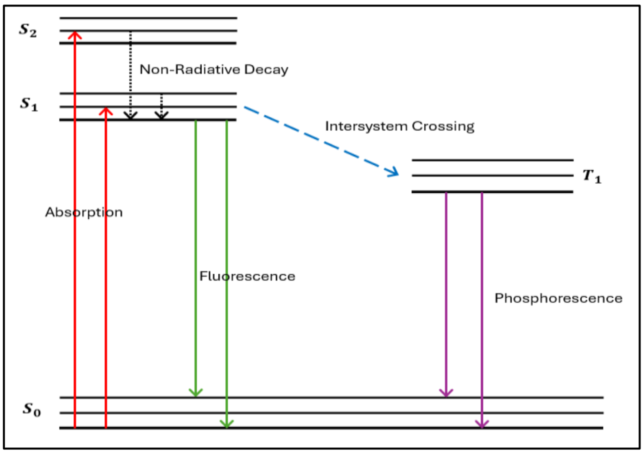

Fig 4.13 Jablonski Diagram

4.4. Heater magnetic stirrers

The heater magnetic stirrer shown in Figure (4.14) was used to increase the solution's temperature by placing the cuvette containing the solution on top of it. The temperature of the solution was measured approximately and is not considered precise.

Fig 4.14 Heater magnetic stirrers

CHAPTER FIVE

5. Results and Discussions

5.1. Absorption spectra

5.1.1. Effect of the Solvents

A set of solutions of the chalcone in different solvents under same concentration (0.05 mM) as mentioned in Figure (4.3). The absorption spectrum was recorded as illustrated in Figure (5.1). The absorbance values of these solutions were found to vary, as illustrated in Figure 5.1. Ethyl acetate exhibited the highest absorbance among the solvents, while glycerin recorded the lowest absorbance for chalcone. Additionally, the absorbance of chalcone in different solvents did not correlate with the dielectric constant, as shown in Table (5.1). The findings suggest that absorbance is primarily influenced by solubility. Notably, a greater portion of chalcone molecules were completely dissolved in ethyl acetate compared to the other solvents. This observation indicates that the compound possesses moderate polarity leaning towards low polarity, consistent with the solubility principle: "like dissolves like."

On the other hand, it is observed that the wavelength increases with an increase in the dielectric constant, which may be attributed to the properties of the solvents' dielectric constant. As the electric field strength of the solvent molecules increases, it influences the solute molecules, leading to a decrease in the energy required for the electron transition from a lower energy level to a higher energy level. This effect arises because the electric field either attracts or repels the electron due to the charges present. As a result, the reduction in the energy required for the electron transition causes a corresponding decrease in the energy of the photon. Consequently, the photon’s wavelength increases.

It is observed that when the solvent's dielectric constant was reduced from 6 to 2, no change in the wavelength occurred. This indicates that the difference in the electric field affecting the solute molecules is negligible when the dielectric constant is altered by a small amount.

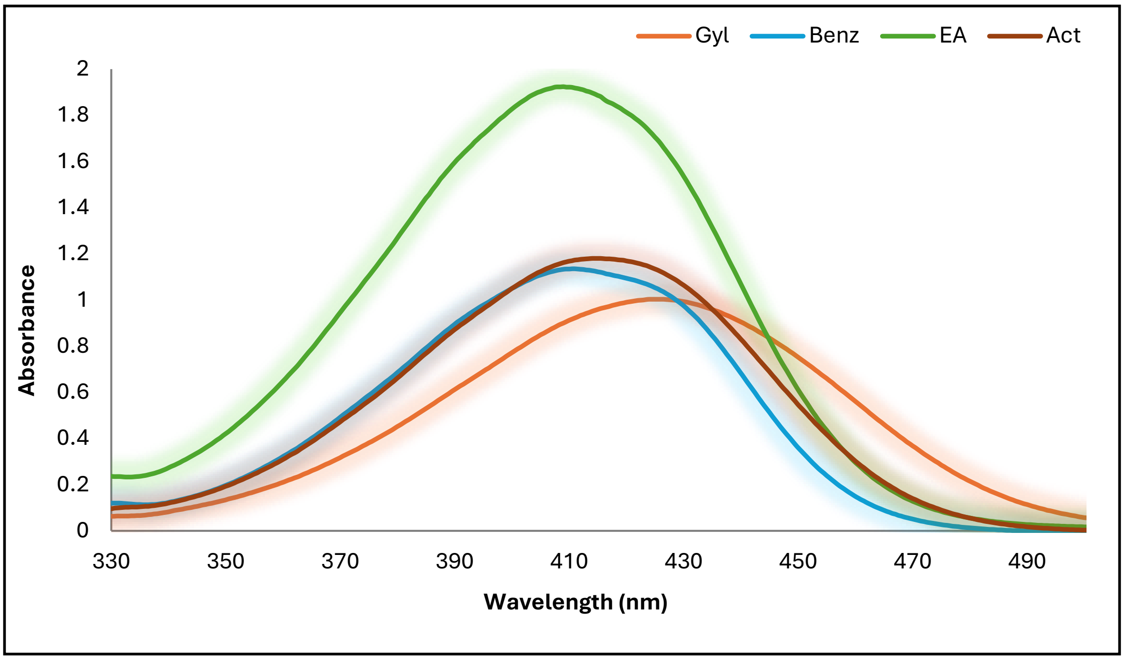

Fig 5.1 Absorption spectra of chalcone at 0.05mM in different solvent

Table 5.1 Absorption spectra of chalcone at 0.05mM in different solvent

Solvent	Dielectric constant	Absorbance	Wavelength (nm)
Glycerin	42.5	1	425
Acetone	20.7	1.18	416
Ethyl Acetate	6.02	1.9	410
Benzene	2.27	1.13	410

5.1.2. Effect of the Concentrations

The chalcone was dissolved in ethyl acetate for different concentrations (0.01, 0.05, and 0.1 mM). The absorbance spectra of these solutions were recorded as shown in Fig. (5.2). From Figure 5.2, it is evident that increasing concentration results in a greater number of absorbed photons while the absorbed wavelength remains constant across all concentrations.

This can be explained by the fact that higher concentrations correspond to an increased number of solute molecules, which are responsible for photon absorption. As the number of solute molecules increases, the total number of absorbed photons also rises.

However, this increase in solute molecules does not affect the energy required for the electron to transition from a lower energy level to a higher energy level. Consequently, the absorbed wavelength remains unchanged.

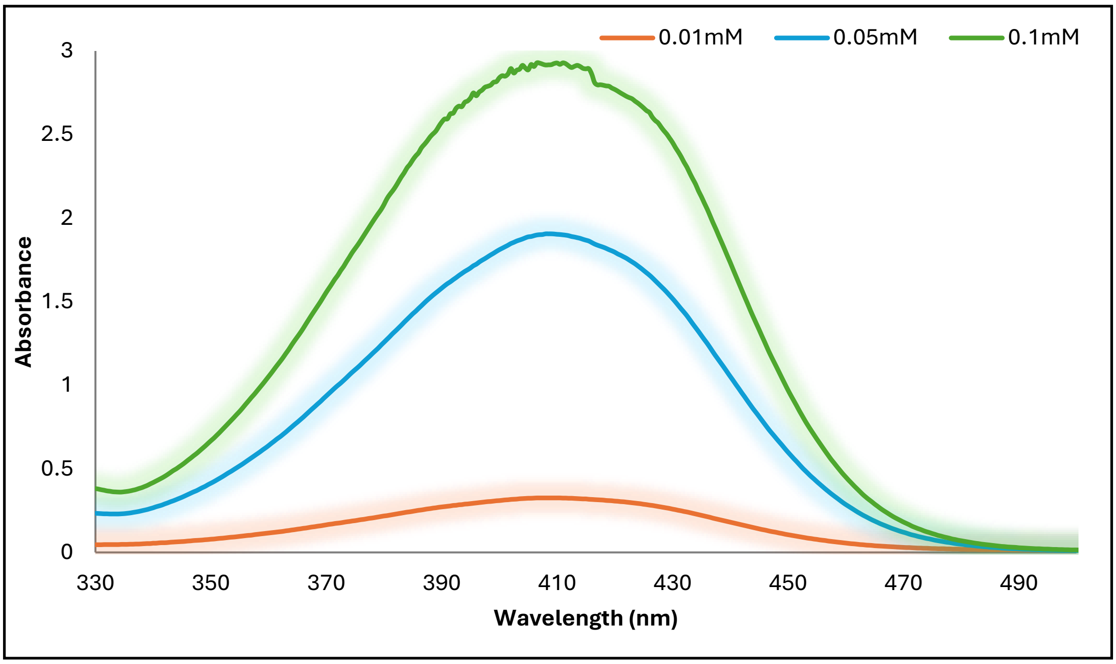

Fig 5.2 Absorption spectra of chalcone at Different Concentrations in ethyl acetate

Table 5.2 Absorption spectra of chalcone at Different Concentrations in ethyl acetate

Concentration (Mm)	Absorbance	Wavelength (nm)
0.5	2.9	410
0.1	1.9	410
0.05	0.326	410

5.1.3. Effect of the Temperatures

The absorption spectra of chalcone in ethyl acetate at a concentration of 0.05 mM were analyzed under varying temperatures (300 K, 310 K, and 315 K). The results indicate that the absorption spectrum is influenced by temperature, as shown in Figure (5.3). As the temperature increased, a decrease in both absorbance and wavelength was observed.

The decrease in the absorbance could be attributed to the effect of temperature on the stability of the molecules, which may disrupt the conjugated orbitals. Additionally, the temperature causes some electrons to transition to higher energy levels, thereby reducing the number of electrons available for absorption, leading to a decrease in the number of absorbed photons.

Moreover, the decrease in the wavelength of the absorbed photons can be attributed to the fact that increasing temperature raises the kinetic energy of molecules, causing them to move further apart. As the molecules become more dispersed, the electric field generated by the solvent molecule, which previously pushed or pulled the electron, weakens. When this electric field decreases, the electron requires more energy than before to transition to a higher energy level. As a result, the energy of the absorbed photon increases, leading to a shorter wavelength.

Temperature also reduces the energy required by the electron for its transition. However, the graph indicates that the dielectric constant provides more energy to the electron than the temperature does.

This is because the increase in temperature decreases the energy contribution of the dielectric constant while adding thermal energy. Despite this, the wavelength does not increase but rather decreases. This indicates that the energy affecting the electron prior to the temperature increase was more significant and had a greater influence on the electron’s behavior.

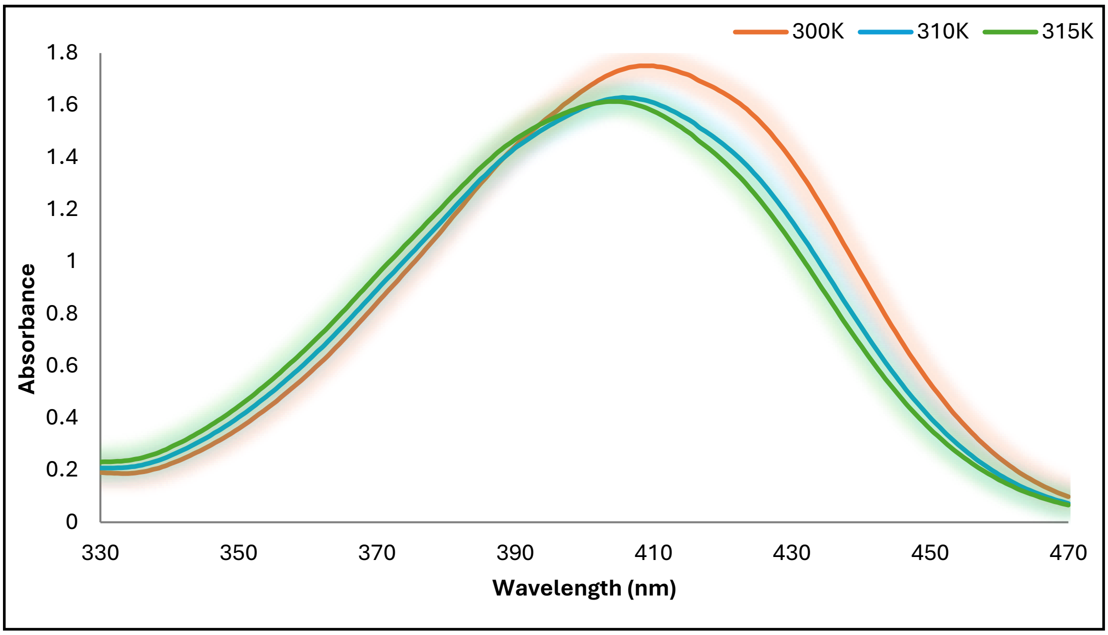

Fig 5.3 Absorption spectra of chalcone at 0.05mM in ethyl acetate at different Temperature

Table 5.3 Absorption spectra of chalcone at 0.05mM in ethyl acetate at different Temperatures

Temperature (K)	Absorbance	Wavelength (nm)
300	1.7	410
310	1.63	405.5
315	1.61	405

5.1.4. extinction coefficient

Table (5.4) shows the calculated extinction coefficient of the chalcone in different solvents using equation (3.3). This coefficient is essential for determining the absorbance value when varying concentration. Based on the obtained results as illustrated in Table 5.1, the extinction coefficient was maximum value for ethyl acetate and minimum value for glycerin, indicating that its value varies depending on the solubility.

Table 5.4 Extinction coefficients of the chalcone in different solvents

Solvent	Absorbance	Extinction coefficient $\left(\frac{L}{mol\cdot cm}\right)(10^3)$
Glycerin	1	20
Acetone	1.18	23.6
Ethyl Acetate	1.9	38
Benzene	1.13	22.7

5.1.5. Optical Band Gaps

The optical band gap is the value that represents the energy difference between the HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) orbitals. The band gap calculation involves plotting two graphs using Tauc's equation, as mentioned in equation (3.8). In the beginning, the optical band gap was calculated for the chalcone in ethyl acetate at a concentration of 0.05 mM and room temperature (300 K) as seen in Figures 5.4 and 5.5.

In the first plot, the transition is assumed to be direct, whereas in the second plot, it is assumed to be indirect. The plot that exhibits a significant and noticeable linear rise along the y-axis, forming a straight line, corresponds to the appropriate transition type and allows for the determination of the band gap value. From the Figur (5.5) , the optical band gap was determined to be 2.77 eV, which represents the energy required for the electron to transition from the HOMO to the LUMO. The plot also revealed that the transition is an indirect.

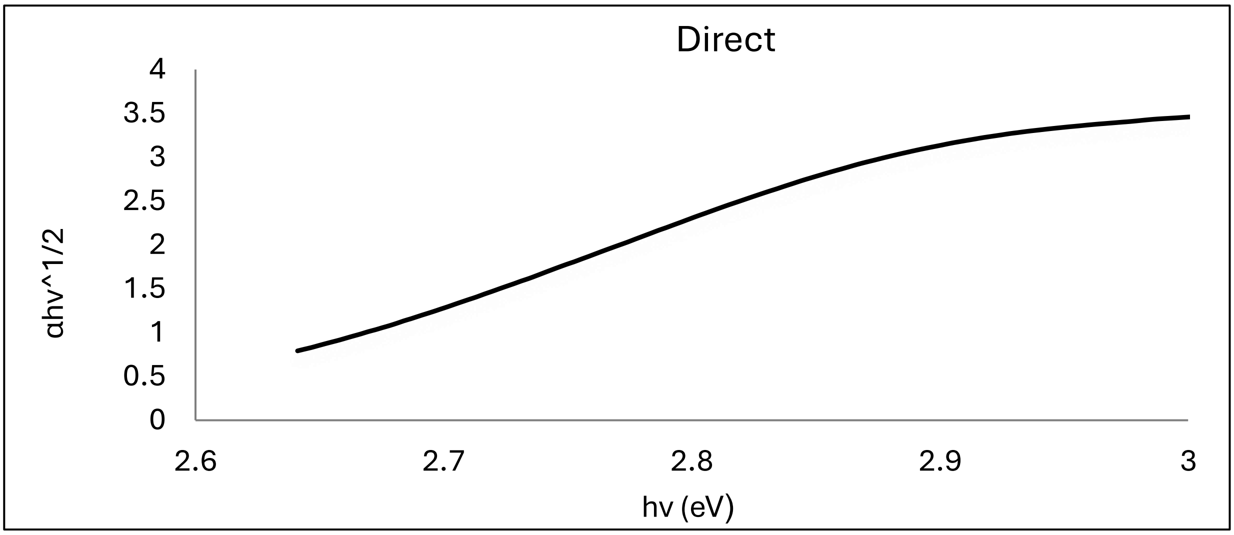

Fig 5.4 Direct optical band gap of Chalcone in ethyl acetate at 0.05mM and temperature of 300K

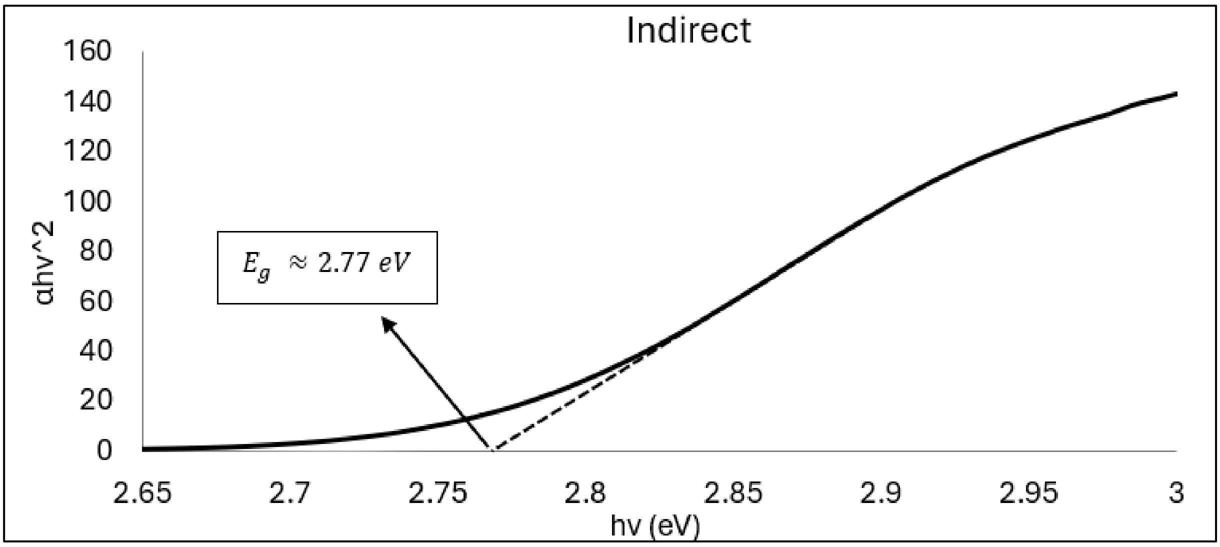

Fig 5.5 Indirect optical band gap of Chalcone in ethyl acetate at 0.05mM and temperature of 300K

When the temperature increases, as previously explained, the energy required for the electron to transition increases. Consequently, the band gap value becomes greater than 2.77 eV as seen in Figure 5.6.

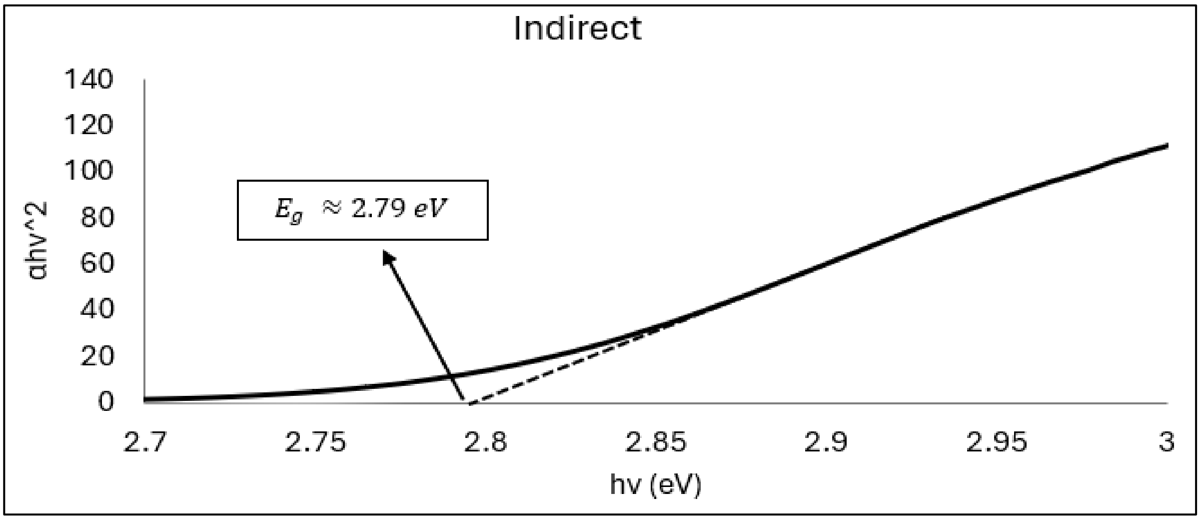

Fig 5.6 Indirect optical band gap of Chalcone in ethyl acetate at 0.05mM and temperature of 310K

When the solvent was changed to Glycerin under identical operational conditions (T=300K); the optical band gap shifted to 2.63 eV (Figure 5.7). The results showed that when the dielectric constant increases, the energy required for the electron to transition decreases. Consequently, the band gap value becomes smaller than its value at Figure (5.5).

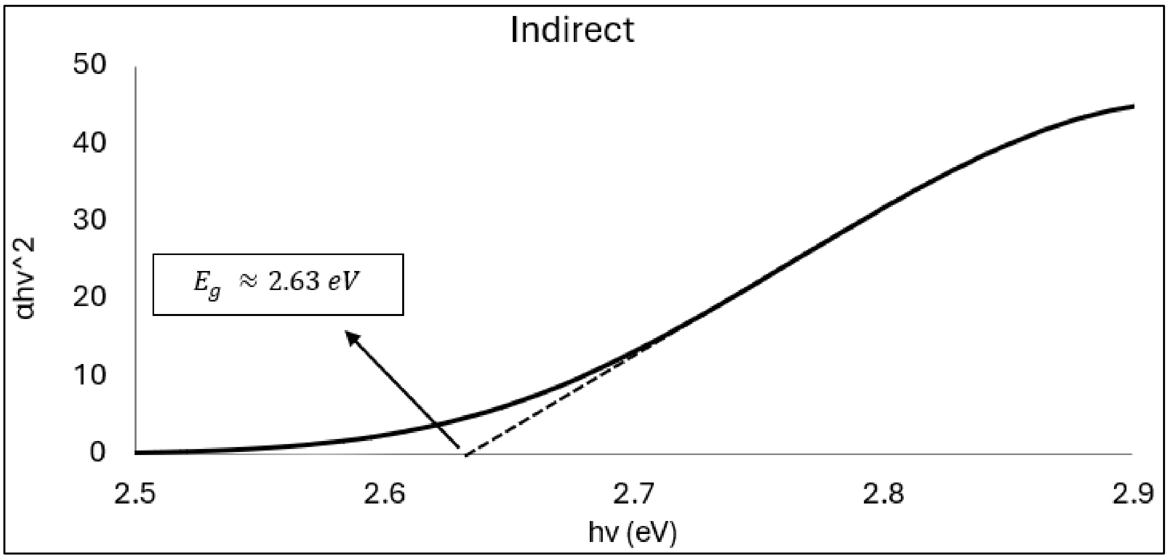

Fig 5.7 Indirect optical band gap of Chalcone in glycerin at 0.05mM and temperature of 300K

5.2. Emission Spectra

5.2.1. Effect of Solvents

A set of solution of the chalcone in different solvents under same concentration (0.05 mM) as mentioned in Figure (4.3). The excitation wavelengths used here based on the max absorption as mentioned in Table 5.1. The emission spectra were recorded as illustrated in Figure (5.8). It is observed that the highest intensity occurs in ethyl acetate, while the lowest intensity is observed in glycerin. This indicates that the intensity varies depending on solubility. Furthermore, it is noted that, unlike absorption, the dielectric constant affects the number of photons. An increase in the dielectric constant enhances molecular collisions in the excited state, leading to the occurrence of non-radiative collisions, which result in a significant decrease in intensity. On the other hand, it is observed that the increase in the dielectric constant correlates with an increase in the wavelength. This is because a higher dielectric constant enhances the polarity of the solvent molecule, and an increase in solvent polarity leads to greater energy loss for the solute molecule due to bond (dipole-dipole interaction) dissociation and collisions in the excited state. The more energy the excited molecule loses, the lower the energy of the emitted photon. Lower energy corresponds to a higher wavelength.

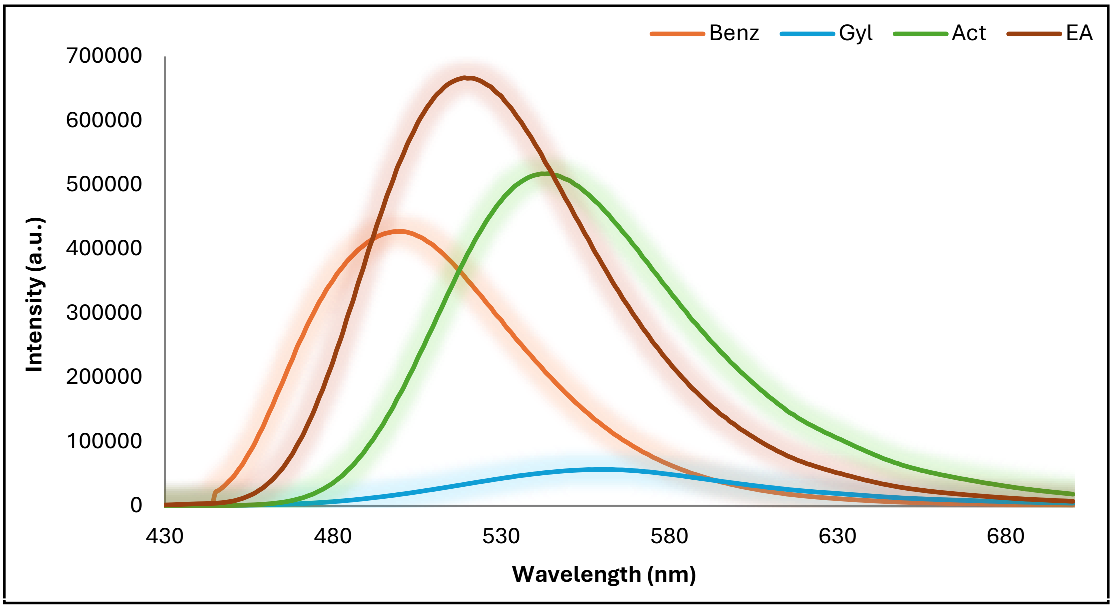

Fig 5.8 Fluorescence spectra of chalcone at 0.05mM in different Solvent

Table 5.5 Fluorescence spectra of chalcone at 0.05mM in different Solvent

Solvent	Dielectric constant	Intensity (a.u.)(10^4)	Wavelength (nm)
Glycerin	42.5	5.6	560
Acetone	20.7	51.7	544
Ethyl Acetate	6.02	66.6	519
Benzene	2.27	42.2	500

5.2.2. Effect of Concentrations

The chalcone was dissolved in ethyl acetate for different concentrations (0.01, 0.05, and 0.1 mM). The emission spectra of these solutions were recorded as shown in Fig. (5.9). It was observed that an increase in concentration initially enhances the intensity, reaching a maximum at an optimal concentration. Beyond this point, further increases in concentration result in a decline in intensity. This behavior can be attributed to the higher population of molecules in the excited state at elevated concentrations, which facilitates non-radiative processes through collisional interactions, thereby reducing the overall intensity. Additionally, it is observed that changing concentration does not affect the wavelength. This is because the increase or decrease in the number of molecules does not influence the energy of the emitted photon.

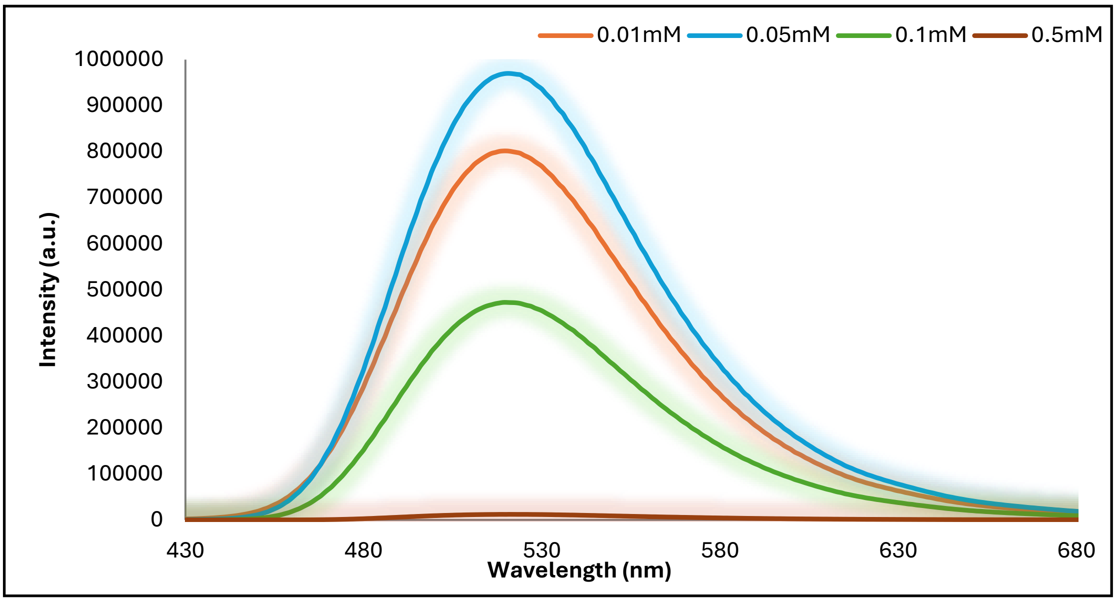

Fig 5.9 Fluorescence spectra of chalcone at different concentrations in ethyl acetate

Table 5.6 Fluorescence spectra of chalcone at different concentrations in ethyl acetate

Concentration (mM)	Intensity (a.u.) (10^4)	Wavelength (nm)
0.5	1.2	520
0.1	47	520
0.05	97	520
0.01	80	520

4.2.3. Effect of Temperatures

The emission spectra of chalcone in ethyl acetate at a concentration of 0.05 mM were analyzed under varying temperatures (300 K, 310 K, and 315 K). The results indicate that the emission spectrum is influenced by temperature, as shown in Figure (5.10). As the temperature increased, a decrease in both intensity and wavelength was observed. The decrease in intensity is attributed to the increase in collisions within the excited state caused by the elevated temperature, leading to non-radiative collisions. The decrease in wavelength, on the other hand, The decrease in wavelength appears to be due to the effect of heat, which causes the solvent molecules to move farther away from the solute molecules in the excited state, thereby weakening their interactions.

This facilitates the transition of solute molecules to the ground state without significant energy loss for bond dissociation. Consequently, the molecule returns with higher residual energy, leading to a shorter wavelength. Although heat also causes the excited molecule to lose energy, the energy loss due to thermal effects is less than the energy loss resulting from bond dissociation.

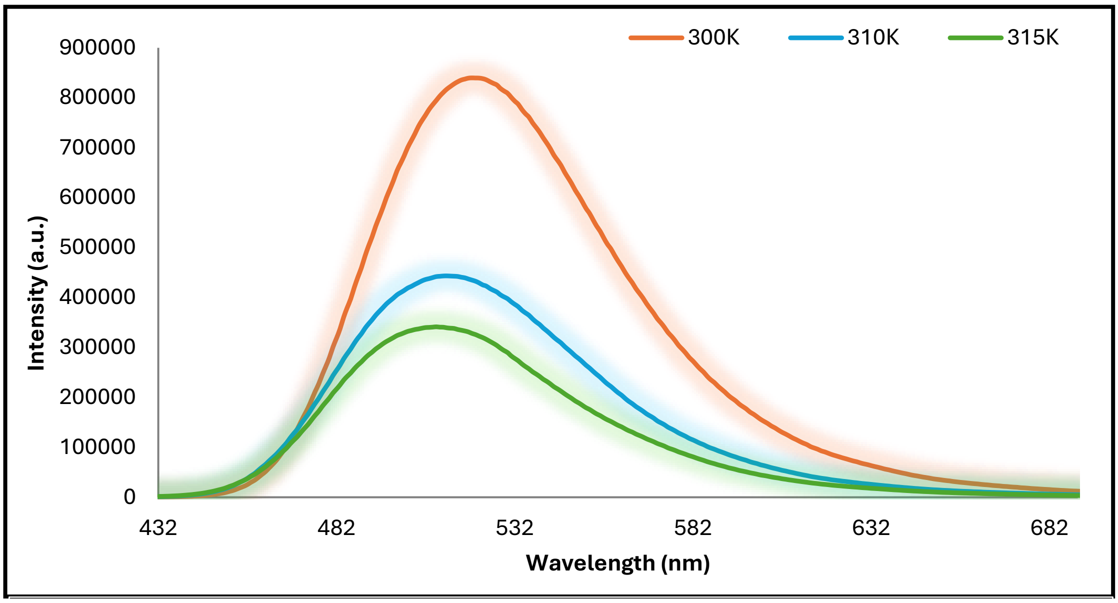

Fig 5.10 Fluorescence spectra of chalcone at 0.05mM in ethyl acetate at different Temperature

Table 5.7 Fluorescence spectra of chalcone at 0.05mM in ethyl acetate at different Temperature

Temperature (K)	Intensity (a.u.)(10^4)	Wavelength (nm)
300	84	519
310	44	513
315	34	510

5.3. Stoke Shift

The Stokes shift was calculated, as shown in Table (5.8), using the equation (3.5) and based on the values presented in Table (5.1) and Table (5.5). Observed that an increase in the dielectric constant leads to an increase in the Stokes shift. This appears to be because the dielectric constant affects the absorbed wavelength in only one way: through the electric field generated by the solvent molecule, which either pushes or pulls the electron. But, for the emitted wavelength, the dielectric constant has two effects:

- The excessive polarity of the solvent molecule increases collisions in the excited state, leading to greater energy loss.
- The excessive polarity of the solvent molecule strengthens the interaction (bond) with the solute molecule, causing the excited molecule to lose more energy while attempting to return to the ground state.

Table 5.8 The spectral properties of Chalcone in different solvents and Values of Stokes' Shift

Solvent	**Dielectric constant**	**Absorption in λ_{max}(nm)**	**Fluorescence in λ_{max} (nm)**	**Stokes' Shift (nm)**
Glycerin	42.5	425	560	135
Acetone	20.7	416	544	128
Ethyl Acetate	6.02	410	519	109
Benzene	2.27	410	500	90

5.4. Lippert-Mataga equation

A graph was plotted, as shown in Figure (5.11), using equation (3.6), which represents a linear relationship between the inverse of the Stokes shift difference and certain solvent properties. The plot demonstrated the validity of our results by confirming the linearity of the relationship. Furthermore, from the plot, we can determine the dipole moment difference by extracting the slope value.

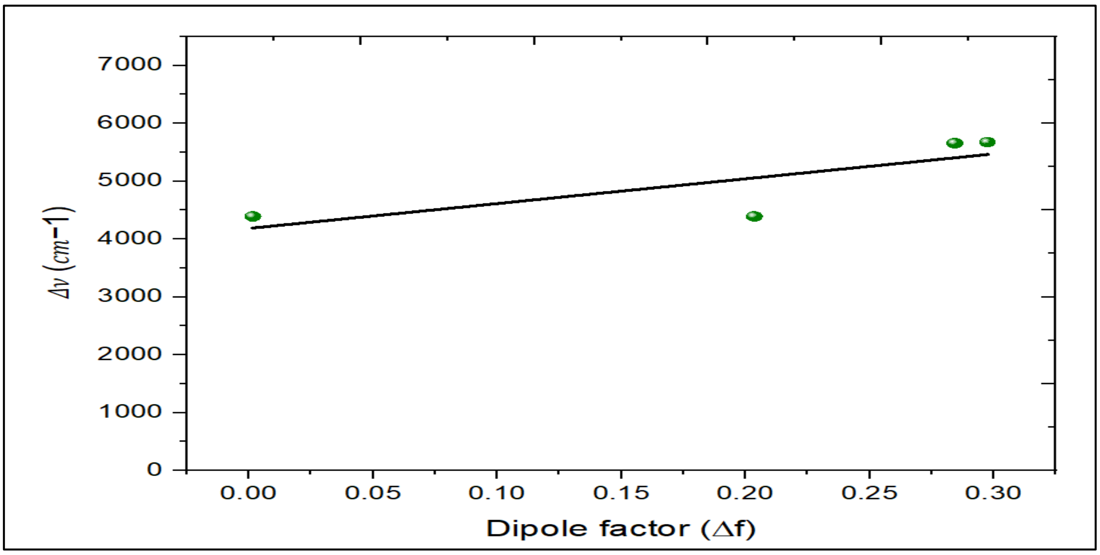

Figure 5.11 Variation in the Stokes’ shift of Chalcone in solution with a dipole factor for different

CHAPTER SIX

6. Conclusions and Recommendations

6.1. Conclusions

Through this research project, it was concluded that the factors influencing the optical properties of the chalcone compound are solubility, concentration, dielectric constant, and temperature. Solubility does not affect the wavelength but influences the intensity, while concentration affects the wavelength only and does not influence the intensity. The dielectric constant impacts both the wavelength and the intensity in emission only, whereas temperature influences both the wavelength and the intensity. It was determined that ethyl acetate is the most suitable solvent for the chalcone compound. Furthermore, the chalcone exhibits moderate polarity, tending towards weak polarity. The highest emission intensity for ethyl acetate was recorded at a concentration of 0.05 mM. It was also found that increasing the temperature leads to an increase in the band gap and a decrease in both the absorbed and emitted intensities. Increasing the dielectric constant decreases the energy required for electron transition, resulting in absorption at a higher wavelength. Additionally, it was observed that an increase in the dielectric constant reduces the photon energy emitted by the excited molecules during their return to the ground state, leading to a higher emission wavelength. Finally, the validity of the measurements obtained was confirmed using an equation (3.6), which demonstrated a linear relationship between the Stokes shift and the solvent properties.

6.2. Recommendations

- I recommend conducting more experiments and further studies on these chalcones to verify and support the obtained results.
- I recommend using ethyl acetate as a suitable solvent for this chalcone.
- I advise against increasing temperatures, as it leads to a decrease in the absorbed and emitted intensities.
- I recommend further investigation into the non-radiative intensity to gain a deeper and more precise understanding of the factors influencing it.
- Based on the high fluorescence compound, I suggest studying the laser properties of this chalcone in ethyl acetate solvent at different concentrations.

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