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## Synthesis an organic dye and investigating its spectral and optical properties for laser active medium application

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### Abstract

The spectral properties, specifically absorption and fluorescence, of Acridone-based compounds dissolved in DMF at various concentrations were thoroughly analyzed. Critical optical characteristics, namely, the absorption coefficient and refractive index were measured. The results demonstrated that increasing concentration led to higher absorbance and reduced transmittance, which in turn caused a rise in both the absorption coefficient and the refractive index. Furthermore, fluorescence intensity was found to increase with concentration, accompanied by a red shift in the emission peak toward longer wavelengths.

**Keywords:** Acridone derivatives dye, dye laser, fluorescence, absorbance

### Introduction

Dye lasers are a class of lasers in which the active medium comprises organic dye compounds dissolved in liquid solvents like ethyl alcohol, methanol, or water<sup>[1]</sup>. These organic dye molecules possess the capability to interact with a wide span of the electro-magnetic spectrum, enabling them to release radiation over an extensive wavelength range, typically shifting toward longer wavelengths compared to the initially absorbed light. This broad emission capability in the visible region has made organic dyes highly effective as active media in tunable dye lasers.

The first tunable lasers to operate within the visible spectrum emerged due to the wide fluorescence bandwidth exhibited by organic dyes, which allows for continuous tuning of the laser output across an extensive spectral range. As a result, dye lasers can emit at various wavelengths, spanning regions of the ultraviolet (UV), visible, and near-infrared spectra, depending on the dye used.

Typically, dye lasers are capable of producing output across a spectral range extending from approximately 340 nm to 1.2  $\mu\text{m}$ . Owing to this spectral coverage, dye lasers have become essential tools in a variety of scientific applications, particularly in spectroscopy and physical chemistry<sup>[2, 3]</sup>.

### The Theoretical Part: Optical Properties

The optical properties of a material arise from its interaction with electromagnetic radiation, which is governed by the arrangement and dynamics of electronic, molecular, or ionic charges within the material<sup>[4]</sup>. When an electromagnetic wave impinges upon a material, several physical processes may arise simultaneously. The material absorbs a portion of the incident light, resulting in the conversion of light energy into heat. Another portion passes through the medium without significant loss of energy and is referred to as the transmitted radiation. The remaining part is reflected off the material's surface<sup>[5]</sup>.

To gain insights into the internal structure and bonding nature of the material, it is essential to examine its optical characteristics namely, transmittance, absorbance, and reflectance under the influence of incident electromagnetic radiation. For instance, ultraviolet (UV) spectroscopy is commonly employed to investigate electronic transitions within the material. In practical applications, materials are often studied and utilized within the visible spectral region<sup>[6]</sup>.

The mathematical parameter that relates the concentration of absorbing particles in a sample to the optical path length (sample thickness) is referred to as the absorbance (A) or optical

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density, which serves as a quantitative measure of light attenuation through the material.

$$A = \log \left( \frac{I_0}{I} \right) \quad (1)$$

Here, (I) represents the light intensity at a particular wavelength ( $\lambda$ ) after it has traversed the sample, while  $I_0$  denotes the incident light intensity before interacting with the sample. When light is absorbed by the material, it can induce electronic excitations that may result in either the dissociation of molecular bonds—if the absorbed photon energy exceeds the bond dissociation energy—or transitions of electrons to upper energy states.

The probability of absorption rises with an increased population of molecules in the lower energy state and a greater number of incident photons [6]. Thus, the probability of photon absorption increases with the population of ground-state absorptive species and the photon flux of the incident radiation.

According to Beer-Lambert's law, the absorption of light by a medium is directly proportional to both the concentration of the absorbing species within the sample and the optical path length (i.e., the thickness of the medium through which the light travels). This law provides an empirical relationship linking the extent of the light absorption to the physical characteristics of the material it traverses.

Specifically, this law indicates that light absorption increases linearly with the concentration of the absorbing entities present in the medium. As light travels through a solution, the absorption intensity exhibits an exponential relationship with solute concentration. This phenomenon is quantitatively described by the Beer-Lambert law, as represented below [7]:

$$I = I_0 \exp(-\alpha_{op} C_m L) \quad (2)$$

$$\ln \left( \frac{I_0}{I} \right) = \alpha_{op} C_m L = A \quad (3)$$

Here, A refers to the absorbance (optical density),  $I_0$  represents the intensity of the incident light, I corresponds to the intensity of light diffused through the sample,  $\alpha_{op}$  is the molar absorptivity expressed in  $L \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ ,  $C_m$  indicates the molar concentration of the absorbing types (mol/L), and L denotes the optical path length traversed by the light within the sample (cm).

The Beer-Lambert law is applicable across a range of spectral regions, including ultraviolet (UV) radiation and photovoltaic applications, provided that the incident light is monochromatic [7]. The absorption coefficient quantifies the fraction of radiation intensity lost per unit length as the electromagnetic wave travels through a material. This coefficient is influenced by the photon energy ( $h\nu$ ) as well as the intrinsic properties of the material [8]. Based on the Beer-Lambert law, the absorption coefficient ( $\alpha_0$ ) can be expressed as:

$$\log \left( \frac{I_0}{I} \right) = 2.303 A = \alpha_0 d \quad (4)$$

$$2.303 \frac{A}{d} = \alpha_0 \quad (5)$$

Where d characterizes the thickness that equals to (1 cm)

Transmittance -T is introduced as the ratio of the transmitted light intensity (I) to the incident light intensity ( $I_0$ ), often expressed as a percentage.

Put differently, it indicates the proportion of the transmitted radiation to the initial incident energy as it passes through the material [8].

$$T = \frac{I}{I_0} \quad (6)$$

As stated by the Beer-Lambert law, transmittance diminishes as the concentration of the molecular rises and as the optical path length (L) over which light travels becomes longer [8]. Transmittance (T) is fundamentally related to absorbance (A) through the following expression:

$$A = -\log \left( \frac{1}{T} \right) = -\log \left( \frac{I}{I_0} \right) = \log \left( \frac{I_0}{I} \right) \quad (7)$$

It is evident that transmittance (T) rises when the medium exhibits lower absorption. The light speed in a vacuum represents the maximum constant value, which is higher than its speed in any other medium. This speed varies depending on the physical properties of the medium and the wavelength of the light passing through it. At a particular wavelength, the refractive index is characterized as the quotient of the light speed in a vacuum to that in the medium [9].

$$n = \frac{c}{v} \quad (8)$$

The refractive index of a material is not a fixed value; rather, it diverges with the wavelength of the incident electromagnetic radiation. Additionally, in some anisotropic materials, the refractive index varies with the direction in which the electromagnetic wave propagates through the medium. Such substances are frequently used in applications requiring the adjustment of electromagnetic wave polarization [10].

The refractive index serves as a measure of the extent to which a material influences the propagation of electromagnetic radiation. When an alternating electric field with frequency ( $\nu$ ) impinges on the material, the molecular electric polarization oscillates in sync with the frequency of the incident electromagnetic wave ( $\nu$ ). Consequently, a portion of the energy carried by the incident electromagnetic wave is converted into vibrational energy of the induced dipoles, which in turn diminishes the energy transmitted by the wave. Assuming that

The energy loss due to molecular dipole oscillations causes a slight delay in the re-emission of radiation, which consequently reduces the speed of light within the medium. This effect is quantitatively described by the refractive index (n), as expressed in Eq. (9). The refractive index of a material can be inferred from the extent of polarization induced by the incoming electromagnetic radiation. Greater polarization corresponds to a longer delay in the propagation of light, resulting in a higher refractive index. Conversely, materials

with negligible polarization exhibit no delay in light propagation, yielding a refractive index of  $n=1$  [11].

Generally, the refractive index of most materials exceeds unity, and its magnitude is directly proportional to the medium's density. That is, a growth in the average density of the material results in a corresponding increase in its refractive index. However, the refractive index cannot be characterized solely by density; it can be calculated using the following relation

$$n = \left( \frac{4R}{1-R^2} - K^2 \right)^{\frac{1}{2}} - \left( \frac{R+1}{R-1} \right) \quad (9)$$

### Spectral properties

Radiative transitions are processes in which photons are emitted as excited molecules return from higher energy states to lower-lying electronic states. These processes include both fluorescence and phosphorescence. Fluorescence is characterized as a direct, radiative transition occurring between states of the same multiplicity.

Specifically, fluorescence arises from electronic transitions between vibrational sublevels of the first excited electronic state ( $S_1$ ) to numerous vibrational levels within the ground electronic state ( $S_0$ ). The fluorescence lifetime, denoted by  $\tau$ (lifetime), typically measures on the order of 10 to 9 Sec for organic molecules [12]. Accordingly, some organic compounds exhibit fluorescence emission that originates from the lowest vibrational level of the second excited electronic state ( $S_2$ ) and transitions to vibrational levels of the ground state ( $S_0$ ). This occurs because the energy gap between  $S_2$  and  $S_1$  is relatively large in these molecules, which suppresses internal conversion from  $S_2$  to  $S_1$  [13]. The structural configuration of organic pigment molecules significantly affects their ability to emit fluorescence efficiently. Fluorescence intensity tends to increase in rigid molecular structures and in molecules exhibiting energy coupling between the singlet excited state ( $S_1$ ) and the triplet state ( $T_1$ ), which results in a reduced rate of intersystem crossing.

The fluorescence spectrum arises when a molecule absorbs an incident photon, promoting an electron to a higher excited state.

Subsequently, these excited molecules tend to stabilize by relaxing to the first excited singlet state, releasing excess energy either as heat or vibrational energy. When the molecules transition back to the ground electronic state, they emit photons. Due to energy losses during relaxation, the emitted radiation possesses lower energy than the absorbed photon, which corresponds to a longer emission wavelength compared to the excitation wavelength [14].

When a molecule absorbs light from an external source, it becomes exciting to a vibrational sublevel within a higher electronic state ( $S_n$ ). In dense-phase media, collisions with surrounding molecules cause the excited molecule to lose part of its vibrational energy, eventually relaxing to the first excited singlet state ( $S_1$ ). From this level, the molecule undergoes a radiative transition to one of the vibrational levels of the ground electronic state ( $S_0$ ). This sequence of events occurs on extremely short time scales [15].

The radiative lifetime ( $\tau_{FM}$ ) refers to the time taken for an electron to transition from the minimum vibrational level of the excited electronic state ( $S_1$ ) to several vibrational levels of the ground state ( $S_0$ ) via photon emission. This lifetime is inversely proportional to the radiative transition probability ( $K_{FM}$ ), typically expressed in units of  $\text{sec}^{-1}$  [13].

$$\tau_{FM} = 1 / K_{FM} \quad (10)$$

Due to the presence of non-radiative processes that compete with the radiative transition probability ( $K_{FM}$ ), the number of molecules capable of emitting fluorescence is reduced. As a result, the overall transition probability ( $K_{FK}$ ) represents the sum of both radiative and non-radiative transition probabilities [15, 16].

### Practical Part: Instruments and Equipment Used

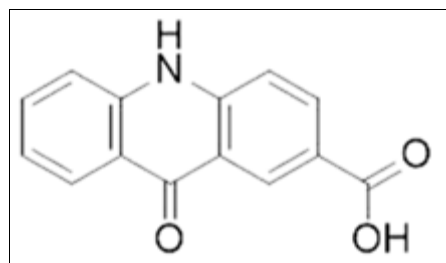
A UV-Visible spectrophotometer was employed to record the absorption spectra, encompassing wavelengths across the ultraviolet to near-infrared regions of the electromagnetic spectrum. The instrument is equipped with two excitation sources: a deuterium lamp, which provides radiation within the wavelength range of 190-360 nm, and a tungsten lamp, which covers the spectral region from 360 to 1100 nm.

The F96PRO Fluorescence Spectrometer had been employed to record the fluorescence spectra of the Acridone derivatives dye solution. The device features the 150-watt xenon arc lamp as the excitation source and operates over an excitation and emission wavelength range of 200-700 nm. It offers selectable scanning speeds (200, 400, and 600 nm/min) and utilizes the highly sensitive photomultiplier tube (PMT) detector for enhanced signal detection.

### Acridone Derivatives Dye

The dye under study appears as a crystalline powder in its pure form. When dissolved in dilute solutions, it exhibits a green color. The dye is thermally stable with a melting point exceeding 279 °C.

The chemical formula of the Acridone derivatives dye is  $C_{14}H_9NO_3$ , with a molecular weight of 239.23 g/mol. Fig. (1) Demonstrates the molecular structure of the corresponding compound, thereby illustrating the arrangement of atoms within the Acridone derivatives dye.



**Fig 1:** Molecular structure of the Acridone derivatives dye

### Dimethylformamide: Description

Dimethylformamide (DMF) is a transparent, color-less, and hygroscopic liquid with a mild, amine-like odor. It is widely appreciated for its exceptional solvent capabilities, which stem from its high dielectric constant, aprotic nature, broad liquid temperature range, and low volatility. These properties make DMF an ideal solvent for various chemical processes that demand strong solvating power. Owing to its capability to dissolve a broad spectrum of both polar and non-polar substances, it is commonly referred to as a “universal solvent.”

Characteristic	Quantity
Molecular formula	$C_3H_7NO$
Molecular weight	73.09 gm/mol
Boiling point	153°C

### Solutions Preparation

To prepare a  $1 \times 10^{-3}$  M solution of the acridone derivative dye, precisely 0.0012 g of the dye powder was measured and dissolved in 10 cm<sup>3</sup> of DMF, which was used as the solvent throughout the experiment. The solution was prepared following the standard molarity formula:

$$W_m = \frac{C \times V \times M.W}{1000} \quad (11)$$

Where

W<sub>m</sub>: Weight of the dye (gm)

C: concentration in (ML)

V: unit size (cm<sup>3</sup>)

From Eq. (12), lighter concentrations ( $1 \times 10^{-4}$ ) ( $1 \times 10^{-5}$ ) ML can be gotten as.

$$C_1V_1 = C_2V_2 \quad (12)$$

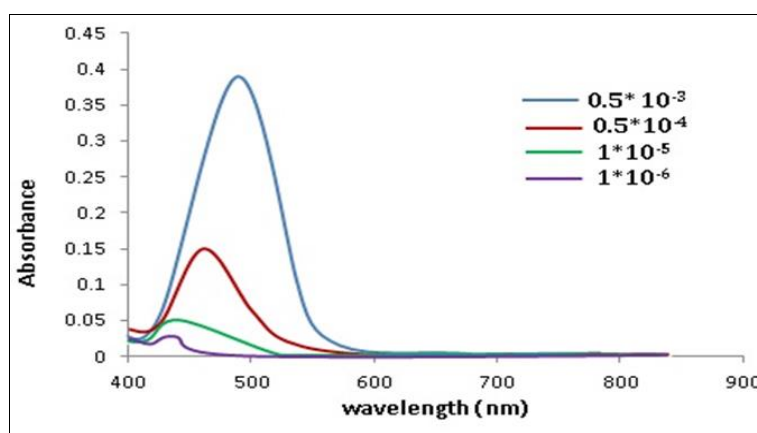
Here:

- C<sub>1</sub> represent focus only

- C<sub>2</sub> represent lighter concentration
- V<sub>1</sub> represent 1<sup>st</sup> concentration volume
- V<sub>2</sub> represent the size which must added to the 1<sup>st</sup> concentration.

### Calculations

The absorption spectra of Acridone derivatives dissolved in DMF at various concentrations ( $1 \times 10^{-3}$ ,  $1 \times 10^{-4}$ ,  $1 \times 10^{-5}$ , and  $1 \times 10^{-6}$  M) had been recorded using a UV-Vis spectrophotometer. As presented in Fig. 2, a progressive decrease in absorbance is detected with the reduction in dye concentration, indicating a direct correlation between concentration and light absorption. This behavior is consistent with the Beer-Lambert law, where absorbance is proportional to both the path length and concentration. The use of ethanol as a solvent lead to a reduction in absorption intensity, accompanied by a redshift in the absorption spectrum toward longer wavelengths. This behavior is consistent with Lambert's law. Table 1 provides a summary of how varying concentrations affect the relative absorption intensity and corresponding wavelengths of acridone derivatives dissolved in DMF.

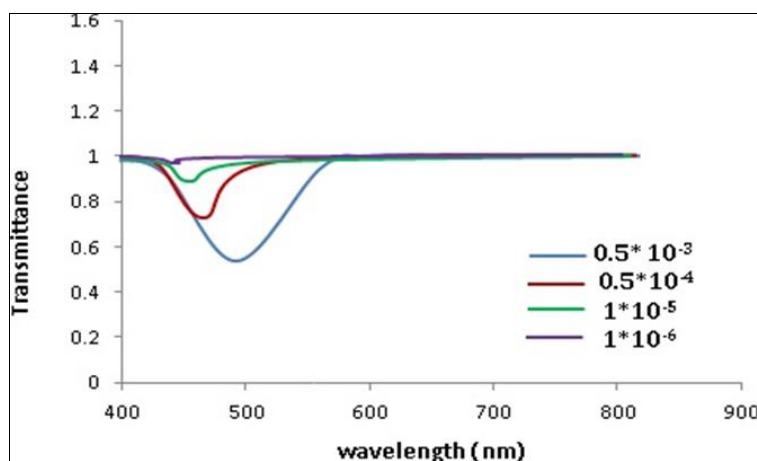


**Fig 2:** Absorption spectra of acridone derivative solutions in DMF at varying concentrations.

**Table 1:** Absorption with maximum wavelengths

C (ML)	$\lambda$ max (nm)	A
$0.5 \times 10^{-3}$	498	0.39
$0.5 \times 10^{-4}$	460	0.15
$1 \times 10^{-5}$	440	0.05
$1 \times 10^{-6}$	438	0.01

From absorption spectra, the transmission spectra were found as presented in Table (2) and Figure (3).



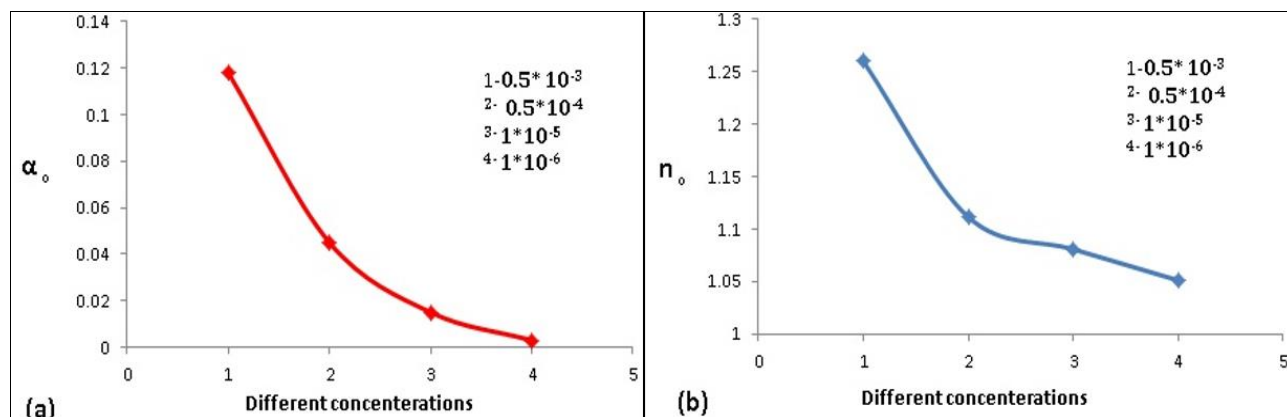
**Fig 3:** UV-Vis transmittance spectra of acridone derivatives dissolved in DMF at various molar concentrations.



**Table 2:** The Transmittance with wavelengths

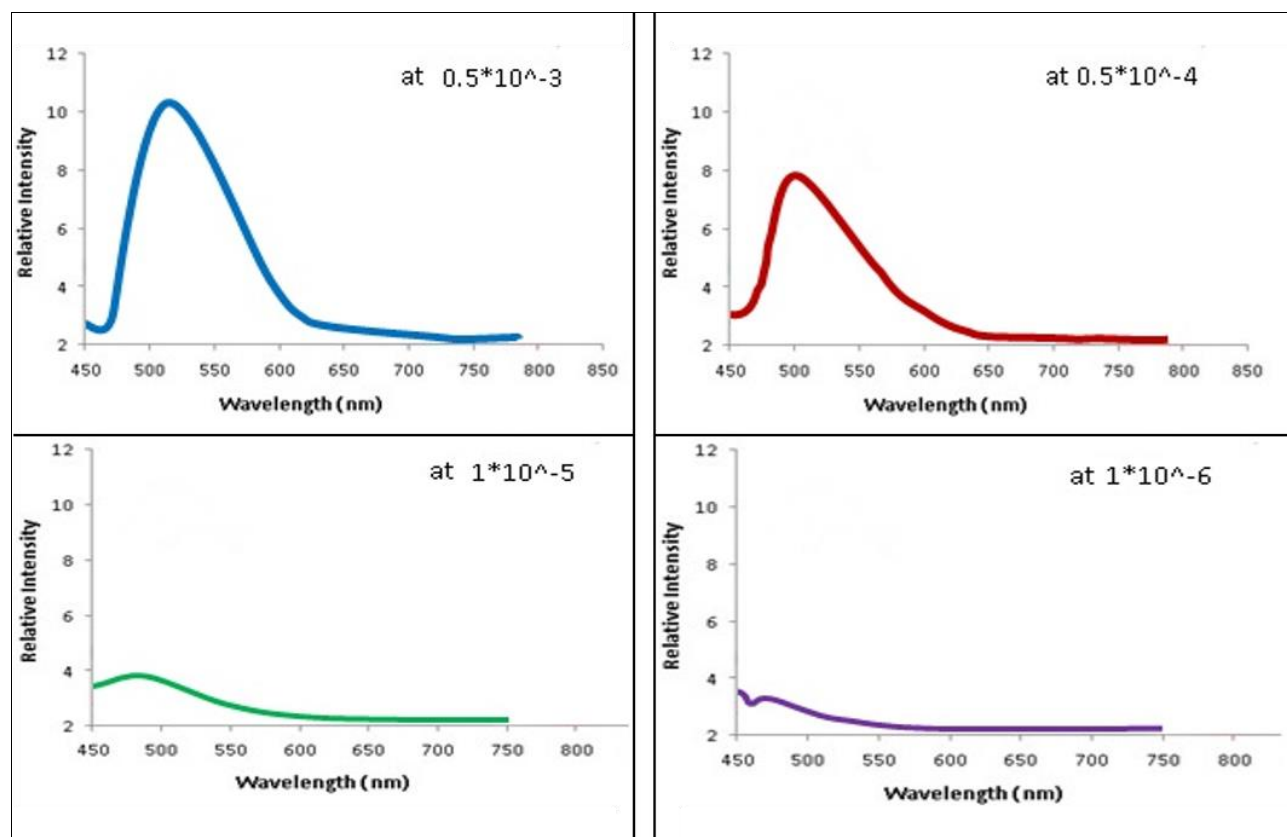
C (ML)	$\lambda$ max (nm)	T
$0.5 \times 10^{-3}$	495	0.4932
$0.5 \times 10^{-4}$	458	0.7922
$1 \times 10^{-5}$	450	0.9112
$1 \times 10^{-6}$	448	0.9401

Following the measurement of transmittance values, the linear absorption coefficient and linear refractive index of the prepared samples were calculated using Equations (5) and (9). As shown in Figure 4 and summarized in Table 3, a reduction in concentration leads to a corresponding drop in the quantity of both parameters.

**Fig 4:** (a) The linear absorption coefficient ( $\alpha_0$ ) (b) the refractive index at different concentrations**Table 3:** Values of linear absorption coefficient and linear refractive index at different concentrations

C (ML)	Linear Absorption ( $\alpha_0$ )	Linear refractive index ( $n_0$ )
$0.5 \times 10^{-3}$	0.118	1.2600
$0.5 \times 10^{-4}$	0.045	1.1115
$1 \times 10^{-5}$	0.015	1.0808
$1 \times 10^{-6}$	0.003	1.0511

Fluorescence spectra of the samples dissolved in DMF were recorded using a spectrofluorometer. The obtained results are presented in Figure 5 and summarized in table 4.

**Fig 5:** Fluorescence spectra at different concentration

**Table 4:** The intensity with maximum wavelengths

C (ML)	$\lambda_{\max}$ (nm)	Relative Intensity
$0.5 \times 10^{-3}$	514	10.50
$0.5 \times 10^{-4}$	502	7.98
$1 \times 10^{-5}$	485	3.95
$1 \times 10^{-6}$	472	3.21

### Conclusion

By examining the optical properties of Acridone derivatives dissolved in DMF, it was observed that decreasing the concentration leads to absorption spectra characterized by peaks of reduced intensity, which also shift towards longer wavelengths. The highest relative absorption intensity was recorded at 498 nm for the concentration of  $1 \times 10^{-3}$  M, whereas lower concentrations, such as  $1 \times 10^{-6}$  M, exhibited diminished absorption intensity with a corresponding redshift to 438 nm. This spectral shift is attributed to the increased molecular population, which raises the likelihood of photon absorption. The observed absorption behavior of pigments is reliable with the Beer-Lambert law, which accounts for the decrease in absorption values as the concentration decreases. Additionally, the results indicate that lowering the concentration causes a decrease in the fluorescence intensity, accompanied by a blue shift in the emission spectra.

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