Oscillator Strength and Quantum Efficiency of Fluoranthene Molecule

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ABSTRACT:

The fluorescence and absorption spectra of Fluoranthene dissolved in cyclohexane and ethanol were studied and analyzed. The effect of the concentration of this molecule and the polarity of the solvents on the spectral shifts and on relative intensity has been investigated. A computational program was written in order to convert the spectra from grapher to data. Some photophysical parameters such as oscillator strength and quantum efficiency have been calculated. Fluorescence quantum efficiency of Fluoranthene was measured relative to Quinine Sulfate (QS) in 1N H_2SO_4. The obtained values were (0.5) in cyclohexane and (0.45) in ethanol.

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الخلاصة:

في هذا البحث تم قياس ودراسة أطياف الامتصاص والتألق لجزئية الفلوراثين في مذيبي السايكلوهكسان و اليثانول وبتركيز مختلفة, وتضمن البحث دراسة تأثير تركيز هذه الجزئية وقطبية المذ يبات المستخدمة على الازاحات الطيفية والشدة النسبية للحزم. تم قياس وحساب بعض الاعلومات الفيزيائية (شدة المهتز، عمر الزمن الإشعاعي والكفاءة الكمية للفلورة) ولأجل هذه الحسابات تم كتابة برنامج خاص لتحويل المنحني إلى بيانات وحساب المساحة تحت حزم الامتصاص والتألق, فقد تم حساب الكفاءة الكمية للفلورة نسبة إلى مركبQuinine Sulfate المذاب في واحد عياري من حامض الكبريتيك وتبين لنا إن قيمة الكفاءة الكمية مذيبي السايكوهكسان واليثانول (0.5) و (0.45) على التوالي.

INTRODUCTION:

The *Fluoranthene* ($C_{13}H_{18}$) is considered as one of aromatic molecules, therefore in this present work the absorption and fluorescence spectra of this molecule in different solvents have been recorded. At dilute solution (10^{-5}) M, certain spectroscopic parameters (Oscillator Strength, Radiative Lifetime and Quantum Efficiency) have been measured and found to be a solvent dependent. For this purpose, computer program was written to convert the spectra from grapher to data and provide a printout of the spectra in units of relative quanta and molar extinction coefficient $\varepsilon(\bar{\upsilon})$ per unit wave number. The measurement of quantum efficiency by using a comparative method which, makes use of a *Quinine Sulfate* as the standard reference. The comparative method for measuring quantum efficiency proposed by Weber and Teale [1] has been used with proper modification by Melhuish [2] as well as by Parker and Rees [3]. Finally, since in this work where we are concerned with relative measurements one must be certain that the

reference and unknown molecules are compared at same optical density or at least under conditions where both optical densities are accurately known.

EXPERIMENTAL:

Spectrofluorophotometer mode –RF-540 supplied by Shimadzu is used for recording the fluorescence and absorption of samples prepared. The instrument computerized and operates in the wavelength range 200 nm to 800 nm and a scanning speed of 480 (nm /min). It consists of two unites [4]:

1-Main unit 2- Recorder unit

Emission spectra are obtained when the excitation monochrometer M_1 is fixed and the emission monochrometer M_2 is scanned. If M_2 is fixed and M_1 is scanned the result is an excitation spectrum.M_1 and M_2: off -plane concave diffraction grating monochromators, F/2.6, and both monochromators have a diffraction gratings of 900 grooves/mm. Also Refractometer type (ABBE) is used to measurements the refractive index of the solutions.

RESULTS AND DISCUSSION:

Figures (1) and (2) show the absorption and fluorescence spectra of *Fluoranthene* in the solvents (cyclohexane and ethanol). The (0-0) bands of the absorption and fluorescence spectra of *Fluoranthene* dissolved in cyclohexane are shifted to shorter wavelengths when the concentration is lowered. When ethanol is used instead of cyclohexane, we find that the solvent change effects are minimal, which is the same as in cyclohexane, the only exception of this result the fluorescence spectra are displaced toward longer wavelengths about (2 nm) compared with cyclohexane. Computer program was used to convert the spectra from grapher to data; this process included first working scanner to all grapher. This scanner converts grapher from features on the paper to images inside the computer. The relationship between the absorbance and concentration is linear given by Beer and Lambert's law [5]:

$$I = I_0 10^{-\varepsilon c L} \quad (1)$$

Where:I and I_0 are the incident and transmitted intensity, c is the *Fluoranthene* concentration(mol.liter^{-1}), L is the cell thickness (cm) and ε is the molar extinction coefficient (l.mol^{-1}.cm^{-1}). After converting the grapher (I_0 and I) to data, the values of (ε) measured and represented graphically in Figs.(3) and (4). From these Figs., one concluded that the maximum (ε) in unit (l.mol^{-1}.cm^{-1}) for *Fluoranthene in* cyclohexane was (4738.181) at (27522 cm^{-1}) and in ethanol was (7718.828) at (27152.81 cm^{-1}). After knowing the molar extinction coefficient (ε) as a function of wave number ($\bar{\upsilon}$), It is necessary to know the strength of an electronic transition is generally expressed in terms of a quantity called "Oscillator Strength", which can be express by [6]:

$$f = \frac{4.39\times10^{-9}}{n}\int \varepsilon(\bar{\upsilon})d\bar{\upsilon} \quad (2)$$

Where n: is the refractive index of the solution, the area under the curve, which represented $\int \varepsilon(\bar{\upsilon})d\bar{\upsilon}$, measured by program known as "graph pad".

The radiative lifetime of the first singlet excited state τ_{FM}, was computed by means of a formula given by Forster [7].

$$1/\tau_{FM} = 2.88\times10^{-9} n^2 \int \frac{(2\bar{\upsilon}' - \bar{\upsilon})^3}{\bar{\upsilon}} \varepsilon(\bar{\upsilon})\, d\bar{\upsilon} \quad (3)$$

Where: $\bar{\upsilon}'$ is the wave number of the mirror symmetry point between the absorption and fluorescence curves.

In our evaluation of the relative fluorescence quantum efficiency, we have assumed that the quantum efficiency of Q*uinine Sulfate* in 1N H_2So_4 is 0.55 [3], as show in Fig. (5) be used as a standard. The quantum efficiency in this work was

calculated by using the formula given by equation (4) including the index of refractor term and that the absorption at λ_{ex} are matched [8].

$$q_{FM_1} = q_{FM_2} \frac{n_1^2 I_2 A_2 \int F_1(\bar{\upsilon}) d\bar{\upsilon}}{n_2^2 I_1 A_1 \int F_2(\bar{\upsilon}) d\bar{\upsilon}} \quad (4)$$

Where: F_1 and F_2 are the area under the fluorescence spectra of the two solutions, I and A are the relative photon output of the light source and optical density of the given solutions at the wave length of excitation.Values of "f",τ_{FM} and q_{FM} have been calculated using Eqs.(2,3 and 4) and given in Table(1).

Table (1): Oscillator strength, Radiative Lifetime and Quantum Efficiency of Fluoranthene.

Concentration 10^{-5}M			**At room temperature**	
Solvent	**F**	**τ_{FM} (ns)**	**q_{FM}**	***Reported*** Work **q_{FM}**
Cyclohexane	0.068	19.12	0.5	0.3[9]
Ethanol	0.113	13.58	0.45	0.25[10]

It is clear from Table (1) that the "f" values are close to (0.1) this means that bands are (P-Bands) according to classification of absorption by Clar [11]. Also the accuracy of quantum efficiency is somewhat improved due to using a standard with a suitable quantum efficiency.

CONCLUSION:

The described measurements and data – analysis technique is applied for (S_0 -- S_1) absorption and (S_1 -- S_0) fluorescence. The effect of the polarity of the solvent is minimal on the absorption and fluorescence spectra of *Fluoranthene* where, the behavior of *Fluoranthene* in cyclohexane and ethanol was similar. It is that the absorption and fluorescence spectra at dilute solution show a rather good mirror image relationship, this is evidence that most of the intensity in absorption bands is due to a single electronic transition (fluorescence). Finally, this molecule is one of the few molecules, which does not exhibit self-absorption in liquids, as a result can be used as a standard instead of *Quinine Sulfate* in evaluation the relative quantum efficiency.

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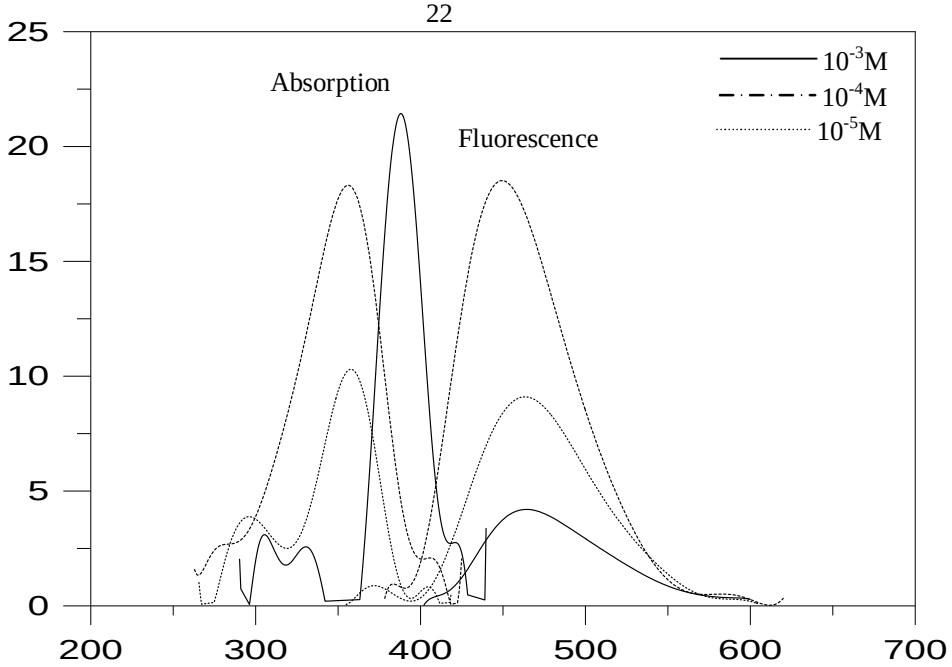

Fig. (1) Absorption and Fluorescence spectra of Fluoranthene dissolved in Cyclohexane at different concentrations.

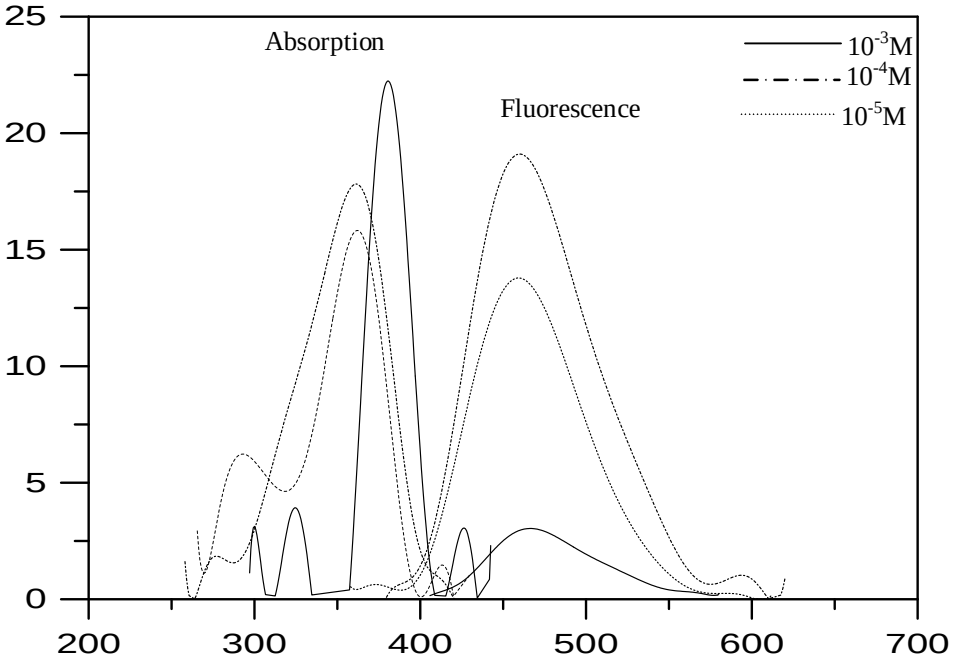

Fig. (1) Absorption and Fluorescence spectra of Fluoranthene dissolved in Cyclohexane at different concentrations.

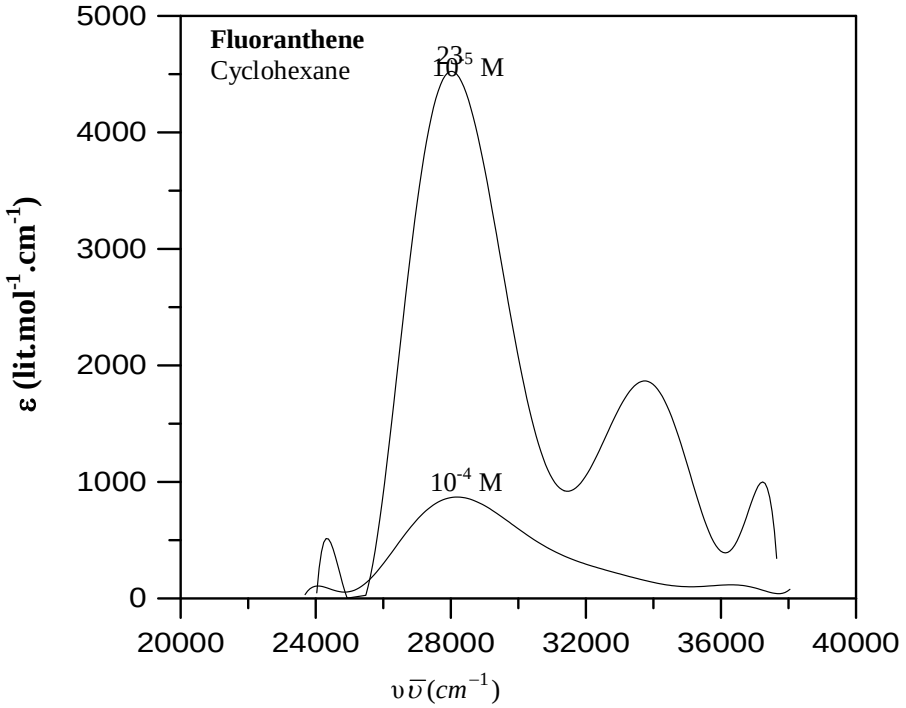

Fig. (3) Molar extinction coefficient ε as a function of the wave number for Fluoranthene dissolved in Cuclohexane at dilute solutions.

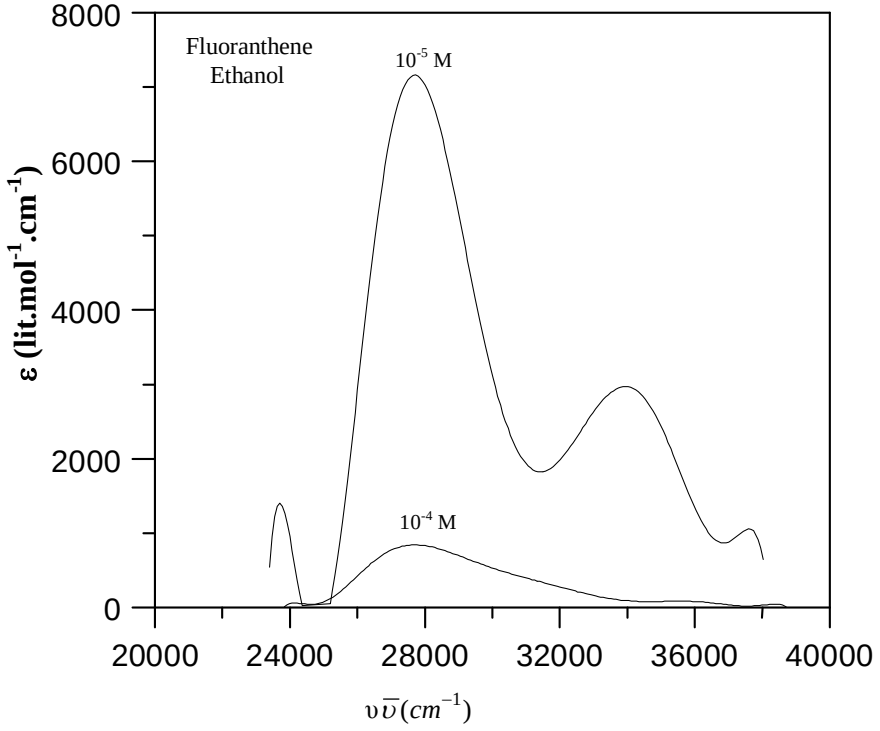

Fig. (4) Molar extinction coefficient ε as a function of the wave number for Fluoranthene dissolved in Ethanol at dilute solutions.