Effect of Solvent on Fluorescence Spectrum of Anthracene

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Abstract
The fluorescence spectra of the anthracene dye dissolved in polar and non-polar solvents (cyclohexane and methanol) were measured and studied at two concentrations [10^{-4}M] and [10^{-5}M]. For anthracene at excited wavelength (λ_{ex}=375 nm). The results showed decreasing of fluorescence intensity of anthracene dye solution with increasing of solvent polarity. Also, a small shift was noticed in fluorescence spectra for the anthracene dye toward the longer wavelength (red shift) in non-polar solvent (cyclohexane). These measurements were done at room temperature (20°C).

Keywords: Anthracene dye; Solvent polarity; Fluorescence; Spectroscopy
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1. Introduction

Anthracene dye is an aromatic organic compound consisting of three fused benzene rings and is classified as a polycyclic aromatic hydrocarbon (PAH). The benzene ring is the simplest aromatic structure, consisting of six carbon atoms and six hydrogen atoms arranged in a stable ring structure, as shown in Fig. (1) [1-3]. Anthracene and its derivatives are semiconducting materials, making them part of the organic semiconductor class, which has received increasing attention in recent years. This interest stems from significant advances in fundamental and applied research related to these materials, due to their distinctive electronic and optical properties. Organic semiconductors are used in the fabrication of a wide range of optoelectronic devices, such as organic light-emitting diodes (OLEDs), organic solar cells, organic field-effect transistors, as well as various memories and sensors [4-6].

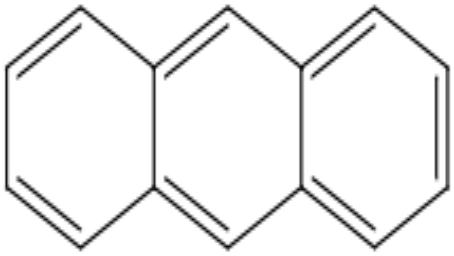

Fig. (1) Chemical composition of anthracene ($C_{14}H_{10}$)

The study of fluorescence is a fundamental topic in physical and analytical chemistry, as it provides precise information about the electronic structure of molecules and their behavior in excited states. The intensity and wavelength of fluorescent radiation emitted by organic compounds depend on several factors, most notably the nature of the solvent and the concentration of the fluorescent substance.

Anthracene is a planar polycyclic aromatic hydrocarbon known for its distinctive fluorescent properties, making it an ideal model for studying the effect of solvents on spectral characteristics.

The polarity of the solvent affects both the absorption and emission energies of molecules. Polar solvents tend to exhibit reduced fluorescence intensity due to strong intermolecular interactions. Conversely, nonpolar solvents show more pronounced emissions due to the limited nature of these interactions [8-11].

The aim of this work is to study the effect of solvent on the fluorescence spectra of anthracene solutions in different solvents.

2. Experimental Part

The anthracene compound of 99.5% purity was dissolved separately in two different solvents (cyclohexane 99% and methanol 99.5%). Anthracene solutions were prepared at two different molar concentrations [10^{-4}M] and [10^{-5}M] at room temperature (20°C). The solutions were prepared using the following relationship [7]:

$$[M] = \frac{1000W}{MW.V} \quad (1)$$

where W is the weight of material (anthracene) in grams, M.W is the molecular weight of the material in g/mol, [M] is the molar concentration of the solution (mol/L), and V is the volume of solvent used to dissolve the material in ml

The prepared solutions were diluted according to the following equation [7]:

$[M]_1V_1 = [M]_2V_2$ (2)

where $[M]_1$ is the primary concentration, $[M]_2$ is the final concentration, V_1 is the volume before dilution and V_2 is the volume after dilution

The fluorescence spectra of the prepared solutions were recorded using a Shimadzu RF-5301pc spectrofluorophotometer in the spectral rang of 200-850 nm.

3. Results and Discussion

The fluorescence spectra of anthracene which consists of four peaks located at different wavelengths are shown in table (1). Figures (2) and (3) show that the decrease in relative fluorescence intensity with increasing molar concentration is caused by the phenomenon of self-absorption and concentration quenching. Also ,we can noticed the increases solvent polarity with decreases in fluorescence intensity because molecule absorbed the light and transitions to the excited electronic state .On the other hand, can observe the fluorescence spectra was a small shifted toward the long wavelength (red shift) in non-polar solvent (cyclohexane). Because anthracene is less sensitive to polarity and may be affected by nonpolar effects. Also methanol interacts with anthracene methanol is a protic solvent and may form hydrogen bonds or interact with the aromatic surface of anthracene, producing a more stable ground state than the excited state, resulting in a relative blue shift. In a nonpolar solvent such as cyclohexane, anthracene may accumulate more density, altering its electronic energies and resulting in a slight red shift. The red shift of the fluorescence spectrum of anthracene in cyclohexane compared to methanol can be explained by the effect of the solvent's dielectric constant (ε) on the stability of the electronic states of the dissolved molecule. The dielectric constant is an indicator of the polarity of the solvent and its ability to stabilize charges in the ground and excited states. The higher the dielectric constant, the more the solvent stabilizes the molecule in both states, with a clearer tendency to stabilize the ground state due to dipole-dipole interactions and hydrogen bonding.

Table (1) Peaks locations for the fluorescence spectra of anthracene in different solutions at concentrations [10^{-4}M] and [10^{-5}M]

Concentrations[10^{-4}M]	Band			
Solvent				
Cyclohexane	381	400.5	424	450
Methanol	380	399.5	423	449
Concentrations[10^{-5}M]	Band			
Solvent				
Cyclohexane	379.5	401.5	424.2	450
Methanol	378.5	400.5	423.2	449

Methanol is a protic solvent with a high dielectric constant (ε≈32.6), which results in strong stabilization of the ground state compared to the excited state, thus increasing the energy difference between the two electron levels and causing a shift toward shorter wavelengths (blue shift). Cyclohexane, on the other hand, is a nonpolar, low-dielectric solvent (ε ≈ 2.0), which has a poor ability to stabilize electronic states. In this environment, the ground state is no more stabilized than the excited state, resulting in a slightly lower energy difference between the two electronic levels and longer-wavelength light emission, a red shift in the fluorescence spectrum. Effect of the refractive Index cyclohexane has a slightly higher refractive index than methanol, which may result in a higher polarization of the environment surrounding the molecule and contribute to a slight red shift.

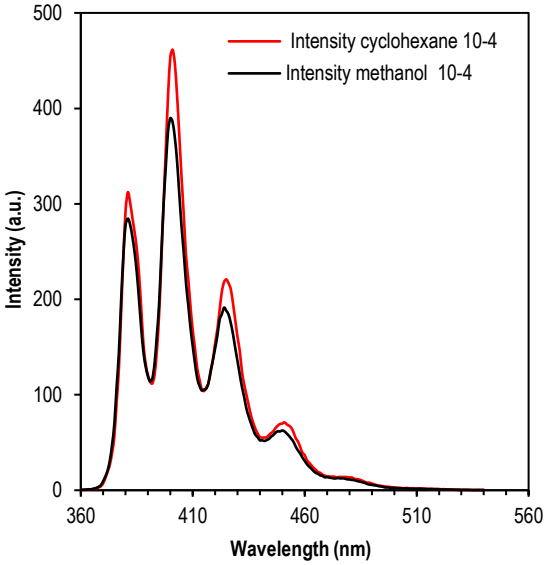

Fig. (2) Fluorescence spectra for anthracene dissolved in cyclohexane and methanol at concentration [10^{-4}M]

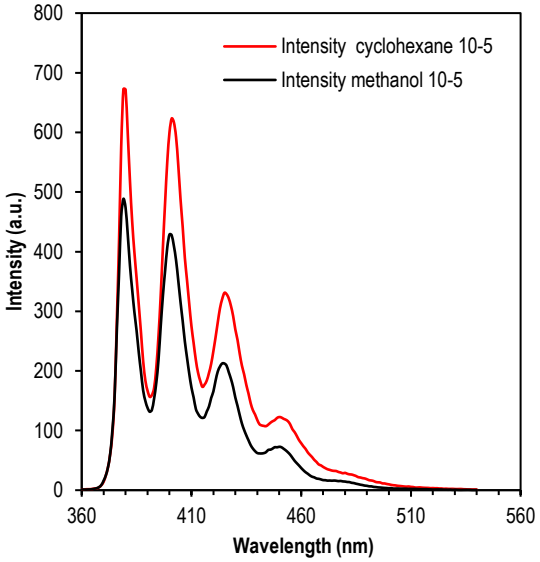

Fig. (3) Fluorescence spectra for anthracene dissolved in cyclohexane and methanol at concentration [10^{-5}M]

4. Conclusions

The comparative analysis of anthracene's fluorescence in cyclohexane versus methanol clearly demonstrates the profound impact of solvent choice. The non-polar cyclohexane provides an ideal environment for strong, structured emission, while the polar protic methanol actively quenches the fluorescence, resulting in a weaker and potentially less structured signal. This underscores the critical importance of solvent selection in fluorometric studies and applications, where maximizing or minimizing emission intensity is desired.

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