Analysis of fluorescence quenching of newly synthesized Coumarin-triazol derivative

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Abstract: Around the world, the number of cases of diabetes has been rising rapidly in recent decades, and one of the most exciting fields of research is the search for small chemicals with strong anti-diabetic properties. Diabetes mellitus (DM) is a chronic metabolic condition characterized by an increase in blood glucose levels due to an imbalance in glucose homeostasis [1, 2]. Two relatively prevalent risk factors that contribute to both neurological diseases and cardiovascular disease are type 2 diabetes and hypertension [3]. With decades of history and potential for growth, heterocyclic chemistry has dominated the field and is essential to the synthesis of new medications. Among the heterocycles, triazoles and coumarins received the most attention due to their significant biological activity and natural occurrence. Coumarins are prepared via Pechmann condensation, catalytic annulation phenolic acetates with acrylates [4], ZnBr₂ catalyzed reaction of salicylaldehyde with ynamides [5], Amberlyst-15 catalyzed reaction of 1,3-dihydroXybenzene and ethyl acetoacetate under micro-wave irradiation in a solvent free conditions [6] etc. Naturally occurring coumarins in the glycoside forms are useful in medicine [7], and coumarins shows antimicrobial [8], anti-HIV [9], radical scavenging [10], and anti-viral [11] properties.

Key Words: AMTCC, Fluorescence quenching, Diffusion Coefficient, Activation Energy

I. Introduction

The compound known as coumarin triazole derivatives has attracted significant attention in the field of medicinal chemistry due to its biological significance and use in the pharmaceutical sectors. According to a recent review [12], they display a variety of biological actions, including antibacterial, analgesic, anti-inflammatory, antipyretic, antihypertensive, and anticancer properties. Fluorescence quenching is a phenomenon that results in a decrease in the lifetime and intensity of fluorescence molecules, resulting in spontaneous emission. In general, it is a process where in the electronic excitation energy of an excited molecule is transferred to a quencher molecule through a variety of methods, including charge transfer and diffusion, resulting in the quencher molecule's non-fluorescent emission [13]. The Stern-Volmer relation is used to study the fluorescence quenching of 3-(4-Amino-5-mercapto-4H-1,2,4-triazol-3-yl)-chloro-2H-6chromen-2-one (AMTCC) molecules by aniline [14]. It is given by

\[
\frac{F}{F_0} = 1 + K_{sv}[Q] \tag{1}
\]

where \(F_0\) and \(F\) represent the fluorescence intensities, respectively, in the absence quencher and quencher conditions. \(K_{sv}\) represents the S-V constant, \(t_0\) denotes the solute lifespan without quencher, and \([Q]\) indicates the quencher concentration.
II. Materials and Methods

The coumarin-triazole derivative are produced a suspension of the potassium salt of coumarin thiocarbazinate in water (5 mL) was dissolved with 10 mmol of hydrazine hydrate. In a water bath, the mixture reacted for eighteen to twenty hours. After the reaction was carried out until a homogenous reaction mixture was obtained, a color shift associated with the release of $\text{H}_2\text{S}$ was noticed. Subsequently, the solution was lowered in temperature and diluted using 20 milliliters of cold water. It was then neutralized using diluted hydrochloric acid to extract the desired chemicals, which were then separated from ethyl alcohol 3-(4-Amino-5-mercapto-4H-1,2,4-triazol-3-yl)-chloro-2H-6chromen-2-one (AMTCC) molecule is Obtained as pale yellow solid in 61% yield with $R=\text{H}$, $R'=\text{H}$ and $R''=\text{Cl}$ as shown in fig.1. The spectroscopic grade solvents methanol, ethanol, propional, heptanol, and ethyl acetate were purchased from S.D Fine Chemicals Ltd. in India. Before usage, the quencher aniline passed a double distilled and a purity test. All five solvents having solutions prepared with the solute with concentration is fixed at $1\times10^{-5}$ M and the quencher concentration ranging from 0.00 to 0.10 M.

![Molecular structure of AMTCC](image)

III. Results and Discussion

At room temperature, the fluorescence spectra of the 3-(4-Amino-5-mercapto-4H-1,2,4-triazol-3-yl)-chloro-2H-6chromen-2-one (AMTCC) molecule are recorded for five different solvents at various quencher concentrations as shown in fig.2.

![Emission spectra of AMTCC with varying quencher concentration](image)

The Stoke's Einstein equation (2) can be used to estimate the diffusion coefficients of the solute $D_S$ and the quencher $D_Q$ [15].and Table 1 displays these results.

$$D = \frac{KT}{a\pi\eta R}$$  \hspace{1cm} (2)

where "a" is the Stoke's Einstein number, which is equal to $a = 6$ for a solute and $a = 3$ for a quencher. $K$, $T$, and $\eta$ represent for the Boltzmann constant, temperature, and solvent viscosity, respectively.

$$k_d = 4\pi N' DR \left[ 1 + \frac{R}{(2D\tau_0)^{1/2}} \right]$$  \hspace{1cm} (3)
The Avogadro's number is N. The Edward method [16] is used to estimate the sum of the radii of the quencher and solute. Equation (3) is used to estimate the diffusion rate parameter \( k_d \),

\[
p = \frac{k_{\text{eff}}}{k_d}
\]  

(4)

Additionally, equation (4) was used to determine the probability of quenching each encounter \( p \) the results are displayed in Table 1. Equation (5) is used to estimate the activation energy of quenching,

\[
E_a = E_d + RT \ln \left( \frac{1}{p} - 1 \right)
\]  

(5)

Table 1: The various quenching rate parameters of for AMTCC molecule.

<table>
<thead>
<tr>
<th>Solvent</th>
<th>( k_{\text{eff}} \times 10^9 ) (M (^-1)s(^{-1}))</th>
<th>( k_d \times 10^9 ) (M (^-1)s(^{-1}))</th>
<th>( DX \times 10^{-5} ) (cm(^3)s(^{-1}))</th>
<th>( p )</th>
<th>( E_d ) (kcal/M)</th>
<th>( E_a ) (kcal/M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>1.59</td>
<td>200.46</td>
<td>3.69</td>
<td>0.0079</td>
<td>3.05</td>
<td>14.68</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.61</td>
<td>139.02</td>
<td>2.12</td>
<td>0.0043</td>
<td>3.02</td>
<td>14.70</td>
</tr>
<tr>
<td>Proponal</td>
<td>1.20</td>
<td>55.01</td>
<td>1.02</td>
<td>0.0218</td>
<td>3.58</td>
<td>21.76</td>
</tr>
<tr>
<td>Heptanol</td>
<td>2.10</td>
<td>315</td>
<td>1.05</td>
<td>0.0066</td>
<td>3.76</td>
<td>22.08</td>
</tr>
<tr>
<td>Ethyl acetate</td>
<td>2.18</td>
<td>324</td>
<td>4.98</td>
<td>0.0067</td>
<td>2.60</td>
<td>5.02</td>
</tr>
</tbody>
</table>

**Conclusion**

In summary, the AMTCC molecule undergoes fluorescence quenching by aniline in five different solvents at room temperature. The value of \( p \) is calculated and also the values of \( E_a \) are greater than \( E_d \) in all five solvents studied. It is in referred that the fluorescence quenching reactions in AMTCC molecule are more significantly affected by activation energy.

**REFERENCES:**


