Fluorescence properties of aromatic asymmetric di-ketone compound in polar and non-polar solvents

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Abstract. Using the quantum chemical and solvatochromic shift technique aromatic unsymmetric di-ketone compound1-(4'-dodecyl-[1,1'-biphenyl]-4-yl)-3-(3,4,5-trimethoxyphenyl)propane-1,3-dione (DK1) fluorescence properties were estimated. The excitation and emission band of recently synthesized DK1 have been examined in various dissolvable. The dipole moments evaluated utilizing Gaussian software and Solvatochromic correlations. Evaluated (μg) value by Gaussian method is comparatively larger than the solvatochromic shift methods. It is seen that the energized state dipole moments (μe) are more prominent than the ground state dipole moment (μg) which authorizes π→π* transition. The (Δμ) were also estimated both from solvatochromic shift method and microscopic solvent polarity parameter (EN) and results are compared. The kinetic stability and chemical reactivity of the selected molecules have been studied with the help of quantum chemical properties of the molecule and Frontier molecular orbital analysis using DFT.

1. Introduction
Diketone derivatives have been extensively used in various regions as of their exclusive important features, durability for heat and light and chemical functionalities as electroluminescence materials [1]. Diketonebyproducts retain a wide-ranging band of biological properties for example antimicrobial and anti-inflammatory activity effects [2].

In real sense when solute molecules dissolve in different solvent media there is an energy associated with it due to the solute-solvent interaction which is known as energy of solvation. When solution matrix is excited with a suitable light there is a difference in the initial and final energy states which is referred to as solvatochromic shift and is of prime importance in various fields of sciences. Experimentally the
solvatochromism of the solute molecules is analyzed by absorption and emission spectroscopic tools and is quite popular. There are many models available for the determination of $\mu_e$ and $\mu_g$ in different solvents, such as electric dichroism, Stark splitting, electric polarization of fluorescence and microwave conductivity give very accurate readings but they have limited usage and restricted to very simple molecules [3]. However, experimentally dipole moments (excited state and ground state) of fluorophore in liquid medium can be evaluated by the equations derived by Bilot and Kawski [4], Bilot and Kawski [5], Bakhshiev [6] and Chamma-Viallet [7] which are simple methods and have provided satisfactory results.

In present work reported a determination of the initial state and energized states of the DK1 [8-13]. An extensive range of (alkane) and (alcohol) dissolvable are used to study the stoke’s shift. The experimental values supplemented with Gaussian calculations. The initial and energized state dipole moments were determined using solvatochromic shift method. Analyzed the result using Bilot-Kawski, Bakhshiev, Lippert, microscopic solvent polarity ($E^P_B$) and Chamma-Viallet-Kawski.

2. Theory

2.1. Dipole moment:
Using the second-order perturbation model and considering Onsager’s model, Bilot and Kawski [4-5] have achieved expressions for the Stokes’s shift given by

$$\bar{\nu}_a - \bar{\nu}_f = m^{(1)} f(\varepsilon, n) + \text{const}$$

$$\bar{\nu}_a + \bar{\nu}_f = -m^{(2)} f(\varepsilon, n) + \text{const}$$

where $\phi(\varepsilon, n) = 2 g (n) + f(\varepsilon, n)$

$$m^{(1)} = \frac{2(\mu_e - \mu_g)^2}{\hbar c a^3}$$

$$m^{(2)} = \frac{2(\mu_e - \mu_g)^2}{\hbar c a^3}$$

$$f(\varepsilon, n) = \frac{2 n^2 + 1}{n^2 + 2} \times \frac{(\varepsilon - 1 - n^2 - 1)}{(\varepsilon + 2 - n^2 + 2)}$$

$$g(n) = \frac{3}{2} \left[ \frac{n^{n-1}}{(n^2+2)^2} \right]$$

Assuming that the symmetry is remains unaffected upon electronic transition and $\mu_e$ and $\mu_g$ are collinear, obtained the following Equations. Using equations (3) and (4).

$$\mu_g = \frac{m^{(2)} - m^{(1)}}{2} \frac{\hbar c a^3}{2 m^{(1)}} \frac{1}{2}$$

$$\mu_e = \frac{m^{(2)} + m^{(1)}}{2} \frac{\hbar c a^3}{2 m^{(1)}} \frac{1}{2}$$

$$\mu_e = \frac{m^{(2)} + m^{(1)}}{m^{(2)} - m^{(1)}} \mu_g \quad \text{for} \quad m^{(2)} > m^{(1)}$$

Commonly, it is assumed that $\mu_e$ and $\mu_g$ are collinear. Angle $\phi$ can be estimated if they are not collinear using Equation. (10) [5].

$$\cos \phi = \frac{1}{2\mu_g \mu_e} \left[ (\mu_g^2 + \mu_e^2) - \frac{m^{(1)}}{m^{(2)}} (\mu_e^2 - \mu_g^2) \right]$$

Using the following equations estimate the energized state dipole moment of diketones derivatives Lippert’s equation [6]

$$\bar{\nu}_a - \bar{\nu}_f = m_1 F_1 (\varepsilon, n) + \text{const}$$

Bakhshiev’s equation [7]

$$\bar{\nu}_a - \bar{\nu}_f = m_2 F_2 (\varepsilon, n) + \text{const}$$
Kawski-Chamma-Viallet’s equation [8]

\[
\frac{1}{2} (\bar{\nu}_a + \bar{\nu}_f) = -m_3[F_3(\varepsilon, n)] + \text{constant}
\]  

(13)

Where,

\[
F_1(\varepsilon, n) = \left[ \frac{\varepsilon - 1}{2 \varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \right]
\]

(14)

\[
F_2 (\varepsilon, n) = \frac{2n^2 + 1}{n^2 + 2} \left[ \frac{\varepsilon - 1}{\varepsilon + 2} - \frac{n^2 - 1}{n^2 + 2} \right]
\]

(15)

and

\[
F_3 (\varepsilon, n) = \frac{2 n^2 + 1}{2(n^2 + 2)} \left[ \frac{\varepsilon - 1}{\varepsilon + 2} - \frac{n^2 - 1}{n^2 + 2} \right] + \frac{3}{2} \frac{n^4 - 1}{(n^2 + 2)^2}
\]

(16)

Where \(F_{1,2}(\varepsilon, n)\) is Lippert’s, \(F_3(\varepsilon, n)\) is Bakshiev’s and \(F_4(\varepsilon, n)\) is Kawski-Chamma-Viallet’s polarity function respectively, \(n\) is the refractive index and \(\varepsilon\) is the dielectric constant of the solvent. Also,

\[
m_1 = \frac{2(\mu_e - \mu_g)^2}{\text{hca}^3}
\]

(17)

\[
m_2 = \frac{2(\mu_e - \mu_g)^2}{\text{hca}^3}
\]

(18)

and

\[
m_3 = \frac{2(\mu_e - \mu_g)^2}{\text{hca}^3}
\]

(19)

Using excitation and emission spectral bands ‘m1’, ‘m2’ and ‘m3’ parameters are determined. The ground (\(\mu_g\)) and energized state dipole moment (\(\mu_e\)) determined from following equations.

\[
\mu_g = \frac{m_3 - m_2}{2} \left[ \frac{\text{h} \cdot \text{a}^3}{2 m_2} \right]^{1/2}
\]

(20)

\[
\mu_e = \frac{m_3 + m_2}{2} \left[ \frac{\text{h} \cdot \text{a}^3}{2 m_2} \right]^{1/2}
\]

(21)

Or

\[
\mu_e = \left[ \frac{m_3 + m_2}{m_3 - m_2} \right] \mu_g \text{ for } (m_3 > m_2)
\]

(22)

Here \(m_1\), \(m_2\) and \(m_3\) slopes are obtained from straight-line plots of \((\bar{\nu}_a - \bar{\nu}_f)\) and \(1/2(\bar{\nu}_a + \bar{\nu}_f)\) versus Stokes shift. The plots of \((\bar{\nu}_a - \bar{\nu}_f)\) and \(1/2(\bar{\nu}_a + \bar{\nu}_f)\) versus solvent polarity functions are straight lines along with their slopes ‘m1’, ‘m2’ and ‘m3’.

2.2 Microscopic solvent polarity \(E_f^N\)

The \(E_f^N\) used to analyze the h-bonding influence or polarization dependence on spectral characteristics. Reichardt [15] proposed the relationship between spectral shift and \(E_f^N\).

\[
\bar{\nu}_a - \bar{\nu}_f = 11307.6 \left[ \left( \frac{\Delta \mu}{\Delta \mu_b} \right)^2 \frac{a b}{a} \right]^{3/2} E_f^N + \text{constant}
\]

(23)

where \(a_b\) and \(\Delta \mu_b\) are the Onsager cavity radius and change in dipole moment of solute on excitation respectively of a betaine dye and \(\Delta \mu\) and ‘a’ are the corresponding quantities for the present solute. The change in dipole moment (\(\Delta \mu\)) can be evaluated from the slope (m) of the Stoke’s shift versus \(E_f^N\) plot and it is given by

\[
\Delta \mu = (\mu_e - \mu_g) = \frac{mX \, 81}{\sqrt{(6.2/a)^3}} \times 11307.6
\]

(24)
3. Materials and methods
The solute 1-(4'-dodecyl-[1,1'-biphenyl]-4-yl)-3-(3,4,5-trimethoxyphenyl)propane-1,3-dione(DK1) was synthesized by standard methods [16-17]. The molecular structure of DK1 is given in Figure 1. Experimental samples of DK1 in various solvents have been prepared with a concentration of 1x10^-4 M by a standard method. The excitation spectrum were recorded using a double UV-VIS Spectrophotometer (Analytic Jenaspeord 210 plus, Germany) with wavelength accuracy of 0.5nm at room temperature. The emission bands of the solute were recorded using a Fluorescence spectrophotometer (Hitachi F 2700, Japan).

\[
\text{C}_{12}\text{H}_{25}\text{-}\text{O}\text{-}\text{O}\text{-}\text{C}_3\text{H}_6\text{OCH}_3\text{-}\text{OCH}_3
\]

Figure 1. Molecular Structures of DK1.

4. Results and discussion:
4.1 Theoretical approach (Computational calculations of dipole moments)
The ground state (\(\mu_g\)) dipole moment of the DK1 are fully optimized and evaluated using DFT with popular hybrid B3LYP/6-31g* functional by Gaussian 16 software [18] and the values are given in Table 4. It is evident that, the ground state dipole moments evaluated by this method are comparatively larger than the solvatochromic shift methods. This is because DFT consider solute molecules in their gaseous phase rather than in solution medium and neglect solvent interactions [19]. The optimized molecular geometries of DK1 are shown in Figure 2 to 4, whereas, the direction of dipole moment in the ground state is represented with an arrow mark.

Figure 2. Optimized ground state molecular structure of DK1
4.2 Experimental approach (Estimation of dipole moments)
Excitation and emission bands were recorded in alkane and alcohols dissolvable of various polarities. Characteristic normalized excitation and emission band of DK1 in propanol are specified in Figure 5. Solvatochromic data obtained from the experimental method is used to analyze the specific and wide-ranging solvent effects. The general effect is due to collective influence of the dielectric constant and refractive index of the dissolvable whereas specific effects are due to formation of H-bond, charge transfer complex, isomerization and exciplex. The solvent polarity functions are calculated using equations (14), (15) and (16) and compared with that available in literature [20-22]. Values like \( \varepsilon \) and \( n \) of the solvents and the microscopic solvent polarity function \( E_N^T \) are obtained from the literature [23] and are listed in Table 1.

Table 2 represents the experimentally obtained values of solvatochromic data such as absorption and emission wavelengths, Stokes’ shift etc for the title molecule. It is observed that, the Stokes’ shift varies from 3903.201cm\(^{-1}\) to 6120.845cm\(^{-1}\) in various solvents. Totally, the increase in Stokes’ shift suggests that a large geometrical change has taken place in the S\(_1\) states. This is an indication of \( \pi \rightarrow \pi^* \) singlet-singlet transition in the excited states. Normally \( \pi \rightarrow \pi^* \) transition refers to an elevation of electron from
a bonding orbital (π) to an anti-bonding orbital (π*). As this transition occurs at longer wavelength side emission spectra show bathochromic effect. It is approximately 55nm for [DK1], in different solvents. This clearly indicates the change in dipole moments in the S1 singlet state and S0 ground state. The title molecule showed bathochromic shift, which suggests that title molecules are sensitive to the polarity of the various solvents used.

![Normalized Absorption and Emission Spectra](image)

**Figure 5.** Typical normalized absorption and emission spectra of DK1 in different solvents at room temperature

Experimentally, using Bilot-Kawaski’s equation (7) we have estimated dipole moments of DK1 molecule in different solvents. A linear progression of \( \bar{\nu}_a - \bar{\nu}_f \) versus \( f(\varepsilon, n) \) and \( \bar{\nu}_a + \bar{\nu}_f \) versus \( \phi(\varepsilon, n) \) have been plotted, then data is fitted to a straight line and are shown in Fig.6(a) and Fig.6(b). The slope \( (m_1, m_2) \) obtained from the Fig.6(a) and Fig.6(b) are given in Table 3. For BilotKawaski method, obtained \( \mu_g \) and excited state \( (\mu_e) \) value is 0.487D and 3.078D for DK1 respectively. Angle between ground state and excited state calculated using equation (10) and it is found to be zero. The values of \( \mu_g \), \( \mu_e \) and \( \phi \) are listed in Table 4.

The three independent equations (20) – (22)are used to determine \( \mu_e \) and \( \mu_g \). Linear progressions for equations (11) – (13) have been plotted for the title molecule. The data is fitted to a straight line and are shown in Figures 6(c) - 6(d). The correlation co-efficient in all fits is found to be above 0.95. Table 3 consists of slopes, correlation factor and data number with respect to the various Solvatochromic methods. The atomic radius is determined from the molecular volume of the molecule [24]. The estimated \( \mu_g \) and \( \mu_e \) values using various solvatochromic methods using equations (20) – (22) are given in Table 4. It is observed that the \( \mu_e \) value is 1.021D for DK1, in various solvents determined. Discrepancy is observed when theoretical and experimental \( \mu_e \) values are compared. This discrepancy may arise because of considering gas phase and not considering the specific solvent-solute interactions for the theoretical calculations. Further it is observed that, \( \mu_e \) values obtained from the experimental calculations (solvatochromic methods) are greater than the theoretical \( \mu_e \) values. This indicates vigorous redistribution of electrons and more polar nature of the solutes in the excited states which confirm the existence of ICT.

However, the values of \( \mu_e \) are different in different models and this may be due to the different assumptions made in the respective models. The maximum differences \( (\Delta \mu) \) calculated using \( \mu_g \) and \( \mu_e \) are found to be 4.994D, for DK1. It is also observed that, as solvent polarity increases there is an increase in the Stokes’s shift. Change in dipole moment of the solute molecules can be studied with the help of possible resonance structures. Figure 7, show the resonance structure of the title molecules.
Figure 6(a) The Stoke’s shift as a function of $f(\varepsilon, n)$

Figure 6(b) The Stoke’s shift as a function of $\phi(\varepsilon, n)$

Figure 6(c) Stoke’s shift as a function of $f_1(\varepsilon, n)$

Figure 6(d) The Stoke’s shift as a function of $f_2(\varepsilon, n)$

Figure 6(e) Stoke’s shift as a function of $f_3(\varepsilon, n)$

Figure 6(f) Plot of Stokes’ shift against $E_N^r$
Table 1. The values of $\varepsilon$, $\eta$, $E^\eta$ polarity parameters $f_1$, $f_2$, $f_3$, $f(\varepsilon, \eta)$ and $\phi(\varepsilon, \eta)$ of different solvents

| Sl.No | Solvents     | $\varepsilon$ | $\eta$ | $f(\varepsilon, \eta)$ | $\phi(\varepsilon, \eta)$ | $F_1$ | $F_2$ | $F_3$ | $E^\eta$ |
|-------|--------------|----------------|--------|------------------------|--------------------------|------|------|------|--------|
| 1     | Pentane      | 1.800          | 1.350  | 0.006                  | 0.471                    | 0.0030 | 0.0056 | 0.2355 | 0.009  |
| 2     | Hexane       | 1.890          | 1.375  | 0.001                  | 0.510                    | 0.0001 | 0.0002 | 0.2550 | 0.009  |
| 3     | Heptane      | 1.900          | 1.388  | 0.006                  | 0.521                    | 0.0034 | 0.0064 | 0.2606 | 0.012  |
| 4     | Decane       | 2.000          | 1.408  | 0.004                  | 0.558                    | 0.0021 | 0.0041 | 0.2792 | 0.009  |
| 5     | Nonane       | 2.000          | 1.405  | 0.006                  | 0.556                    | 0.0031 | 0.0061 | 0.2782 | 0.009  |
| 6     | Cyclohexane  | 2.020          | 1.426  | 0.003                  | 0.575                    | 0.0016 | 0.0031 | 0.2875 | 0.006  |
| 7     | 1,4 Dioxane  | 2.220          | 1.421  | 0.045                  | 0.616                    | 0.0220 | 0.0445 | 0.3080 | 0.164  |
| 8     | Toluene      | 2.400          | 1.496  | 0.034                  | 0.703                    | 0.0153 | 0.0337 | 0.3516 | 0.099  |
| 9     | Octanol      | 10.30          | 1.428  | 2.240                  | 2.821                    | 0.2259 | 0.6272 | 0.6039 | 0.537  |
| 10    | Hexanol      | 13.30          | 1.418  | 2.482                  | 3.050                    | 0.2444 | 0.6910 | 0.6293 | 0.559  |
| 11    | Pentanol     | 13.90          | 1.490  | 2.541                  | 3.096                    | 0.2497 | 0.7036 | 0.6296 | 0.568  |
| 12    | Butanol      | 17.40          | 1.399  | 2.722                  | 3.265                    | 0.2633 | 0.7494 | 0.6459 | 0.586  |
| 13    | 1-Propanol   | 20.45          | 1.380  | 2.872                  | 3.389                    | 0.2761 | 0.7818 | 0.6493 | 0.617  |
| 14    | Ethanol      | 24.30          | 1.361  | 3.018                  | 3.509                    | 0.2886 | 0.8117 | 0.6516 | 0.654  |
| 15    | Methanol     | 33.70          | 1.328  | 3.257                  | 3.704                    | 0.3094 | 0.8578 | 0.6523 | 0.762  |

Table 2. Solvatochromic data of DK1

| Sl No. | Solvents     | $\lambda_a$(nm) | $\lambda_e$(nm) | $\bar{\nu}_a$(cm$^{-1}$) | $\bar{\nu}_f$(cm$^{-1}$) | $(\bar{\nu}_a - \bar{\nu}_f)$(cm$^{-1}$) | $\left(\frac{\bar{\nu}_a + \bar{\nu}_f}{2}\right)$(cm$^{-1}$) | $\nu_a$ + $\nu_f$ |
|--------|--------------|-----------------|-----------------|--------------------------|--------------------------|---------------------------------------------|---------------------------------------------------------------|---------------------|
| 1      | Pentane      | 366             | 427             | 27322.40                 | 23419.20                 | 3903.201                                    | 25370.804                                                   |                     |
| 2      | Hexane       | 365             | 425             | 27397.26                 | 23529.41                 | 3867.849                                    | 25463.336                                                   |                     |
| 3      | Heptane      | 366             | 426             | 27322.40                 | 23474.18                 | 3848.226                                    | 25398.291                                                   |                     |
| 4      | Decane       | 367             | 429             | 27247.96                 | 23310.02                 | 3937.933                                    | 25278.990                                                   |                     |
| 5      | Nonane       | 366             | 428             | 27322.40                 | 23364.49                 | 3957.918                                    | 25343.445                                                   |                     |
| 6      | Cyclohexane  | 366             | 426             | 27322.40                 | 23474.18                 | 3848.226                                    | 25398.291                                                   |                     |
| 7      | 1,4 Dioxane  | 370             | 436             | 27027.03                 | 22935.78                 | 4091.247                                    | 24981.403                                                   |                     |
| 8      | Toluene      | 369             | 439             | 27100.27                 | 22779.04                 | 4321.228                                    | 24939.657                                                   |                     |
| 9      | Octanol      | 371             | 452             | 26954.18                 | 22123.89                 | 4830.284                                    | 24539.036                                                   |                     |
| 10     | Hexanol      | 371             | 457             | 26954.18                 | 21881.84                 | 5072.340                                    | 24418.008                                                   |                     |
| 11     | Pentanol     | 370             | 457             | 27027.03                 | 21881.84                 | 5145.189                                    | 24454.433                                                   |                     |
| 12     | Butanol      | 369             | 460             | 27100.27                 | 21739.13                 | 5361.141                                    | 24419.701                                                   |                     |
| 13     | 1-Propanol   | 370             | 460             | 27027.03                 | 21739.13                 | 5287.897                                    | 24383.079                                                   |                     |
| 14     | Ethanol      | 370             | 461             | 27027.03                 | 21691.97                 | 5335.053                                    | 24359.501                                                   |                     |
| 15     | Methanol     | 371             | 480             | 26954.18                 | 20833.33                 | 6120.845                                    | 23893.756                                                   |                     |
Table 3. Statistical treatment of the correlations of solvents spectral shifts of DK1

| Correlations          | Slope     | Correlation factor ‘r’ | Number of data |
|-----------------------|-----------|------------------------|----------------|
| m₁                   | 505.778   | 0.96                   | 15             |
| BilotKawasaki         | m₂        | 695.804                | 0.95           | 15             |
| m₃                    | 5321.941  | 0.96                   | 15             |
| Lippert               | m₄        | 1877.036               | 0.96           | 15             |
| Bakhshiev’s           | m₅        | 2644.507               | 0.96           | 15             |
| Kawski-Chamma-Viallet’s | m₆    | 2401.785               | 0.97           | 15             |
| E⁷ᴺ correlation      | m         |                        |                |

Debye (D) = 3.33564x10⁻³⁰ cm = 10⁻¹₈ esu cm.

1. The µₑ calculated using Gaussian software
2. The µₑ calculated using BilotKawasaki Eq. 7
3. The µₑ dipole moments calculated using Eq.20
4. The µₑ dipole moments calculated using BilotKawasaki Eq. 8.
5. The µₑ dipole moments calculated using Eq. 21.
6. The µₑ dipole moments calculated from Lippert’s equation.
7. The µₑ dipole moments calculated from Bakhshiev equation.
8. The µₑ dipole moments calculated from Kawski-Chamma-Viallet equation.

Table 4. Ground state µₑ and excited state µₑ dipole moments of DK1

| R ‘a’ (Å) | µₑ¹ (D) | µₑ² (D) | µₑ³ (D) | µₑ⁴ (D) | µₑ⁵ (D) | µₑ⁶ (D) | µₑ⁷ (D) | µₑ⁸ (D) | Aμ¹⁰ (D) | Aμ¹¹ (D) | (µₑ/µₑ)¹² | ϕ³¹ |
|-----------|---------|---------|---------|---------|---------|---------|---------|---------|----------|----------|------------|------|
| 5.11      | 3.39    | 0.48    | 1.02    | 3.07    | 6.01    | 9.42    | 6.01    | 4.12    | 4.99     | 3.10     | 5.89       | 0.0 |

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5. Conclusion

It is noticed that as the solvent polarity has been increased in general solvents band maxima of the fluorescent spectra is shifted towards the longer wavelength side. This indicates a strong solute-solvent interaction and π→π* singlet- singlet transition. Experimentally, excited state dipole moments are found to be greater than the ground state dipole moments in different solvatochromic shift methods except microscopic solvent polarity parameter (E⁷ᴺ). This is due to the fact that, microscopic solvent polarity parameter method incorporates specific solvent-solute interactions which are ignored in other methods. Specific solvent effects like H-bonding effect in case of different solvents are confirmed by microscopic solvent polarity parameter E⁷ᴺ.
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