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 (μ_g) value by Gaussian method is comparatively larger than the solvatochromic shift methods. It is seen that the energized state dipole moments (μ_e) are more prominent than the ground state dipole moment (μ_g) which authorizes $\pi \rightarrow \pi^*$ transition. The ($\Delta\mu$) were also estimated both from solvatochromic shift method and microscopic solvent polarity parameter (E_T^N) 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

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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 $\mu_g$and μ_e 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 Kawaski [4] Lippert [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 BilotKawaski, Bakshiev, Lippert, microscopic solvent polarity (E_T^N) and ChammaViallet-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

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

$$\bar{v}_a + \bar{v}_f = -m^{(2)} \varphi(\varepsilon, n) + const \quad (2)$$

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

$$m^{(1)} = \frac{2(\mu_e - \mu_g)^2}{\mathrm{hca}^3} \quad (3)$$

$$\mathrm{m}^{(2)} = \frac{2(\mu_e - \mu_g)^2}{\mathrm{hca}^3} \quad (4)$$

$$f(\varepsilon, n) = \frac{2\,n^2 + 1}{n^2 + 2} * \left[\frac{\varepsilon - 1}{\varepsilon + 2} - \frac{n^2 - 1}{n^2 + 2}\right] \quad (5)$$

$$g(n) = \frac{3}{2}\left[\frac{n^4 - 1}{(n^2+2)^2}\right] \quad (6)$$

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

$$\mu_g = \frac{m^{(2)} - m^{(1)}}{2}\left[\frac{h\,c\,a^3}{2\,m^{(1)}}\right]^{1/2} \quad (7)$$

$$\mu_e = \frac{m^{(2)} + m^{(1)}}{2}\left[\frac{h\,c\,a^3}{2\,m^{(1)}}\right]^{1/2} \quad (8)$$

$$\mu_e = \left[\frac{m^{(2)} + m^{(1)}}{m^{(2)} - m^{(1)}}\right]\mu_g \qquad for\ \left(m^{(2)} > m^{(1)}\right) \quad (9)$$

Commonly, it is assumed that μ_e and μ_g are collinear. Angle ϕ can be estimated if they are not collinear using Equation. (10) [5].

$$cos\phi = \frac{1}{2\mu_g\mu_e}\left[\left(\mu_g{}^2 + \mu_e{}^2\right) - \frac{m^{(1)}}{m^{(2)}}\left(\mu_e{}^2 - \mu_g{}^2\right)\right] \quad (10)$$

Using the following equations estimate the energized state dipole moment of diketones derivatives

Lippert's equation [6]

$$\bar{v}_a - \bar{v}_f = m_1 F_1(\varepsilon, n) + const \quad (11)$$

Bakshiev's equation [7]

$$\bar{v}_a - \bar{v}_f = m_2 F_2(\varepsilon, n) + const \quad (12)$$

Kawski-Chamma-Viallet's equation [8]

$$^{1}/_{2}\,(\bar{\nu}_a + \bar{\nu}_f) = -m_3[F_3(\varepsilon, n)] + constant \quad (13)$$

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

$$F_3(\varepsilon, n) = \frac{2\,n^2 + 1}{2\,(n^2 + 2)} * \left[\frac{\varepsilon - 1}{\varepsilon + 2} - \frac{n^2 - 1}{n^2 + 2}\right] + \frac{3}{2}\left[\frac{n^4 - 1}{(n^2 + 2)^2}\right] (16)$$

Where $F_1(\varepsilon, n)$ *is*Lippert's , $F_2(\varepsilon, n)$ *is* Bakshiev'sand $F_3(\varepsilon, n)$ is Kawski-Chamma-Viallet's polarity function respectively, *n* is the refractive index and ε is the dielectric constant of the solvent. Also,

$$\mathrm{m}_1 = \frac{2(\mu_e - \mu_g)^2}{\mathrm{hca}^3} \quad (17)$$

$$\mathrm{m}_2 = \frac{2(\mu_e - \mu_g)^2}{\mathrm{hca}^3} \quad (18)$$

and

$$\mathrm{m}_3 = \frac{2(\mu_e^2 - \mu_g^2)}{\mathrm{hca}^3} \quad (19)$$

Using excitation and emission spectral bands 'm_3', 'm_4' and 'm_5'parameters are determined. The ground (μ_g) and energized state dipole moment (μ_e) determined from following equations.

$$\mu_g = \frac{m_3 - m_2}{2}\left[\frac{h\,c\,a^3}{2\,m_2}\right]^{1/2} \quad (20)$$

$$\mu_e = \frac{m_3 + m_2}{2}\left[\frac{h\,c\,a^3}{2\,m_2}\right]^{1/2} \quad (21)$$

Or

$$\mu_e = \left[\frac{m_3 + m_2}{m_3 - m_2}\right]\mu_g \quad for\ (m_3 > m_2) \quad (22)$$

Here m_3, m_4 and m_5 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 'm_3', 'm_4' and 'm_5'.

2.2 Microscopic solvent polarity(E_T^N

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

$$\bar{\nu}_a - \bar{\nu}_f = 11307.6\left[\left(\frac{\Delta\mu}{\Delta\mu_B}\right)^2\left(\frac{a_B}{a}\right)^3\right]E_T^N + constant \quad (23)$$

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_T^N plot and it is given by

$$\Delta\mu = (\mu_e - \mu_g) = \sqrt{\frac{mX\,81}{(^{6.2}/_{a})^3\,11307.6}} \quad (24)$$

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 jenaspecord 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).

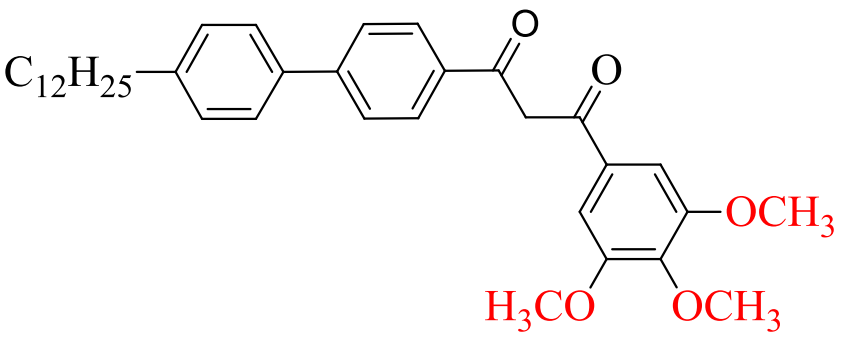

Figure 1. Molecular Structures of DK1.

4. Results and discussion:

4.1 Theoretical approach (Computational calculations of dipole moments)

The ground state (μ_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.

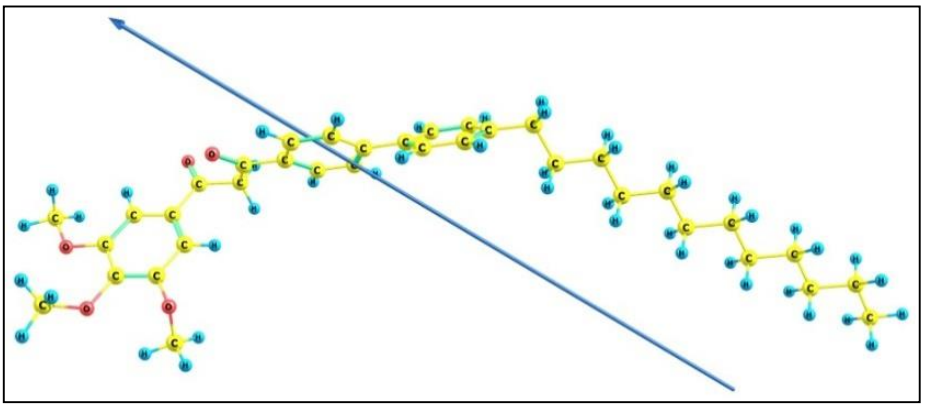

Figure 2. Optimized ground state molecular structure of DK1

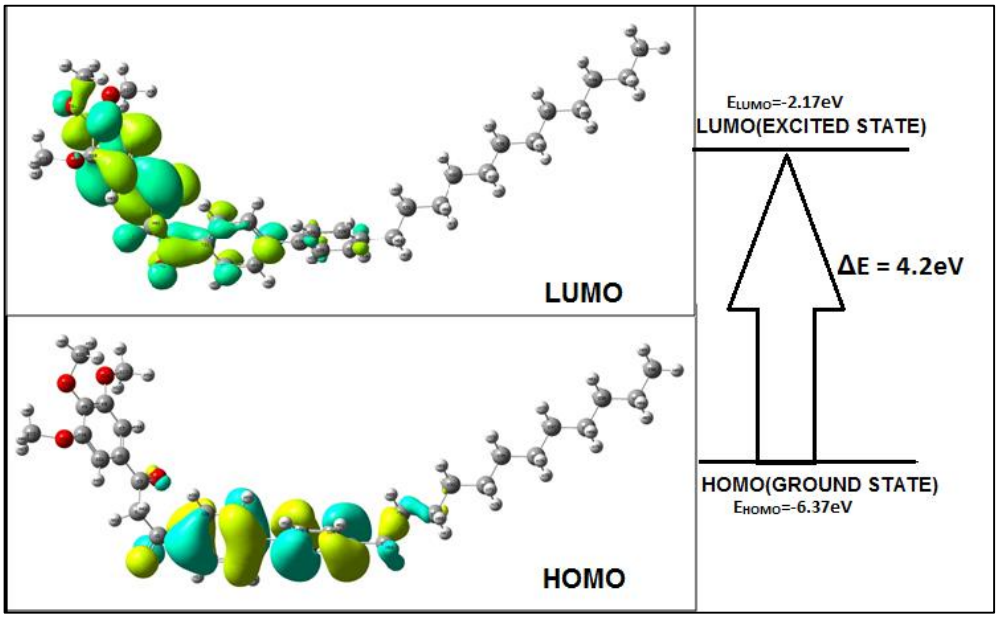

Figure 3.HOMO LUMO Plots of DK1

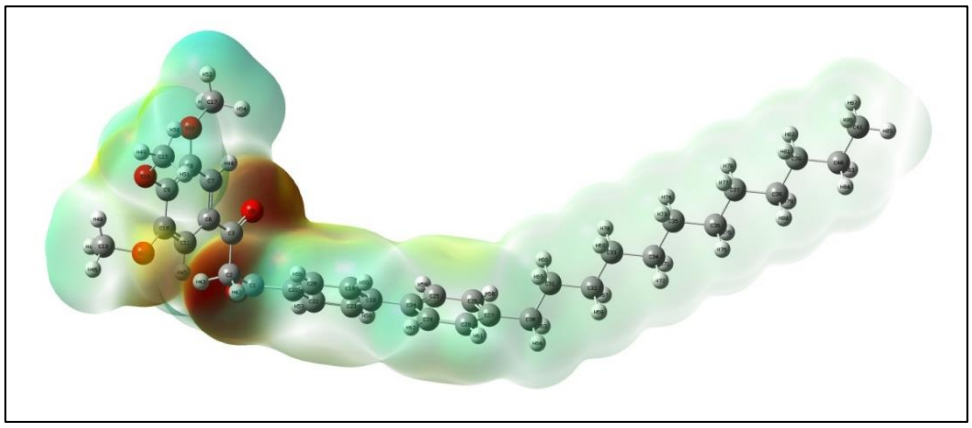

Figure 4. Electrostatic potential (ESP) of DK1

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 ε 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 π→π* singlet-singlet transition in the excited states. Normally π→π* 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 S_1 singlet state and S_0 ground state. The title molecule showed bathochromic shift, which suggests that title molecules are sensitive to the polarity of the various solvents used.

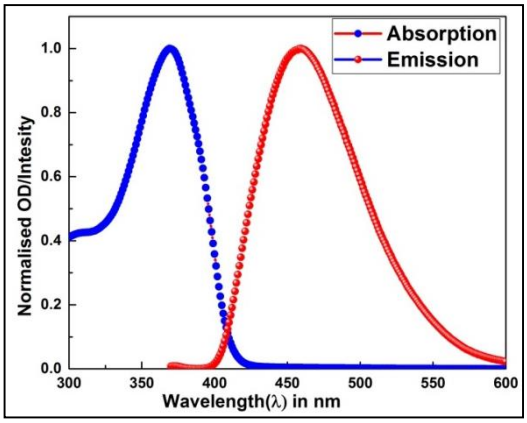

Figure 5. Typical normalized absorption and emission spectra of DK1 in different solvents at room temperature

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(ε,n) and $(\bar{\nu}_a + \bar{\nu}_f)$ versus ϕ(ε, 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 μ_g and excited state (μ_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 μ_g, μ_e and $\phi$are listed in Table 4**.**

The three independent equations (20) – (22)are used to determine μ_g and μ_e. 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 μ_g value is 1.021D for DK1, in various solvents determined. Discrepancy is observed when theoretical and experimental μ_g 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, μ_e values obtained from the experimental calculations (solvatochromic methods) are greater than the theoretical μ_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 (Δμ) calculated using $\mu_e$and $\mu_g$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.

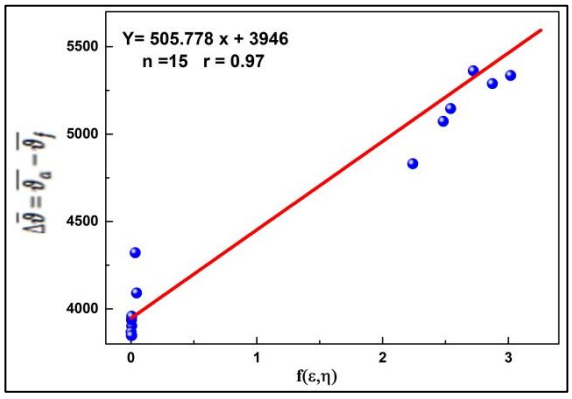

Figure 6(a) The Stoke's shift as a function of f(ε, n)

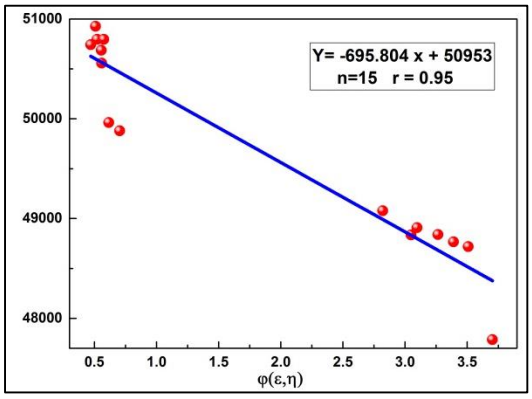

Figure 6(b) The Stoke's shift as a function of ϕ(ε,n)6.2

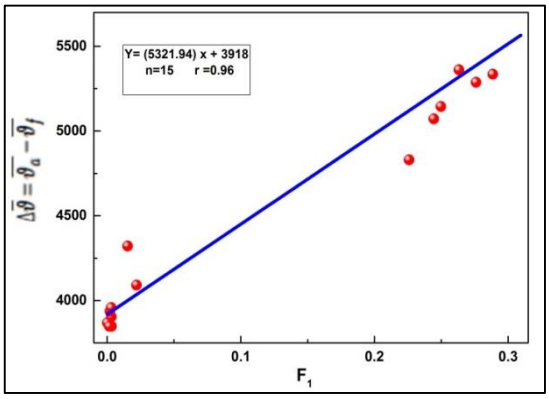

Figure 6(c) Stoke's shift as a function of $f_1(\varepsilon,n)$

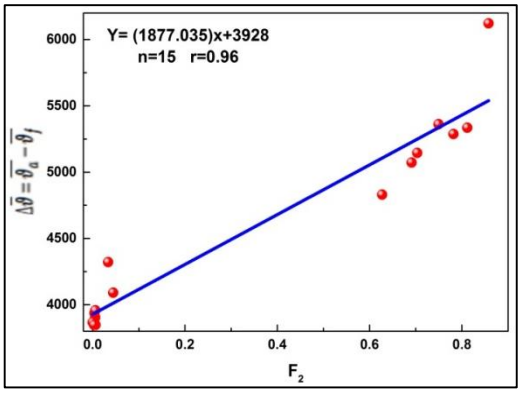

Figure 6(d) The Stoke's shift as a faction of $f_2(\varepsilon,n)$

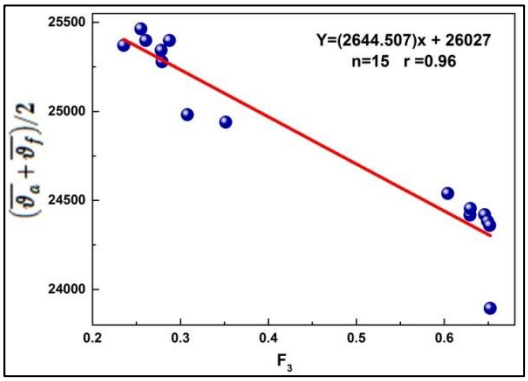

Figure 6(e) Stoke's shift as a function of $f_3(\varepsilon, n)$

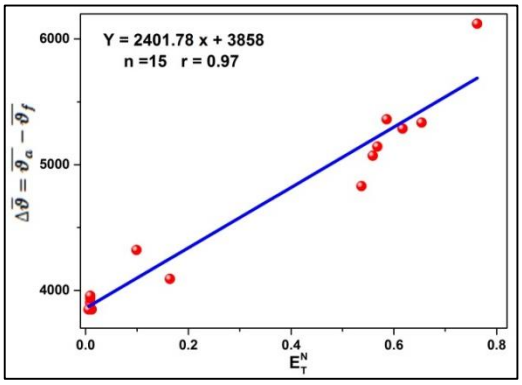

Figure 6(f) Plot of Stokes' shift against E_T^N

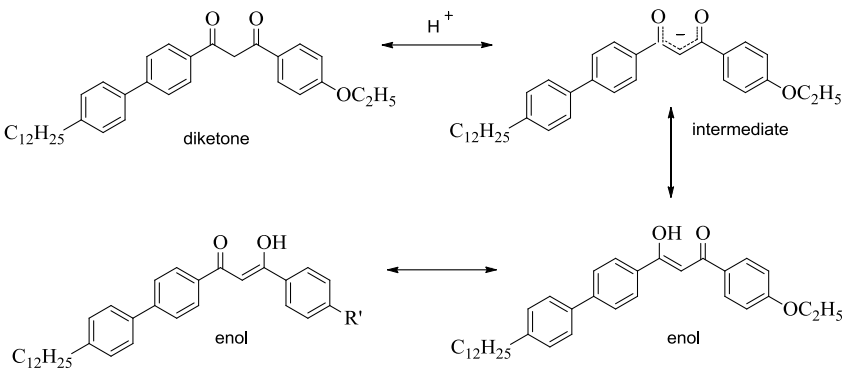

Figure 7 The possible Resonance structure of DK1

Table 1. The values of ε, η, E_T^N polarity parameters f_1, f_2, f_3, $f(\varepsilon,n)$ and $\phi(\varepsilon, \eta)$ of different solvents

Sl.No.	Solvents	ε	H	f (ε,η)	φ(ε,η)	F_1	F_2	F_3	E_T^N
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	1.409	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	λ_a(nm)	λ_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})
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
BilotKawaski	m_1	505.778	0.96	15
	m_2	695.804	0.95	15
Lippert	m_3	5321.941	0.96	15
Bakhshiev's	m_4	1877.036	0.96	15
Kawski-Chamma-Viallet's	m_5	2644.507	0.96	15
E_T^N correlation	m	2401.785	0.97	15

Table 4. Ground state $\boldsymbol{\mu_g}$ and excited state $\boldsymbol{\mu_e}$ dipole moments of **DK1**

Debye (D) = 3.33564×10^{-30}cm = 10^{-18}esu cm.
[1] The $\boldsymbol{\mu_g}$ calculated using Gaussian software
[2] The $\boldsymbol{\mu_g}$ calculated using BilotKawaski Eq. 7
[3] The $\boldsymbol{\mu_g}$ dipole moments calculated using Eq.20
[4] The $\boldsymbol{\mu_e}$ dipole moments calculated using BilotKawaski Eq. 8.
[5] The $\boldsymbol{\mu_e}$ dipole moments calculated using Eq. 21.
[6] The $\boldsymbol{\mu_e}$ dipole moments calculated from Lippert's equation.
[7] The $\boldsymbol{\mu_e}$ dipole moments calculated from Bakshiev equation.
[8] The $\boldsymbol{\mu_e}$ dipole moments calculated from Kawaski-Chamma-Vialletequation.

R 'a' (A^o)	μ_g[1] (D)	μ_g[2] (D)	μ_g[3] (D)	μ_e[4] (D)	μ_e[5] (D)	μ_e[6] (D)	μ_e[7] (D)	μ_e[8] (D)	μ_e[9] (D)	$\Delta\mu$[10] (D)	$\Delta\mu$[11] (D)	(μ_e/μ_g)[12]	ϕ[13]
5.113	3.396	0.487	1.021	3.078	6.015	9.428	6.014	6.012	4.127	4.994	3.106	5.891	0^0

[9] The excited state dipole moments calculated from E_T^N equation
[10] The change in dipole moments $\boldsymbol{\Delta\mu}$for μ_e and μ_g
[11] The change in dipole moments $\boldsymbol{\Delta\mu}$ calculated from Eq. 24
[12] The ratio of excited state and ground state dipole moment
[13]The angle between ground and excited statedipole moments calculated using Eq.10.

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 $\pi \rightarrow \pi^*$ 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 (E_T^N). 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 parameterE_T^N.

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