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# ORIGINAL ARTICLE

# Solvent effect and photo-physical properties of 2,3-diphenylcyclopropenone

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**Abstract** The photo-physical properties of the strained ring 2,3-diphenylcyclopropenone (DPCP) containing donor–acceptor moieties in polar and non-polar solvent are reported. The transition dipole moment ($\Delta\mu$), transition polarizability ($\Delta\alpha$), oscillator strength ($f_{ij}$) and molar absorptivity ($\varepsilon_{(\bar{v})}$) of its different transition bands were determined using solvatochromic shifts theory. The determined $\Delta\alpha$ is positive, signifying the strong activity of this compound and its excited states being more polar than ground states. Its $\Delta\mu$ follows the trend observed for the $f_{ij}$ and $\Delta\alpha$. This conforms to the expectations that the more allowed a transition, the higher the probability that the transition dipole moments will be greater than zero. The transition dipole moment shows gradation of values, being smallest for the weak and forbidden transitions but increases considerably for the fully allowed transitions. The solvents perturbation allows the assignment of the transitions in this compound to be both n→π* and π→π* transitions.

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## 1. Introduction

The study of molecular systems in the liquid phase is important for understanding a large number of chemical, physical and biological processes. Solvent–solute interactions can change the geometry, the electronic structure, and the dipole moment of a solute. UV/Vis absorption or/and emission (fluorescence) band positions of solvent-sensitive molecules will vary with the polarity of the medium and can thus be used judiciously in modelling intermolecular interaction. This phenomenon is called solvatochromism (Thomas et al., 2008; Praveen and Ojha, 2012).

The electrostatic properties of molecules in their electronically excited states are of considerable interest since they determine many observable properties that contain information on the nature of their excited states. Upon excitation of molecules, both dipole moment and polarizability of a molecule can change. Changes in dipole moment alter the electrostatic interaction with the solvent in the ground and excited state, with a shift in the absorption maximum. Also, the changes in polarizability cause changes in the dispersion interaction (van der Waals attraction) between the molecule and its surroundings (Denisio et al., 2004). Therefore, the changes in polarizability and dipole moment upon excitation which contain valuable

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information on the nature of molecules in their electronically excited state, as well as, the course of any photochemical transformation are of interest in the research of many $\pi$-conjugated molecules (Nadaf et al., 2002).

2,3-Diphenylcyclopropenone (2,3-DPCP), a planar molecule investigated in this work belongs to the class of intra-molecular electron-donor-acceptor (EDA) systems with the electron donor and acceptor groups being connected through the $\pi$-electron system and presents mirror symmetry. 2, 3-DPCP, owing to its strained ring, acts as an ambient electrophile with the potential for nucleophilic addition at the carbonyl group or conjugate addition. These factors allow participation in a wide variety of synthetically useful reactions, and the use of 2,3-DPCP in the preparation of a plethora of heterocyclic systems has been systematically studied over the past few decades (Aly et al., 2008; Andrei and Vladimir 2003, 2005; Hemming et al., 2006). Outside the field of synthetic chemistry, it finds utility in medicine as a single agent in the treatment of cutaneous metastatic melanoma and as combination chemotherapy with radiotherapy where it is often referred to as diphencyprone or DCP (Damian and Thompson, 2007; Trefzer and Sterry, 2005). The characteristic features of this EDA (electron-donor-acceptor) system are the low lying charge transfer states which relates to the transfer of electronic charge from the donor to the acceptor moiety as introduced and advanced by Milliken in his theory of intermolecular complexes (Pearson and Mulliken, 1960). Reported Ultra-violet absorption spectra of the parent compounds (cyclopropenone) have shown that, despite its highly strained ring, it is relatively stable compound (characteristics of aromatic system) but fails to give many reactions of ketone. But, 2,3-DPCP has been said to be highly sensitive to ultraviolet light degradation (Firooz et al., 2005).

The assumed configurations of many compounds and their corresponding derivatives are governed by ranges of factors, such as: the type, number and position of the substituent whose effects can be mesomeric (delocalization), inductive and or steric; solvent preferential stabilization of a particular configuration or set of configurations and charge transfer with structural change through the process of absorption of photon (Natasa et al., 2006; Praveen and Ojha, 2012). The varying degrees of perturbation of the potential energy surfaces of ground and excited state by these factors manifest itself by the observed differences in the electronic polarizability ($\alpha$) and dipole moment ($\mu$) of the excited state relative to ground state of molecules. Since these two spectral parameters of the excited molecules often aid the revealing of excited state configuration or structures of molecules and their reactivities (Kawski, 2002; Nadaf et al., 2002). In this work, these factors are studied qualitatively to determine the extent to which they have contributed in determining the assumed molecular configuration by means of solvent and substituent perturbation of band shapes, transition intensities and frequency of electronic spectra of this molecule. These molecular properties help in understanding the mode of action and determine its relative activity in order to help produce more effective drugs.

But, the life time of the excited states of molecules is short ($\sim 10^{-8}$ s), the generation of qualitative and quantitative acceptable description of their excited state properties directly is a much challenging task. Therefore, the photo-physical properties which qualitatively describe the nature of excited states of molecules (i.e. transition dipole moment and transition polarizability of molecules) are estimated indirectly using various approaches to the theoretical and experimental treatments of solvent and substituent effects. These include solvent frequency shift of electronic spectra method (solvatochromism), Electro-optical methods of absorption and the effect of external electric field on the fluorescence anisotropy (i.e. Labhart–Liptay molecular electrochromism) and theoretical treatment/computational technique. However, none of these methods have gained general acceptance and applicability, as most of them suffer various difficulties in the operation of their theories or experiment or their applicability to larger molecules (Helgerker et al., 2000; Schrimer and Trifimov, 2004). These setbacks pave ways to the development of cheaper and more acceptable models for determining these parameters by different researchers, which eventually led to the development of the equations which consistency and validity are being tested in this work.

Hence, in this investigation, a quantum–mechanical perturbation theory that accommodates intensity parameters such as solvent molecular polarizability ($\alpha$), the molar refraction ($R$), stark term ($\mu/r^3$), Einstein coefficient ($k$) and oscillator intensity ($f$), using the scope of Abe (AbdulRaheem et al., 2010) and adopting partly, the Louguett-Higgins and Salem (1961) mode of intermolecular forces, which is effective in revealing the factors governing intensity enhancement was employed. These were used in developing a linear regression model which was then applied in determining the transition polarizabilities ($\Delta\alpha$) and transition dipole moment ($\Delta\mu$) of 2,3-DPCP with the principle of absorption spectrophotometry. This research also correlates the properties of the solvated solutes of interest to those of the vapour and in part identifies the key terms that contribute to oscillator parameter in solution. The effect of solvents on the transition energies of the compounds is also investigated. The choice of this compound is based on the available literature data on the parameters to be used in the application of scope of modified Longuett–Higgin and Salem model.

## 2. Experimental section

### 2.1. Materials and method

The selected solvents used, $n$-heptane, methanol, and dichloromethane, were obtained from British drug House Limited (BDH). These were further purified by re-distillation twice under reduced pressure before use. The compound studied, 2,3-DPCP, was of a spectroscopic grade, a product of British drug house Limited (BDH), and was used without further purification. Diluted solutions of the compound being studied were prepared in the concentration range of $10^{-6}$–$10^{-5}$ M. Its spectral analysis was carried out using a computerized Shimadzu UV-1650 double beam spectrophotometer coupled with UV-probed 2.31 version (software) and operated in the wave length range of 190–400 nm. A pair of matched quartz cuvettes, each of 1 cm path length was in the sample compartment, one containing the pure reference solvent of choice and the other the sample solution in the solvent. The sample compartment was thermo-stated at 20 °C. The spectra were recorded with the instrumental band set at 0.2–1.0 nm and ran with the scan speed of 2 nm per second. At first, the spectra scan over the required wavelength was taken for the pair

**Table 1** Summary of the transition energies $\bar{v}_{max}$ (cm$^{-1}$), molar absorptivities, $\varepsilon_{max}$ (M$^{-1}$ cm$^{-1}$) and other transition properties for the observed absorption bands of the 2,3-diphenylcyclopropenone studied in polar and non-polar solvents.

| Transitions | $\bar{v}_{max}$ (cm$^{-1}$) | $\varepsilon_{max}$ (M$^{-1}$ cm$^{-1}$) | $f_{(s)}$ | $f_{(v)}$ | $X_1$ | $X_2$ (10$^{-1}$Ccm$^2$) | $K \times 10^{19}$ |
|---|---|---|---|---|---|---|---|
| *Methanol* | | | | | | | |
| $S_0 \rightarrow S_1$ | – | – | – | – | | | – |
| $S_0 \rightarrow S_2$ | 33,557 | 2,154 | 0.038 | 0.037 | | | 0.038 |
| $S_0 \rightarrow S_3$ | 45,455 | 1,305 | 0.023 | 0.022 | 1.51 | 4.1 | 0.023 |
| $S_0 \rightarrow S_4$ | 49,505 | 1,396 | 0.018 | 0.017 | | | 0.018 |
| *Dichloromethane* | | | | | | | |
| $S_0 \rightarrow S_1$ | 32,051 | 4,814 | 0.034 | 0.033 | | | 0.42 |
| $S_0 \rightarrow S_2$ | – | – | – | – | 0.92 | 7.38 | – |
| $S_0 \rightarrow S_3$ | 35,461 | 20,355 | 0.37 | 0.36 | | | 4.19 |
| $S_0 \rightarrow S_4$ | 43,234 | 10,895 | 0.13 | 0.12 | | | 1.16 |
| *Heptane* | | | | | | | |
| $S_0 \rightarrow S_1$ | – | – | – | – | | | – |
| $S_0 \rightarrow S_2$ | 33,784 | 6,615 | 0.16 | 0.58 | | | 1.91 |
| $S_0 \rightarrow S_3$ | 44,248 | 8,641 | 0.15 | 0.14 | 1.97 | 0 | 1.31 |
| $S_0 \rightarrow S_4$ | 50,000 | 8,462 | 0.013 | 0.013 | | | 0.1 |
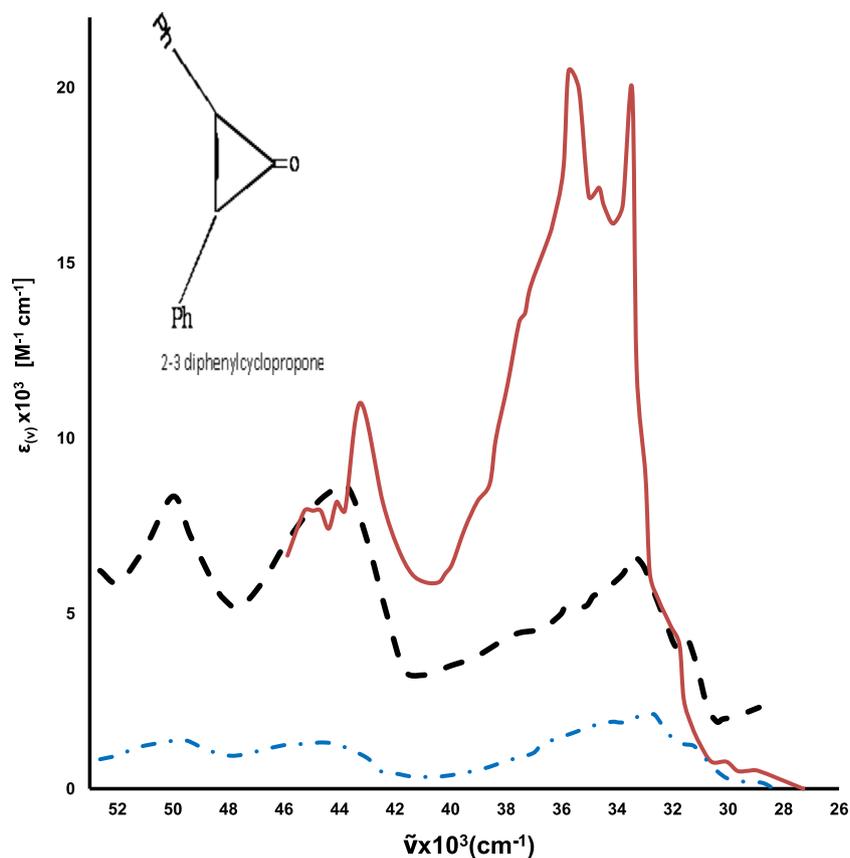


**Figure 1** Electronic absorption spectra of 2,3-diphenylcyclopropenone in methanol (-·-·-), dichloromethane (——) and heptane (——).

of cuvette containing pure solvent only to obtain the solvent baseline. Then, the content of the cuvette in the sample compartment was replaced with an appropriate solution of known concentration of a particular compound. The spectra scan process was repeated to obtain the absorption spectra of the compounds. This process was repeated for the compound in different solvents. Under this condition, it was observed that 0.02 absorbance, corresponding to a 20 cm graphical full scale recording yielded spectra of satisfactory sensitivity and resolution.

**Table 2** Summary of the calculated ground state electric dipole polarizabilities $\alpha$ (Å$^3$), transition polarizabilities $\Delta\alpha$ (Å$^3$) and transition dipole moments $\Delta\mu$ (D) for 2,3-diphenylcyclopropenone in polar and non-polar solvents by the use of Eqs. (2.5b) and (2.6).

| Compounds 2,3-diphenylcyclopropenone | $\alpha$ | $\Delta\alpha$ (Å$^3$) | $\alpha^*$ | $\Delta\mu$ (D) | $\frac{\Delta E_{solute}}{\Delta E_{solution}} = x(10^{-3})$ |
|---|---|---|---|---|---|
| *Methanol* | | | | | |
| $S_0 \rightarrow S_1$ | – | – | | – | – |
| $S_0 \rightarrow S_2$ | 0.10 | 0.18 | 0.28 | 0.13 | 2.1 |
| $S_0 \rightarrow S_3$ | 0.061 | 0.23 | 0.29 | 0.15 | 2.00 |
| $S_0 \rightarrow S_4$ | 0.047 | 0.39 | 0.44 | 0.2 | 1.56 |
| *Dichloromethane* | | | | | |
| $S_0 \rightarrow S_1$ | 0.008 | 0.20 | 0.21 | 0.18 | 2.39 |
| $S_0 \rightarrow S_2$ | – | – | – | – | – |
| $S_0 \rightarrow S_3$ | 0.089 | 0.013 | 0.1 | 0.61 | 1.39 |
| $S_0 \rightarrow S_4$ | 0.03 | 0.14 | 0.17 | 0.35 | 4.60 |
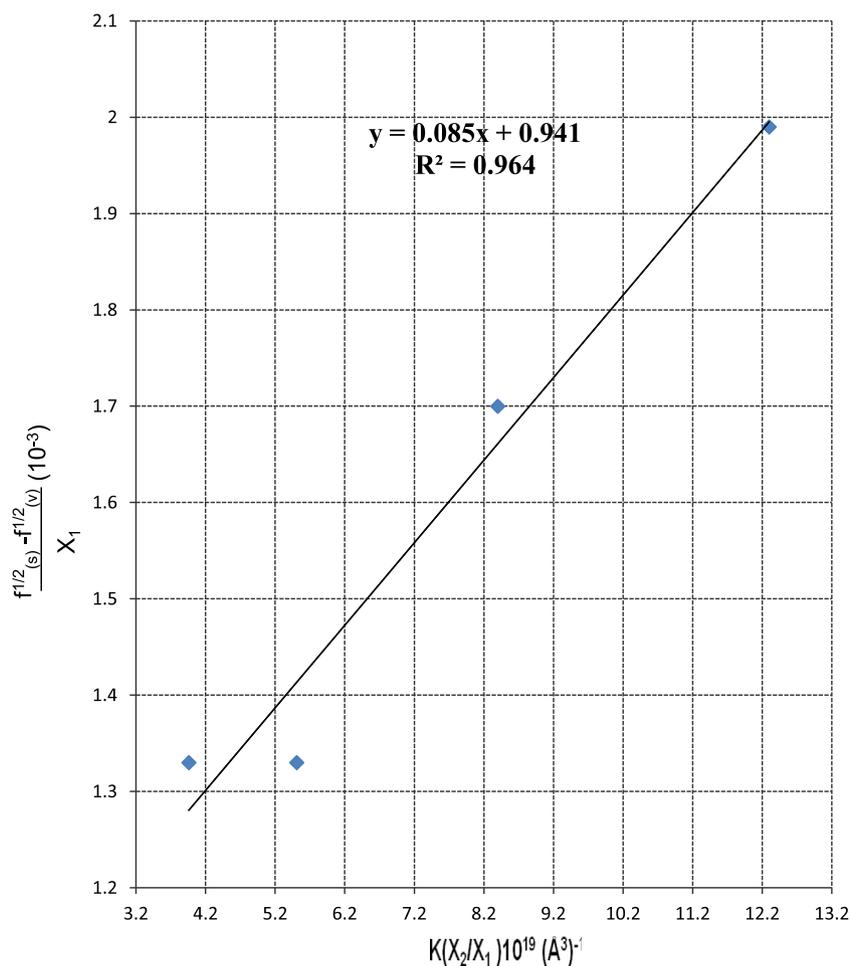


**Figure 2** Plots of data on intensity perturbation of the bands of 2,3-diphenylcyclopropenone in methanol.

## 2.2. Data analysis

### 2.2.1. Computation of oscillator strength

The experimental oscillator strength in solution $f_{(s)}$ and the molar extinction coefficient ($\varepsilon_{(v)}$) for each absorption band in the spectra of the molecules studied were calculated as a measure of the intensity of absorption of the molecules by means of Eq. (2.1). The integral $\int \varepsilon_{\bar{v}} \partial v$ were calculated using the assumptions of symmetrical bands in conformity with Gaussian distribution (Ahmed et al., 2011). The vapour phase oscillator strength $f_{(v)}$ values were also computed using the reaction field model of Eq. (2.2), the Shuyer's expression for the classical extension of Lorentz field effect (Oscar and Weigang, 1963).

$$f_{(s)} = \frac{2.303 m_e c^2 \varepsilon_0}{N_o e^2 n} \int_{vi}^{vj} \varepsilon_v \partial v_j = \frac{4.321 \times 10^{-9}}{n} \int_{vi}^{vj} \varepsilon_v \partial v_j \qquad (2.1)$$
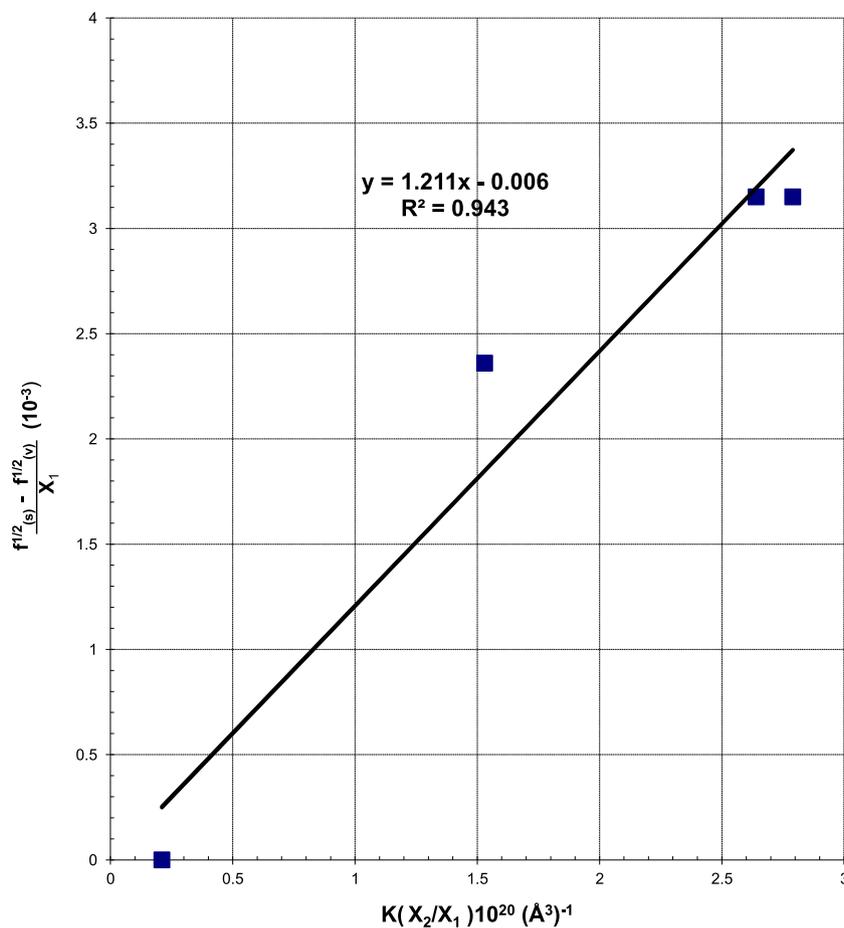
**Figure 3**    Plots of data on intensity perturbation of the bands of 2,3-diphenylcyclopropenone in dichloromethane.

$$\frac{f_{(s)}}{f_{(v)}} = \phi \tag{2.2}$$

where $\phi = \frac{9n^3}{(2n^2+1)^2}$, the correction factor on changing from solution phase to vapour phase and $n$, the refractive index of the solvent of choice.

### 2.2.2. Determination of transition polarizability and transition moments

Using Clausuis–Mossotti expression (Weast et al., 1985–1986) of Eqs. (2.3) and (2.4) below, the theoretical ground state electric polarizability ($\alpha_g$) for the solutes was calculated from the molar refraction ($R$) of bond atoms in a molecule of compound in different solvents in accordance with Schuyer, Blom and Van krevelen (Choingwain and Iweibo, 1991) while the theoretical ground state electric dipole moment ($\mu_g$) of the selected solvents used was computed where necessary from the measurement of stark effect in the microwave spectroscopy of gas.

$$R = \left(\frac{n^2-1}{n^2+2}\right)\frac{M}{d} \tag{2.3}$$

$$\alpha = \frac{3}{4\pi N_0}(R) \tag{2.4}$$

$N_0$ the Avogadro's number (mol$^{-1}$), $M$ being the molecular weight of the molecule under investigation and $d$, the density of solvent in which the molecule is dissolved.

### 2.2.3. Determination of transition dipole moment ($\Delta\mu$) and transition polarizability ($\Delta\alpha$)

$$f_{(s)}^{\frac{1}{2}} = f_{(v)}^{\frac{1}{2}} + \frac{3x}{1-x^2}f_{(v)}^{\frac{1}{2}}\left[\frac{\alpha_b}{r_{\alpha\beta}^3}\right] + \Delta\alpha K\left(\frac{\mu_b}{r_{\alpha\beta}^3}\right) \tag{2.5a}$$

$$\frac{f_{(s)}^{\frac{1}{2}} - f_{(v)}^{\frac{1}{2}}}{X_1} = \frac{3xf_{(v)}^{\frac{1}{2}}}{1-x^2} + \Delta\alpha K\frac{X_2}{X_1}. \tag{2.5b}$$

$$f_{(s)}^{\frac{1}{2}} = \Delta\mu + \frac{3}{2}\Delta\alpha + \left(\frac{\mu_b}{r_{\alpha\beta}^3}\right) + \left(\frac{3x}{1-x^2}f_{(v)}^{\frac{1}{2}}k^{-1}\right)\frac{\alpha_b}{r_{\alpha\beta}^3} \tag{2.6}$$

The expressions in 2.5a, its rearranged form of 2.5b and Eq. (2.6), developed from the intensity perturbation approximation relate the square root of oscillator strength in solution $f_{(s)}^{\frac{1}{2}}$ to that of the vapour $f_{(v)}^{\frac{1}{2}}$ to the stark terms ($\mu_b/r_{\alpha\beta^3}$), the integral Einstein co-efficient ($K$), electric polarizability of the solvent ($\alpha_b$), ($\Delta\mu$), ($\Delta\alpha$) as well as, the ratio of the change in the transition energies of the solute to that of the solvent ($\Delta E_{\text{solute}}/\Delta E_{\text{solvent}}$) where $\frac{\alpha_b}{r_{\alpha\beta}^3} = X_1$, $\mu_b/r_{\alpha\beta^3} = X_2$ and $r_{\alpha\beta}$, the inter-nuclear distance between the solute and the solvent molecule. These show that a number of data on the solvent and the solute were required to enable one to use these equations reliably in determining the change in the transition dipole moment and polarizability of molecules, from where the excited state dipole

moment ($\mu^*$), the excited state polarizability ($\alpha^*$) and ratio of the change in transition energies of the solute to that of the solvent ($x$) may be computed. Table 1 summarizes the data used in this way.

## 3. Results and discussion

The representative electronic absorption spectra of 2,3-DPCP depicting the effects of polar and non-polar solvents on its spectra properties are as shown in Fig. 1. The summarized data of the average transition frequencies (energies) and the corresponding molar absorptivities of this compound in the protic polar, aprotic polar and non-polar solvents (i.e. methanol, dichloromethane and heptane respectively) are as shown in Tables 1 and 2, while the regression plots from where the transition dipole moment and transition polarizability for the compound are obtained are as shown in Figs. 2 and 3.

### 3.1. Absorption spectra, transition energies, maximum molar absorptivity [$\varepsilon_{(\mu_{max})}$] solution and vapour phase oscillator strength, transition dipole moments ($\Delta\mu$) and transition polarizabilities ($\Delta\alpha$)

The absorption spectra of this compound in the representative solvents showed three prominent bands. Band I ($S_o \rightarrow S_1$), a low intensity shoulder around 33,557 cm$^{-1}$ in dichloromethane is absent in the spectra of the compound in the methanol and heptane. This band is both quantum–mechanically and overlap forbidden as reflected by its low intensity. Red shifts are observed for spectra of the compound with increasing solvent polarity for Band II while for Bands III and IV, blue shifts were observed. The slight shifts to longer wavelength (red shift) with increasing solvent polarity for Band II show that the first singlet state of the compound is a $\pi$ -$\pi^*$ transition. Band II ($S_o \rightarrow S_2$) and Band 1($S_o \rightarrow S_1$) are fused together and are not decomposable in dichloromethane due to intensity borrowing phenomena and the special nature of the chloro-substituted solvent which are slightly transparent to the compound in the spectra region of interest. Dichloromethane acts as filters and shields the molecule from UV-light thereby reducing the level of its interaction with this compound. This leads to mixing of the excited states of this compound which is manifested by overlap of bands.

Band III ($S_o \rightarrow S_3$) is more sensitive to solvent perturbation than Band II ($S_o \rightarrow S_2$). Its increase in intensity indicates that the transition is allowed by symmetry. Bands III ($S_o \rightarrow S_3$) and IV ($S_o \rightarrow S_4$) are blue-shifted in polar solvent relative to non-polar solvent, showing that the ground state of this compound is more stable than its excited states in polar solvent. This indicates an n–$\pi^*$ transition in the spectra of 2,3-DPCP as a result of protonation of carbonyl oxygen by methanol (probably, hydrogen bonding). Little diffused vibrational structures which manifest itself in the spectra of the 2, 3-DPCP in heptane, as well as the band III of the compound in dichloromethane show that the compound is a rigid molecule. The level of its interaction, which can be ascribed to dipole–Van-der Waal forces interaction with these solvents is low. On the other hand, the spectrum of 2,3-DPCP in methanol do not show any diffused vibrational fine structure, showing that there is a specific interaction (dipole–dipole) of the compound with methanol. The intensities of absorption, as indicated by the calculated molar

absorptivities values (Tables 1 and 2) therefore allow Band I to be assigned $^1A \rightarrow ^1L_a$, Band II as $^1A \rightarrow ^1L_b$, Band 111 as $^1A \rightarrow ^1B_b$ while Band IV is assigned $^1A \rightarrow ^1B_a$ transitions.

### 3.2. Electronic transition dipole moments and transition polarizabilities

As observed in Tables 1 and 2, the $\Delta\alpha$, a measure of sensitivity of different transitions to applied electric field for the compound in chloro substituted solvent follows the order of oscillator strengths ($f_{ij}$) of each transition. This trend conforms to the expectations as submitted by Iweibo et al. (1990) and supported by the approximate theory which relates the polarizability $\alpha$ of any state $i$, $j$ to the transition frequency $\omega_{ij}$ between the state $i$ and $j$, and the $f_{ij}$ by:

$$\alpha_{ij} = \frac{e^2}{m_e} \sum_j \frac{f_{ij}}{\omega_{ij}} \qquad (3.1)$$

where $e$ and $m_e$ denote the electronic charge and mass respectively, and $\omega_{ij} = 2\pi\upsilon_{ij}$ denotes the circular frequency. These trends are reflective of the oscillator strength values for these transitions, and also confirm the positive correlation between $\Delta\alpha$ and the integral Einstein coefficient $k$ (a measure of the probability of electronic transition per unit time, per unit radiation density) as seen in Eqs. (3.2) and (3.3).

$$k = \frac{D^2}{6\varepsilon_0 \hbar^2} \qquad (3.2)$$

$$f = \frac{4M_e \pi v}{3e^2 \hbar} D^2 \qquad (3.3)$$

where $D = \int \psi_i \mu \psi_j$ is the electric dipole moment operator which determines the strength of transitions, and $\hbar = h/2\pi$. $\varepsilon_0$, $v$, and $h$ are the vacuum permeability, frequency in wave number and Planck's constant respectively.

The deviation from the order of increasing $\Delta\alpha$ with $f_{ij}$ for the different transitions of 2,3-DPCP in methanol is due to the mixing of its allowed states with its forbidden states; the latter thus acquiring the characters of the allowed states (Itamer et al., 2005). The extent of mixing of the states by the substituents reflects the extent of the deviations. Also, in this compound, there is intra-molecular donor–acceptor charge transfer in which there is shift of electron from the phenyl ring through the cyclopropenyl ring to the oxygen atom of the carbonyl carbon (CO) or the second phenyl ring of the compound.

The determined $\Delta\alpha$ is positive and very small ($<1$) for the compound. It small values indicate a little change in the potential energy surface of the ground and the excited state, which is in agreement with the conclusion that the equilibrium nuclear position (from the consideration of shape of Franck–Condon envelop) of the excited states is only a little shifted relative to the ground states. This shows that there is only a slight reorientation of the solvent molecule to produce a reaction field which in turn results in a shift between the energies of ground and the excited states. These results are consistent with the reaction field formulation of Liptay (Thomas et al., 2008). Moreover, the observed positive values for $\Delta\alpha$ show the strong activity of the compound and its excited states being more polar than its corresponding ground states.

The transition moment (measure of the amount of charge transfer associated with transitions) of the compounds in this study follows similar trend observed for the $f_{ij}$ and $\Delta\alpha$. This order conforms to the expectation as it agrees perfectly with the expression that relates the intensity $I$, of a transition to the square of integral of transition moment, $M$ i.e.

$$I\alpha|M_{ij}|^2 = <\mu_i|e_ir_i|\mu_j>^2 \tag{3.4}$$

This implies that the more allowed a transition, the higher the probability that $\Delta\mu$ will be greater than zero. Hence, the transition moment integral shows a gradation of values, being smallest for the weak and forbidden transitions but increases considerably for the fully allowed transitions. The small values of $\Delta\mu$ observed for all the transitions in this compound, as seen in Table 2 also point to the conclusion that the equilibrium nuclear position of the excited state is a little shifted relative to the ground state. This result confirms the selection rule which states that for electronic transition to occur, transition moment integral must not be zero.

## 4. Conclusion

This work has successfully used solvatochromic shift theory that accommodates intensity parameters to determine the $\Delta\mu$ and $\Delta\alpha$ simultaneously for the compound studied in polar solvent. This provides insight into the nature of electrostatic interactions between these solvents and 2,3-DPCP and its activity. The values of oscillator strength in vapour ($f_v$) and solution phase ($f_s$) have also verified the facts on intensity borrowing phenomena from solvents. The method gave results that showed minimal dispersion in the values of $\Delta\mu$ and $\Delta\alpha$. It can therefore serve as a supplementary method for the determination of photo-physical parameters in polar solvents. Moreover, the observed positive values of $\Delta\mu$ and $\Delta\alpha$ attest to its high relative activity and its usefulness as starting material for many novel drug preparations.

In addition, the $\Delta\mu$ and $\Delta\alpha$ determined for this compound in this research are expected to form a database for comparison with the results of their future determinations by electro-optical or molecular orbital calculation methods. The molecule exhibits both n→π* and π→π* transitions in the UV range.

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