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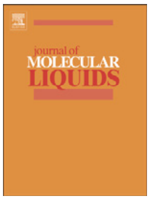

Estimation of ground and excited state dipole moments of synthesized coumarin derivative [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl-phosphorane

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ABSTRACT

Electronic absorption and fluorescence spectra of coumarin derivative [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl phosphorane have been recorded at room temperature in wide range of solvents of different polarities. The absorption maximum remains almost unchanged with the increase in solvent polarity, whereas, a red shift in fluorescence emission maximum was observed. Synthesized compound [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl phosphorane was characterized by ^{1}H and ^{13}C NMR, and FT-IR spectral studies. The ground and excited state dipole moments of molecule were obtained from Bakhshiev's and Bilot–Kawski's equations by means of the solvatochromic shift method. Very high value of dipole moment is observed for excited state as compared to ground state value and this is attributed to more polar excited state of the molecule. Numerical calculations are performed using B3LYP/6-31G+(d) and B3LYP/6-31G(d) level of theory for ground state in Gaussian 03. Studies in different solvents are also done using the CPCM method and UA0 radii with the same level of theory. A critical analysis between the values of dipole moment in gas phase and various solvents is also carried out for ground state.

1. Introduction

Coumarins have been extensively studied due to their practical applications [1–5], which include uses as biological and chemical sensors, fluorescent probes and laser dyes [6–9]. Coumarins possess anti-inflammatory, antiallergic, hepatoprotective, spasmolitic, antiviral, anticarcinogenic and anticoagulant activities [10]. They also constitute an important group of organic compounds that are used as additives to cosmetics, as optical brightening agents [11–13]. Due to their inherent physicochemical and photophysical characteristics, such as reasonable relative ease of synthesis, coumarin derivatives have been extensively investigated for electronic and photonic applications such as charge-transfer complexes, laser dyes, fluorescence whiteners, solar energy collectors, and non-linear optical materials [14–17].

Studies on the photophysical properties of the coumarin and its derivative have been the subject of intense research in photochemistry for quite a long time [18]. In spite of significant amount of literature reports, many of the photophysical characteristics are still not explored [19–26].

Excitation of a molecule by photon causes a redistribution of charges leading to conformational changes in the excited state. This can result in increase or decrease of dipole moment of the excited state as compared to ground state. The dipole moment of an electronically excited state of a molecule is an important property that provides information on the electronic and geometrical structure of the molecule in short-lived state. Knowledge of the excited-state dipole moment of electronically excited molecules is quite useful in designing nonlinear optical materials [27], elucidating the nature of the excited states and in determining the course of photochemical transformation. For a chromophore, the tunability range of the emission energy as a function of polarity of the medium is also determined by excited state dipole moment [28].

Solvent affects the equilibria, absorptions, emissions and the mechanisms of reactions for many compounds. Understanding solute–solvent interactions and measuring them quantitatively are an active area of research. The emission and absorption spectroscopy is the widely used method for investigating the solvatochromism with the help of various solvent parameters.

A number of techniques e.g. electronic polarization of fluorescence, electric-dichroism, microwave conductivity and stark splitting [29–32] are available for determination of excited-state dipole moment, but their use is limited because they are considered equipment sensitive and studies have been related to very simple molecules. As the solvatochromic method does not use any external field [33,34], it is experimentally much simpler and widely accepted. The solvatochromic method is based on the shift of absorption and fluorescence maxima in different solvents of varying polarity. The solvent dependence of

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absorption and fluorescence maxima is used to determine the excited-state dipole moments of different molecules. Several workers have made extensive experimental and theoretical studies on ground (μ_g) and excited state (μ_e) dipole moments using different techniques in variety of organic fluorescent compounds like coumarins [35,36], indoles [37,38], purines [39,40], exalite dyes [41,42], quinazolines [43], quinine sulfate [44,45], quinidine [46], 6-methoxyquinoline [47] etc.

In this paper, we have estimated the ground and excited state dipole moments of synthesized coumarin derivative [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl phosphorane by the solvatochromic shift method using Bakhshiev [48] and Bilot–Kawski [49,50] correlations. Although this compound is described in the literature, Saito et al. [51] have carried out some thermal studies on this compound and they have used very different synthesis methods than ours. To the best of our knowledge there are no reports available in literature on the determination of ground and excited state dipole moments of this compound.

2. Experimental

2.1. Materials

4-hydroxycoumarin, $POCl_3$, NaN_3 and triphenylphosphine were procured from Spectrochem and SRL, India and were used without further purification. All the solvents used were of HPLC grade or AR (purchased from Alfa Aesar).

2.2. Synthesis of coumarin derivative

*2.2.1. 4-chlorochromen-2-one (**2**)*

A solution of 4-hydroxycoumarin (**1**) (3.0 g, 1 eq.) in $POCl_3$ (6 mL) was refluxed at 90 °C for 2 h. The completion of the reaction was monitored via TLC. The reaction mixture was allowed to attain room temperature and was added drop-wise to an ice bath with continuous stirring. The precipitated yellow solid was filtered and washed with cold water (3 × 20 mL). The dried crude solid was washed with hot hexane (3 × 30 mL) and filtered from the remaining solid. Evaporation of the combined hexane filtrates under reduced pressure yielded 4-chlorocoumarin (**2**) as a white solid.

Yield: 2.2 g, 65%; m.p. 86–88 °C ([52] 87–89 °C); IR (KBr) cm^{-1} 1755, 1720, 1601, 1450, 1271, 1176.

*2.2.2. 4-azidochromen-2-one (**3**)*

To a solution of 4-chlorocoumarin (**2**) (2.0 g, 1 eq.) in anhydrous DMF (10 mL), NaN_3 (2 eq.) was added at room temperature. The stirring was continued for about 10 h, until the consumption of the starting material as monitored by TLC. After the completion of the reaction, the reaction mixture was added drop-wise to crushed ice and the resultant precipitate was filtrated, washed with cold water (3 × 15 mL) and dried to pure 4-azidocoumarin (**3**) as a light yellow solid.

Yield: 2.03 g, 98%; m.p. 161–162 °C ([53] 160 °C); IR (KBr) cm^{-1} 2175 (N_3) and 1736 (C═O).

*2.2.3. [N-(2-oxo-2H-chromen-4-yl)imino]triphenyl-phosphorane (**4**)*

To a solution of 4-azidocoumarin (**3**) (2.0, 1 eq.) in THF (20 mL) at room temperature, a solution of triphenylphosphine (2 eq.) in THF (10 mL) was added drop-wise. The reaction mixture was stirred for 4 h at room temperature and the progress of the reaction was monitored via TLC. After the completion of the reaction, solvent was evaporated under reduced pressure and re-crystallization of the residue using diethyl ether gave [*N*-(2-oxo-2H-chromen-4-yl)imino] triphenyl-phosphorane (**4**) as a colorless solid.

Yield: 4.4 g, 99%; m.p. 238–239 °C ([51] 239.2–240.5 °C).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.81–7.73 (m, 6H), 7.61 (td, *J* = 7.2, 1.4 Hz, 3H), 7.55–7.44 (m, 7H), 7.31–7.23 (m, 2H), 5.09 (s, 1H).

IR (KBr) cm^{-1}: 1697 (C═O), 1535, 1384.

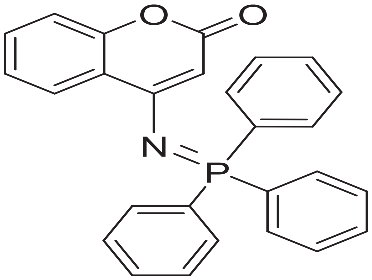


Fig. 1. Molecular structure of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane.

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 161.7, 154.0, 154.0, 132.8, 132.8, 132.7, 132.6, 130.9, 129.2, 129.1, 128.4, 127.4, 125.5, 122.9, 122.5, 122.2, 116.6, 94.6, 94.4.

2.3. Measurements

The melting point was found out using the capillary method in a melting point apparatus. The ^{1}H NMR was recorded on a Bruker AMX 400 MHz spectrometer and ^{13}C NMR spectra were recorded on a Bruker AMX 100 MHz solid state NMR spectrometer. IR spectra (KBr) were recorded on ABB Bomen MB 3000 FTIR. TLC analysis was carried out on pre-coated silica gel glass plates using the solvent system ethyl acetate:hexane (40:60).

Absorption spectra were taken using dual beam Thermo Evolution 201 UV/Vis/NIR spectrophotometer and fluorescence spectra were recorded using a Shimadzu RF-5301PC spectrofluorometer. The data were analyzed using a related software. The spectral shifts obtained with different sets of samples were identical in most of the cases and values were within ±1.0 nm. Data were analyzed and were fitted to a straight line using Origin 6.1 software. Molecular radius a_0 (Å) of the spherical cavity is obtained for optimized geometry calculated at the B3LYP/6-31G(d) level of theory (in liquid phase) using Gaussian 03.

The concentration of compound in all the solutions prepared in different solvents was 10^{-4} M and the molecular structure of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane is shown in Fig. 1.

3. Method

Most theories of solvent effect on the location of absorption and fluorescence spectra, in spite of different assumptions, lead to similar expressions for the Stokes shift. We have used the following two formulae to determine the ground and excited state dipole moments by the solvatochromic method. These equations have been obtained by employing the simplest quantum-mechanical second order perturbation

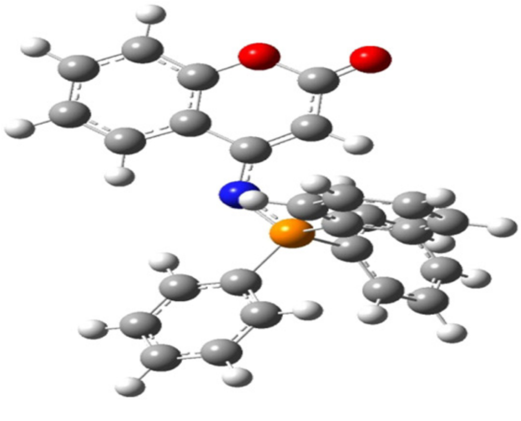


Fig. 2. Optimized molecular geometry of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane using B3LYP/6-31G(d) level of theory in gas phase.

Table 1
Ground state dipole moment evaluated at B3LYP/6-31+G(d) level of theory.

Solvent	Dielectric constant	Dipole moment (μ_g)[a]
Dimethyl sulfoxide	46.4	12.51
Acetonitrile	35.9	12.48
Dichloromethane	8.9	12.13
Tetrahydrofuran	7.6	12.04
Diethyl ether	4.3	11.65
Toluene	2.3	11.02
Carbon tetrachloride	2.2	10.93
Gas	–	9.20

[a] μ_g is the ground state dipole moment evaluated at B3LYP/6-31+G(d) level of theory for gas phase and also the same level of theory using the CPCM model along with UA0 radii for solvents.

theory and taking into account the Onsager reaction field for a polarisable dipole.

Bakhshiev's formula [48]

$$\overline{\nu_a}-\overline{\nu_f} = S_1 F_1(\varepsilon,\eta) + \text{const.} \tag{1}$$

here, $\overline{\nu_a}$ and $\overline{\nu_f}$ are the wavenumbers of the absorption and emission maxima respectively.

F_1 the bulk solvent polarity function and S_1 the slope are defined as follows:

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

and

$$S_1 = \frac{2\left(\mu_e-\mu_g\right)^2}{hca_0{}^3} \tag{3}$$

here, h denotes the Planck's constant, c is the velocity of light in vacuum, μ_g is the dipole moment in the excited singlet state, a_0 is the Onsager cavity radius, ε is the solvent dielectric constant and η is the solvent refractive index.

Bilot–Kawski formula [49,50]

$$\frac{\overline{\nu_a}+\overline{\nu_f}}{2} = -S_2 F_2(\varepsilon,\eta) + \text{const.} \tag{4}$$

here, the meaning of symbols is the same as given above except for F_2 and S_2 which are defined as follows

$$F_2(\varepsilon,\eta) = \frac{2\eta^2+1}{2(\eta^2+2)}\left[\frac{\varepsilon-1}{\varepsilon+2}-\frac{\eta^2-1}{\eta^2+2}\right]+\frac{3}{2}\left[\frac{\eta^4-1}{(\eta^2+2)^2}\right] \tag{5}$$

and

$$S_2 = \frac{2\left(\mu_e{}^2-\mu_g{}^2\right)}{hca_0{}^3}. \tag{6}$$

The parameters S_1 and S_2 are the slopes which can be calculated from Eqs. (1) and (4) respectively. Assuming the ground and excited states are parallel, the following expressions are obtained using Eqs. (3) and (6) [49]

$$\mu_g = \frac{S_2-S_1}{2}\left[\frac{hca_0{}^3}{2S_1}\right]^{1/2} \tag{7}$$

$$\mu_e = \frac{S_1+S_2}{2}\left[\frac{hca_0{}^3}{2S_1}\right]^{1/2} \tag{8}$$

and

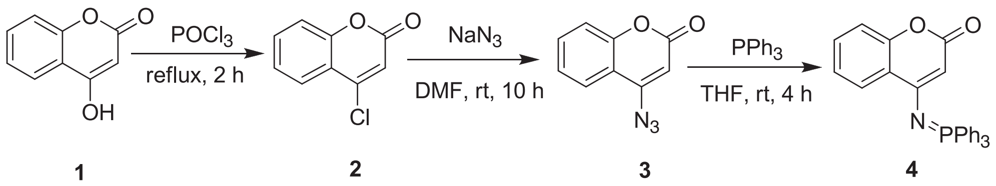
$$\mu_e = \frac{|S_1+S_2|}{|S_2-S_1|}\mu_g. \tag{9}$$

3.1. Computational calculations

Density functional theory (DFT) [54,55] cuts down the steep rise in computational cost efficiently compared to ab initio wave function techniques and it is also proved to be accurate for calculating several important physical properties of molecules. Systematic and critical comparisons of DFT theories with experiment and also with HF and Møller–Plesset (MP2) treatments are carried out by many researchers over years [56]. In this paper, geometry optimizations were carried out at B3LYP/6-31G(d) [57–59] level of theory for ground state of coumarin derivative [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl phosphorane. Harmonic frequencies are simultaneously checked to ensure the minimum energy structure. Subsequently, single point calculations are done for different solvents and also for gas phase with higher level of theory, i. e., B3LYP/6-31G+(d) to obtain the ground state dipole moment μ_g. The basis set 6-31G+(D) (which has polarization functions on nonhydrogen atoms and diffuse functions are added to heavy atoms) can efficiently determine the properties of moderately large organic molecules. To take care of the solute–solvent interaction, the solute is placed in a cavity (via a set of overlapping spheres) within the solvent reaction field using a conductor-like polarizable continuum model (CPCM) [60,61]. To build the cavity, UA0 radii are used where the United Atom Topological Model is applied on atomic radii of the UFF force field for heavy atoms. Hydrogens are enclosed in the sphere of the heavy atom to which they are bonded. The SCF density is used for all ground state calculations. All calculations were carried out using Gaussian 03 suite of program [62]. The optimized structure is given in Fig. 2.

4. Results and discussion

Dipole moment bears a close relation with the degree of charge distribution and thus it reflects the net molecular polarity. Usually, it is exploited to determine a variety of physical and chemical properties. The dipole moment of coumarin derivative [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl phosphorane is computed at the B3LYP/6-31+G(d) level of theory in different environments (various solvents with varying polarities and gas phase) and are shown in Table 1. A distinct variation in dipole moment is observed while going



Scheme 1. Synthesization methodology of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane.

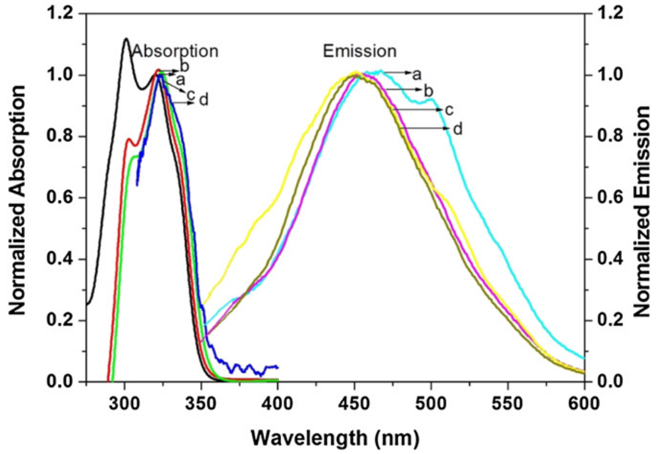


Fig. 3. Normalized absorption spectrum and fluorescence spectra of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane in (a) acetonitrile, (b) ethylacetate, and (c) toluene, (d) CCL4.

Table 2
Different solvent parameters and spectral data of [*N*-(2-oxo-2*H*-chromen-4-yl)imino] triphenyl-phosphorane in different solvents.

Solvent	ε	η	F_1	F_2	$\overline{\nu_a}-\overline{\nu_f}$ (cm^{-1})	$\frac{\overline{\nu_a}+\overline{\nu_f}}{2}$ (cm^{-1})
Dimethyl sulfoxide	46.4	1.4770	0.8410	0.7440	9015.44	26461.6
Acetonitrile	35.9	1.3442	0.8660	0.6560	9360.99	26452.8
Dichloromethane	8.9	1.4241	0.5900	0.5820	8803.22	26683.3
Tetrahydrofuran	7.6	1.4070	0.5450	0.5490	9292.04	26352.1
Ethylacetate	6.1	1.3720	0.4890	0.4970	9034.52	26500.1
Diethyl ether	4.3	1.3526	0.3730	0.4260	9019.14	26623.7
O-xylene	2.4	1.5054	0.0270	0.3540	8816.31	26551.7
Toluene	2.3	1.4969	0.0330	0.3510	8628.94	26502.2
Carbon tetrachloride	2.2	1.4610	0.0144	0.3190	8716.50	26639.9

from gaseous to solvent phases. Higher values of dipole moments are obtained in the solvent phases compared to the gas phase. This is due to the intermolecular interactions between the solvent molecules and the studied compound (i. e., the coumarin derivative). The value of the dipole moment increases with the polarity of the solvent, i. e., the higher the dielectric constant, the higher is the observed dipole moment (Table 1).

[*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane (**4**) used in the present studies was synthesized in a methodology shown in Scheme 1. Commercially available 4-hydroxychromen-2-one (**1**) on reaction with $POCl_3$ under refluxing conditions gave 4-chlorochromen-2-one (**2**), which on azidation using sodium azide in DMF gave 4-azidochromen-2-one (**3**). **3** on reaction with triphenylphosphine in THF at room temperature gave (**4**) in pure form as a colorless solid.

The absorption and fluorescence spectra of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane were recorded in nonpolar and aprotic polar solvents at ambient temperature and are shown in Fig. 3. No significant change in absorption spectrum with solvent polarity for this coumarin compound is observed while markedly emission maximum shifts towards lower frequencies with the increase in polarity of the solvent.

The emission spectrum has only a structure-less broad band with maximum around 448 nm in carbon tetrachloride and 460 nm in acetonitrile on excitation at 320 nm. The variation of wavenumber of absorption and emission maxima with the solvent polarity function, F_1 (ε, η), is shown in Fig. 4. The absorption maximum for different solvents studied remains constant with the polarity function, whereas, the emission maximum shifts towards lower frequencies with the increase in polarity of the solvent.

The red shift in fluorescence spectrum is more in the case of acetonitrile aprotic solvent as compared to nonpolar solvents. This trend in the fluorescence spectra is a bathochromic shift with increase in polarity and is an indication of π, π* transition. The shift of the fluorescence wavelengths towards longer wavelengths could be caused, if the excited state charge distribution in the solute is markedly different from the ground-state charge distribution, and is as to give rise to stronger interactions with polar solvents in the excited state. Solvent polarity functions F_1 (ε, η) and F_2 (ε, η) have been calculated in order to ascertain the ground and excited state dipole moments of the molecule and are given in Table 2.

The spectral shifts $\overline{\nu_a}-\overline{\nu_f}$ versus the solvent polarity function F_1 (ε, η) and $\frac{\overline{\nu_a}+\overline{\nu_f}}{2}$ versus F_2 (ε, η) are shown in Figs. 5 and 6, respectively. The linear behavior of Stokes shift versus solvent polarity function indicates general solvent effects as a function of dielectric constant and refractive index. Using software origin 6.1, the data were fitted to a straight line. Slopes were found to be $S_1 = 560.78\ cm^{-1}$ and $S_2 = -289.84\ cm^{-1}$ from Figs. 5 and 6, respectively. Using Gaussian 03 software, we calculated ground state dipole moment for the probe at B3LYP/6-31G+(d) level. The ground state dipole moment obtained was 9.20 D in gas phase which matched well with the experimental one.

Further by making use of Eqs. (7) and (8), we calculated $\mu_g = 7.86$ D and $\mu_e = 24.90$ D. The change in dipole moment from excited state to

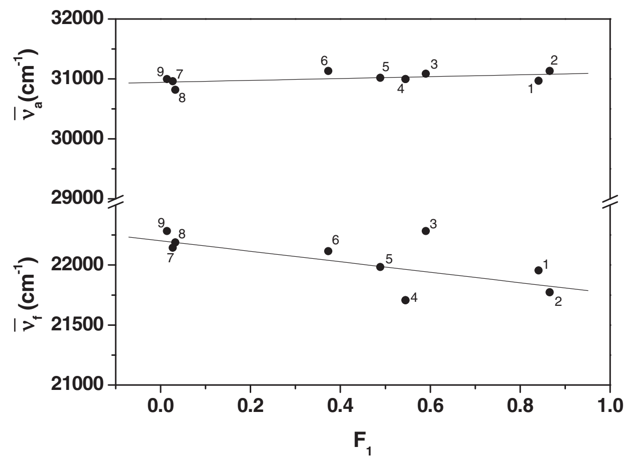


Fig. 4. Variation of absorption and emission maxima of [*N*-(2-oxo-2*H*-chromen-4-yl) imino] triphenyl phosphorane with solvent polarity function. (1) DMSO, (2) acetonitrile, (3) dichloromethane, (4) THF, (5) ethyl acetate, (6) diethyl ether, (7) O-xylene, (8) toulene, (9) CCL4.

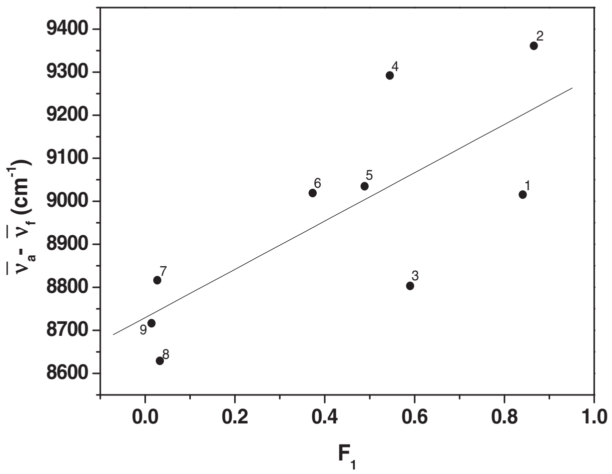


Fig. 5. Plot for Stokes shift versus solvent polarity function F_1. (1) DMSO, (2) acetonitrile, (3) dichloromethane, (4) THF, (5) ethyl acetate, (6) diethyl ether, (7) O-xylene, (8) toulene, (9) CCL4.

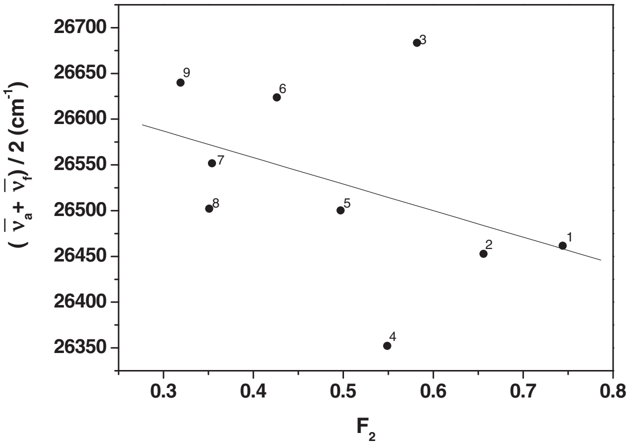


Fig. 6. Plot for arithmetic average of absorption and fluorescence wavenumbers versus solvent polarity function F_2. (1) DMSO, (2) acetonitrile, (3) dichloromethane, (4) THF, (5) ethyl acetate, (6) diethyl ether, (7) O-xylene, (8) toulene, (9) CCL_4.

Table 3
Dipole moment of [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane molecule in ground and excited states.

a_0 (Å)	S_1 (cm^{-1})	S_2 (cm^{-1})	μ_g (D)	μ_e (D)	$\Delta\mu$ (D)	μ_e/μ_g
5.96	560.78	289.84	7.86	24.90	17.04	3.16

ground-state is 17.04 D. All the data related to dipole moment are summarized in Table 3. Clearly, the dipole moment in excited state is significantly larger than the dipole moment in the ground state for the probe molecule studied. The dipole moments of a molecule in the ground and excited states are different due to changes in electron densities in these states. The invariance of absorption spectra with solvent polarity and continuous variation of emission spectra suggests that the excited state is more sensitive to solvent polarity than the ground state and change in fluorescence peak position with solvent polarity is responsible for the observed Stokes shift in [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane.

5. Conclusions

We have calculated ground state and excited state dipole moments of synthesized [*N*-(2-oxo-2*H*-chromen-4-yl)imino]triphenyl-phosphorane coumarin derivative. The ground (μ_g) and excited (μ_e) state dipole moments estimated from the solvatochromic shift method are 7.86 D and 24.90 D respectively. This large variation of the dipole moment value between the ground state and the excited state suggests that fluorescence originates from highly polar excited state. In the excited state it is likely that the charge separation increases, resulting in a large dipole moment than in the ground state. The value of computationally calculated ground state dipole moment 9.20 D (in gas phase) correlates well with that of the experimental one. A comparative analysis between the values of dipole moment in gas phase and various solvents is also provided for ground state.

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