



## Estimation of Ground State and Excited State Dipole Moments of (5-Amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone

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The fluorescence and absorption properties of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone were studied at room temperature in 15 solvents with dissimilar polarities. The impacts of solvent and GCRD parameters on the properties of the spectra are discussed. By utilizing the Gaussian 09 program, the ground-state dipole moments ( $\mu_g$ ) were have been measured experimentally and compared with theoretical values. After determining the ground-state dipole moments, the Kawski-Chamma-Viallet, Bakhshiev and Lippert equations were utilized to calculate the excited-state dipole moments ( $\mu_e$ ). It was observed that  $\mu_e$  has been greater than the ground state for the dye. In this work, the impact of solvent on the absorption and emission spectra of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone was computed and estimated their dipole moments. For every molecule studied, there was a substantial change in the Stokes shift values increasing polarity.

**Keywords:** Dipole moment, Stokes shift, Absorption, Emission, Spectra.

### INTRODUCTION

The analysis of the ground-state dipole moments ( $\mu_g$ ) and the excited-state dipole moments ( $\mu_e$ ) of the molecules is significant because it provides data regarding the variation in the dipole moment, polarizability and electronic distribution of molecules in a solvent environment upon excitation [1-7]. The simplest technique for determining dipole moments is the solvatochromic technique, which is based on the shift in the fluorescence and absorption maxima in many solvents and yields satisfactory results [8-12]. The solvatochromic method relies on a linear relationship between a solvent's polarity functions and the wavenumbers of its fluorescence and absorption maxima. To understand a molecule's structure "in an electronically excited state", it is crucial to estimate the dipole moments of the molecule using solvatochromic shifts [12-14]. The importance of these studies has increased significantly as dye photoscience has progressed both historically and recently. The value provides details on the optical properties of the substance. Utilizing the solvatochromic method was utilized to determine  $\mu_e$  and results

of multiple approaches were compared using different equations [15-19].

One intriguing field of study has been how solvents affect the absorption as well as fluorescence properties of the organic molecules [9,11,20-23]. The excited state of a molecule undergoes conformational modifications as a result of the redistribution of charges caused by photon stimulation. This may cause the  $\mu_e$  to change from the ground state to an increased or decreased value. The molecular dipole moment in the electrically excited state is a crucial characteristic that reveals the details of about the geometric and electronic structure of a molecule throughout its short lifetime. The  $\mu_e$  of an electronically excited molecule can be utilized to produce nonlinear materials, understand the nature of the excited state and observe the progression of photochemical transformation. The  $\mu_e$  of fluorescent dye molecules, such as those under investigation, also controls the tunability of the emission energy's range in relation to the medium.

All the existing methods rely on the spectrum shift produced by either internal solvatochromism or external electrochromic

effects to determine the singlet  $\mu_e$  [10,20,21,24,25]. Although electrooptic techniques such as microwave conductivity, electric-dichroism, stark splitting and electronic polarization of fluorescence are usually considered as be extremely accurate, their utilization is limited because their studies have focused only on relatively simple molecules and they are considered to be equipment-sensitive. Changes in the fluorescence maxima and absorption in a variety of solvents with variable polarities are the basic of the solvatochromic technique. The  $\mu_e$  values of various compounds are estimated by utilising the solvent dependency of absorption and also the fluorescence maxima.

The nature of a dissolved dye's surroundings affects its photophysical behaviour *i.e.*, the solvent-solute interactions and solvent nature have a vital influence on the dye's absorption as well as the fluorescence band's maximum absorption or emission wavelength, intensity and shape in solution. This effect is directly correlated with the type and strength of dye-solvent interactions. There are two forms of solvent-solvent interactions that might cause solvent-dependent spectrum shifts: non-specific and specific. The solvatochromic parameters or solvent polarity scale, can be utilized to determine the solvent effect.

This study presents the dipole moments of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in the ground and excited states. The current research goal is to investigate and compare the ground-state dipole moments ( $\mu_g$ ) and the excited-state dipole moments ( $\mu_e$ ) of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone by multiple techniques and study the GCRD parameters.

**Theory:** The solvent effect of dye in various solvents is essential aspect of studying the spectroscopic parameter. An electron is moved to a new electronic level in less time compared to what it takes for the molecule as a whole to rearrange itself inside the solvent environment. The molecule is stimulated in a similar structural environment as it is in the ground state upon excitation. The emission and absorption spectra of the solute reveal differences in its chemical properties. The standard equations for the solvatochromism of fluorophores are usually examined with linear correlations *viz.* Bakhshiev, Lippert-Mataga, Reichardt and Kawski-Chamma-Viallet [11,23,26-28]. According to Lippert-Mataga, the Stokes shift ( $\Delta\nu = \nu_a - \nu_f$ ) of solute molecule is related to the refractive index ( $n$ ) and permittivity ( $\epsilon$ ) of solvent as:

$$\bar{\nu}_a - \bar{\nu}_f = m_1 F_1(\epsilon, n) + \text{Constant} \quad (1)$$

here  $\bar{\nu}_a$  and  $\bar{\nu}_f$  indicate the fluorescence and absorption emission maxima wavenumbers ( $\text{cm}^{-1}$ ),  $F_1(\epsilon, n)$  is known as the Lippert solvent polarity function (eqn. 2) and the standard equation is provided as:

$$F_1(\epsilon, n) = \frac{\epsilon - 1}{2\epsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$

$$F_1(\epsilon, n) = \frac{2n^2 + 1}{n^2 + 2} \left( \frac{\epsilon - 1}{\epsilon + 2} - \frac{n^2 - 1}{n^2 + 2} \right) \quad (2)$$

$m_1 = 2(\mu_e - \mu_g)^2/hca^3$ ,  $\mu_e$  and  $\mu_g$  represent the  $\mu_e$  and  $\mu_g$  of solute molecule, respectively and  $a$  represent the solute molecule's Onsager cavity radius, which may be computed using eqn. 3:

$$a = \left( \frac{3M}{4\pi\delta N_A} \right)^{1/3} \quad (3)$$

where  $M$  = molecular weight and  $\delta$  = density.

The Bakhshiev equation provides the dependency of the solute Stokes shift on the  $\epsilon$  &  $n$  of the solvent as:

$$\bar{\nu}_a - \bar{\nu}_f = m_2 F_2(\epsilon, n) + \text{Constant} \quad (4)$$

where  $m_2 = 2(\mu_e - \mu_g)^2/hca^3$  and  $F_2(\epsilon, n)$  indicates the Bakhshiev solvent polarity function (eqn. 5):

$$F_2(\epsilon, n) = \frac{2n^2 + 1}{2(n^2 + 2)} \left( \frac{\epsilon - 1}{\epsilon + 2} - \frac{n^2 - 1}{n^2 + 2} \right) + \frac{3(n^4 - 1)}{2(n^2 - 1)^2} \quad (5)$$

The average of solute emission and absorption maximum is associated with solvent  $\epsilon$  and  $n$  by the Kawski-Chamma-Viallet equation as:

$$\frac{\bar{\nu}_a + \bar{\nu}_f}{2} = -m_3 F_3(\epsilon, n) + \text{Constant} \quad (6)$$

where  $m_3 = 2(\mu_e^2 - \mu_g^2)/hca^3$  and  $F_3(\epsilon, n)$  denote the Kawski-Chamma-Viallet solvent polarity function as presented in eqn. 7:

$$F_3(\epsilon, n) = \frac{2(\epsilon - 1)}{\epsilon + 2} \quad (7)$$

$F_4(\epsilon)$  presents the Suppan's polarity parameter and expressed in eqn. 8:

$$F_4(\epsilon, n) = \frac{2(\epsilon - 1)}{2\epsilon + 2} \quad (8)$$

The computed values of  $F_1(\epsilon, n)$ ,  $F_2(\epsilon, n)$ ,  $F_3(\epsilon, n)$  and  $F_4(\epsilon, n)$  and  $E_N^T$  are presented in Table-1.

TABLE-1  
SUMMARY OF SOLVENT PROPERTIES WHICH IS  
REFRACTIVE INDEX, DIELECTRIC CONSTANT AND  $E_N^T$

Solvent	Dielectric constant ( $\epsilon$ )	Refractive index ( $n$ )	$E_N^T$
Toluene	2.38	1.4970	0.099
Methanol	33.7	1.3290	0.762
N-Butyl alcohol	17.4	1.3993	0.586
Ethyl acetate	6.08	1.3720	0.228
DMSO	47.2	1.4790	0.444
Acetonitrile	36.64	1.3440	0.460
Benzene	2.28	1.4990	0.111
Isopropyl alcohol	20.2	1.3772	0.617
Water	80.4	1.3330	1.000
DMF	38.25	1.4300	0.386
DCM	8.9	1.4240	0.321
Dioxane	2.3	1.4210	0.164
THF	7.5	1.4040	0.207
Ethanol	24.3	1.3610	0.654
Octanol	10.3	1.4290	0.537

Assuming that the molecule exhibits stable symmetry upon excitation and that the dipole moments are oriented parallelly,  $\mu_g$ ,  $\mu_e$  as well as  $\mu_e/\mu_g$  can be estimated from the slopes ( $m_2$  &  $m_3$ ) of the plots of  $\nu_a - \nu_f$  versus  $F_2(\epsilon, n)$  and  $(\bar{\nu}_a + \bar{\nu}_f)/2$  versus  $F_3(\epsilon, n)$  as:

$$\mu_g = \frac{m_3 - m_2}{2} \left( \frac{hca^3}{2m_2} \right)^{1/2} \quad (9)$$

$$\mu_e = \frac{m_3 + m_2}{2} \left( \frac{hca^3}{2m_2} \right)^{1/2} \quad (10)$$

$$\frac{\mu_e}{\mu_g} = \frac{m_2 + m_3}{m_3 - m_2} \quad \text{for } m_3 > m_2 \quad (11)$$

If  $\mu_g$  &  $\mu_e$  subtend an angle  $\phi$ ,

$$\cos\phi = \frac{1}{2\mu_g\mu_e} \left[ (\mu_g^2 + \mu_e^2) - \frac{m_2}{m_3} (\mu_e^2 - \mu_g^2) \right] \quad (12)$$

$\mu_e$  can also be calculated utilizing the empirical relation:

$$\bar{\nu}_a - \bar{\nu}_f = 11307.6 \left( \frac{\Delta\mu}{\Delta\mu_B} \right)^2 \left( \frac{a_B}{a} \right)^3 E_T^N + \text{Constant} \quad (13)$$

where  $a_B$  indicates the Onsager cavity radius of the reference molecule;  $\Delta\mu$  and  $\Delta\mu_B$  represents the variations in the dipole moments of the reference and sample (betaine dye) molecules on the excitation; and  $E_T^N$  signifies the minute solvent polarity function.  $\Delta\mu$  may be estimated by employing the slope of  $\bar{\nu}_a - \bar{\nu}_f$  vs.  $E_T^N$  plot and the stated values of  $\Delta\mu_B$  and  $a_B$  (9 D and 6.2 Å, respectively) for betaine dye. Additionally, by utilizing  $\Delta\mu$  &  $\mu_g$  from eqn. 9,  $\mu_e$  may be ascertained. The solvent polarity function and Stokes shift are more closely correlated with eqn. 13, which takes into considering more intermolecular interactions than with the other relations.

## EXPERIMENTAL

The (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone was synthesized using standard method. The solvents used in the present study namely toluene, methanol, *n*-butyl alcohol, ethyl acetate, DMS, acetonitrile, benzene, isopropyl alcohol, water, DMF, DCM, DIO, THF and ethanol. All the chemicals were obtained from S.D. Fine Chemicals Ltd., India and were of spectroscopic grade. The molecular structure of the molecule is shown in Fig. 1.

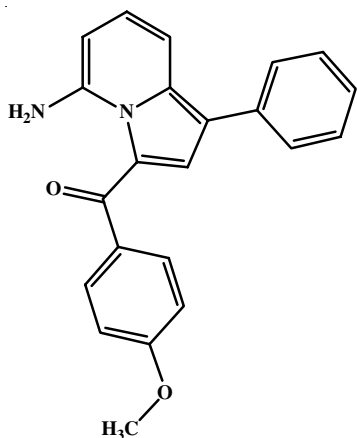


Fig. 1. Molecular structure of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone

A Hitachi UH5300 UV/VIS spectrophotometer was used to record the absorption spectra of 5-amino-1-phenylindolizin-3-yl (4-methoxyphenyl)methanone throughout the wavelength range of 200-700 nm. A Hitachi F-7000 FL spectrophotometer

was used to observe the fluorescence spectrum using a standard quartz cuvette. All the measured values were obtained at room temperature. The observed fluorescence wavelength and absorption maxima have an uncertainty of  $\pm 1$  nm. For all of the organic solvents, concentrations of  $1 \times 10^{-5}$  M were selected. The observed wavelengths of the fluorescence and absorption maxima have an error of  $\pm 1$  nm. For all of the organic solvents, concentrations of  $1 \times 10^{-5}$  M were selected. To observe the absorption and fluorescence spectra, fresh homogenous solutions have been prepared each time. (5-Amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone has a significant vibrational structure and a mirror image relation in its absorption and fluorescence spectrum.

## RESULTS AND DISCUSSION

The experimental ground-state dipole moments ( $\mu_g$ ) served as the basis for the experimental methods used to assess the excited-state dipole moments ( $\mu_e$ ). The interpretation of the experimental data is frequently aided by the findings of theoretical computations. This work provides a detailed summary of the solvent properties of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone. The interpretation of experimental data is frequently facilitated by the outcomes of theoretical calculations. The detailed overview of solvent characteristics of 5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone is given in Table-1.

The computed solvent polarity parameters function values in several solvents in the current research are shown in Table-2. The solubility of the chosen molecule resulted in the selection of several solvents.

TABLE-2  
SOLVENT POLARITY PARAMETERS  $F(\epsilon, n)$ ,  $F_1(\epsilon, n)$ ,  $F_2(\epsilon, n)$ ,  $F_3(\epsilon)$ , &  $F_4(\epsilon)$  VALUES IN DIFFERENT SOLVENTS WERE CALCULATED

Solvent	$F(\epsilon, n)$	$F_1(\epsilon, n)$	$F_2(\epsilon, n)$	$F_3(\epsilon)$	$F_4(\epsilon)$
Toluene	0.013	0.029	0.349	0.630	0.479
Methanol	0.309	0.857	0.652	1.831	0.956
N-Butyl alcohol	0.263	0.749	0.646	1.690	0.916
Ethyl acetate	0.200	0.492	0.499	1.257	0.772
DMSO	0.263	0.841	0.744	1.878	0.968
Acetonitrile	0.304	0.861	0.664	1.844	0.959
Benzene	0.003	0.007	0.340	0.598	0.460
Isopropyl alcohol	0.276	0.780	0.646	1.729	0.927
Water	0.320	0.913	0.683	1.927	0.981
DMF	0.275	0.839	0.711	1.850	0.961
DCM	0.216	0.589	0.582	1.449	0.840
Dioxane	0.029	0.061	0.316	0.604	0.464
THF	0.209	0.547	0.548	1.368	0.812
Ethanol	0.288	0.811	0.651	1.771	0.939
Octanol	0.225	0.626	0.604	1.512	0.861

The fluorescence and absorption spectra of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone molecule are shown in Fig. 2. The absorption and fluorescence peaks were found to be 262 nm and 404.2 nm, respectively. For molecules, shorter absorption wavelength maxima are produced by minimally extended conjugations. At shorter wavelengths, the fluorescence excitation spectrum sometimes has only one

TABLE-3  
ABSORPTION MAXIMA AND FLUORESCENCE MAXIMA, STOKES SHIFT, ARITHMETIC MEAN OF THE STOKES VALUES OF (5-AMINO-1-PHENYLINDOLIZIN-3-YL)(4-METHOXYPHENYL)METHANONE

Solvent	Absorption maximum (nm)	Fluorescence maximum (nm)	$\bar{\nu}_a$ (nm)	$\bar{\nu}_f$ (nm)	Stokes shift ( $\Delta\bar{\nu}$ ) ( $\text{cm}^{-1}$ )	$(\nu_a + \nu_f)/2$ ( $\text{cm}^{-1}$ )
Toluene	245	386	40816	25893	14923	33354
Methanol	252	382	39682	26123	13559	32902
N-Butyl alcohol	250	381	40000	26191	13808	33095
Ethyl acetate	240	385	41666	25947	15719	33806
DMSO	240	390	41666	25627	16038	33647
Acetonitrile	254	386	39370	25853	13516	32611
Benzene	235	385	42553	25920	16633	34236
Isopropyl alcohol	250	380	40000	26274	13725	33137
Water	262	404	38167	24740	13427	31454
DMF	240	388	41666	25773	15893	33719
DCM	256	385	39062	25920	13142	32491
Dioxane	250	398	40000	25087	14912	32543
THF	252	385	39682	25947	13735	32814
Ethanol	254	382	39370	26136	13233	32753
Octanol	255	381	39215	26205	13010	32710

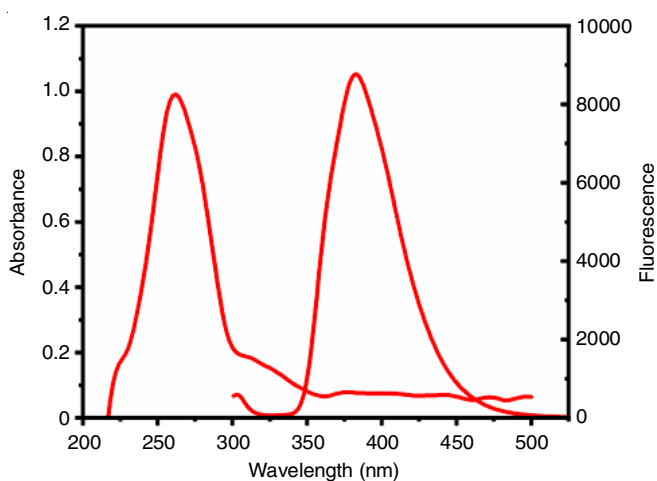


Fig. 2. Absorption and fluorescence spectrum of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone

band with a shoulder. The wavelengths of excitation and absorption are typically near each other. For each solvent, a greater spectral shift is seen in the spectrum of emission in comparison to the molecule's absorption spectrum.

The variations in values of absorption and fluorescence were found according to the medium of solvent. Simultaneously, the Stokes shift for the same has been calculated from the absorption and fluorescence data in Table-3. In every case, the large slope values indicate a significant variation between the values of  $\mu_e$  and  $\mu_g$ . Table-4 provides the intercept, slope as

TABLE-4 SLOPE, INTERCEPT ALONG WITH CORRELATION COEFFICIENT DATA OF (5-AMINO-1-PHENYLINDOLIZIN-3-YL)(4-METHOXYPHENYL)METHANONE			
Method	Slope	Intercept	Correlation coefficient
Lippert's	4978	12088	0.94
Bakshiev's	1446	12294	0.99
Kawski-Chamma-Viallet's	5054	36205	0.93
McRae's	5293	31191	0.92
Suppan's	21566	20707	0.93
$E_{tr}^N$	2141	12486	0.94

well as correlation coefficient of the fitted lines. The correlation coefficients in the majority of the published data are adequate and show linearity with the chosen number of Stokes shift points.

The values of  $\mu_e$  and  $\mu_g$ , which are determined using Edward's approach, depend on the Onsager cavity radius and are shown in Table-5. Eqns 9 and 10 are applied to assess the  $\mu_e$  and  $\mu_g$ , respectively. None the less, the  $\mu_e$  was also computed utilizing the Kawski-Chamma-Viallet, Bakshiev and Lippert equations. The polarity function of the microscopic solvent is applied to examine the  $\mu_e$ . Here, the ratio between the  $\mu_e$  and  $\mu_g$  was determined. The angle between the  $\mu_e$  and  $\mu_g$  was simultaneously studied using the solvatochromic data.

Fig. 3 plot shows the Stokes shift vs.  $F(\epsilon, n)$  namely Lippert's and Bakshiev's polarity parameters of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in different solvents,

TABLE-5  
GROUND-STATE DIPOLE MOMENTS ( $\mu_g$ ), EXCITED-STATE DIPOLE MOMENTS ( $\mu_e$ ) OF (5-AMINO-1-PHENYLINDOLIZIN-3-YL)(4-METHOXYPHENYL)METHANONE

Onsager cavity radius 'a' (Å)	$\mu_g^a$ (D)	$\mu_e^b$ (D)	$\mu_e^c$ (D)	$\mu_e^d$ (D)	$\mu_e^e$ (D)	$\mu_e^f$ (D)	$\mu_e/\mu_g^g$	$\phi^h$
4.20	4.05	7.32	10.11	7.32	10.15	2.18	1.08	0

Debye (D) =  $3.33564 \times 10^{-30} \text{ cm} = 10^{-18} \text{ esu cm}$

<sup>a</sup>Ground state dipole moment computed from eqn. 9; <sup>b</sup>Excited state dipole moment computed from eqn. 10; <sup>c</sup>Excited state dipole moment computed from Lippert's equation; <sup>d</sup>Excited state dipole moment computed from Bakshiev equation; <sup>e</sup>Excited state dipole moment computed from Kawski-Chamma-Viallet equation; <sup>f</sup>Excited state dipole moment computed from microscopic solvent polarity function  $E_{tr}^N$ ; <sup>g</sup>Ratio of excited to ground state dipole moment; <sup>h</sup>Angle between excited state to ground state dipole moment with solvatochromic data

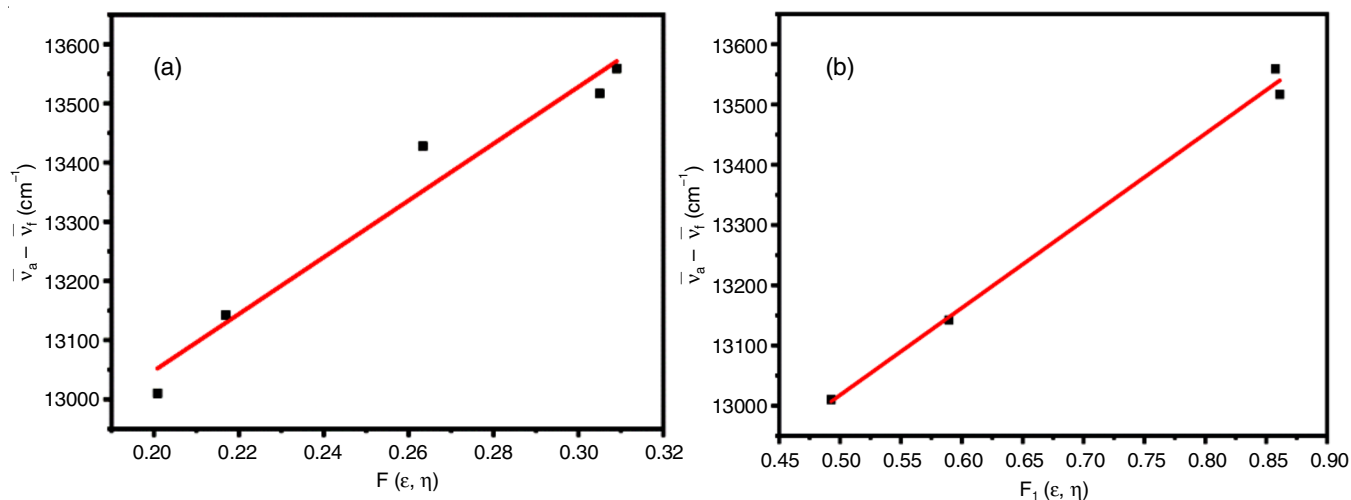


Fig. 3. Plots of Stokes shift vs. (a)  $F(\epsilon, \eta)$  [Lippert's polarity] and (b)  $F_1(\epsilon, \eta)$  [Bakshiev's polarity] of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in different solvents

whereas Fig. 4 shows the nature using Kawaski-Chamma-Viallet's, McRae's and Suppan's polarity parameter of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in different solvents.

**Analysis of global chemical reactivity descriptor (GCRD) parameters:** The geometry optimization has been carried out in vacuum using a semi-empirical method for the PM6 basis set on an Intel i7/2.11 GHz personal computer using the Gaussian

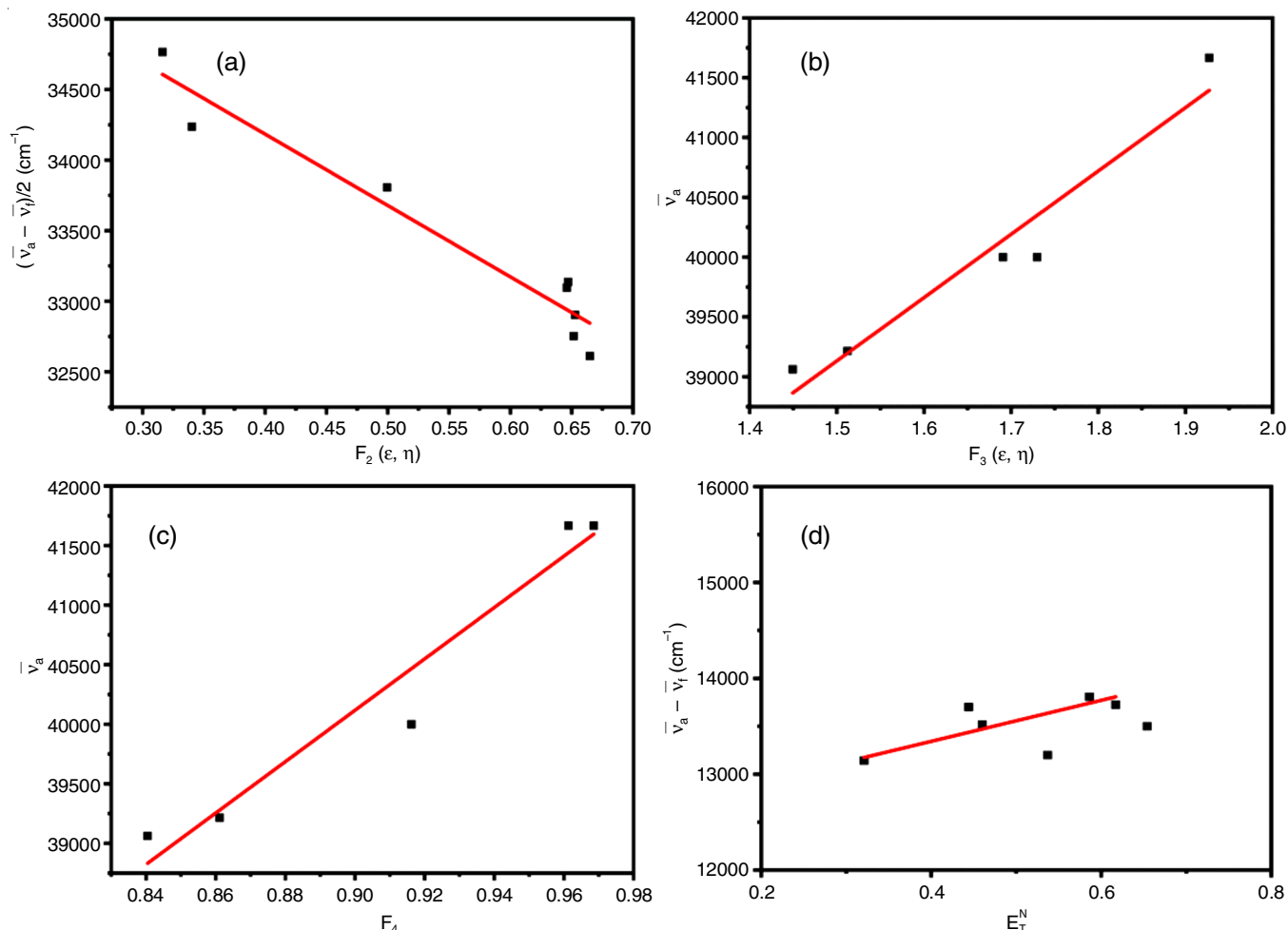


Fig. 4. Plots of  $(\bar{\nu}_a + \bar{\nu}_f)/2$  vs.  $F_2(\epsilon, \eta)$  [Kawaski-Chamma-Viallet's polarity] (a),  $\bar{\nu}_a$  vs.  $F_3(\epsilon)$  [McRae's polarity] (b),  $\bar{\nu}_a$  vs.  $F_4(\epsilon)$  [Suppan's polarity] (c) and  $\bar{\nu}_a - \bar{\nu}_f$  versus  $E_T^N$  [solvent polarity] (d) of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in various solvents

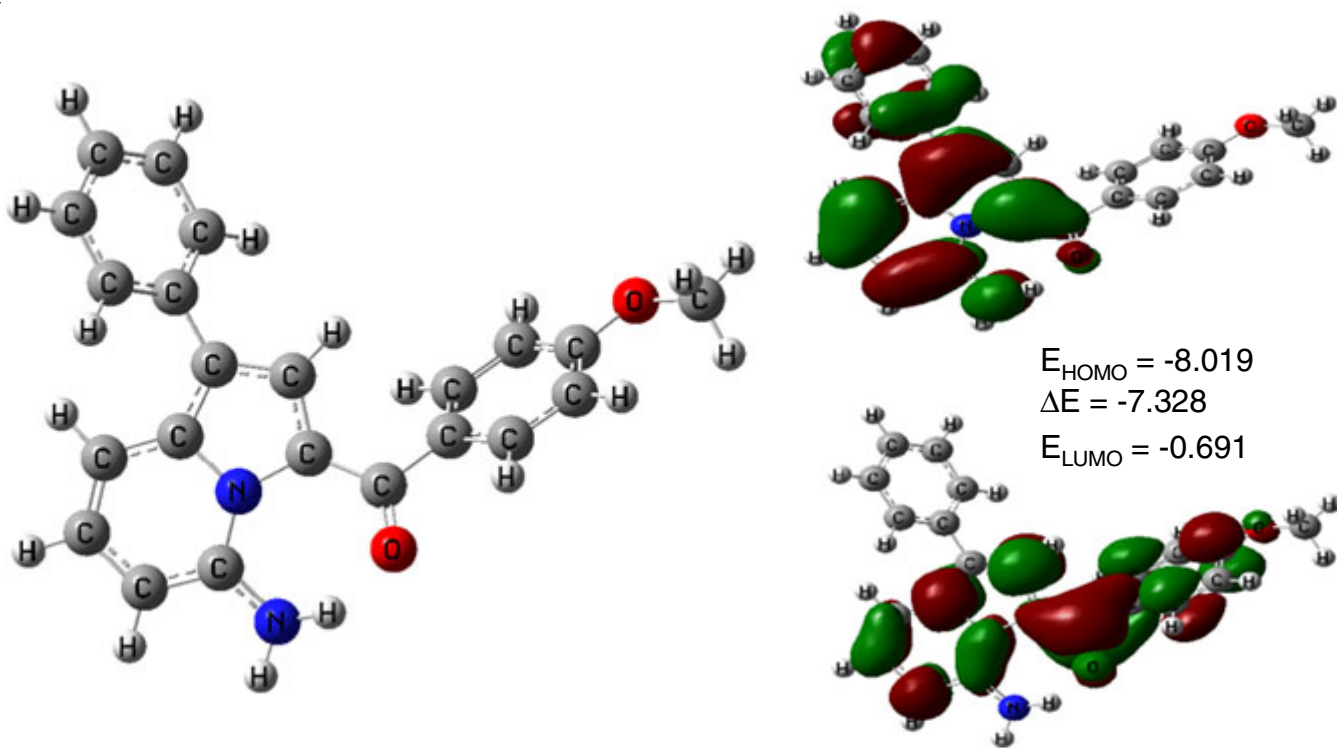


Fig. 5. Optimized geometry and HOMO-LUMO surfaces of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone molecule

09 W program package [29]. The optimized geometry of the title molecule and the optimized ground-state molecular geometry are shown in Fig. 5. The theoretical ground state dipole moment is 1.58 D using Gaussian software in the gas phase and the experimental ground state dipole moment is estimated from the solvatochromic shift method. There exists a slight discrepancy between the theoretical value and the experimental value of the ground-state dipole moments. The variation in values may be attributed to variations in the experimental and theoretical values of the dipole moments [18,22,23,26,28,30]. A measurement of the solute molecule's radius is necessary for the ground state dipole moment to differ. As compared to experimental and theoretical values obtained from *ab initio* calculations, they are based on the gaseous phase.

The reason may be that the experimental method considers solvent and environmental effects, while *ab initio* calculations only give a value of  $\mu_g$  for the gas phase molecule. The HOMO-LUMO values were found to be -8.019 and -0.691, respectively, with the  $\Delta E$  value being -7.328. The negative chemical potential of HOMO-LUMO shows that molecule (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone is highly stable. This shows optimization in the geometrical structure of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone with the GCRD parameters (Table-6) [26]. This shows a wider gap in HOMO-LUMO with stability and hardness, which signifies a more reactive soft molecule with high polarization [26,29,30].

The process in mapping the active sites of a given chemical structure, which helps in measure the electrophilic and nucleophilic sites as well as hydrogen bonding interactions of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone molecule. An electrostatic potential map is a representation where

the molecular surface is indicated by different colours as shown in Fig. 6. This map allow for an easy to understand visualization of the distribution of charge in a chosen molecule.

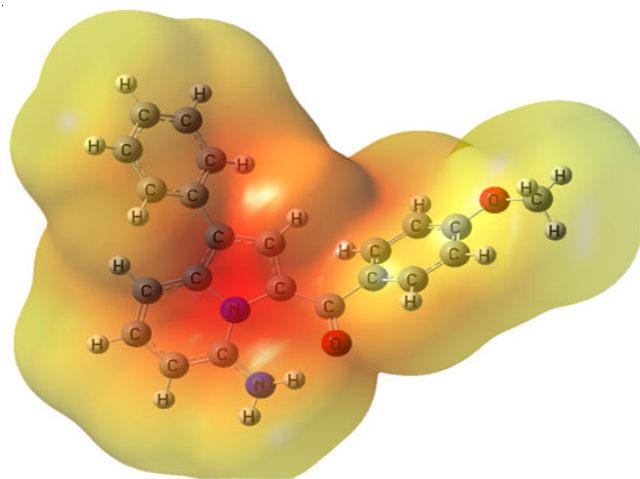


Fig. 6. ESP map of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone

The global chemical reactivity descriptors (GCRD) provide the key characteristics for determining the chemical reactivity and stability of the studied molecule. The GCRD parameters like electrophilic index ( $\omega$ ), electronegativity ( $\chi$ ), chemical softness ( $s$ ), chemical hardness ( $\eta$ ), chemical potential ( $\mu$ ), electron affinity (EA) and ionization potential (I) for (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone have been calculated with the following expressions and these values (Table-6) provide the chemical properties and stability of the chosen molecule in various solvents.

TABLE-6  
PARAMETER FOR GLOBAL CHEMICAL REACTIVITY DESCRIPTORS (GCRD)

$E_{\text{HOMO}}$ (eV)	$E_{\text{LUMO}}$ (eV)	Ionization potential, IP (eV)	Electron affinity, EA (eV)	Electronegativity, $\chi$ (eV)	Chemical hardness, $\eta$ (eV)	Chemical potential, $\mu$ (eV)	Chemical softness, S (eV)	Electrophilic index, $\omega$ (eV)
-8.019	-0.691	8.019	0.691	4.355	3.664	-4.355	0.136	2.588

$$\text{IP} = -E_{\text{HOMO}}$$

$$\text{EA} = -E_{\text{LUMO}}$$

$$\chi = \frac{\text{IP} + \text{EA}}{2}$$

$$\mu = -\chi, \eta = \frac{\text{IP} - \text{EA}}{2}$$

$$s = \frac{1}{2\eta}$$

## Conclusion

In present work, the dipole moments of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in different 15 solvents were studied and characterized the solvent effect on their emission and absorption spectra. The molecule's photo physical characteristics were determined in a series of solvents with progressively higher polarity. In different solvent, there was a substantial change in the values of Stokes shift with increasing polarity, which suggested the  $\pi$ - $\pi^*$  transitions as the cause of the bathochromic change in the fluorescence and absorption spectrum. It suggests that as compared to the ground state, the molecule was more solvated in the singlet excited state. The ground state dipole moments of (5-amino-1-phenylindolizin-3-yl)(4-methoxyphenyl)methanone in different solvents were successfully calculated by quantum chemical calculations.

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## CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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