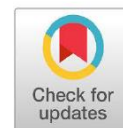




Original Research article

Evaluation of Ground and Excited State Dipole Moments of 2(3)-tetra(*tert*-butylphenoxy)phthalocyaninato Zinc(II) from Solvatochromic Data



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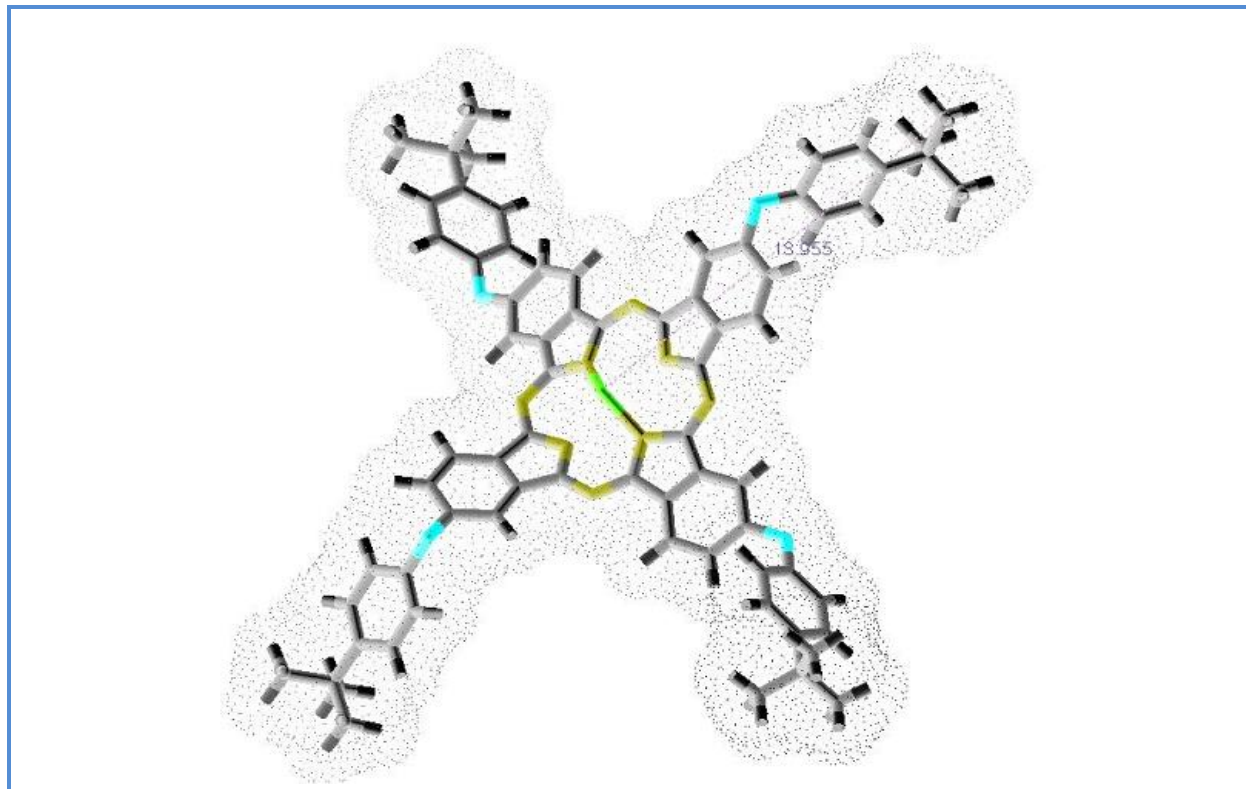
Solvatochromic

ABSTRACT

This article presents a semi-empirical determination of ground state dipole moment (μ_g) and excited state dipole moment (μ_e) of 2(3)-tetra(*tert*-butylphenoxy)phthalocyaninato zinc(II) (ZnTBPC) using the solvatochromic shift method, which is based on the Onsager's reaction field theory. A combined application of the Bakshiev's equation and the Kawski-Chamma-Viallet's equation was used to determine the ratio μ_e/μ_g while the use of the molecular-microscopic solvent polarity parameter yielded the term $\Delta\mu$ ($\mu_e - \mu_g$). The dipole moment of ZnTBPC in its excited singlet state ($\mu_e=4.46D$) is more than twice as much as that in its ground state ($\mu_g=2.14D$). These values suggest that the higher charge separation is greater in the excited state of ZnTBPC than in its ground state.

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Graphical Abstract



Introduction

The phthalocyanine (Pc) molecule is made up of four isoindole groups connected by four nitrogen atoms to form a symmetrical 18 π -electron conjugated aromatic macrocycle. Pc is related to the naturally occurring porphyrins which possess exceedingly high thermal and chemical stability. Pcs which can be systematically described as *tetra-aza tetra-benzoporphyrins* possess distinctive physicochemical properties that have provoked wide-reaching interest in academics and in the chemical industry. These robust properties have been exploited in molecular metals [1], chemical sensors [2], pollution control [3], fuel cells [4] and information technology [5]. The Pc molecule is planar and fairly symmetrical with a four-fold principal axis of rotation, four perpendicular two-fold axes and a horizontal mirror plane (Figure 1); these attributes suggest that the molecule might possess a roughly zero dipole moment. However, modifications to the Pc structure result in different degrees of non-planarity and symmetry loss.

The insertion of a metal (whose diameter does not fit into the Pc's cavity, and therefore forms a dome [6]) leads to symmetry reduction and introduces a dipole parallel to the principal axis, while

an unsymmetrical peripheral or non-peripheral ring substitution could bring about a dipole moment perpendicular to the principal axis.

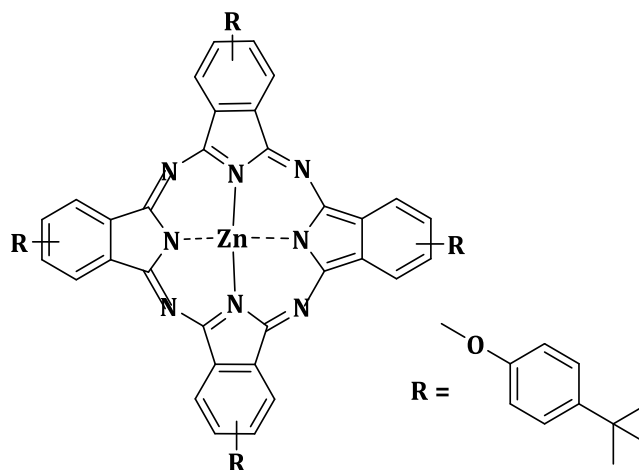


Figure 1. Structure of 2(3)-tetra-(tert-butylphenoxy phthalocyaninato) zinc (ZnTBPC)

Pcs are significantly photoactive; the excited states are well-populated upon absorption of UV-Vis radiation, and the absorption and emission spectra are very informative because they are related to the energies of Franck-Condon and the relaxed excited states, respectively. Following the excitation, the dipole moment and the polarizability of a molecule are significantly changed. In polar solvents, these changes cause shifts in absorption and fluorescence positions when compared to spectra in a non-polar solvent. These shifts in molecular properties depend strongly on the natures of both the molecule and the solvent as this solvent's dependence of absorption and emission frequencies has been widely exploited in the determination of ground and excited state dipole moments of molecules. Knowledge of the dipole moments is valuable for the appreciation of the nature of the absorbing states and also in the estimation of the dielectric friction contribution to the rotational reorientation of the polar solutes in solvents [7]. In addition, dipole moment is a direct measure of electron distribution in a molecule of the known geometry [8]. A prior knowledge of the dipole moments of the electronically excited species is often useful in the design of non-linear optical materials [9] and in the elucidation of the nature of the excited states. Experimental and theoretical studies on ground and excited state dipole moments of organic fluorophores using different techniques are well documented [10-13]. The determination of the ground- and excited-state dipole moments of molecules is very desirable, as the values offer information about the change in the electronic charge distribution following excitation. Many techniques are known for determining the excited state dipole moment; *e.g.*, electrochromic of absorption and fluorescent bands [14], Stark splitting of

rotational levels of the 0-0 vibrational bands and the effect of an external electric field on the fluorescence anisotropy [15, 16]. These methods, though more accurate, are restricted only to relatively simple molecules. In order to study the changes in electronic distribution in the excited states of larger molecules, the solvent-induced shifts of electronic bands of molecules have found to be of use [17]. However, literature is very scanty on the use of solvent-induced shifts for the determination of dipole moments of Pcs. In the present study, a semi-empirical estimation of the ground and excited-state dipole moments of 2(3)-tetra(*tert*-butylphenoxy)phthalocyaninato zinc(II) is presented using the solvatochromic shift method [18-21], which is based on the Onsager's reaction field theory [22].

Experimental

Materials and equipment

Tetra(*tert*-butylphenoxy)phthalocyaninato zinc(II) (ZnTPc) was synthesized according to the literature procedure [23]. Solvents—acetone, tetrahydrofuran (THF), dichloromethane (DCM), *N,N'*-dimethylformamide (DMF), chloroform, dimethyl sulphoxide (DMSO), toluene, and benzene were obtained from SAARCHEM; while pyridine and 1-chlorophthalene (1-CN) were obtained from FLUKA. UV-Vis absorption spectra were recorded on a Varian 500 UV/visible/NIR spectrophotometer, and fluorescence spectra on a Varian Eclipse spectrofluorometer.

Method

Semi-empirical determination of dipole moment

Ground- and excited-state dipole moments of ZnTBPC are determined *via* a quantitative assessment of solute-solvent interactions (involving the use of solvent-induced spectral shifts, solvent polarity functions and the molecular-microscopic solvent polarity parameter).

A combined application of the Bakshiev's equation [24] and the Kawski-Chamma-Viallet's equation [25, 26] is used to determine the ratio μ_e/μ_g , while the use of the molecular-microscopic solvent polarity parameter yielded the term $\Delta\mu$ ($\mu_e - \mu_g$); where μ_g and μ_e are the ground-state and excited-state dipole moments, it is assumed that $\mu_e > \mu_g$ is usually the case, especially for polar fluorophores.

Bakshiev and Kawski-Chamma-Viallet polarity functions

Bakshiev [24] and Kawski-Chamma-Viallet [25, 26], obtained a simple quantum-mechanical second-order perturbation theory and taking cognizance of the Onsager's model, from which these equations emerge:

$$\bar{\nu}_a - \bar{\nu}_f = m_1 F_1(\varepsilon, n) + k_1 \quad \text{Bakshiev's equation} \quad (1)$$

$$\frac{\bar{\nu}_a + \bar{\nu}_f}{2} = m_2 F_2(\varepsilon, n) + k_2 \quad \text{Kawski-Chamma-Viallet's equation} \quad (2)$$

$\bar{\nu}_a$ and $\bar{\nu}_f$ are absorption and fluorescence maximum wavenumbers (cm^{-1}), respectively; ε and n are the solvent's dielectric constant and refractive index, respectively; k_1 and k_2 are constants

The expressions $F_1(\varepsilon, n)$ and $F_2(\varepsilon, n)$ are defined as:

$$F_1(\varepsilon, n) = \left[\frac{\varepsilon-1}{\varepsilon+2} - \frac{n^2-1}{n^2+2} \right] \left[\frac{2n^2+1}{n^2+2} \right] \quad (\text{Bakshiev's polarity function}) \quad (3)$$

$$F_2(\varepsilon, n) = \frac{2n^2+1}{2(n^2+2)} \left[\frac{\varepsilon-1}{\varepsilon+2} - \frac{n^2-1}{n^2+2} \right] + \left[\frac{3(n^4-1)}{2(n^2+2)^2} \right] \quad (\text{Kawski-Chamma-Viallet's polarity function}) \quad (4)$$

It follows that plots of $\Delta\bar{\nu}$ (i.e., $\bar{\nu}_a - \bar{\nu}_f$) versus $F_1(\varepsilon, n)$, and $\frac{\bar{\nu}_a + \bar{\nu}_f}{2}$ versus $F_2(\varepsilon, n)$ should give straight lines. The parameters m_1 and m_2 occurring in Eqs. 1 and 2 can be determined from the slopes of the straight lines. m_1 and m_2 are also defined as follows:

$$m_1 = \frac{2(\mu_e - \mu_g)^2}{hc a^3} \quad (5)$$

$$m_2 = \frac{2(\mu_e^2 - \mu_g^2)}{hc a^3} \quad (6)$$

h is the Planck's constant, c is the velocity of light in vacuum, and a is the Onsager's cavity radius of ZnTBPC. The dye's Onsager cavity radius is assumed to be equal to molecular radius R , and is obtained using the ACD/ChemSketch software [27] ($R=13.95 \text{ \AA}$).

Analysis of Eqs. 5 and 6 yielded the ratio μ_e/μ_g given as:

$$\frac{\mu_e}{\mu_g} = \frac{m_1 + m_2}{m_2 - m_1} \quad (7)$$

Molecular-microscopic solvent polarity parameter (E_T^N)

Reichardt [28, 29] proposed an empirical scale, which brought forth the molecular-microscopic solvent polarity parameter (E_T^N). E_T^N values are defined according to Eq. 8 as dimensionless figures, using water ($E_T^N=1.0$) and trimethylsilane ($E_T^N=0.0$) as extreme polar and non-polar reference solvents, respectively. Hence, the E_T^N scale ranges from 0.0 to 1.0.

$$E_T^N = \frac{E_T(\text{Solvent}) - E_T(\text{TMS})}{E_T(\text{Water}) - E_T(\text{TMS})} = \frac{E_T(\text{Solvent}) - 30.7}{32.4} \quad (8)$$

The relationship among Stokes' shift $\Delta\bar{\nu}$ ($\bar{\nu}_a - \bar{\nu}_f$), the dipole moment difference term ($\Delta\mu$) and E_T^N is given by Eq. 9a [30]:

$$\Delta\bar{\nu} = \bar{\nu}_a - \bar{\nu}_f = 11307.6 \left[\left(\frac{\Delta\mu}{\Delta\mu_B} \right)^2 \left(\frac{a_B}{a} \right)^3 \right] E_T^N + \text{constant} \quad (9a)$$

Where $\Delta\mu$ and $\Delta\mu_B$ (=9D) are the differences between the excited- and ground-state dipole moments of ZnTBPC and betaine dyes, respectively; a (13.95 Å) and a_B (6.2 Å) are the Onsager cavity radii of ZnTBPC and betaine dyes, respectively.

A plot of $\Delta\bar{\nu}$ against E_T^N should give a straight line with slope m given as:

$$m = 139.6 \left(\frac{6.2}{a} \right)^3 \cdot (\Delta\mu)^2 \quad (9b)$$

$\Delta\mu$ can then be calculated as:

$$\Delta\mu = \sqrt{\frac{m \cdot \left(\frac{6.2}{a} \right)^{-\frac{3}{2}}}{139.6}} \quad (9c)$$

Results and discussion

Ground state electronic absorption and fluorescence (emission) spectra

The ground state electronic absorption spectra of ZnTBPC in four solvents (acetone, THF, DMSO and 1-CN) are shown in Figure 2a. The assignment of absorption bands in Pcs and their metallated derivatives (MPcs) may be done qualitatively in terms of the Gouterman's model [31, 32]. MPcs typically have a Q band near 670 nm with extinction coefficient greater than 10^5 L/mol· $1/\text{cm}^{-1}$, and accompanied by a series of vibrational bands. Figure 2b shows the overlaid absorption and fluorescence spectra of ZnTBPC in DMSO.

In this work, the Q-band position of ZnTBPC ranges between 670 nm in acetone and 688 nm in 1-CN (Table 1). The bands are well-defined, which is expected for monomeric phthalocyanine complexes [33].

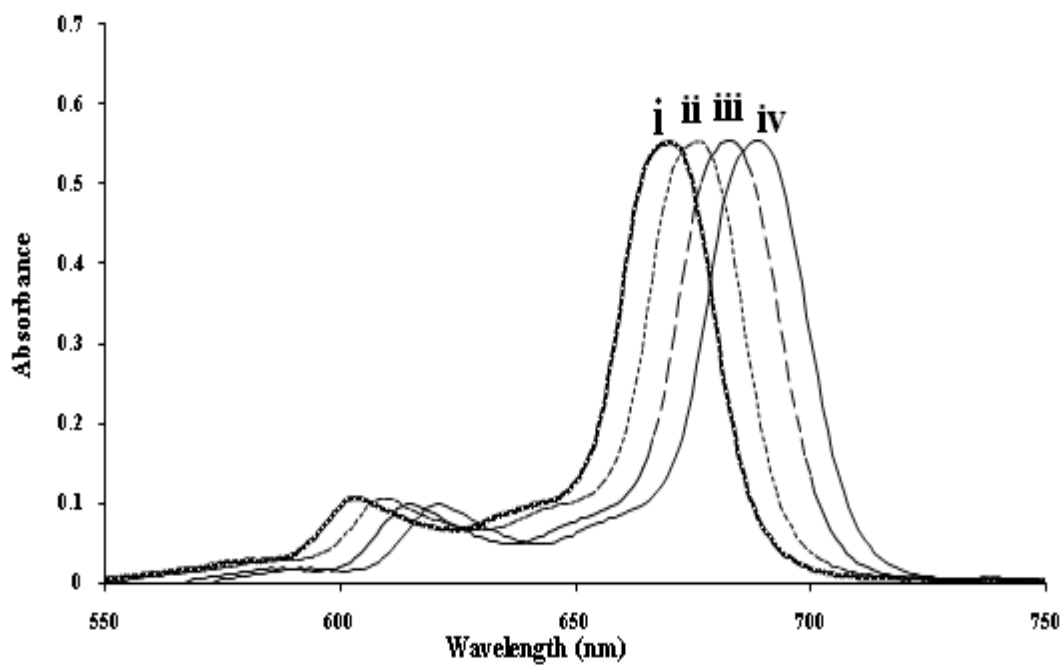


Figure 2a. Ground state electronic absorption spectra of ZnTBPC in (i) Acetone, (ii) THF, (iii) DMSO and (iv) 1-chloronaphthalene. $[ZnTBPC] \sim 4.50 \times 10^{-6} M$

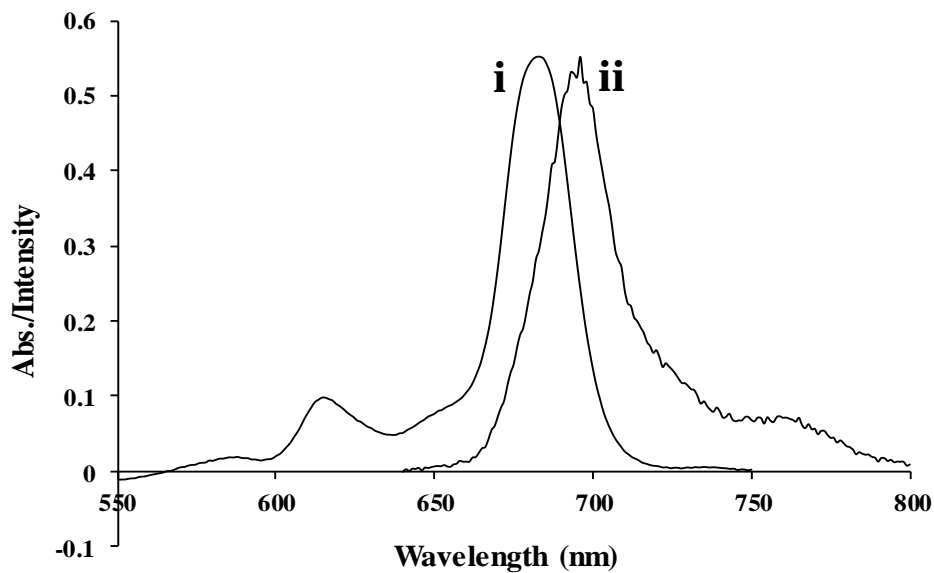


Figure 2b. Absorption (i) and fluorescence (ii) spectra of ZnTBPC in DMSO

Table 1. Spectral data for ZnTBPC in various solvents

	n	ε	λ_{Abs} (nm)	λ_{Ems} (nm)	ū_{Abs} (cm⁻¹)	ū_{Ems} (cm⁻¹)	Δū/cm⁻¹
Acetone	1.359	21.36	670	688	14925	14535	390.49
THF	1.406	7.47	676	693	14793	14430	362.88
DCM	1.424	9.02	679	697	14728	14347	380.34
DMF	1.43	37.06	679	696	14728	14368	359.72
Chloroform	1.446	4.89	681	698	14684	14327	357.64
DMSO	1.479	46.71	682	692	14663	14451	211.89
Toluene	1.497	2.43	679	695	14728	14388	211.89
Benzene	1.501	2.274	679	696	14728	14368	339.05
Pyridine	1.509	13.22	683	698	14641	14327	314.64
1-CN	1.633	5.00	688	707	14535	14144	390.61

λ_{Abs} and λ_{Ems} are the wavelengths of maximum absorption and fluorescence, respectively; while ū_{Abs} and ū_{Ems} are the wave numbers of maximum absorption and fluorescence, respectively

However, it can be observed that the Q bands are not as sharp as those observed for the unsubstituted zinc phthalocyanine (ZnPc) in the same solvents [34]; the bands are slightly broadened (~26 nm half-width in DMSO compared to ~20 nm for ZnPc in the same solvent). This broadening could have arisen from two causes: (i) steric effects of the *tert*-butylphenoxy substituents at the peripheral positions, which results in a slight deviation of the Pc skeleton from planarity, as observed for tetraphenyl porphyrins [35]; and (ii) the existence of ZnTBPC as a mixture of isomers, as it is known that band broadening is a characteristic of all tetrasubstituted Pcs [36].

There are 149 atoms in a ZnTBPC molecule (compared to 57 in ZnPc), therefore it is expected to exhibit a complex vibrational structure. Consequently, many vibrations of differing frequencies are coupled to an electronic transition following excitation. As a result of the solvation shell and the corresponding interactions between ZnTBPC and solvent molecules, the resulting vibrational transitions are considerably broadened, leading to longer Stokes' shifts. For instance, the Stokes' shifts associated with ZnTBPC in the various solvents used in this work range between 10 (in DMSO) and 18 (in 1-CN). These values are more than twice as much as those associated with ZnPc in the same solvent set. The variation of Stokes' shift can be correlated with solvent parameters like dielectric constant (ε), refractive index(n), Kosower-Z value *etc.* The plots of Stokes' shift of ZnTBPC (Δū) against the refractive index function, $n^2-1/2n^2+1$ and the dielectric constant function, $\epsilon-1/2\epsilon+1$ of the different solvents are shown in Figures 3 and 4, respectively.

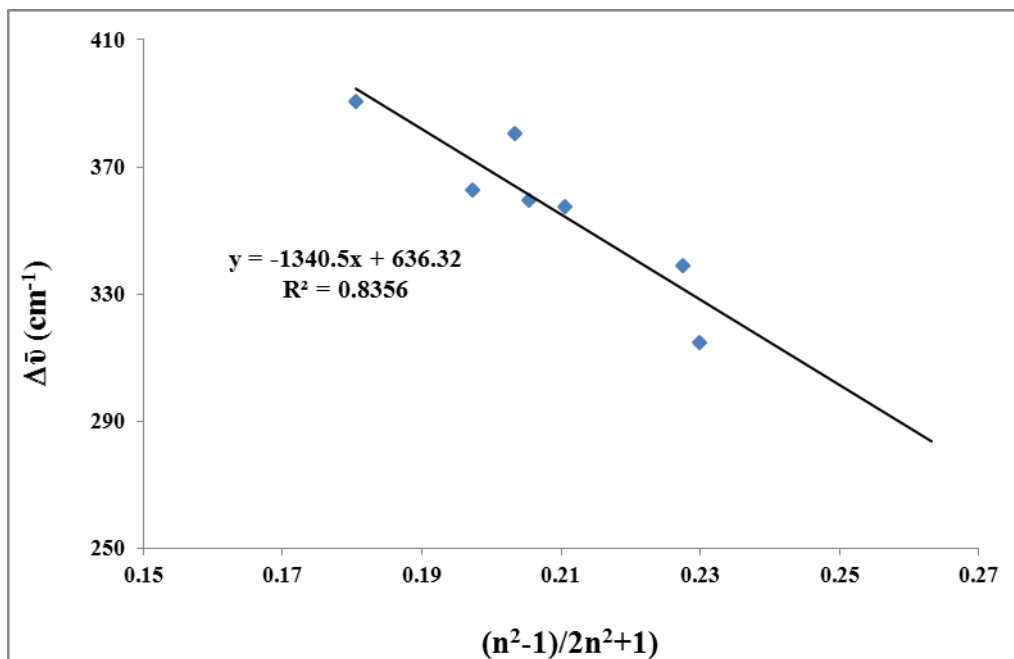


Figure 3. Dependence of ZnTBP's Stokes shifts on solvents' refractive index functions

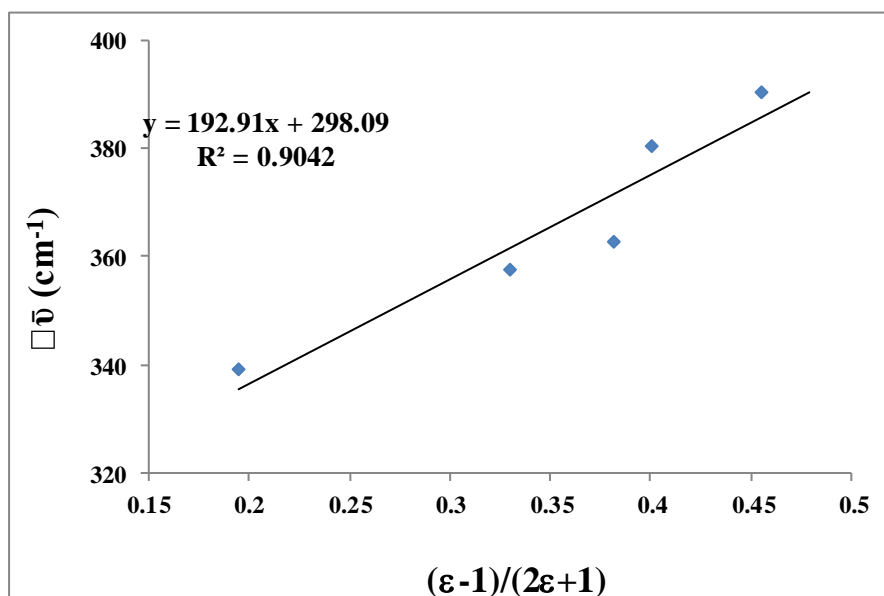


Figure 4. Dependence of ZnTBP's Stokes shifts on solvents' dielectric constant functions

The linearity of these plots is usually regarded as the proof for the overriding significance of the general solvent effect in spectral shifts. The plot of Stokes' shift ($\Delta\bar{\nu}$) versus solvent polarity

(Lippert) function $\frac{\epsilon-1}{2\epsilon+1} - \frac{n^2-1}{2n^2+1}$ is also shown in Figure 5.

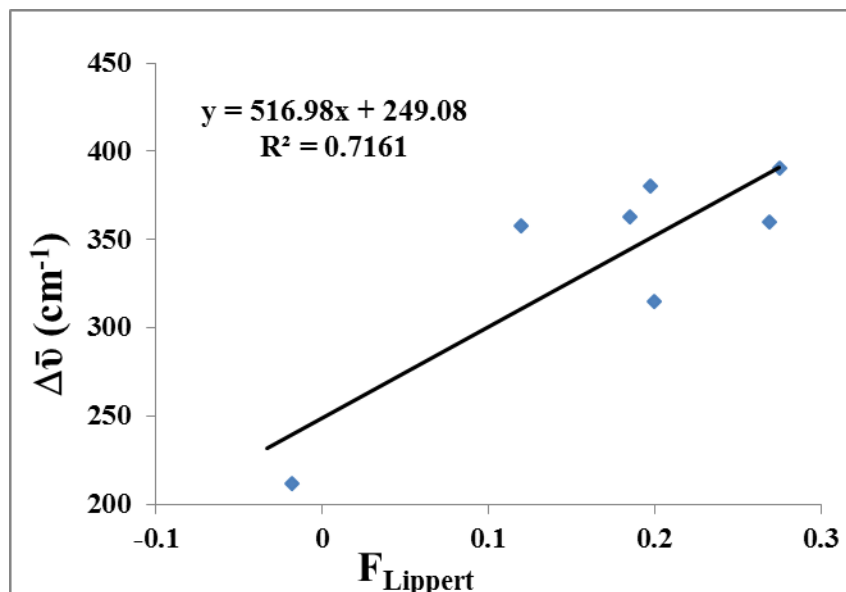


Figure 5. Dependence of ZnTBPC's Stokes shifts on solvents' polarity (Lippert's) functions

The refractive index and the dielectric constants have opposite effects on the Stokes' shift; and the low correlation coefficients of these plots suggest specific solvent effects. The dielectric constant of a solvent depends on both electronic and molecular motions, but a reorientation of the solvent dipoles as well as redistribution of the electrons in the solvent molecules around the excited state occurs; hence an increase in dielectric constant results in an increase in Stokes' shift (Figure 4). On the other hand, the refractive index (n), which depends on motion of electrons within the solvent molecules, accounts only for the redistribution of electrons; and an increase in refractive index decreases the energy losses in the absorption band (Figure 3).

Ground- and excited-state dipole moments of ZnTBPC

Metallation and ring substitution are among the factors that could impart non-planarity, and therefore appreciable polarity unto the Pc skeleton. In the present study, the protrusion of the central metal (zinc) 45 pm out of the aromatic ring plane [37, 38], coupled with the presence of *tert*-butylphenoxy substituents should impart a considerable dipole moment on the molecule. The dipole moments of a molecule in the ground state and an excited state depend on the electron distribution in these states. The excited state dipole moment reveals information on the electronic and geometrical structures of the molecule in the transient excited-state.

Figures 6-8 show the plots of $\Delta\bar{\nu}$ vs F_1 ; $V_A + V_F/2$ vs F_2 ; and $\Delta\bar{\nu}$ vs E_T^N (with corresponding slopes m_1 , m_2 and m , respectively); resulting from the analysis of solvatochromic data. The slopes of the respective plots are $m_1=201.6$; $m_2=1288$ and $m=574.4$ (Table 2).

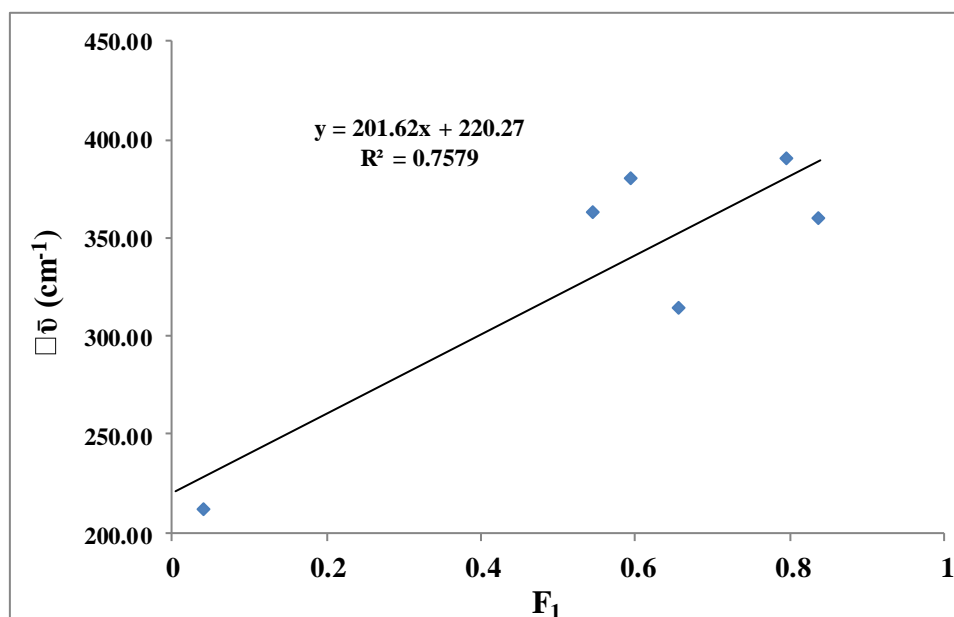


Figure 6. Plot of ZnTBPC's Stokes' shift on the Bakshiev's solvent polarity function (F_1 , Eq. 3)

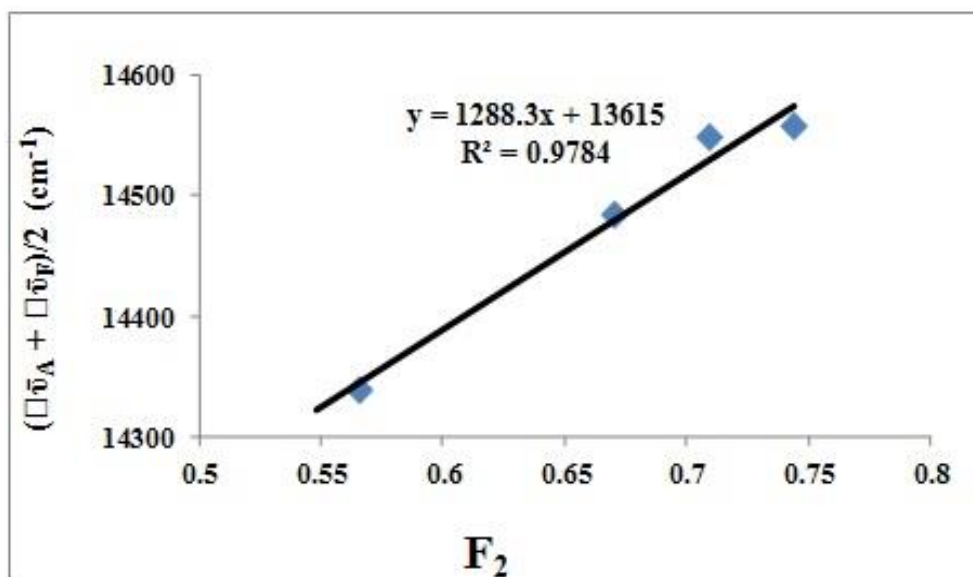
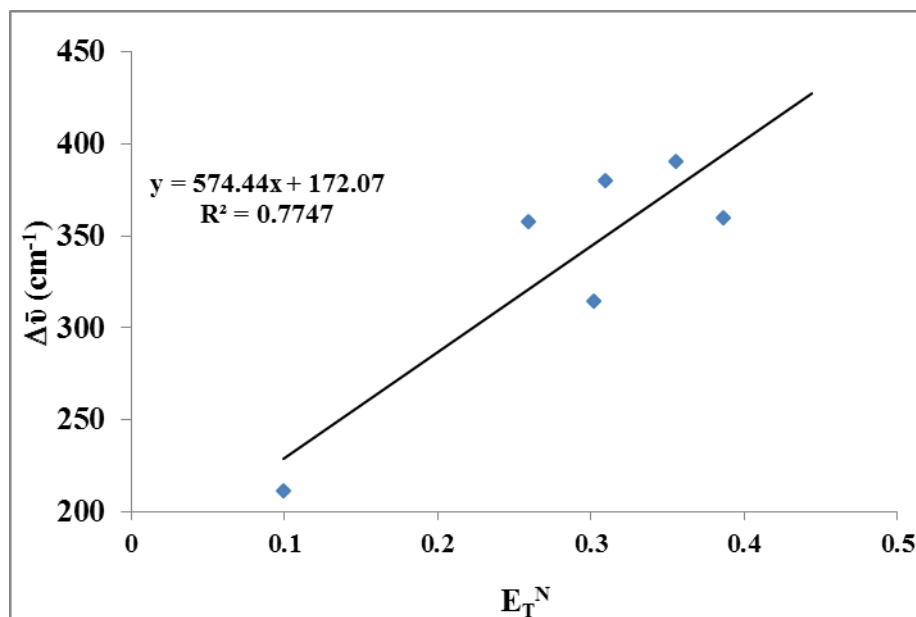


Figure 7. Plot of ZnTBPC's Stokes' shift on the Kawski-Chamma-Viallet's solvent polarity function (F_2 , Eq. 4)

Table 2. Solvatochromic data for the determination of ground state and excited state dipole moments of ZnTBPC

	$\Delta\bar{\nu} / \text{cm}^{-1}$	$(\bar{\nu}_a + \bar{\nu}_f) / \text{cm}^{-1}$	F_1	F_2	E_T^N	m_1	m_2	m
Acetone	390.49	14730.13	0.794838	0.641799	0.355	201.6	1288	574.4
THF	362.88	14611.46	0.545062	0.54833	0.207			
DCM	380.34	14537.37	0.593189	0.584323	0.309			
DMF	359.72	14547.68	0.836622	0.710003	0.386			
Chloroform	357.64	14505.47	0.377364	0.490906	0.259			
DMSO	211.89	14556.81	0.840533	0.744045	0.444			
Toluene	211.89	14558.01	0.039009	0.354939	0.099			
Benzene	339.05	14547.68	0.004487	0.340258	0.111			
Pyridine	314.64	14483.97	0.654882	0.670605	0.302			
1-CN	390.61	14339.58	0.290813	0.566329	0.194			

$(\mu_e/\mu_g)=1.37$, $(\mu_e-\mu_g)=2.32\text{D}$, $\mu_g=2.14\text{D}$, $\mu_e=4.46\text{D}$

**Figure 8.** Plot of ZnTBPC's, Stokes' shift on the molecular-microscopic solvent polarity parameter (E_T^N , Eq. 9a)

The ratio of excited state to ground state dipole moments of ZnTBPC (μ_e/μ_g) is 1.37; while the difference between the ground and excited state dipole moments ($\Delta\mu$) is 2.32D. The values of ground state and excited state dipole moments were then calculated to be $\mu_g=2.14\text{D}$, and $\mu_e=4.46\text{D}$ (Table 2), signifying a significant reorganization of the π -electron densities in the more polar excited state. When a molecule is excited, its dipole moment changes because of the change in

electronic distribution of the molecules. A sizeable intramolecular charge transfer in the excited state makes the molecule more polar in this state as compared to the ground state.

It is of interest to note that the values of μ_g and μ_e determined for ZnTBPC are significantly greater than those obtained for ZnPc ($\mu_g=1.50D$; $\mu_e=3.12D$) in an earlier work [19]. In ZnPc, it was suggested that the drop in symmetry from D_{4h} to C_{4v} in the molecule is responsible for its observed polarity. Even in the C_{4v} symmetry, the molecule could not have had a component of the dipole moment perpendicular to the symmetry axis, but only parallel to the molecular axis.

In ZnTBPC however, the additional polarity could have arisen from the non-symmetrical arrangement of the *tert*-butylphenoxy substituents at the peripheral positions of the molecule. It has been proposed that ZnTBPC is a mixture of isomers; a peripheral substituent could be attached to either position-2 or position-3 of the Pc ring; hence at any given time, the substituents may not be symmetrically positioned.

Conclusions

In conclusion, this work presents a semi-empirical estimation of the ground- and excited-state dipole moments of ZnTBPC using the solvatochromic shift method. The linearity of the plots of Stokes' shifts against the refractive index, dielectric constant and polarity functions is usually regarded as the proof for the overriding significance of general solvent effect in spectral shifts. The electronic absorption spectra of ZnTBPC showed that the Q bands are not as sharp as those observed for unsubstituted zinc phthalocyanine (ZnPc) in the same solvents, which was attributed to steric effects from the substituents and the existence of ZnTBPC as a mixture of isomers. In this work, it has been suggested that metallation and ring substitution could impart non-planarity, and therefore appreciable polarity unto the Pc skeleton. The appreciably higher dipole moment of ZnTBPC in the excited singlet state ($\mu_e=4.46D$) than in the ground state ($\mu_e=2.14D$) implies that charge separation is higher in the excited state than in the ground state. Some solvents were left out of the plots leading to the evaluation of the dipole moments; it appears that specific fluorophore-solvent interactions cannot be overlooked in these treatments. The solvatochromic shift procedure for the estimation of the ground and excited state dipole moments is easily accessible as it involves only the measurement of absorption and fluorescence maxima; and so it is not void of inaccuracies due to approximations and oversimplifications.

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