

# Estimation of Dipole Moments and Quantum Yield of 5-chloro-2-methoxyphenyl Boronic Acid in Different Solvents Environment

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**Abstract** The Photophysical properties like ground state and excited state dipole moments, change in the dipole moment and fluorescence quantum yield of a boronic acid derivative 5-chloro-2-methoxy phenyl boronic acid (5CMPBA) are characterized. The study is carried out in various solvents at room temperature using absorption and steady-state fluorescence technique. The emission wavelength of 5CMPBA is quite sensitive to the polarity of solvents. With the increase in solvent polarity red shift or bathochromic shift of about 9 nm has been observed. The excited state and ground state dipole moments are estimated using solvatochromic shift method and effect of solvents on spectral properties of the molecule are investigated using Kamlet-Taft multiple linear regression approach. The changes in dipole moment ( $\Delta\mu$ ) are calculated both from solvatochromic shift method and microscopic solvent polarity parameter ( $E_T^N$ ), and the values are compared. The ground state dipole moment is also evaluated using quantum chemical calculations. The bathochromic shift of the emission spectra and the increase in the excited state dipole moment indicates  $\pi \rightarrow \pi^*$  transitions as well as the possibility of intramolecular charge transfer (ICT) character in the emitting singlet state of 5CMPBA. The relative quantum yield ( $\Phi$ ),

radiative and non-radiative decay constants are calculated using single point method. It is found that the quantum yield of the molecule varies from 11 to 64 % with the change in the solvent polarity indicating the dependency of fluorescence nature on the solvent environment.

**Keywords** Boronic acid derivative · Solvatochromic shift method · Dipole moment · Relative quantum yield

## Introduction

Boronic acids have emerged as one of the most useful class of organo boron molecules, with application in synthesis, catalysis, analytical chemistry, biology, and medicine [1]. Highly water soluble monoboronic acid probes display the more desirable OFF-ON fluorescence response. They show a remarkable sensitivity for glucose rather than fructose and galactose [2]. A wide range of boronic acid probes for the detection and determination of mono saccharides in contact lens polymers have been developed [3]. In chemical biology, boronic acids are used in the detection and sensing of peroxides, recognition and sensing of the tetra serine motif in protein, development of new MRI contrast agents [4]. Further, Boronic acids exhibit strong fluorescence in the UV and VISIBLE region which makes them suitable for used as colorants, dye laser media and as nonlinear optical chromospheres [5].

In this paper we present the behavior of 5CMPBA by means of UV fluorescence technique in different solvents environment and by determining the increase in the dipole moment, relative quantum yield, radiative and non-radiative decay constants. We have estimated the ground state and excited state dipole moments using solvatochromic shift

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5-chloro-2-methoxyphenyl boronic acid (5CMPBA)

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method. The solvatochromic method has been proved to be the most useful method to make both experimental and theoretical studies on ground state and excited state dipole moments [6–9]. The experimental results are analyzed using Lippert, Bakshiev, Chamma Viallet-Kawski, microscopic solvent polarity ( $E_T^N$ ) parameters and solvatochromic parameters given by Kamlet and coworkers [10–12]. The Theoretical calculations are carried out by using Gaussian 03 program [13, 14] to supplement the experimental results. We have adopted single point method for the determination of relative quantum yield [15, 16].

## Theory

### Dipole Moment

When a molecule absorbs UV light, its electrons get promoted from the ground state to higher energy state. In the ground state, the spins of electrons in each molecular orbital are essentially paired. The higher energy orbitals are designed as anti-bonding molecular orbitals. The highly probable transition due to absorption of quantized energy involves the promotion of one electron from the highest occupied molecular orbital (HOMO) to lowest available unfilled molecular orbital (LUMO). Hence the electron charge cloud around the atom or molecule is disturbed. This distortion of charge cloud produces a dipole in the direction of the incident radiation. On absorption of light either a dipole is created or destroyed. This leads to either increase or decrease in the dipole moment of the excited state compare to that of the 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 the short-lived state. An understanding of dipole moments not only helps one to get an idea of the charge distribution, it also provides information on the sites of attack by electrophilic – nucleophilic in some photochemical reactions. In addition it is a very useful probe for ab-initio calculations of the efficiencies of the related properties such as quantum chemical derivations, electron correlation treatments and the electron density distribution in the singlet and triplet states. The spectral shift caused internally by solvatochromic or externally by electrochromic forms the underlying basis of all the methods applicable till today for determination of the dipole moment of the singlet excited state.

In the literature for the solvatochromic shift method, there exist three formulae to determine excited state dipole moments of different molecules. These formulae were proposed by Lippert [17], Bakshiev [18] and Chamma - Viallet [19]. The three independent equations, which are derived on the basis of different assumptions, for the calculation of the

excited state dipole moments of the solute molecule are as follows.

Lippert's equation [17]

$$\bar{\nu}_a - \bar{\nu}_f = m_1 F_1(D, n) + const \quad (1)$$

Bakshiev's equation [18]

$$\bar{\nu}_a - \bar{\nu}_f = m_2 F_2(D, n) + const \quad (2)$$

Chamma-Viallet-Kawski's equation [19]

$$1/2(\bar{\nu}_a + \bar{\nu}_f) = -m_3[F_3(D, n)] + constant \quad (3)$$

Where,

$$F_1(D, n) = \left[ \frac{D-1}{2D+1} \frac{n^2-1}{2n^2+1} \right] \quad (4)$$

And

$$F_3(D, n) = \frac{2n^2+1}{2(n^2+2)} \left[ \frac{D-1}{D+2} \frac{n^2-1}{n^2+2} \right] + \frac{3}{2} \left[ \frac{n^4-1}{(n^2+2)^2} \right] \quad (6)$$

Where  $F_1(D, n)$ ,  $F_2(D, n)$  and  $F_3(D, n)$  are known as Lippert's polarity function, Bakshiev's polarity function and Chamma-Viallet-Kawski's polarity function respectively,  $D$  is the dielectric constant and  $n$  is the refractive index of the solvent. Also,

$$m_1 = \frac{2(\mu_e - \mu_g)^2}{hca^3} \quad (7)$$

$$m_2 = \frac{2(\mu_e - \mu_g)^2}{hca^3} \quad (8)$$

And

$$m_3 = \frac{2(\mu_e^2 - \mu_g^2)}{hca^3} \quad (9)$$

'h' being Planck's constant 'a' is the Onsager cavity radius and 'c' is the speed of light in vacuum. The parameters 'm<sub>1</sub>', 'm<sub>2</sub>' and 'm<sub>3</sub>' can be determined from absorption and fluorescence band shifts. The values of ground state dipole moment ( $\mu_g$ ) and excited state dipole moment ( $\mu_e$ ) from Eq. (7) to (8) can be given as.

$$\mu_g = \frac{m_3 - m_2}{2} \left[ \frac{hca^3}{2m_2} \right]^{1/2} \quad (10)$$

$$\mu_e = \frac{m_3 + m_2}{2} \left[ \frac{hca^3}{2m_2} \right]^{1/2} \quad (11)$$

Or

$$\mu_e = \left[ \frac{m_3 + m_2}{m_3 - m_2} \right] \mu_g \quad \text{for } (m_3 > m_2) \quad (12)$$

The plots of  $(\bar{\nu}_a - \bar{\nu}_f)$  and  $1/2 (\bar{\nu}_a + \bar{\nu}_f)$  versus solvent polarity functions are straight lines and their slopes are nothing but the parameters 'm<sub>1</sub>', 'm<sub>2</sub>' and 'm<sub>3</sub>'. The validity of the use of these equations is based on certain assumptions like considering both the dipole moments collinear and have same Onsager cavity radius in both ground and excited state. They do not consider the polarizability, hydrogen bonding effect and complex formation and also ignores molecular aspects of solvation. For understanding polarization dependence or hydrogen bonding effect on spectral characteristics, normalized value called microscopic solvent polarity  $E_T^N$  is employed which includes not only solvent polarity but also the protic hydrogen bond effect. The theoretical basis for the correlation as the spectral shift with  $E_T^N$  was proposed by Reichardt [20]

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

Where  $\Delta\mu_B$  and  $a_B$  are the change in dipole moment on excitation and Onsager cavity radius of molecule respectively of a betaine dye and  $\Delta\mu$  and 'a' are the corresponding quantities for the present solute molecule. The change in dipole moment ( $\Delta\mu$ ) can be evaluated from the slope (m) of the Stoke's shift versus  $E_T^N$  plot and it is given by

$$\Delta\mu = (\mu_e - \mu_g) = \sqrt{\frac{mX 81}{(6.2/a)^3 11307.6}} \quad (14)$$

### Kamlet-Taft Multiple Regression

Kamlet and co-workers suggested multiple linear regression approach to correlate various spectral properties like absorption maxima ( $\bar{\nu}_a$ ), emission maxima ( $\bar{\nu}_f$ ), Stoke's shift ( $\Delta\bar{\nu}$ ) and quantum yield ( $\Phi$ ) with the indices of solvents hydrogen bond donor (HBD) strength ( $\alpha$ ), Hydrogen bond acceptor (HBA) strength ( $\beta$ ) and solvent dipolarity/polarizability ( $\pi^*$ ) through the equation

$$y = y_0 + A\alpha + B\beta + C\pi^* \quad (15)$$

Where y is the desired spectral property,  $y_0$  is the corresponding spectral property in gas phase and A, B and C are the calculated values of HBD ability, HBA ability and dipolarity/polarizability respectively. The magnitudes of the values of these parameters are evaluated using multiple linear regression method. The signs of  $A\alpha$  and  $B\beta$  coefficients may vary from one compound to another.

### Quantum Yield

The fluorescence quantum yield ( $\Phi$ ) is the ratio of photons emitted through fluorescence to number of photons absorbed [4]. In other words the quantum yield gives the probability of the excited state being deactivated by fluorescence rather than by another, non-radiative mechanism.

$$\Phi = \frac{\text{photons}_{EM}}{\text{photons}_{AB}}$$

The quantum yield  $\Phi$  can also be described by the relative rates of the radiative  $k_r$  and non-radiative  $k_{nr}$  relaxation pathways, which deactivate the excited state.

$$\Phi = \frac{k_r}{k_r + \sum k_{nr}}$$

The quantum yield can be close to unity if the rate of non-radiative decay constant ( $k_{nr}$ ) is much smaller than rate of radiative decay constant ( $k_r$ ).

Quantum yields provide important information regarding excited electronic states, radiation less transitions, and coupling of electronic to vibronic states. Moreover they are used in the determination of chemical structures, sample purity, and appropriateness of laser media. While measurements of the "absolute" quantum yield do require more sophisticated instrumentation [21], it is easier to determine "relative" quantum yield of fluorophore by comparing it to a standard with a known quantum yield. The relative quantum yield measurements of samples using single point method include a standard reference. There are number of standard references available in literature [22]. The standard should be chosen to ensure maximum overlap of the absorption and emission between sample and reference. In our study we have taken Tryptophan in water at 20 °C as standard reference whose absorption maxima is 280 nm and quantum yield is 0.13 and measured the relative quantum yield of our solute molecule in different solvents especially in alcohols and alkanes. The general equation used in the determination of relative quantum yields from earlier research is given in Equation [23].

$$\Phi = \frac{\Phi_s F_u (OD_s) n_u^2}{F_s (OD_u) n_s^2} \quad (16)$$

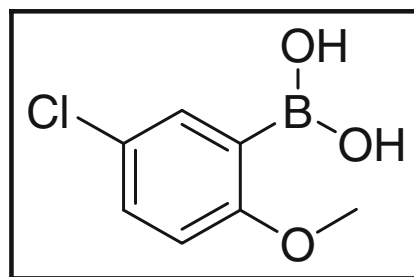


Fig. 1 Molecular structure of 5CMPBA

**Table 1** Photophysical parameters of 5CMPBA molecule in different solvents

Solvent	$\lambda_a$ (nm)	$\lambda_f$ (nm)	$F_1$ (D,n)	$F_2$ (D,n)	$F_3$ (D,n)	$E_T^N$	$\overline{\nu}_a - \overline{\nu}_f$ (cm <sup>-1</sup> )	$\frac{1}{2}(\overline{\nu}_a + \overline{\nu}_f)$ (cm <sup>-1</sup> )
TCE	293.00	328.30	0.1930	0.5478	0.6009	0.1600	3669.74	32,294.82
THF	292.50	325.50	0.2092	0.5495	0.5519	0.2070	3466.06	32,455.00
DMF	292.80	329.50	0.2753	0.8408	0.7215	0.3860	3803.99	32,251.01
EA	292.00	325.00	0.1740	0.4930	0.4990	0.2280	3477.33	32,507.90
DCM	294.15	328.00	0.2182	0.5952	0.5859	0.3210	3508.45	32,242.00
AN	292.43	328.72	0.3100	0.8700	0.6700	0.4600	3775.19	32,308.62
CYHX	292.55	320.45	-0.0350	-0.00213	0.2880	0.0060	2976.07	32,694.15
GL	294.00	332.22	0.2600	0.8400	0.7400	0.8120	3913.06	32,057.07
DMSO	292.6	329.00	0.2590	0.8420	0.7440	0.4440	3781.21	32,285.73

$\lambda_a$ =absorption maxima,  $\lambda_f$ =emission maxima,  $F_1$  (D,n) - Lippert's polarity function,  $F_2$  (D,n) - Bakshiev's polarity function,  $F_3$  (D,n) - Chamma Viallet – Kawski polarity function,  $E_T^N$  - Microscopic solvent polarity function

Where  $\Phi$ - quantum yield, F- integrated area under the corrected emission spectrum (in Ep units), OD- absorbance at the excitation wavelength, n- the refractive index of the solvent used and the subscripts u refer to the unknown and s refers to standard. Quantum yield is also given in terms of average life time ( $\tau_0$ ) and radiative decay rate constant ( $k_r$ ) as [1, 24]

$$k_r = \frac{\Phi}{\tau_0} \quad (17)$$

And the non-radiative decay rate constant is given by the equation

$$k_{nr} = \frac{1}{\tau_0} - k_r \quad (18)$$

## Experimental Methods

The molecule 5CMPBA was synthesized by standard methods [25]. Its molecular structure is as shown in Fig. 1. We have

used a wide range of solvents. The list includes tetrachloroethane (TCE), tetrahydrofuran (THF), dimethylformamide (DMF), ethyl acetate (EA), cyclohexane (CYHX), glycerol (GL) and dimethylsulphoxide (DMSO) for dipole moment measurements and methanol, ethanol, isopropanol, butanol, heptanol, hexane, heptane and decane for quantum yield measurements. They all are of HPLC grade and used without further purification. Water used for the preparation of standard solution in the relative quantum yield measurement is double distilled. The absorption spectra are measured at room temperature using Shimadzu UV –1800 Spectrophotometer with a wavelength accuracy of 0.5 nm. The concentration of the solution in all the solvents is kept as low as  $1 \times 10^{-4}$  mol L<sup>-1</sup>. The absorbance (OD) of the solutions at the excited wavelength is less than 0.15. The fluorescence intensities of the solutions are measured on Hitachi F-2700 Spectrofluorimeter in Dept. of Physics, MSRIT, Bangalore-54 at room temperature with perpendicular geometry. Fluorescence lifetime ( $\tau_0$ ) measurements are done using TCSPC nanosecond fluorescence lifetime spectrometer, ChronosBH, USA at USIC,

**Table 2** Radius of the molecule (a), calculated values of ground state ( $\mu_g$ ) and excited state ( $\mu_e$ ) dipole moments and change in the dipole moments

Solute	Radius (A <sup>0</sup> )	$\mu_g^a$ (D)	$\mu_g^b$ (D)	$\mu_e^c$ (D)	$\mu_e^d$ (D)	$\mu_e^e$ (D)	$\mu_e^f$ (D)	$\Delta\mu^g$	$\Delta\mu^h$
5CMPBA	3.4849	4.2480	0.1533	2.1856	3.6627	2.1860	1.2828	2.0323	1.1298

D=Debye= $3.33564 \times 10^{-30}$  cm=10<sup>-18</sup> esu cm

<sup>a</sup> Ground state dipole moment calculated using B3LYP functional with 6-31 g\* basis using DFT

<sup>b</sup> Experimental ground state dipole moments calculated from Eq. 10

<sup>c</sup> Experimental excited-state dipole moments calculated from Eq. 11

<sup>d</sup> Excited state dipole moments calculated from Lippert's Eq. 7

<sup>e</sup> Excited state dipole moments calculated from Bakshiev's Eq. 8

<sup>f</sup> Excited state dipole moments calculated from  $E_T^N$  parameter Eq. 14

<sup>g</sup> Change in dipole moments for  $\mu_e$  and  $\mu_g$

<sup>h</sup> Change in dipole moments calculated from  $E_T^N$  parameter Eq. 14

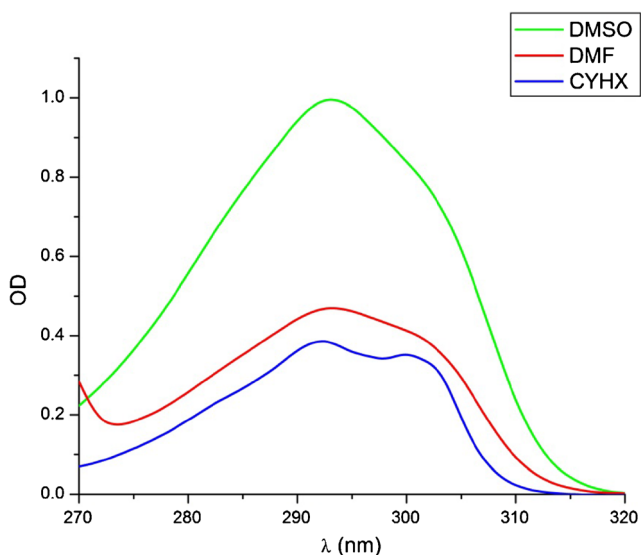


Fig. 2 Absorption spectra of 5CMPBA in different solvents

Karnataka University, Dharwad, India. Standard reference solution is prepared by dissolving Tryptophan in distilled water. The concentration of this solution is also kept at  $1 \times 10^{-4}$  M.

## Results and Discussions

### Solvent Effect on Dipole Moment

Typical absorption and emission spectra of 5CMPBA in different solvents are shown in Figs. 2 and 3. The Lippert's plot, Bakhshiev's plot and Kawski-Chamma-Viallet's plot and plot of Stoke's shift as a function of microscopic solvent polarity parameter ( $E_T^N$ ) are constructed for normal fluorescence spectrum of 5CMPBA. These plots are represented in Figs. 4, 5, 6 and 7. The least square fit analysis gives good correlation in each case. The values of slope (m) and correlation coefficient

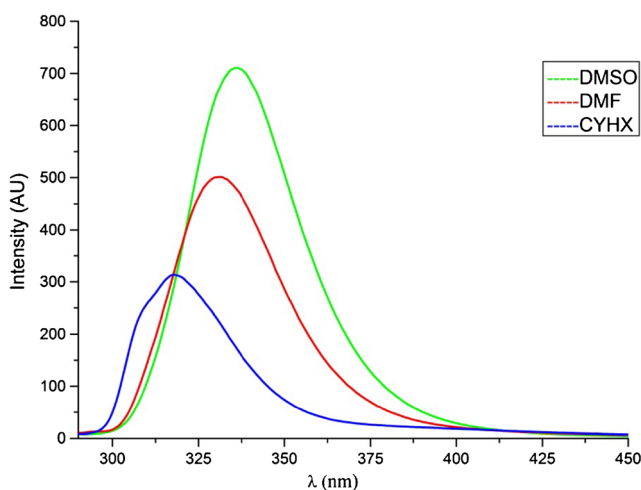


Fig. 3 Emission spectra of 5CMPBA in different solvents

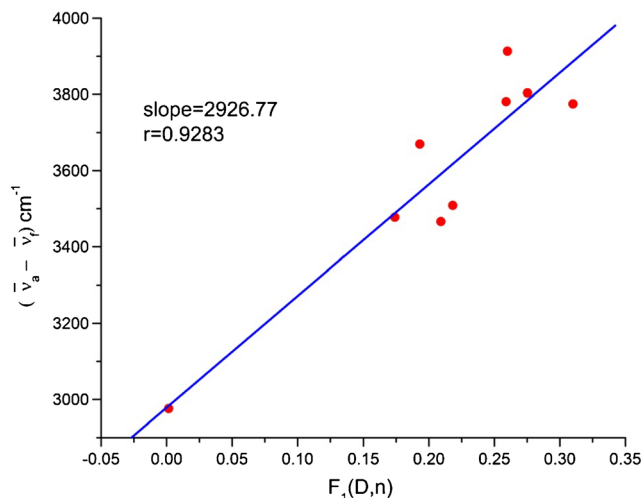


Fig. 4 Plot of Stoke's shift versus Lippert's solvent polarity function ( $F_1$ )

( $r$ ) are mentioned in the respective plots. The value of  $r$  is around 0.9 in the case of Lippert's plot, Bakhshiev's plot and Kawski-Chamma-Viallet's plot and about 0.8 in the case of plot of Stoke's shift versus  $E_T^N$ . We found in literature that the calculations done using this type of correlation values yielded good results [26]. The deviation from the linearity may be attributed to short range specific interactions between solute and solvents such as hydrogen bonding. Photophysical parameters like absorption maxima ( $\lambda_a$ ), emission maxima ( $\lambda_f$ ) and Stoke's shift ( $\bar{\nu}_a - \bar{\nu}_f$ ) in different solvents are presented in Table 1. The radius of the solute molecule is calculated from the molecular volume of molecule (<http://www.molinspiration.com/cgi-bin/properties>) and the ground state dipole moment is calculated using quantum calculations. These values are tabulated in Table 2. Further, the dipole moments calculated using above mentioned equations, changes in dipole moment ( $\Delta\mu$ ) calculated both from solvatochromic

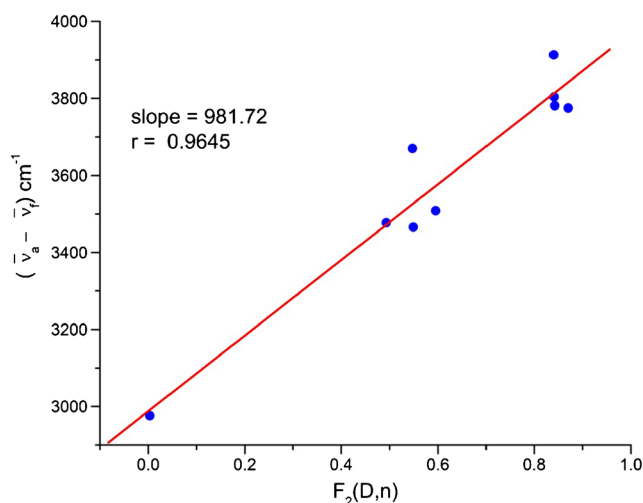
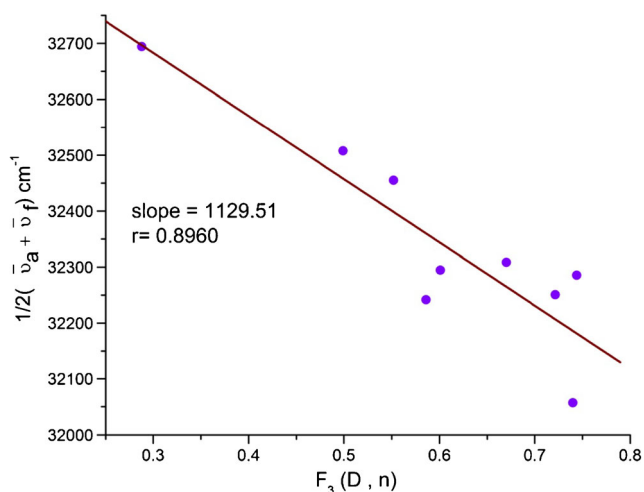


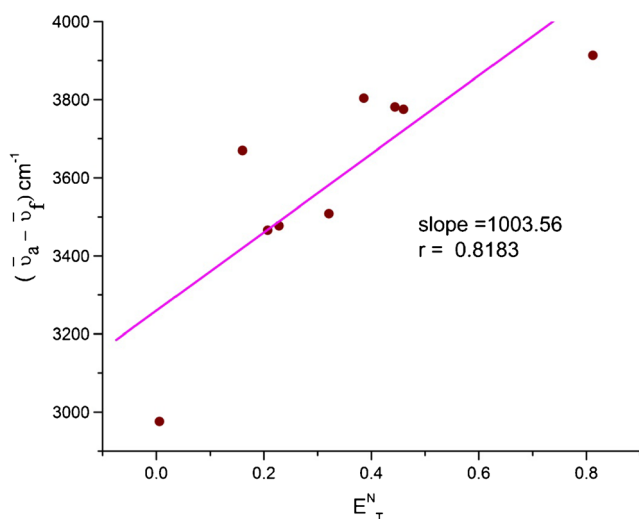
Fig. 5 Plot of Stoke's shift versus Bakshiev's solvent polarity function ( $F_2$ )





**Fig. 6** Plot of arithmetic mean of Stokes shift versus Chamma-Viallet-Kawski solvent polarity function ( $F_3$ )

shift method and microscopic solvent polarity parameter ( $E_T^N$ ) are also listed in Table 2. There is no observable change in the absorption maxima with the change in polarity of the solvent. However we have noticed a red shift in the emission peak with increase in the dielectric constant of the solvent. The emission peak shifts from 320 nm in CYHX, to 329 nm in DMF and DMSO. The shift could be attributed to the existence of hydrogen bond in the solute molecule (Fig. 8) as well as hydrogen bonding characteristics of solvents [9]. The Stoke's shift of  $805.14 \text{ cm}^{-1}$  from lower polar solvent to higher polar solvent indicates that there is a  $\pi \rightarrow \pi^*$  transitions. This could be due to marked difference between excited state charge distribution and ground state charge distribution. The increase in the dipole moment by about 3.51D in the excited state gives the evidence about the intramolecular charge transfer (ICT) [27] character in the emitting singlet state of 5CMPBA. The ground state dipole moment of this molecule is calculated by

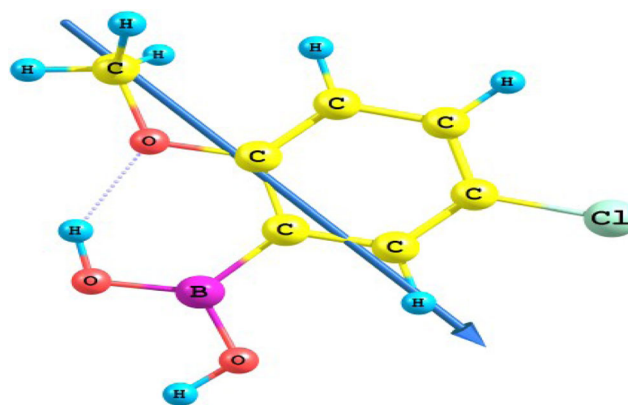


**Fig. 7** Plot of Stoke's shift versus  $E_T^N$  solvent polarity function

quantum chemical calculations using Gaussian 03 program on a Pentium- 4 PC and the basis set level used is B3LYP/6-31 g\*. Corresponding optimized molecular geometries of the molecule is shown in Fig. 8. The arrow mark indicates the direction of the dipole moment. The value of ground state dipole moment obtained using this model is 4.2480D. This kind of calculation assumes that molecules are involved in the gas phase and does not include solvent interactions [28].

### Solvent Effect on Relative Quantum Yield

We have adopted single point method for the determination of relative quantum yield of 5CMPBA. The solutions are prepared using above mentioned solvents. The concentration of the solution is kept as low as  $1 \times 10^{-4} \text{ M}$  in each solvent, in order to achieve the least absorbance or optical density ( $OD < 0.15$ ) and to avoid aggregation and dimer formation. For such a low concentration, the possibility of self-quenching can be ruled out. Each time a fresh solution is prepared using stock solution and the experiment is conducted at room temperature. Standard reference solution is prepared by dissolving tryptophan in distilled water. All the solutions including the reference are excited at 281 nm. The slit width, PMT voltage and scanning range are respectively 5 nm, 400 V and 280–600 nm. It is found that the optical density varies between 0.04 (in ethanol) to 0.13 (In decane). The absorption spectra and emission spectra of the molecule in methanol are as shown in Fig. 9. The corresponding spectra for the standard reference Tryptophan+water are as shown in Fig. 10. The life time decay profile in methanol is as shown in Fig. 11. The fluorescence integrated intensity is more in heptanol. The relative quantum yield in different solvent environment calculated using Eq. (16) and the values of radiative decay constant ( $k_r$ ) and non-radiative decay constant ( $k_{nr}$ ) calculated using Eqs. (17) and (18) are listed in Table 3. Absorbance (OD) and fluorescent integrated intensity of the standard reference are given at the bottom of Table 3. The relative quantum yield is found to be high in heptanol and heptane. This is further supported by more  $k_r$  and less  $k_{nr}$  values. It is found that as the



**Fig. 8** Optimised geometry of 5CMPBA

**Table 3** The values of Refractive index (RI), Absorbance (OD), Fluorescence integrated intensity ( $F_{int}$ ), excited state life time ( $\tau_0$ ), relative quantum yield ( $\Phi$ ),  $k_r$ , and  $k_{nr}$  of 5CMPBA

Solvents	RI (n)	OD	$F_{int}$	$\Phi$	$\tau_0$ (ns)	$k_r 10^9(s^{-1})$	$k_{nr} 10^9(s^{-1})$
Methanol	1.328	0.066	30,561.33	0.1823	0.525	0.3472	1.5575
Ethanol	1.361	0.040	30,251.96	0.3128	0.479	0.6530	1.4346
Isopropanol	1.386	0.090	23,139.59	0.1103	0.394	0.2799	2.2581
Butanol	1.399	0.080	34,434.08	0.1881	0.579	0.3248	1.4023
Heptanol	1.423	0.060	85,864.13	0.6470	0.494	1.3097	0.2358
Hexane	1.375	0.070	34,453.73	0.2078	1.160	0.1791	0.6829
Heptane	1.457	0.050	53,843.20	0.5104	0.910	0.5608	0.5381
Decane	1.408	0.130	65,575.13	0.2233	1.260	0.1772	0.6164

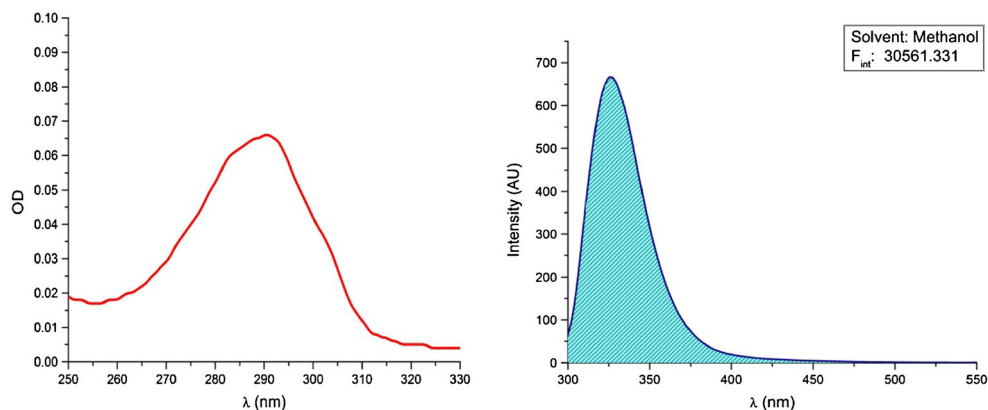
$(OD)_S=0.061, (F_{int})_S=19,988.44$

solvent polarity varies, the relative quantum yield varies from 11 to 64 %. This confirms that the excited energy states as well as fluorescence emission species of the studied molecule strongly depends on the solvent environment. The high values of  $\Phi$  and short  $\tau_0$  probably shows the absence of twisted intermolecular charge transfer (TICT) character in the excited state. Hence the fluorescence is from intramolecular charge transfer (ICT).

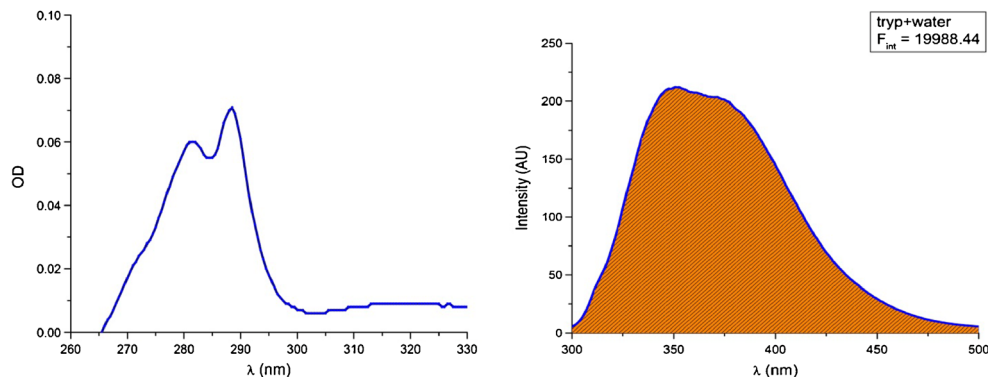
The molecule is examined for the individual contributions of HBD and HBA abilities of solvents on spectral properties.  $\bar{\nu}_f$  and  $\bar{\Delta\nu}$  values are correlated with Kamlet – Taft parameters  $\alpha$ ,  $\beta$  and  $\pi^*$  using multiple regression. The analyzed data with correlation co-efficient ( $r$ ) is given in the following equation.

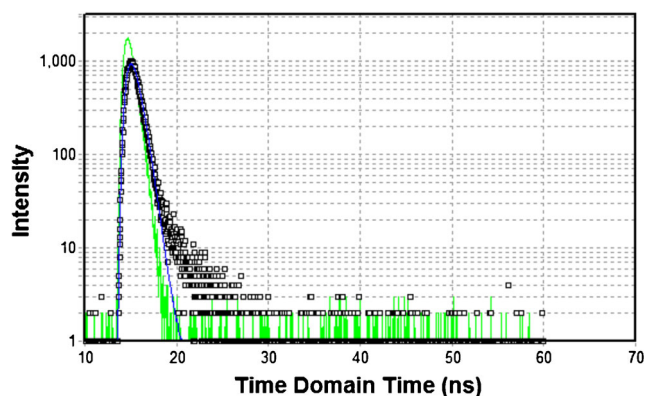
$$\left. \begin{aligned} \bar{\nu}_f(cm^{-1}) &= 31281.07 - 791.66(\alpha) + 7.68(\beta) - 706.86(\pi^*), r = 0.97 \\ \bar{\Delta\nu}(cm^{-1}) &= 3030.57 + 1269.10(\alpha) + 251.56(\beta) + 800.73(\pi^*), r = 0.98 \end{aligned} \right\} \quad (19)$$

**Fig. 9** Absorption (with  $OD < 0.15$ ) and emission spectra of 5CMPBA in methanol with fluorescence integrated intensity



**Fig. 10** Absorption (with  $OD < 0.15$ ) and emission spectra of standard reference (tryptophan in water) with fluorescence integrated intensity





**Fig. 11** Life time decay profile of 5CMPBA in methanol

From these equations, it is clear that the contribution of HBD ( $\alpha$ ) is higher than that of HBA ( $\beta$ ) in the studied molecule. The molecule is less subtle to HBA features of solvents as the value of  $\beta$  is low compare to  $\alpha$  and  $\pi^*$ . However, the contribution of nonspecific dielectric interactions (dipolarity/polarizability) cannot be neglected.

## Conclusions

The boronic acid derivative 5CMPBA shows a bathochromic shift. The bathochromic shift of the emission spectra and the increase in the excited state dipole moment indicates  $\pi \rightarrow \pi^*$  transitions as well as the possibility of intramolecular charge transfer (ICT) character in the emitting singlet state. We have estimated the relative quantum yield in alkane solvents as well as alcohol solvents and noticed the variation of quantum yield from 0.1103 to 0.6470 with the change in the solvent environment. This strongly suggests that the excited state energy levels of 5CMPBA are perturbed by the solvent polarity. The influence of HBD is more compare to HBA and nonspecific dielectric interactions.

## Compliance with Ethical Standards

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