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Journal:	<i>Canadian Journal of Physics</i>
Manuscript ID	cjp-2018-0116.R3
Manuscript Type:	Article
Date Submitted by the Author:	18-Jun-2018
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Keyword:	Electronic spectra, Kamlet-Taft, Catalan, Acidity Basicity, OLED
Is the invited manuscript for consideration in a Special Issue? :	Not applicable (regular submission)

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Photophysical Properties of Novel Fluorescent 1-(3-Hydroxy-benzofuran-2-yl)-benzo[f]chromen-3-one Derivative: Models for Correlation Solvent Polarity Scales

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Abstract

Photophysical and spectral properties of a new benzofuran derivative based fluorescent probe 1-(3-Hydroxy-benzofuran-2-yl)-benzo[f]chromen-3-one (1-HBBC) were considered in various parameters of solvents, making use of UV-Vis absorption and fluorescence emission spectroscopy. The absorption and fluorescence emission peak maxima were observed between 260-349 nm and 400-485 nm respectively, prompting stokes' shift between 13993 – 18495 cm⁻¹. Diverse solvent parameters have been utilized to understand the Solvatochromism of 1-HBBC. This information is applied to understand the effects of the solvent, on the shifting in the spectra of 1-HBBC and access the execution of empirical solvatochromic models: the well-known Kamlet-Taft model and two recent Catalan models. Linear solvation energy relationships proposed by Kamlet-Taft treatment for 1-HBBC molecule appealing as a molecule for hydrogen bond and solvent polarity properties has been exhibited, models offer good statistical execution for all solvents studied in this work. The general decency of fit for Benzofuran information about the models contractions whereas, these solvents are incorporated into the solvatochromic analysis. These reductions are comparable for the Kamlet -Taft and Catalan 4P models but

important for Catalan 3P model. Propositions portrayal can be abused for outlining new luminescent tests for nonpolar and polar microenvironment.

Keywords: Electronic spectra, Kamlet-Taft, Catalan, Acidity Basicity, OLED

1. Introduction

A deliberate examination of the solvent impacts is basic in the comprehension of the excited state conduct of the molecule. Some photophysical and photochemical qualities of coumarins were researched by few specialists [1-5]. These properties were contemplated as an element of centralization of the colour, thickness, polarizability polarity of the solvents and also the pH level of the solution. The solvent shifts can be elucidated as far as the general impact of the communication forces, which are fundamental of van derWaal's kind on the π electron arrangement of the molecules. It is notable that as the π electron system turns out to be less limited. The shifts in energy wind up little high and consequently brings about a bathochromic move (red shift) and its inverse impact offer to ascend to a hypsochromic move (blue shift). A band ($\pi \rightarrow \pi^*$) displays a red move when in the solvents of polarity get increases while $n \rightarrow \pi^*$ band demonstrates a blue move The solvent satisfies a few capacities amid a compound responses and reagents with the goal that they break up [6-10]. This encourages impacts between the reactants and reagents, that must happen to keep in mind the end goal to change the reactants to products. The solvents additionally give a method for temperature control, either to expand the energy of the impacting particles, so that they will respond all the more rapidly, or to retain warm that is created amid an exothermic response.

The Solvatochromic shifts were utilized for the determination of dipole moments in the excited state are reported [11-17]. The Solvatochromic shifts prove about the change in energy. Spectra of emission in this regard frequently more useful than the spectra of absorption since they are identified with the energy loss in the excited state. These exploratory perceptions of the solvent reliance on the energy of excited states should not be mistaken for the different speculations of Solvatochromic shifts. Such hypotheses are intriguing on the ground state that they attempt to correlate the Solvatochromic shifts to the dissemination of the electron when the probe is in the excited states, particularly to the aggregate dipole moments as well as to the normal polarizability. This information is imperative for the portrayal of the intramolecular

charge transfer in the molecule excited states and also intermolecular charge transfer in exciplexes.

Among the different nitrogen-containing heterocyclic compound, quinolines happen predominately in nature apparent to their dependability and simplicity of the era. The heterocyclic compounds are broadly disseminated in nature. For instance, sugars and their subordinates exist to a great extent as five membered (furan) or six membered (pyran) ring containing one oxygen particle. The vitamin B aggregate contain heterocyclic ring with nitrogen. The anti-infection agents including penicillin additionally have a heterocyclic moiety. An expansive number of manufactured heterocyclic compounds have profitable properties as, antiviral, invigorating, antimicrobial, pain relieving chemotherapeutic operators, dyestuffs, copolymers, and so on. The Benzofuran is moderately less investigated at the point when contrasted with other heterocyclic frameworks. And still, voluminous work has been done on Benzofurans and a few monographs committed to the investigation of both regular and manufactured Benzofurans have shown up in writing [18-22]. The physicochemical and hypothetical examinations of Benzofurans based 1-HBBC (1-(3-Hydroxy-benzofuran-2-yl)-benzo[f]chromen-3-one) pull in unique consideration close to their properties of excited and ground state, as a result, the nearness of acceptor and donor moieties in 1-HBBC. The solvents can essentially impact the substance and physical characteristics of the solute. The solvents actuate resolves in the electronic transition of solutes (Solvatochromism) in view to the nature and the degree of the solute solvent connections in the ground and first excited energized conditions of solutes [23-25].

1-HBBC in various solvents by utilizing diverse experimental Solvatochromic model to try the association between 1-HBBC with perfect solvents. The distinctive Solvatochromic were used like that of the Dimorth model [26, 27] Lippert model [28, 29] Kamlet–Taft model [30, 31], Catalan 3P model [32, 33] and Catalan 4P model [34] to go through the impact of the specific and non-specific interaction of molecules with these encompassing solvents. The Kamlet–Taft model exhibits particular solute solvent hydrogen bonding associations to account, in which Dimorth and Lippert simulates are barred. The Kamlet–Taft classic considerations π^* , a , b are comparative with these SPP, SA, SB parameters of Catalan 3P. The Catalan model in particular is utilized to recognize the specific and non-specific solvent-solute relation from models Kamlet–

Taft. Also to be noted is that the Catalan model gives appropriate outcomes in nearness of non-polar or similarly solvents of fewer polar properties. The utilization of various models Solvatochromic, on the frequency spectra of 1-HBBC, confer the best learning to appreciate the solute solvent dynamics [35, 36].

Benzofuran derivatives are additionally of significance for morphological functionalization [37, 38]. Therefore, the comprehension of the impact of environment polarity on the UV/Vis absorption property is likewise to modify the structure of the molecule for a particular application [39]. The aim of this work is to know the solvent impacts on the position of the UV/Vis absorption band of a progression of Benzofuran derivatives to demonstrate and the sort of solvent interaction instigates a revealing shift on the position of the absorption spectra. In this work, we report an orderly Solvatochromic investigation of the photophysical properties of Benzofurans based 1-HBBC for the first time, in various solvents polarity parameters. We have additionally exhibited the specific and non-specific interaction of 1-HBBC with a few perfect solvents utilizing distinctive observational Solvatochromic models.

2. Material and Methods

The Benzofuran derivative 1-(3-Hydroxy-benzofuran-2-yl)-benzo[f]chromen-3-one (1-HBBC) was synthesized in our laboratory (Fig.1), the detailed synthesis method are reported [1, 40] and was vacuum dried up finished 1-HBBC before the utilization since the hygroscopic idea of the compound. All solvents including acetone, acetonitrile, chloroform, dichloromethane, N,N-dimethylformamide (DMF), 1,4-dioxane, ethanol, methanol, ethyl acetate, chloroform, propanol, hexane, ethyl benzoate and tetrahydrofuran were of HPCL grade of 99.9% purity. The solvents used in this study grouped as polar protic, polar aprotic and non-polar solvents. Solvents were acquired from business providers were of spectroscopic virtue and utilized as gotten. Estimation of 1-HBBC solution, an industrially accessible double beam high determination UV/vis spectrophotometer (Shimadzu UV-1800 spectrophotometer) was utilized to decide the maximum peak position of the transition for 1-HBBC in the solvents. The solvent was set in a 1cm quartz reference cuvette, a little measure of 1-HBBC was set in the coordinated cuvette sample and filled with a solvent. The arrangement in the cuvette sample was stirred up to the point that a consistent value absorbance is required.

The stock solution of samples was prepared independently in every solvent and afterwards diluted to the concentration 2.5 μM . Every solution was scanned in the spectrum range of 330-600 nm and every solution have been performed at the room temperature. 1-HBBC solution was then diluted with the solvent to alter the absorbance value to in between the 0.2 and 1.8 units of absorbance. The spectrum range of 1-HBBC in different solvents was scanned at a resolution of 0.05 nm for every information point. The maximum peak was resolved by a peak recognition calculation of the spectrophotometer programming and visual affirmation by the administrator utilizing an unsmoothed spectrum range. All spectra are determined for 1-HBBC in every solvent and the average value of the maxima peak absorption computed. Fluorescence emission estimations were recorded on (Hitachi F-2700 fluorescence spectrophotometer) utilizing 1.0 cm quartz cells and matched double silicon photodiode detectors. The concentration used was 2.5 μM for Solvatochromism contemplate. The values of dielectric constant ' ϵ ', refractive index ' n ' and Solvatochromic parameters ' α , β and π^* ' were collected from literature [41]. Fluorescence quantum yields (QY) were obtained by integrating the area under the fluorescence curves using the following equation,

$$QY = QY_s * \left[\frac{A_u}{A_s} \right] * \left[\frac{F_s}{F_u} \right] * \left[\frac{n_u}{n_s} \right]^2$$

where ' A_u ' is the area under the fluorescence spectral curve, ' F_u ' is optical density of the compound at the excitation wavelength and n_u was the refractive indices of the solvent. In this equation, the subscripts u and s denotes sample and standard. This, we used Tryptophan (quantum yield is 0.13 in water) [23, 60] as quantum yield standard for measuring the quantum yields of 1-HBBC at 280 nm and we measured the relative quantum yield of studied the sample in different solvents and the results are presented in Table 1.

3. Results and Discussion

3.1 Influence of solvents on the UV/Vis absorption spectra

Absorption spectra of 1-(3-Hydroxy-bezofuran-2-yl) benzo[f]chromen-3-one (1-HBBC) were measured at 25° C in fifteen solvents of different polarities in the range of 200-700 nm and Fig. 2 shows the Uv-vis absorption spectra of chosen compound. The absorption maxima of 1-

HBBC and Solvatochromic shifts $\Delta\nu$ for all studied solvents in this experiment are tabulated in Table 1. In this study, the solvents are distinguished as three types of solvents commonly encountered: nonpolar, polar protic and polar aprotic. Solvents selection are made based on their dielectric constants. On increasing the solvent polarity, from non-polar to polar solvent, the absorption spectra of 1-HBBC shows redshift. Along with redshifts, the molecule shows splitting in the absorption band, this is due to hydrogen bond arrangement and deprotonation. This shows exceptionally solvation behaviour of the benzofuran derivatives as a component of the encompassing intermediate. The positions of the UV/Vis maximum wavelength of absorption positions are free from the compound concentration. As the dielectric constant of the solvent increases, the wavelength of maximum absorption peak slowly shifts to the red, whereas the splitting nature remains same. We observed that the absorption peak positions of 1-HBBC in all solvents are very contrast to that of non-polar to polar solvents. Because, of its extremely weak dissolvability in nonpolar solvents indicates little absorbance value of 1-HBBC is indicated. Its interaction with non-specifically to non-polar solvents, having non-hydrogen bond and in this manner do not influence charge exchange character. The spectral shift of 1-HBBC absorption peak position and their shape remain practically identical if there has to arise an occurrence of non-polar solvents like 1,4-dioxane, chloroform and hexane. Krystkowiak et al. recently [42] revealed a definite report on 6-amino coumarin with non-specific interactions with non-polar solvents.

In polar condition, the marginal change in peak positions of absorption spectra is owing to more degree stabilization in the excited state of 1-HBBC. The intermolecular hydrogen bond forming ability in the presence of π -electrons between 1-HBBC and polar solvent is responsible for bathochromic shifting in UV/Vis absorption spectra. The largest red shift of UV/Vis absorption maxima is noticed in polar protic solvents like $\lambda_{\max} = 260$ nm for butanol and polar aprotic solvent say $\lambda_{\max} = 349$ nm for tetrahydrofuran. The Stoke shifts of the UV/Vis absorption bands are positive Solvatochromic with scales of $\Delta\nu = 13993 - 18495 \text{ cm}^{-1}$, this may be due to π - π^* electronic transition. Banibarata Maity et al. [36] recommended that, this kind of behaviour does not just depends upon their solvent properties (dielectric constant values). The Stokes shift $\Delta\nu = \nu_{\text{absorp}} - \nu_{\text{emiss}}$ ($\Delta\nu = [2(\mu_e - \mu_g)^2 / hca^3] \Delta F + \text{const.}$) of identical energized transits has been related with directional polarizability $[\Delta F]$ of the solvents accordingly, $\Delta F = [(\epsilon-1) / (2 \epsilon +$

1) $-(n^2 - 1) / (2n^2 + 1)$] where, ν_{emiss} (in cm^{-1}), ν_{absorp} (in cm^{-1}) denotes the wavenumber for maxima emission and maxima absorption of spectra respectively, μ_g and μ_e denotes the ground and excited electronic states of dipole moments respectively, 'h' Planck's constant, 'c' speed of light in vacuum, 'a' is the radius of Onsager cavity for molecule. The plots of absorption maximum versus solvent directional polarizability (ΔF) for sample with different solvents are shown in Fig. 3. For 1-HBBC plot indicates linear dependency with residual square $R^2 = 0.912$ that evaluates the Lippert-Mataga relation, which includes solvents like 1,4 Dioxane, Hexane, Butylacetate, Ethylacetate and DMF. The widespread character of few groups is apparently because of blending of the lowest electronic condition of the hydrogen reinforced complex with distinct electronic states, due to charge exchange from the electron donor particle. It is also found in Table 1, the results show lower values of the relative quantum yield. These observations can be described as follows, Benzopyran basically has a lower quantum yield, but appropriate substitution leads to the fluorescent compound blue green region of wavelength. The substitution in position 4 leads to more fluorescent nature. because there is no substitution in position 4 in our studied compound, the relative quantum yield may be less in value [61].

3.2 Influence of Solvents on the Fluorescence emission spectra:

The fluorescence emission spectra of 1-HBBC in non-polar, polar protic and polar aprotic solvents are shown in Fig. 4. These spectra companions indicate the absorption spectra and reveal the nearness of dual peak. Excitation spectra checked at the wavelength of maximum emission of all these dual peaks are indistinguishable and this indicate that both peaks arises as the same electronic states are likely vibronic. From nonpolar solvents to polar solvents 1-HBBC in hexane is 408 nm, whereas in polar solvent of butanol it is 488 nm and the emission peak position of 1-HBBC in butanol is on small scale redshift contrasted to methanol. The relationship with other polar protic solvent, the stability of intermolecular charge transfer character of benzofuran in existence of butanol is upgraded because to the value of dielectric constant. From literature, butanol is the higher polar solvent compared to methanol [43, 44], comparable kind of behaviour of coumarins was likewise revealed in the reviews [45, 46]. When the solvent polarity is increased, the fluorescence emission peak position of 1-HBBC experiences (85 nm) bathochromic shifts from non-polar to polar solvents, directing that the π - π^* transition is included. In nonpolar solvents the Stokes shift (85 nm) is not as much as that in polar solvents

(54 nm), demonstrating that 1-HBBC experiences a less affected conformational change upon electronic excitation, these observations follow the same trend for other Solvatochromic coumarins in non-polar solvents are believed to show Twisted Intermolecular Charge Transfer (TICT) character [47, 48]. In reality, the state TICT is only stabilized in polar solvents, rather it is understood that a locally excited state from where emission happens, is a state that develops directly upon excitation state in direct and occurs promptly without any solvent role [1, 23].

In this manner, the wavelength of Uv/Vis absorption and fluorescence emission are quite large in nonpolar solvents and Stokes shift are substantially lower compared to polar solvents. Increasing solvent polarity of the surrounding media in 1-HBBC the absorption and emission peak is redshifted (Table 1). Thus, within the sight of polar solvents, the Twisted Intermolecular Charge Transfer state formation of 1-HBBC is favourable [36, 49, 50]. From increasing the solvent polarity promotes improve the capacity Intramolecular Charge Transfer (ICT) character of the excited state of 1-HBBC, thus delocalising the charge within the sight of molecules of a polar solvent. In addition, very high polar solvents with the energetic character of hydrogen bond acceptor encourage the charge separation in 1-HBBC. An analogous plot of fluorescence max. versus directional polarizability (ΔF) (Fig. 5) for 1-HBBC too reveals a nearly linear dependency with residual square $R^2 = 0.833$ when Hexane, Chloroform, Butylacetate, Decanol, Propanol, Butanol and Ethanol are accommodated. The plot of Fig. 6 Stokes shift ($\Delta\nu$) versus solvent directional polarizability (ΔF) for sample in chosen solvents for 1-HBBC plot indicates linear dependency with residual square $R^2 = 0.934$, that evaluates the Lippert-Mataga relation, which indicates solvents like Tetrahydrofuran, Acetone, DMF, Ethanol, Acetonitrile and Methanol. Hence, hereby linearity affirms that the gradient relies upon the modifications in electric dipole moment takes place upon excitation.

3.3 Different Solvatochromic model analysis

We have examined the Solvatochromic investigation of 1-HBBC within the sight of different solvents using Solvatochromic models which deals the solute-solvent interaction. We used Kamlet-Taft (KT) model [27]

$$\nu = \nu_0 + s\pi^* + a\alpha + b\beta \quad (1)$$

where ' ν ' is the spectral peak frequency molecule in solvents, ' ν_0 ' for frequency peak position of the solute in vapour state, ' π^* ' signifies polarity, ' α ' for hydrogen bond donor (HBD) and β for hydrogen bond acceptor (HBA) properties of the solvents ' s ,' ' a ' and ' b ' are the coefficients obtained from linear regression method. Solvents parameters ' π^* ', ' α ' and ' β ' are taken from literature report [51]. The second model Catalan 3P [32] Solvatochromic

$$\nu = \nu_0 + c_{spp} SPP + c_{sa} SA + c_{sb} SB \quad (2)$$

where ' ν ' remains for the peak frequency of the molecular spectra in the solvent, ' ν_0 ' is solute peak frequency of in vapour state. SPP, SA and SB signify also for solvent polarity parameters, Solvent Acidity and Solvent Basicity parameters Catalan respectively. The values of c_{spp} , c_{sa} and c_{sb} co-efficient are derived by multilinear regression method.

The last Catalan et al. [34] indicated the solvent polarity parameters (SPP) in addition to new two parameters are modified as solvent polarizability (SP) and solvent dipolarity parameter (SDP). Concurring into Catalan 4P model,

$$\nu = \nu_0 + C_{sp} SP + C_{sdp} SDP + C_{SA} SA + C_{SB} SB \quad (3)$$

The values of c_{sp} , c_{sdp} , c_{sa} and c_{sb} coefficients are acquired by multiple linear regression method.

In this section, the classification of solvents was done as two Groups A and B based on the energies, frequency transition sorts and solvents that are used in this study. In first Group A, the solvents exclude solvents which are free from either benzene ring (or) chlorine atom it should be noted in Group A, solvents whose polarizability are slightly different from aromatic and polychlorinated solvents, are used to represent the effect of nonhydrogen bond and of specific solvent effects. In second, Group B includes all solvents in this investigation used aromatic, polychlorinated solvents are also added.

3.4 Assessment of Solvatochromic models for 1-HBBC in Group A solvents

In the Group A solvent, the transition energy according to Moog et al. [52]

$$\nu = \left(\frac{\frac{1}{\lambda_S} + \frac{1}{\lambda_L}}{2} \right) \quad (4)$$

where ' λ_s ' and ' λ_L ' corresponds to the shorter wavelength and longer wavelength for the spectra of absorption (or) fluorescence is equivalent to half of its peak intensity. Based on the Group A solvent which Moog's apprizes, the energies transition of 1-HBBC are obtained using Eq. (4) in 14 non-aromatic and non-chlorinated solvents. Computing the transition energy along these lines, as opposed to specifically utilizing the $1/\lambda_{\max}$ thinks about of coneruiable changes of the shapes of 1-HBBC, diffused within the various solvents [53-55].

In any case, marginally difference solvent constant in the Kamlet-Taft model is adopted as part of our analysis. Regression coefficient analysis of steady state absorption maximum and fluorescence maximum peak along with three empirical Solvatochromic models within the sight of Group A solvent accords best statistical results as summarized in Table 2. A statistically treatment of each of three models shows phenomenal execution with Adj R^2 averaged at 0.921, 0.952 and 0.993 respectively. Their decency of fitting is comparable with each other. From the consequences of all three models have the negative co-efficients related for π^* , Spp, SP and SdP proposing a general red spectral shift of 1-HBBC as greater solvent polarity. In all cases negative co-efficients for SA showing 1-HBBC capable of performing as HBA and coming about 1-HBBC solvent interacts considering the decrement of transition energies. The zero terms in Kamlet-Taft and Catalan 3P model clearly suggest that interaction between 1-HBBC and HBA solvents, this confirms the presence of HBD moieties has in 1-HBBC compound. Das et al [56], found the same trend results for C35 laser dye. From the above, the ability of hydrogen to donate 1-HBBC at the ground and excited state must be zero because of the vacancy of a hydrogen atom. We found that, from Table 2, the co-efficients of 'b' term in the ground and excited state value is zero. The high total value of 'b' term in the excited state looks quiet stranger due to the inconceivability of hydrogen formation, where the molecule gives hydrogen bond to the solvents for accepting its nature. The presence of non-zero 'b' parameter additionally revealed in the article [56, 52], where the solute molecule does not contain hydrogen bond for concurrence in hydrogen bond interaction.

There are three unexpected terms in C_{SB} in the best fit condition got from Catalan 3P and Catalan 4P model as highlighted in bold fonts in Table 2. Interestingly, statistical analysis associated with physical approval based on absolute solvent-solution interactions prompts diverse dependable results. Along with these lines which increases the agreement of Moog and

coworkers by forcing the unphysical parameters that fit to zero and that afford a view of the modified parameters in Table 3. This requirement inconvenience around different issues related to these three Solvatochromic models. For instance in the fluorescence data of 1-HBBC, in the fitting equation Catalan 4P model coefficient C_{sp} has an uncertain by value (Table 3) complexity to the zero values in the best-fits of the rest of the fluorescence data (Table 2). It merits promoting that, with this conditioning by the limitation of the Adj R^2 each of three Solvatochromic models continue to high averaging values 0.995 for the Kamlet-Taft model, 0.985 for Catalan 3P and 0.997 for Catalan 4P models respectively. The re-examined best fit terms are generally physically substantial in foreseeing the red or blue spectral shifts divine to solvent effects of diverse qualities.

Three parameters were taken from every polarity scale separately (Kamlet-Taft and Catalan) for comparable estimation: α and SA (acidity); β and SB (basicity); π^* and SPP (dipolarity/polarizability). By contrasting the Adj R^2 coefficient of determination values, the parameter and obviously, the solvent scale which best depicted the solute-solvent interaction can be obviously resolved. For 1-HBBC fluorescence emission, Solvatochromic parameter π^* the fit to the single has a very low 'F' value (Table 3). An expansion of the Adj R^2 expression brings about a great increment in 'F' value. At the point when the two Adj R^2 and ' α ' terms are included into the fit, be that as it may, 'F' decreases significantly compared with the value Adj R^2 only. This conclusion shows, the consideration of the ' α ' parameter is not compelling in fitting the data, dependable with the structure of the molecule. In 1-HBBC there are no hydrogen bond-donating locales, in a way that there is no desire the electronic transition energy be forced to build upon the solvent hydrogen bond that has an accepting capability. In 1-HBBC, Kamlet-Taft scale is by all accounts more precise in anticipating acidity and basicity of solute-solvent interaction (Table 2), while Catalan appears to be more compelling in foreseeing dipolarity and polarizability interaction. At 95 % confidence level utilized, ' β ' and SB gave factually critical correlation with Adj R^2 of 0.995 and 0.997 respectively. Contrasting the two Adj R^2 values, ' β ' is higher incentive than SB showing more precision and consistency for the regression model. Additionally, the 'F' number could be likewise used to analyze two models portraying the same exploratory information: the higher 'F', the more sufficient the relating model.

Table 3 demonstrates, the after effect of all methods for Group A solvents transition energies suggestive that Solvatochromic parameters from Eq. (2) are represented in addition to the relating values of 'F' and Adj R² value. These values of Adj R² greater than 0.980. Along these lines, two groups data are a good fit by Eq. (2) all inclusive π^* and either of Adj R² and ' α '. In everything except one example, the following equations consist of Solvatochromic terms that are sensible accordingly molecule sort structure. For this situation, the 'step-forward' method brings about an equation that incorporates ' α ', ' α ' captions although there is no Hydrogen bond donating moiety in 1-HBBC. Table 3 confirms the point of interest of the 'step-forward' study for 1-HBBC. The fitting including ' α ' has the highest 'F' value. This is an unforeseen (non-physical) conclusion. Anyhow, it is observed that the value of the 'b' term in this fit is little low, pointing to moderately weakly dependence, demonstrating a relatively frail reliance and the detailed instability is quite more than half of its magnitude [57, 36].

The 'F' number for Catalan 3P model is 4503 while that of Kamlet-Taft, Catalan SB parameter is 251 and 1550 (Table 3). Looking at Adj R² acquired for ' α ', SA and Sdp the value for SA is higher than that of ' α ' and Sdp despite the fact that both were statistically insignificant at the level of confidence used. This demonstrates that the estimation of acidity of solute-solvent interaction can be viably clarified by Catalan 3P model. Looking at π^* , SPP and SP it can be seen that Kamlet-Taft parameter, π^* indicates a poor correlation (Adj R² = 0.994) while Catalan 3P and 4P parameter, SPP and SP demonstrated a better relationship (Adj R² = 0.999). In this manner, Catalan solvent scale shows a better assurance of dipolarity and polarizability interactions than Kamlet-Taft scale.

3.5 Assessment of the Solvatochromic models for 1-HBBC in Group B Solvents.

In Group B, solvent transition energies ' ν ' are derivative by the $1/\lambda_{\max}$ and all aromatic and polychlorinated solvents are incorporated as shown in Table 1. Thusly, the related transition energies in Group B consist of larger noise than that of Group A, inferable from the probable disruption in bandgaps of 1-HBBC in various solvents. The Catalan 3P model executes inadequately, whereas information from aromatic and polychlorinated solvents are combined. An extraordinary care is in a way required while applying for aromatic and polychlorinated solvents to all models and prescribed to function best-fits to all type of solvents separately, contributing the sufficient spectral information. The distinctive execution of all three models during managing

with aromatic and polychlorinated solvents may likely be analysed by review according to polarity range is built. In an inhomogeneous mixture of π^* scale comprises of dipolarity and polarizability solvent, although the same inhomogeneous mixture in the spp parameter range is the same [52, 34]. Anyhow, polarity polarizability can convey diverse measurements in the general solvent effects, over the various distinction of solvents. The better results are choicing may be systematically mixed within π^* scale. By isolating the two polarizability and polarity as, SP and SdP in the Catalan 4P model can be executed satisfactorily.

The best fit results from statistically analysed are shown in Table 4, we observed repeatedly starting parameters are negative coefficients for no existing hydrogen bond types of interactions. The Catalan 4P model creates conclusive determination, when prohibited with the aromatic and polychlorinated solvents. In this model, two invalid terms are obtained. Coefficients then set to zero. Based on the solvent solute interactions from revised best fit equations are outlined in Table 5. Initially, the best fit equations to all Solvatochromic models are resolved on the basis of 'F' values. After crosschecking of the best fitting parameters of 1-HBBC in the Group A and Group B solvents and their comparative results, they are similar to one another with the expectation of best fits for the fluorescence emission. It is fascinating to take note that the best-fit of 1-HBBC in Group B solvents has generally less value of Adj R^2 and seems to be less dependable. The Adj R^2 values are improved from the best fit results as 0.992 to 0.999 when we avoided taking the aromatic and polychlorinated solvents; and this recent best fitting equation obtains by greater understanding the Group A solvents. Generally nonetheless the fair understanding among the best fitting parameters from both Group A and Group B proposes that the disorder in bandgap of 1-HBBC when in various solvents are comparably small-scale, and applying the $1/\lambda_{\max}$ direct determine 'v' is a sensible decision, even though less perfect than Moog's analysis or more other advanced treatment. In conclusion, we reach for some fascinating determinations. In the first place, hydrogen bond shows major contribution in 1-HBBC to cause the red shifting. By taking the $1/\lambda_{\max}$ directly, the proportion between a, b and s measures in Kamlet-Taft model their corresponding contribution directly depends on the solvent properties [27]. Table 4 and 5, the fitting equation to the absorption of 1-HBBC in which there are two HBD moieties, due to which 's' is noticeably greater than 'a' and 'b'. This is due to effects of hydrogen bond that is supported by many molecular structures or quantum mechanical estimations. For instance, Sakata et al. presumed [58] that, the structure of solvent around the

amino group (hydrogen bond), cause the main role of red shifting of spectra. Secondly, it is to be noticed that in Catalan 4P model the shifting of the absorption spectra of 1-HBBC is easily affected to both polarizability and dipolarity of solvents.

The moderately more essential part of dipolarity solvent of showing in fluorescence emission than in absorption is noticeable. In 1-HBBC with the solvent molecules, during the fluorescence emission process have sufficient time to revamp themselves aligning with the excited state of solute [23]. This alignment promotes effectively dipole-dipole interactions between 1-HBBC and solvents; and results, red shift of solute due to the decreases in energy levels in excited 1-HBBC. By studying the Catalan 4P it is confirmed that there exists better understanding of the various performance of dipolarities and polarizability of solvents in 1-HBBC spectral shifts. Nonetheless, clear one extra parameter in the Catalan 4P in contrast with the Kamlet-Taft and Catalan 3P models, deeper spectral information is necessary for a good fit in the previous model. In summary, each of these models determines excellent statistic role in explaining the Solvatochromism of 1-HBBC, when excluded the aromatic and polychlorinated solvents and when included, both aromatic and polychlorinated with other aliphatic solvents the Adj R^2 values decrease slightly for Kamlet-Taft and Catalan 4P models. The precise explanation of spectral shifting in 1-HBBC in this regard Catalan 3P model fails. Besides, the bestfittings co-efficients of all the models enable to appreciate the significance of various conditions of solvent effects, and pick up a more profound knowledge of the solute-solvent interactions. The verification of best fitting results for all three models purely depends on structures of the solvents, the structures of solutes and their interactions are basic with a specific end goal to verify the best fit condition. It is important to validate the best fitting results, based on the molecular structures of both solutes-solvents and their corresponding interactions of hydrogen-bond. Upon such validations, the resulting best fits remain high and their parameters are physically valid. Considering the validated best fit parameters, we notice that, among nonspecific solvent effects, dipolarity plays an important role in the red shifting of the fluorescence spectra than in absorption spectra of 1-HBBC.

3.6 Colour space chromaticity of 1-HBBC with CIE coordinates

Organic Light Emitting Diodes (OLED) advancement will create a fundamental cutting edge development for the showcases and the lighting. It is currently used as a part of cell phones,

TV screens, mp3 players, propelled camera, PC appears and various other things. It can moreover be used as a light hotspot for general space lighting up. A champion among the most generally perceived inclinations over LCDs is that OLED does not require backdrop light. This suggests they draw less power, which is greatly useful when the unit is managed by a battery. As there is no background light required slenderer introductions can be made. There are some unique central focuses over LCDs. Extended wonder and higher separations are one of them. Others have lighter weight, speedier response time for full-development video and more broad working temperature ranges. As to shading, the human vision responds to trichromatic lifts on the virtual cortex [59, 62], assessed by the Commission Internationale de L'Eclairage (CIE) in three coordinating limits or powerful spectral bands, $a(\lambda)$, $b(\lambda)$ additionally $c(\lambda)$, open as free-get to tables.

The 'a' and b' CI facilitates the fluorescence emission of 1-HBBC in different polarity solvents, Fig. 7 were figured by Eq. (5) and (6) from their x, y and z tristimulus integrals of Eq. (7-9).

$$a = x/(x+y+z) \quad (5)$$

(6)

$$b = y/(x+y+z)$$

$$x = \int_{200}^{800} I(\lambda) \bar{a}(\lambda) d\lambda \quad (7)$$

$$y = \int_{200}^{800} I(\lambda) \bar{b}(\lambda) d\lambda \quad (8)$$

$$z = \int_{200}^{800} I(\lambda) \bar{c}(\lambda) d\lambda \quad (9)$$

At 255-285 nm excitation, a CIE chromaticity coordinates value for 1-HBBC in all alcohols solvents ($X = 0.16 - 0.23$, $Y = 0.22 - 0.23$) generates bluish colour. For other solvents ($X = 0.16 - 0.24$, $Y = 0.23 - 0.33$) in the studied compound which is near bluish green colour with CIE coordinates with the almost same range between $X = 0.16 - 0.24$ to $Y = 0.23 - 0.33$ (Table 6). The colour difference observed in the CIE graph probably photophysical characteristics of the

different solvent environment with different polarities of molecular network structure. The emission shading tuning is more featured and obviously reacts to the pulling back of electrons of the substituents. These outcomes are profoundly thorough of emission tuning methodologies and the molecular design of advanced particles along desirable scenery.

4. Conclusions

Electronic absorption and fluorescence emission properties of 1-(3-Hydroxy-benzofuran-2-yl)-benzo[f]chromen-3-one are dominated by solvent polarity. The absorption peak maxima and fluorescence peak maxima spectra show a bathochromic shift as the increases of the solvent polarity. According to the solvent polarity scale to Kamlet-Taft, Catalan 3P and 4P were analyzed and compared based on their individual parameters. adopting of linear regression helps to investigate the spectroscopic property of the 1-HBBC, Kamlet scale is used for evaluating the solvent effect and is more adapted for hydrogen bond donor basicity and hydrogen bond acceptor acidity interactions although Catalan scale is more suitable for dipolarity and polarizability interactions. Proposals for more itemized photophysical portrayal in various media with various polarities can be for put forward to outline the new luminescent studies.

Acknowledgement

The authors are thankful to Prof. Sharath Ananthmurthy, Coordinator DST-PURSE Program Bangalore University Bengaluru, for providing the financial assistance to conduct the experiment.

References

- [1] C. G. Renuka, K. Shivashankar, P. Boregowda, S. S. Bellad, M. V. Muregendrappa Y. F. Nadaf. *J. Sol. Chem.* **46**, 1 (2017)
- [2] K. Aggarwal, J. M. Khurana. *A Chem.* **276**, 71 (2014)
- [3] K. B. Akshaya, V. Anitha, L.L. Prajwal, K. Rekha, G. Louis. *J. Mol. Liq.* **224**, 247 (2016)
- [4] G. J. Amol, S. S. Suvidha, S. P. Dinesh, N. Sekar. *Struct. Chem.* **4**, 1 (2017)
- [5] L. C. Benjamin, G. M. Dannielle, No. Rodrigo, B. P. Samuel, D. Milan, D. D. David, M. Sukrit, S. D. Timothy, S. G. Naomi. *ACS Energy Lett.* **2**, 1526 (2017)
- [6] B. Bhattacharya, A. Samanta. *Chem. Phys. Lett.* **442**, (4 – 6) 316–321 (2007)
- [7] C. Gasbarri, G. Angelini. *J. Mol. Liq.* **229**, 185 (2017)

- [8] M. Cigan, J. Filo, H. Stankovicova, A. Gaplovsky, M. Putala. *Spectrochim. Acta. A Mol. Biomol. Spectrosc.* **89**, 276 (2012)
- [9] M. S. Mehata, A. K. Singh, R. K. Sinha. *J. Mol. Liq.* **231**, 39 (2017)
- [10] R. Kumari, A. Varghese, L. George, Y.N. Sudhakar. *RSC Adv.* **7**, 24204 (2017)
- [11] I. Sidir, Y. Gulseven, H. Berber, E. Ta. *J. Mol. Liq.* **178**, 127 (2013)
- [12] M.S. Masoud, S.S. Hagagg, A.E. Ali, N.M. Nasr. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **94**, 256 (2012)
- [13] J. Beata, M. Józefowicz. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **171**, 258–267 (2017)
- [14] R. Kumari, A. Varghese, L. George. *J. Lumin.* **179**, 518 (2016).
- [15] M. Panigrahi, S. Patel, B.K. Mishra. *J. Mol. Liq.* **177**, 335 (2013)
- [16] M. Avadanei, V. Cozan, O. Avadanei. *J. Mol. Liq.* **227**, 76 (2017)
- [17] A.G. Al-Sehemi, M. Pannipara, A. Kalam, A.M. Asiri. *J. Fluoresc.* **26**, 1357 (2016)
- [18] R. Dolique. *Masson.* **18**, 222 (1935)
- [19] V. B. Meyer.: *Heterocyclic compound*. Elderfield ed, Wiley, New York, (1951)
- [20] T. S. Stevens.: *Chemistry of carbon compounds*. IV A. Elsevier, Ed, By E.M. Rodd, Amsterdam, (1957)
- [21] F.M. Dean.: *Naturally occurring oxygen ring compounds*. First ed, London, (1963)
- [22] A. Mustafa.: *Fuopyrans and fuopyrones*. interscience Publisher, Ed, By Weissberger, London (NY), (1967)
- [23] J.R. Lakowicz.: *Principles of fluorescence spectroscopy*. Third ed. Plenum, New York, (2006)
- [24] M. Sowmiya, A.K. Tiwari, S. K. Saha. *J. Photochem Photobiol A Chem.* **218**, 76 (2011)
- [25] V. Balachandran, G. Santhi, V. Karpagam, B. Revathi, M. Karabacak. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **136**, 451 (2015)
- [26] C. Reichardt, K. Dimroth. *Fortsch. Chem. Forsch.* **11**, 1 (1968)
- [27] J. Kamlet, J. L. M. Abboud, M. H. Abraham, R. W. Taft. *J. Org. Chem.* **48**, 2877 (1983)
- [28] E. Lippert. *Z. Naturforsch. Teil A.* **10a**, 541 (1955)
- [29] C. Reichardt. *Chem. Rev.* **94**, 2319 (1994)
- [30] J. L. Abboud, M. J. Kamlet, R. W. Taft. *J. Am. Chem. Soc.* **99**, 8325 (1977)
- [31] J. Catalan, V. Lopez, P. Perez, R. Martin-Villamil, J. G. Rodriguez. *Liebigs Annalen.* **2**, 241 (1995)
- [32] J. Catalan, C. Diaz, V. Lopez, P. Perez, J.L.G. De Paz, J. G. Rodriguez. *Liebigs Annalen.* **11**, 1785 (1996)
- [33] J. Catalan, C. Diaz. *Liebigs Annalen.* **9**, 1941 (1997)
- [34] J. Catalan. *J. Phys. Chem. B.* **113**, 5951 (2009)
- [35] T. Higashijima, T. Fuchigami, T. Imasaka, N. Ishibashi. *Anal. Chem.* **64**, 711 (1992)
- [36] B. Maity, A. Chatterjee, D. Seth. *Photochem Photobiol.* **90**, 734 (2014)
- [37] M. D. Shultz, J. U. Reveles, S. N. Khanna, E. E. Carpenter. *J. Am. Chem. Soc.* **129**, 2482-2487 (2007)

- [38] J.Y. Wach, B. Malisova, S. Bonazzi, S. Tosatti, M. Textor, S. Zurcher, K. Gademann. *Chem. Eur. J.* **14**, 10579 (2008)
- [39] F. Riedel, S. J. Spange. *Phys. Org. Chem.* **25**, 1261–1268 (2012)
- [40] K.B. Puttaraju, K. Shivashankar, M.C. Mahendra, V.P. Rasal, P.N.V. Vivek, K. Rai, M.B. Chanu. *Eur. J. Med. Chem.* **69**, 316 (2013)
- [41] R. C. Weast.: *CRC Handbook of chemistry and physics*. First ed. CRC press, Florida, (1988)
- [42] E. Krystkowiak, K. Dobek, A. Maciejewski. *Photochem. Photobiol. Sci.* **12**, 446 (2013)
- [43] C. Marek, J. Donovalova, S. Vojtech, J. Gaspar, K. Jakusova, A. Gaplovsky. *J. Phys. Chem. A.* **117** (23), 4870 (2013)
- [44] A. Kowski. *Z. Naturforsch.* **57A**, 255 (2002)
- [45] N. Sanjukta, P. Haridas. *J. Phys. Chem. A.* **105**, 1097 (2001)
- [46] C. Marek, F. Juraj, S. Henrieta, G. Anton, P. Martin. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **89**, 276 (2012)
- [47] N. Sanjukta, K. Manoj, P. Haridas. *J. Phys. Chem. A.* **107**, (24), 4808 (2003)
- [48] K. Robert, J. Wlodzimierz. *J. Phys. Chem. A.* **106**, 1708 (2002)
- [49] Z. R. Grabowski, K. Rotkiewicz, W. Rettig. *Chem. Rev.* **103**, 3899 (2003)
- [50] M. Cigan, J. Filo, H. Stankovicova, A. Gaplovsky, M. Putala. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **89**, 276 (2012)
- [51] C. Reichardt.: *Solvent and solvent effect in organic chemistry*. Wiley-VCH, Weinheim, Germany, (2001)
- [52] R. S. Moog, D. D. Kim, J. J. Oberle, S. G. Ostrowski. *J. Phys. Chem. A.* **108**, 9294 (2004)
- [53] R. S. Moog, W. W. Davis, S. G. Ostrowski, G. L. Wilson. *Chem. Phys. Lett.* **299**, 265 (1999)
- [54] S. M. Richard, D. K. Daniel, J. O. Jessica, G. O. Sara. *J. Phys. Chem. A.* **108**, (42), 9294 (2004)
- [55] L. Xiaogang, M. C. Jacqueline, S. L. Kian. *J. Phys. Chem. C.* **117**, 14731 (2013)
- [56] K. Das, B. Jain, H. S. Patel. *J. Phys. Chem. A.* **110**, 1698 (2006)
- [57] R. J. Cave, K. Burke, E. W. Jr Castner. *J. Phys. Chem. A.* **106**, 9294 (2002)
- [58] T. Sakata, Y. Kawashima, H. Nakano. *J. Chem. Phys.* **134**, 014501 (2011)
- [59] Thiago Moreira Pereira, Felipe Vitorio, Ronaldo Costa Amaral, Kassio Papi Silva Zanoni, Neyde Yukie Murakami Iha, Arthur Eugen Kummerle, Microwave-assisted synthesis and photophysical studies of novel fluorescent N-acylhydrazone and semicarbazone-7-OH-coumarin dyes. *New J. Chem.* **40**, 8846 (2016)
- [60] H.S. Geethanjali, D. Nagaraja, R. M. Melavanki. *J Fluoresc.* **25**, 745 (2015)
- [61] C.V. Bindhu, S.S. Harilal, G.K. Varier, R.C. Issac, V.P.N. Nampoori, C.P.G. Vallabhan. *J Phys D: Appl Phys.* **29**, 1074 (1996)

- [62] Jun Choi, Se Hun Kim, Woosung Lee, Chun Yoonb, Jae Pil Kim.: Synthesis and characterization of thermally stable dyes with improved optical properties for dye-based LCD color filters. *New J. Chem.* **36**, 812 (2012)

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Fig. 1. Molecular structure of 1-(3-Hydroxy-benzofuran-2-yl)-benzo[f]chromen-3-one.

Fig. 2. UV-Vis absorption spectra of 1-HBCC in a) Non-polar, b) Polar protic and c) Polar aprotic solvents.

Fig.3. The Absorption Max. versus solvent directional polarizability (ΔF) for 1-HBBC in selected solvents.

Fig. 4. Fluorescence emission spectra of 1-HBBC in a) Non-polar, b) Polar protic and c) Polar aprotic solvents.

Fig. 5. The Fluorescence Max. versus solvent directional polarizability (ΔF) for 1-HBBC in selected solvents.

Fig. 6. The Stoke shifts ($\Delta\nu$) versus solvent directional polarizability (ΔF) for 1-HBBC in selected solvents.

Fig. 7. CIE chromaticity plot for colour coordinates of 1-HBBC.

Table 1

Summary of Absorption and Fluorescence spectral data of 1-HBBC in various solvents.

Solvent	$\lambda_{\text{max}}(\text{abs})$ $\text{cm}^{-1}(\text{nm})$	$\lambda_{\text{max}}(\text{em})$ $\text{cm}^{-1}(\text{nm})$	Stokes shift $\Delta\nu \text{ cm}^{-1}$	Quantum Yield	Absorption Coefficient $\epsilon \times 10^4 (\text{L} \text{ mole}^{-1} \text{ cm}^{-1})$
1,4-Dioxane	39093.1 (255.8)	20597.4 (485.5)	18495.7	0.049	6.00
Acetone	29027.6 (344.5)	21810.3 (458.5)	7217.32	0.045	4.40
Acetonitrile	38971.2 (256.6)	21949.1 (455.6)	17022.0	0.027	6.00
Butyl acetate	35790.9 (279.4)	20850.7 (479.6)	14940.2	0.094	3.28
Butanol	38124.3 (262.3)	20479.2 (488.3)	17645.0	0.032	5.60
Chloroform	29316.9 (341.1)	21547.1 (464.1)	7769.83	0.083	7.20
Chloromethane	38669.8 (258.6)	23121.4 (432.5)	15548.3	0.157	4.40
DMF	35087.7 (285.0)	24943.9 (400.9)	10143.8	0.132	3.20
Decanol	39077.7 (255.9)	20846.4 (479.7)	18231.4	0.062	5.60
Ethyl acetate	35511.4 (281.6)	35186.5 (420.2)	11713.1	0.067	2.12
Ethanol	36258.2 (275.8)	20721.1 (482.6)	15537.0	0.017	9.60
Hexane	48449.6 (260.0)	35026.3 (408.7)	13993.7	0.090	6.80
Methanol	39323.6 (254.3)	20959.9 (477.1)	18363.6	0.012	9.20
Propanol	38804.8 (257.7)	35186.5 (484.2)	18152.1	0.064	5.60
Tetrahydrofuran	28653.3 (349.0)	24709.7 (404.7)	3943.63	0.053	2.40

Table 2

Statistical regression fit to Group A solvents for different empirical solvatochromic polarity scales of absorbance and fluorescence of 1-HBBC

Group A	Taft Kamlet Method (n=12)					Catalan's 3P Model (n=15)					Catalan's 4P Model (n=12)					
	ν_0	α	β	π^*	Adj.R ²	ν_0	Cspp	Csa	Csb	Adj.R ²	ν_0	Csp	Csdp	Csa	Csb	Adj.R ²
1-HBBC(abs)	37.49	-	-	-3.48	0.923	67.28	-43.20	-9.58	-5.59	0.979	277.31	-349.1	-10.9	-110.6	51.53	0.993
1-HBBC(flu)	15.56	-	3.94	6.92	0.920	2.380	21.23	-	2.75	0.924	5.390	17.20	4.61	0.350	2.750	0.993

Bold terms indicates with larger uncertainty: n is number of solvents used

Table 3

Revised best regression fit to Group A solvents in all the models subjected to 95% confidence limits for their corresponding fitting coefficients.

GroupA	Taft Kamlet Method						Catalan's 3P Model						Catalan's 4P Model						
	v ₀	α	β	π*	F	Adj.R ²	v ₀	Cspp	Csa	Csb	F	Adj.R ²	v ₀	Csp	Csdp	Csa	Csb	F	Adj.R ²
1-HBBC(abs)	35.2	-2.5	2.9	7.80	251	0.994	66.2	-38.2	9.5	-33.5	4503.2	0.999	39.41	71.8	-9.8	14.19	-58.3	1550.2	0.999
1-HBBC(flu)	15.4	-1.1	5.9	5.80	423	0.995	2.49	19.39	-1.0	5.73	58.500	0.972	5.300	17.5	4.64	0.410	2.50	242	0.995

Valid best fits are highlighted in Italic bold; F-Fisher test

Table 4

Statistical regression fit to Group B solvents for solvatochromic polarity scales of absorbance and fluorescence of 1-HBBC.

Group B	Taft Kamlet Method (n=15)					Catalan's 3P Model (n=15)					Catalan's 4P Model (n=15)					
	ν_0	α	β	π^*	Adj.R ²	ν_0	Cspp	Csa	Csb	Adj.R ²	ν_0	Csp	Csdp	Csa	Csb	Adj.R ²
1-HBBC(abs)	-389.29	-121.69	188.8	1271.7	0.988	82.21	-69.12	-	16.51	0.911	134.10	-140.79	-24.62	-	18.44	0.918
1-HBBC(flu)	16.340	-	-	8.900	0.860	20.70	3.680	-	-	0.891	3.590	20.00	5.470	-0.98	1.210	0.973

Bold terms indicates with larger uncertainty: n is number of solvents used

Table 5

Revised best regression fit to Group B solvents in all the models subjected to 95% confidence limits for their corresponding fitting coefficients.

Group B	Taft Kamlet Method						Catalan's 3P Model						Catalan's 4P Model							
	v ₀	a	b	s	F	Adj.R ²	v ₀	Cspp	Csa	Csb	F	Adj.R ²	v ₀	Csp	Csdp	Csa	Csb	F	Adj.R ²	
1-HBBC(abs)	231	23.7	-101	204	3725.5	0.999	75.4	-53.40	9.8	3.38	241.37	0.992	48.45	-6.77	-5.34	17.33	-9.87	832.5	0.998	
1-HBBC(flu)	17.7	-2.2	1.80	6.73	269.87	0.993	8.09	16.69	-7.0	1.92	367.57	0.996	4.350	18.94	5.61	-1.10	1.16	335.9	0.995	

Valid best fits are highlighted in Italic bold; F-Fisher test

Table 6

CIE colour coordinates of 1-HBBC in various solvents.

Solvents	CIE colour coordinates	
	X	Y
1,4-Dioxane	0.17	0.29
Acetone	0.17	0.24
Butyl acetate	0.17	0.27
DMF	0.16	0.23
Decanol	0.17	0.23
Ethyl acetate	0.19	0.30
Ethanol	0.19	0.25
Hexane	0.24	0.27
Methanol	0.17	0.24
Propanol	0.33	0.39