J Fluoresc (2011) 21:2111–2116
DOI 10.1007/s10895-011-0911-6

ORIGINAL PAPER

Mathematical Representation of Fluorescence Intensity of Probes in Aqueous Binary Solvent Mixtures

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Received: 20 May 2011 / Accepted: 4 July 2011 / Published online: 12 July 2011

Abstract Fluorescence intensities of propranolol and atenolol in binary solvent mixtures at various temperatures are measured and mathematical models are proposed to represent the fluorescence intensity data. The results showed that the proposed models are able to correlate/predict the data with reasonable error. The fluorescence intensity of pyridoxal HCl in binary solvents at 25 °C is also determined and represented by the proposed model as an additional test probe.

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Keywords Fluorescence intensity · Mixed solvent · Jouyban-Acree model · Mathematical representation

Introduction

Water-organic solvent mixtures are used in many chemical applications such as synthesis and separation processes. Most of photochemistry subjects are investigated in liquid solutions, and intermolecular solute—media interactions affect the energy of the electronic states. As the interaction energy depends on the nature and the properties (e.g. the charge distribution or the dipole moment) of the respective state, it will be different for ground and excited state molecules and hence gives rise to spectral shifts, normally referred to as solvatochromic shifts. Solvatochromy can be an excellent measure for variations of the relative energies of the molecular states in different environments [1]. Two kinds of interactions can be defined; 1) Physical (non-specific) solute—solvent interactions such as ion–dipole, dipole–dipole, dipole–induced dipole interactions [2]. Generally these interactions, mostly cause a red shift of the spectra on increasing solvent polarity, because excited state dipole moments are more often larger than in the ground state. In many media shifts of the UV–Vis absorption and fluorescence emission spectrum (band position) of the solute can additionally be attributed to specific chemical effects of the solvent on one or both electronic states. 2) Specific interactions include hydrogen bonding, proton or charge transfer, solvent dependent aggregation, etc. Specific interactions could influence the energy of the initial and final state of an electronic transition in the same or in opposite way, causing thus a red or a blue shift of the spectrum [3].

In many cases the solutes are dissolved in solvent mixtures instead of the mono-solvents in chemical analysis

to overcome a number of problems such as solubility or resolution of analytes in chromatographic systems. An important factor in mixed solvents is the preferential solvation. Solvation of a solute depends on the interaction of the solute with solvent molecules in the vicinity of the solute. In a mixed binary solvent the microenvironment near the solute may be different from the bulk environment owing to the difference between the nature and extent of the interaction of the solute with component solvents. This phenomenon, known as preferential solvation (PS), has been studied in recent years. PS in binary solvent mixtures has been studied using absorption and steady-state fluorescence spectroscopy [4].

A large range of different processes are involved in the excited state decay. The most extensive experimental and theoretical treatments are available for the dynamic solvent effect (e.g. the bulk dielectric properties of the solvent) on charge transfer rate [5]. Such short range interactions between substrate and medium molecules become often evident in a strongly non-linear dependence of spectral or photophysical properties on the composition of binary solvent mixtures. The addition of small amounts of a polar solvent to an inert medium (e.g. adding alcohol to a hydrocarbon) can result in large spectral shifts, which can be attributed to the formation of molecular clusters. Studies of spectroscopic and photophysical properties in such binary mixtures allows us to separate the effects of relaxation mechanism caused by solute-solvent complexes from long range electrostatic interactions. Furthermore, information on the stoichiometric structure of such clusters, the interaction strength and structural changes upon excitation can be obtained from such investigations. In this context, fluorescence-based techniques can be immensely useful in providing both microscopic and macroscopic structural information, in addition to probing dynamical processes that occur on the timescale of the fluorescence decay. Fluorescent molecules are often extremely sensitive to their local environment with many fluorophores being profoundly influenced by surrounding solvent molecules [6–8]. For example, solvent effects on excited state relaxation phenomena in binary solvent mixtures, using steady state and time-resolved fluorescence and absorption spectroscopy, was studied in the frame of electrostatic interactions, PS, weak associations with defined stoichiometry, structure and strongly bonded ground and excited state complex formation [8]. The theoretical results demonstrating the role of solvent dynamics in fluorescence quenching of polar compounds in polar solutions has been reported [7]. Spectral shifts in fluorescence have been correlated with several solvent parameters, such as the solvatochromic parameter, $E_T(30)$ [9], solvent index for hydrogen bond donor, solvent index for hydrogen bond acceptor and solvent polarity/polarizability [10, 11].

The aim of this work is to report a mathematical model for representing the effects of solvent composition and temperature on the fluorescence intensity of some probes. As indicated above, mixed solvents are used in many application fields and mathematical representation of the fluorescence in these mixtures could facilitate the process optimization when different variables such as solvent composition and temperature should be optimized. To show the practical applicability of the proposed model, experimental fluorescence intensities of two beta-blocker drugs in aqueous mixtures of methanol, ethanol and 1-propanol at 15, 20, 25, 30, and 35 °C and also pyridoxal HCl in aqueous mixtures of 2-propanol, acetonitrile, ethanol and methanol at 25 °C were determined.

Experimental

Reagents

All reagents and solvents were of analytical grade and used without further purification. Methanol, 1-propanol and 2-propanol were obtained from Caledon (Caledon, Canada), ethanol and acetonitrile were purchased from Merck (Germany). Double distilled water was used throughout these experiments.

A 0.01 M tris-(hydroxymethyl) aminomethane-hydrochloric acid (Tris- HCl) buffer solution was prepared by dissolving a desired amount of Tris-base (Merck, Germany) in 90 mL of water, adjusting the pH to 7.0 with HCl and making up the volume to 100 mL with water.

Solutions of 2 g/L of propranolol (Daru-Pakhsh, Iran), 1 g/L of atenolol (Daru-Pakhsh, Iran) and 0.01 g/L pyridoxal HCl (Merck, Germany) in the mono-solvents were prepared and appropriate volumes of the solutions were mixed.

Apparatus

Fluorescence spectra and intensity measurements were performed using a Jacso FP 750 spectrofluorimeter (Japan) equipped with a 150 W xenon lamp, using 1.0 cm quarts cell. The excitation and emission monochromator bandwidths were 5 nm. The excitation wavelength was set at 280 nm for propranolol, at 240 nm for atenolol and at 323 nm for pyridoxal HCl, then the fluorescence intensity was measured using the peak heights at 340 nm for propranolol, 303 nm for atenolol and 382 nm for pyridoxal HCl. All measurements were performed at the given temperature ±0.1 °C using a temperature control set of ETC-272T. The pH of solutions was measured using a Metrohm pH meter (Herisau, Switzerland).

Methods

All measurements were corrected for the background fluorescence of blank which was taken as the solution containing all reagents except the analytes under investigation.

Experimental Procedure

Computational Procedure

The Jouyban-Acree model was derived from a thermodynamic mixing model that includes contributions from both two-body and three-body interactions. The model was presented for solubility calculations in mixed solvents by our group [12, 13] and was expressed as:

$$\log X_m = f_1 \log X_1 + f_2 \log X_2 + f_1 f_2 \sum_{i=0}^{2} S_i (f_1 - f_2)^i \qquad (1)$$

where X_m, X_1 and X_2 are the solute solubility in mixed solvent, solvents 1 and 2, f_1 and f_2 are the volume (weight or mole) fractions of solvents *1* and *2* in the mixture, and S_i stands for the model constants. The model was used to calculate multiple solubility maxima and also solute solubility in mixed solvents at various temperatures [14]. The model was also used to correlate other physico-chemical properties (*PCP*) in mixed solvent systems; including the electrophoretic mobility of analytes in mixed solvent electrolyte systems [15], the instability rate constants in binary solvent systems [16], the acid dissociation constants in water-organic solvent mixtures at a fixed and various temperatures [13, 17], the capacity factor of analytes in HPLC [18], the dielectric constant [19], surface tension [20], viscosity [21], density [22], solvatochromic parameter [23], refractive index [24], ultrasound velocity [25] and molar volumes [26] in the solvent mixtures. The theoretical basis of the model for describing the chemical potential of solutes dissolved in mixed solvents [12] and the acid dissociation constants in aqueous-organic mixtures [13] have been provided in earlier papers. The constants of the Jouyban-Acree model represent differences in the various solute-solvent and solvent-solvent interactions in the mixture [12]. Therefore, the model should be able to calculate any *PCP* in mixed solvents, which is a function of solute-solvent and/or solvent-solvent interactions. The general form of the Jouyban-Acree model is:

$$\log PCP_{m,T} = f_1 \log PCP_{1,T} + f_2 \log PCP_{2,T} + f_1 f_2 \sum_{i=0}^{2} \frac{A_i (f_1 - f_2)^i}{T} \qquad (2)$$

where $PCP_{m,T}$, $PCP_{1,T}$ and $PCP_{2,T}$ are the numerical values of the physico-chemical property of the mixture and solvents *1* and *2* at temperature *T*, respectively and A_i represent the model constants. The model for representing the fluorescence intensity (*FI*) of probes in mixed solvents at various temperatures is:

$$\log FI_{m,T} = f_1 \log FI_{1,T} + f_2 \log FI_{2,T} + f_1 f_2 \sum_{i=0}^{2} \frac{J_i (f_1 - f_2)^i}{T} \qquad (3)$$

in which J_i is the model constant calculated using a no intercept least square analysis. The model could be simplified to Eq. 3 for representing the *FI* at a given temperature as:

$$\log FI_m = f_1 \log FI_1 + f_2 \log FI_2 + f_1 f_2 \sum_{i=0}^{2} M_i (f_1 - f_2)^i \qquad (4)$$

however, we prefer to use Eq. 3 since the trained model at a given temperature could be used to calculate the *FI* of the same probe at different temperatures.

The van't Hoff type model could be used to represent the effects of temperature at a given solvent composition as:

$$\log FI_T = A + \frac{B}{T} \qquad (5)$$

where A and B are the model constants.

To check the accuracy of the *FI* calculations, the mean percentage deviation (MPD) between the calculated *FI* and experimental *FI* is computed using:

$$MPD = \frac{100}{N} \left(\frac{|Calculated - Experimental|}{Experimental} \right) \qquad (6)$$

in which N is the number of data points.

Results and Discussion

Table 1 lists the fluorescence intensity of analytes in aqueous mixtures of organic solvents at various temperatures. For the investigated systems, fluorescence intensity is increased with increaseing concentrations of the organic solvents, it reaches to a maximum value and decreases with further increase in the concentration of organic solvents. The maximum intensities for propranolol in 1-propanol + water, atenolol in methanol + water and atenolol in ethanol + water mixtures were observed at 0.30, 0.80, and 0.80 volume fractions of the organic solvents, respectively. There are possibilities of excitation and emission wavelengths shifts in different solvent compositions [27], however this has not been considered in this work, since in many applications, these wavelengths were fixed at given wavelengths.

Table 1 Fluorescence intensity of probes in organic solvent + water mixtures at 15–35 °C

f_1	15	20	25	30	35
	Propranolol in 1-propanol + water				
0.00	352.2	344.5	335.1	333.1	326.6
0.10	415.6	420.7	406.9	400.0	387.9
0.20	496.4	486.0	478.1	472.2	467.8
0.30	529.9	524.3	514.8	501.8	483.0
0.40	524.2	506.0	489.2	475.0	470.5
0.60	487.2	482.0	472.0	449.6	436.7
0.70	476.2	466.3	449.0	436.3	425.5
0.90	421.3	416.6	399.8	393.8	376.0
1.00	390.7	371.9	356.1	342.6	327.0
	Atenolol in methanol + water				
0.00	546.7	505.8	472.9	441.6	412.8
0.20	680.9	649.8	608.0	563.7	531.1
0.30	733.3	694.5	665.3	645.6	604.3
0.40	780.5	772.6	746.6	685.5	647.7
0.50	810.0	795.3	779.8	697.5	667.9
0.60	900.9	849.0	819.7	798.5	743.3
0.80	997.6	976.2	952.4	885.6	827.2
0.90	861.0	844.6	798.0	766.8	740.0
1.00	817.0	783.2	777.7	760.3	735.7
	Atenolol in ethanol + water				
0.00	546.7	505.8	472.9	441.6	412.8
0.10	560.6	529.1	493.8	475.1	458.8
0.20	600.8	567.5	541.2	524.9	499.0
0.30	651.9	610.3	594.5	559.6	547.1
0.40	682.1	658.3	648.9	600.9	580.2
0.60	732.1	696.6	654.0	598.9	581.0
0.80	735.5	724.5	706.0	671.4	655.5
0.90	726.8	710.5	694.4	658.4	649.6
1.00	706.5	698.7	661.8	648.8	626.5

With respect to a given solvent composition, the fluorescence intensity of the solutions is decreased with an increase in temperature. This observation is confirmed by other reports [28] and indicates an increase in the radiationless deactivation of the excited state. A number of mechanisms could be considered for temperature quenching effect; a) an increase in conversion rate of electronic into vibrational energy (internal conversion), b) a change-over from an excited singlet-state to a higher triplet state (inter-system crossing) and c) loss of planarity in molecular structure and dissociation of molecular complexes at higher temperatures [28].

Table 2 reports the fluorescence intensity of pyridoxal HCl in 2-propanol + water, acetonitrile + water, ethanol + water and methanol + water mixtures at 25 °C. The intensity increases for all investigated organic solvents,

Table 2 Fluorescence intensity of pyridoxal HCl in organic solvents + Tris buffer (0.1 M, pH 7.0) at 25 °C

f_1	2-Propanol	Acetonitrile	Ethanol	Methanol
0.0	40.6	40.6	40.6	40.6
0.1	125.6	85.0	110.0	105.0
0.2	202.0	148.7	174.1	234.1
0.3	319.9	204.1	282.7	320.1
0.4	447.6	287.2	423.5	416.3
0.5	582.5	382.1	566.5	526.0
0.6	700.7	491.7	702.4	648.0
0.7	836.4	596.5	812.9	731.0
0.8	868.8	707.7	833.5	764.4
0.9	828.0	759.2	824.0	774.3
1.0	739.2	734.5	752.4	755.6

until it reaches to the maximum values (at 0.80 for 2-propanol, ethanol and methanol, and 0.90 for acetonitrile), then decreases with further increase in the organic solvent concentrations in the mixture. For a given f_1, the 2-propanol mixture produced higher intensity when compared with other organic solvents.

The $FI_{m,T}$ data of the systems reported in Tables 1 and 2 was fitted to Eq. 3 and the calculated J terms, the correlation coefficients (R), and the MPD values are listed in Table 3. The R values for all systems investigated is >0.98 and the overall MPD of 2.5% is obtained revealing that the proposed model represents the $FI_{m,T}$ data accurately. As noted above, Eq. 3 could be trained using $FI_{m,T}$ data at one temperature and the $FI_{m,T}$ data at other temperatures could be predicted using the trained model and employing the FI data in mono-solvents at the temperature of interest. As an example, the trained model for propranolol in 1-propanol + water mixtures using FI data at 25 °C is:

$$\log FI_{m,T} = f_1 \log FI_{1,T} + f_2 \log FI_{2,T} + \frac{415.846 f_1 f_2}{T} - \frac{219.822 f_1 f_2 (f_1 - f_2)}{T} + \frac{209.441 f_1 f_2 (f_1 - f_2)^2}{T} \quad (7)$$

and using Eq. 7, the MPD of the predicted $FI_{m,T}$ data at other temperatures is 2.5% (N=36). Similar analyses for atenolol in methanol + water and ethanol + water mixtures produced the prediction MPDs of 2.7 and 2.0%, respectively.

The FI_T data of beta-blockers in a given solvent composition at various temperatures was fitted to Eq. 5, and the computed A and B values are listed in Table 4. High R and low MPD values reveal that Eq. 5 is able to represent the temperature effects on the fluorescence intensity of probes.

The data prediction is one of the main aims of data modeling and *in silico* models which predict the data without using any experimentally determined values as

Table 3 The model constants, correlation coefficient (R), number of data points in each set (N) and mean percentage deviation (MPD) of the investigated systems

	J_0	J_1	J_2	R	N	MPD
Propranolol in 1-propanol + water	403.560	−214.136	208.097	0.995	45	1.7
Atenolol in methanol + water	287.109	115.041	153.099	0.982	45	2.3
Atenolol in ethanol + water	304.622	202.738	NS	0.987	45	2.0
Pyridoxal HCl in 2-propanol + water	1424.547	−511.871	803.795	0.998	11	3.6
Pyridoxal HCl in acetonitrile + water	937.748	−221.596	566.631	0.999	11	1.2
Pyridoxal HCl in ethanol + water	1382.695	−339.901	412.622	0.998	11	3.3
Pyridoxal HCl in methanol + water	1331.769	−722.142	657.420	0.999	11	3.3
						2.5

NS Not statistically significant

input data is highly in demand in practical applications. Because of the lack of deep understanding from fluorescence phenomenon in mixed solvents and at different temperatures, there is no *in silico* model to predict the $FI_{m,T}$ data. On the other hand, an experimental trial and error approach is time-consuming and as an alternative method, it is possible to train the Jouyban-Acree model using a minimum number of experimental data points and predict the data at other solvent compositions and temperatures using interpolation technique. To test this hypothesis, the experimental $FI_{m,T}$ data of propanolol in 1-propanol + water mixtures, i.e. f_1=0.00, 0.10, 0.40, 0.70 and 1.00, at 15 and 35 °C is fitted to a combined version of Eqs. 3 and 5, and the trained model is:

$$\log FI_{m,T} = f_1\left(3.598 + \frac{682.128}{T}\right) + f_2\left(5.008 + \frac{243.726}{T}\right) + \frac{414.333 f_1 f_2}{T} - \frac{162.646 f_1 f_2 (f_1 - f_2)}{T} - \frac{7.786 f_1 f_2 (f_1 - f_2)^2}{T} \quad (8)$$

Using Eq. 8, the $FI_{m,T}$ data of propranolol at other solvent compositions and temperatures are predicted in which the MPD of 1.6% (N=35) is obtained. Similar equations are trained (equations are not reported here) for $FI_{m,T}$ data of atenolol in methanol + water and ethanol + water mixtures and the MPDs of 3.2, and 2.9% are obtained.

As a conclusion, the proposed models are able to represent the effects of solvent composition and temperature on the *FI* data of the probes and could be used to speed up the optimization of analytical and/or detection processes in chemical/pharmaceutical analysis. The addition of organic solvents to the aqueous solutions is a common method to modify the resolution, peak shape and other analytical parameters in chromatographic or electromigration methods where similar algorithms have been used to represent the solvent and temperature effects on retention factor in HPLC [29]. The proposed models in this work could be used to model the *FI* data of a fluorescent analyte in chromatographic separation cou-

Table 4 The model constants, correlation coefficients (R) and mean percentage deviation (MPD) of the fluorescence intensity of probes in different solvent compositions

f_1	Propranolol in 1-propanol + water				Atenolol in methanol + water				Atenolol in ethanol + water			
	A	B	R	MPD	A	B	R	MPD	A	B	R	MPD
0.00	4.718	329.299	0.986	0.3	2.002	1239.170	>0.999	0.1	2.002	1239.170	>0.999	0.1
0.10	4.893	331.724	0.922	1.0	–	–	–	–	3.180	905.379	0.993	0.7
0.20	5.293	262.346	0.991	0.3	2.599	1133.750	0.996	0.7	3.622	798.491	0.997	0.5
0.30	4.876	405.050	0.970	0.8	3.764	816.210	0.993	0.6	3.772	777.805	0.989	0.9
0.40	4.530	497.567	0.987	0.6	3.665	870.447	0.958	1.9	3.985	734.748	0.974	1.1
0.50	–	–	–	–	3.551	913.818	0.946	2.2	–	–	–	–
0.60	4.431	509.812	0.970	0.9	4.056	790.974	0.986	0.8	4.726	543.084	0.981	0.8
0.70	–	–	–	–	–	–	–	–	–	–	–	–
0.80	–	–	–	–	4.033	833.715	0.962	1.6	4.741	533.820	0.982	0.7
0.90	4.307	502.699	0.978	0.8	4.308	708.620	0.991	0.6	4.631	558.036	0.983	0.7
1.00	3.265	778.440	0.999	0.2	5.226	424.892	0.979	0.7	4.270	621.012	0.978	1.0
				0.6				1.0				0.7

pled with fluorescence detector in which the addition of the organic solvent alters the detector's response, retention factor and peak shape.

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