

# Two Sensitive Fluorescent BOPIM Probes with Tunable TICT Character for Low-Level Water Detection in Organic Solvents

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**Abstract** Two novel Boron-fluorine derivatives bearing dimethylamino moieties, BOPIM-1 and BOPIM-2, were proposed as sensitive fluorescent sensors for low-level water quantification in organic solvents. Two BOPIMs exhibit typical phenomenon for an emission from a twisted intramolecular charge transfer (TICT) state, the emission red shift and intensity weakening with solvent polarity. Introduction of trace amount of water to solvent resulted in fluorescent quenching, accompanied by the red shift of the emission, which was attributed to the formation of TICT excitation of BOPIMs by hydrolysis. A quantification method to detect water content was developed, described by a linear equation  $\lg \frac{I}{I_0}$  vs.  $\lg \varphi_w$  in the range of  $\varphi_w$  (volume fraction of water) 0.001~0.01, 0.01~0.1, respectively. The experiment results of determination of water in real 1, 4-dioxane (Diox) samples proved that this method can be used in practical application.

**Keywords** BOPIMs · Twisted intra-molecular charge transfer (TICT) · Fluorescent sensor · Water determination · Solvent

## Introduction

Determination of water contents in organic solvents is essential for many practical applications, such as pharmaceutical

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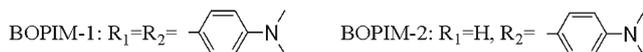
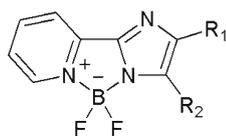
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manufacturing, food processing, biomedical and environmental monitoring, since water is generally considered as the most common impurity in many organic solvents. The Karl-Fischer method is most frequently used because of its absolute measurement, low capital cost, high sensitivity, applicability to both liquid and solid samples, as well as large dynamic range [1, 2]. Unfortunately, this method is less sensitive in aprotic and non-alcoholic solvents, and can hardly be performed to continuously monitor any occurrence of water in the sample media [3, 4].

It is urgently needed to develop effective techniques for ultra sensitive water content determination. Many advanced techniques, for example, NMR, IR, UV/Vis and also fluorescence spectrometry have been proposed [5–8]. Among them, fluorescent probes such as electron sensors and optical sensors have demonstrated the advantages of high sensitivity, easy operation and low cost, flexibility in readout, possibility of remote and in situ monitoring [9]. A novel approach to the quantification of relatively small amounts of water present in low polarity has been proposed by Kłucińska, using 4-methylumbelliferone as a fluorescence probe [10]. Optical-fiber chemical sensor based on a fluorescence dye, 10-allylacridine orange [11], a series of anthracene–boronic acid ester [12–14], 4-(2-dimethylaminoethoxy)-N-octadecyl-1, 8-naphthalimide (DON) with AIEE [15] were also developed for determining water content in organic solvents.

Many organic dyes possessing both electro donor and acceptor groups exhibit positive solvatochromism caused by an intra-molecular charge transfer (ICT) or twisted ICT (TICT) process [16, 17]. Their fluorescence characteristics in organic solvent could be affected by the increase of water content because of the change in the polarity of the solvent mixture [18], suggesting a new kind of chemosensor for trace water detection in solvent. Recently, we reported a BOPIM derivate, BOPIM-1 [19] (Scheme 1), which exhibited extremely weak



**Scheme 1** Structure of BOPIMs

fluorescence in polar solvent due to the TICT mechanism. Meanwhile, we noticed that BOPIM-1 is an efficient “off-on” switcher for pH between 4.0 and 2.4 ascribed to the inhibition of TICT upon protonation [20]. Based on the above mentioned considerations, we employed another BOPIM derivative, BOPIM-2 (Scheme 1), which possessed the same parent structure with BOPIM-1, but contained only one electron donor group -Ph-N(CH<sub>3</sub>)<sub>2</sub>. In this work, our investigation found that two BOPIMs (BOPIM-1 and BOPIM-2) both showed TICT characteristic, verified by their positive solvatochromism of fluorescence spectra and frontier MOs of at the equilibrium geometries. They can act as fluorescence sensors for monitoring the water content in organic solvent, for their sensitive response in fluorescence intensities and wavelengths. Compared with Karl-Fischer method, our fluorescence sensor shows more sensitive and visible for measurement application, especially for medium polarity organic solvents. Five organic solvents, 1,4-dioxane (Diox), tetrahydrofuran (THF), acetonitrile (MeCN), iso-propanol, acetone, as representatives, were investigated in this paper.

## Experimental

### Materials and Apparatus

Solvents were purchased from Aldrich Chemical, purified by normal procedures and dried over freshly activated molecular sieves (MS 4A). All starting materials used to synthesize BOPIMs were obtained from commercial supplies and used as received. <sup>1</sup>H-NMR and <sup>13</sup>C-NMR were recorded on Bruker

400 NMR spectrometers. Chemical shifts are reported in ppm with TMS as reference. Fluorescence spectra were obtained using a Hitachi F-4500 fluorescence spectrometer.

### Synthesis of two BOPIMs

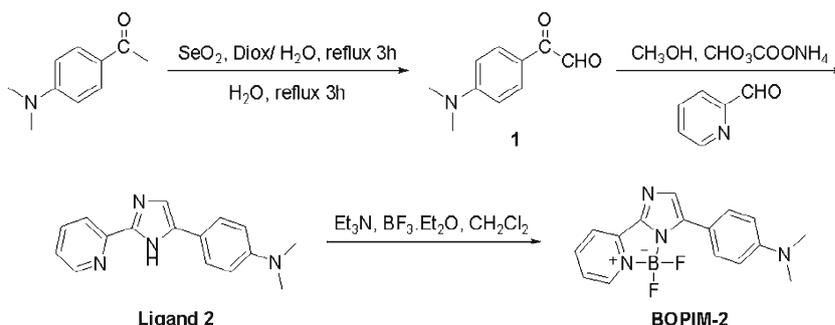
The BOPIM-1 was synthesized and characterized according to literature procedure [19].

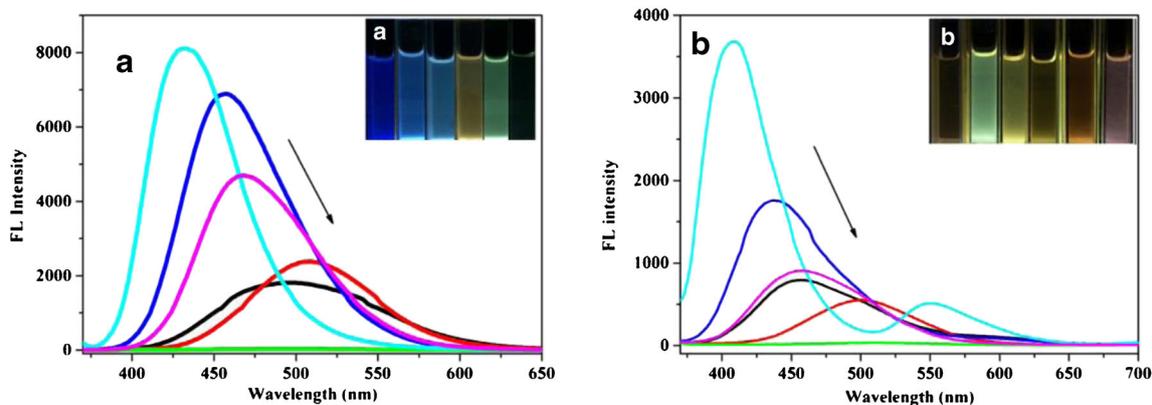
The BOPIM-2 was synthesized as Scheme 2. First, dimethyl amine acetophenone (1.3 g), 1, 4-dioxane (10 mL), water (0.5 mL), selenium dioxide (1.11 g) was added in a round bottom flask, heated to reflux for 3 h, filtered. Then water (20 mL) was added into the organic phase, refluxed for 3 h, cooling and crystallization, 1 was obtained. 1 (6.2 mmol, 1.1 g) in 32 mL methanol was mixed with 2- aldehyde pyridine (6.2 mmol, 0.66 g) and ammonium acetate (2.30 g, 30.0 mmol) in 30 mL methanol, stirred at room temperature overnight. The crude product was subjected to column chromatography. Then the resulting ligand 2 was mixed with Et<sub>3</sub>N (5 mL) in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (25 mL) and stirred, and BF<sub>3</sub>·OEt<sub>2</sub> (7.0 mL) was added dropwise at 0 °C. After the addition of BF<sub>3</sub>·OEt<sub>2</sub>, the reaction mixture was allowed to warm to room temperature and stirred at room temperature overnight to obtain a orange solid, which was purified by silica gel column chromatography to afford product. Yield: 20 %. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.41 (d, J=5.6 Hz, 1H), 8.13 (t, J=1.20 Hz, 1H), 7.96 (d, J=8.00 Hz, 1H), 7.71 (d, J=2.00 Hz, 2H), 7.46 (s, 1H), 7.41(m, 1H), 6.78 (d, J=2.20 Hz, 2H), 3.00 (s, 6H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 149.30, 143.28, 140.02, 130.80, 126.91, 125.92, 120.97, 117.06, 116.33, 11.57, 39.36. The NMR spectra were shown in supplementary information (Fig. S1).

### General Measurements

The stock solution of BOPIMs was prepared in various anhydrous solvents (5.0 mmol) and working solutions were freshly prepared from the stock solutions. The fluorescence spectra were scanned 10 min later after working solutions prepared. The excitations were carried out at 365 nm while both

**Scheme 2** Synthesis of BOPIM-2





**Fig. 1** Fluorescence spectra of BOPIM-1 (a), BOPIM-2 (b) ( $5.0 \times 10^{-5}$  M) in different solvents at room temperature, from left to right: *n*-hexane,

Diox, THF,  $\text{CHCl}_3$ , MeCN,  $\text{CH}_3\text{OH}$ . The insets show the fluorescence photographs of compounds in corresponding solvents

excitation and emission slit widths were 5 nm. All experiments were carried out at 298 K.

Elucidation of the molecular orbitals (HOMO and LUMO) of BOPIMs has been accomplished by optimizing the geometry of the molecule on the software package GAMESS platform [21], using B3LYP hybrid functional and 6-311G (d, p) basis set [22].

## Results and Discussion

### Fluorescence and TICT Properties of Two BOPIMs

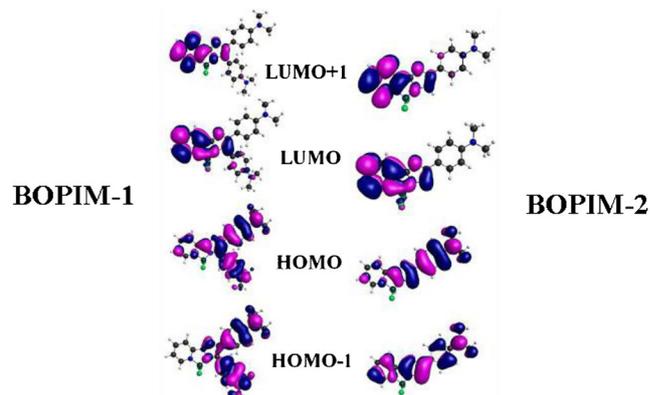
The emission spectra of BOPIMs in different solvents are shown in Fig. 1. The emission maximum of BOPIM-1 was changed from 433 nm in *n*-hexane to 521 nm in methanol while BOPIM-2 was changed from 408 nm in *n*-hexane to 508 nm in methanol, indicative of the charge transfer nature of the emitting state. As the solvent polarity increased, there was a decrease in transition energy and a positive solvatochromism effect was observed. The emission red shift and intensity weakening with solvent polarity were typical phenomenon for an emission from a TICT state [23]. Both BOPIM-1 and BOPIM-2 in various solvent exhibited dramatic fluorescent color variations under illumination with 310 nm light (insets), which were consistent with the fluorescence spectra.

Theoretical calculation has also been shown to correlate well to the experimental findings in the light of the TICT model. As shown in Fig. 2, the highest occupied molecular orbital (HOMO) is mainly localized on the substituent  $-\text{PhN}(\text{CH}_3)_2$ , the electron donor, and the lowest unoccupied molecular orbital (LUMO) is localized predominantly on BOPIM precursor, limited flexibility, the electron acceptor. What's more, a visible separated charge state can be observed from HOMO-1 to LUMO + 1, that means this compound is prone to be a twisted geometrical state afford a clear view for the

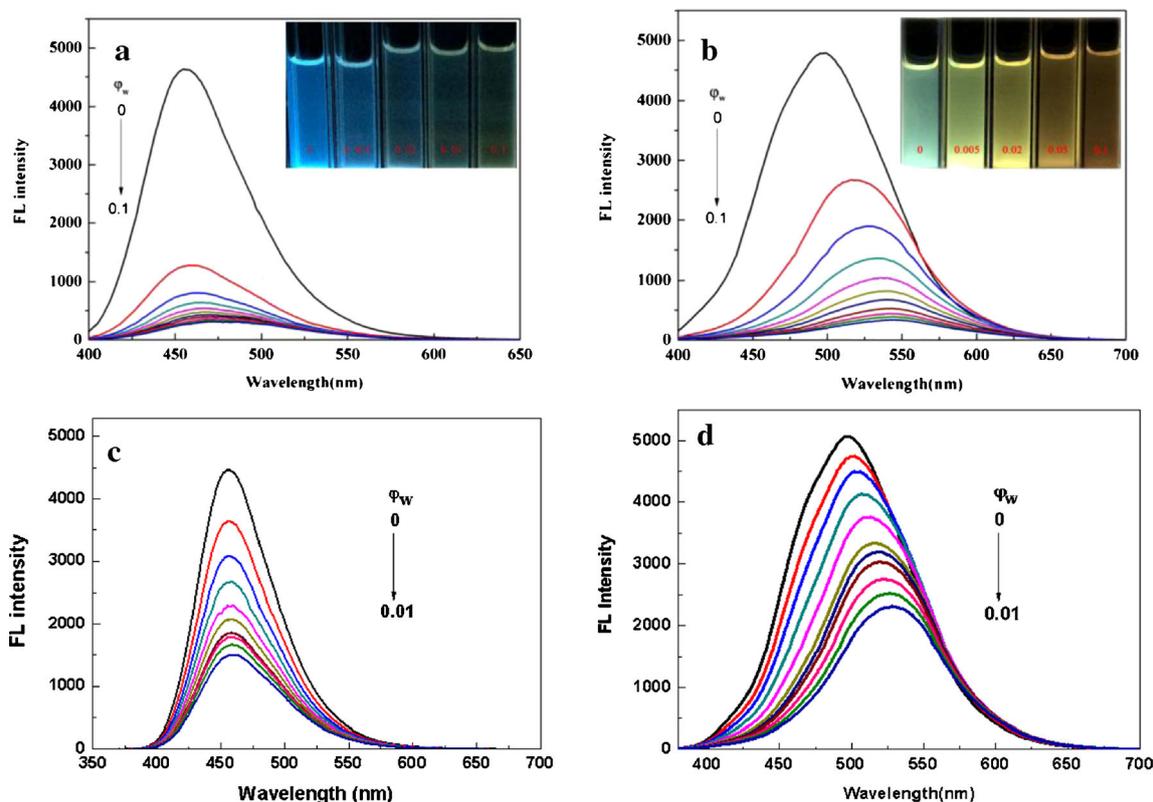
photoinduced TICT formation in excited state in both BOPIM-1 and BOPIM-2.

### Spectral Changes Induced by Addition of Water in Organic Solvents

Introduction of water to organic solvent results in the characteristic emission bands effectively quenching along with bathochromic shifts for polarity changes. As it can be seen from Fig. 3, introduction of even relatively small amount of water, reaching  $\varphi_w$  0.01 (volume fraction of water) to pure Diox, the characteristic emission intensity at 450 nm (excitation 360 nm) drop dramatically to 28 % of that from the water-free solution, with 5 nm spectra red-shift for BOPIM-1, and the emission at 500 nm (excitation wavelength 360 nm) drop to 55 %, with 23 nm red-shift for BOPIM-2, respectively. The emission decrease and red shift will proceed on with the increase of the amount of water (Fig. 3a, b; Table 1). Furthermore, BOPIM-2 exhibited dramatic fluorescent color variations under illumination with 310 nm light: green to brown, with the increase of water



**Fig. 2** Frontier molecular orbital contours of BOPIMs on the B3LYP 6-311G (d, p) level



**Fig. 3** Water-dependent fluorescence emission spectra of BOPIM-1 (a, c) and BOPIM-2 (b, d) ( $5.0 \times 10^{-5}$  M) in Diox with increasing amount of water (a, b:  $\varphi_w=0-0.1$ ; c, d:  $\varphi_w=0-0.01$ ); inset: a BOPIM-1 and b

BOPIM-2 fluorescence photographs of Diox (3.0 mL) in pure Diox to Diox containing water ( $\varphi_w$ , from left to right: 0, 0.005, 0.02, 0.05, and 0.1)

content, along with a significant decrease in the fluorescence intensity (inset of Fig. 3b). The illumination of blue almost quenched completely for BOPIM-1 when  $\varphi_w > 0.02$  (inset of Fig. 3a). It was found that the red shift of BOPIMs occurred with the introduction of water to pure Diox is so similar to their emission change and the TICT states prominent with the increasing of solvent polarity.

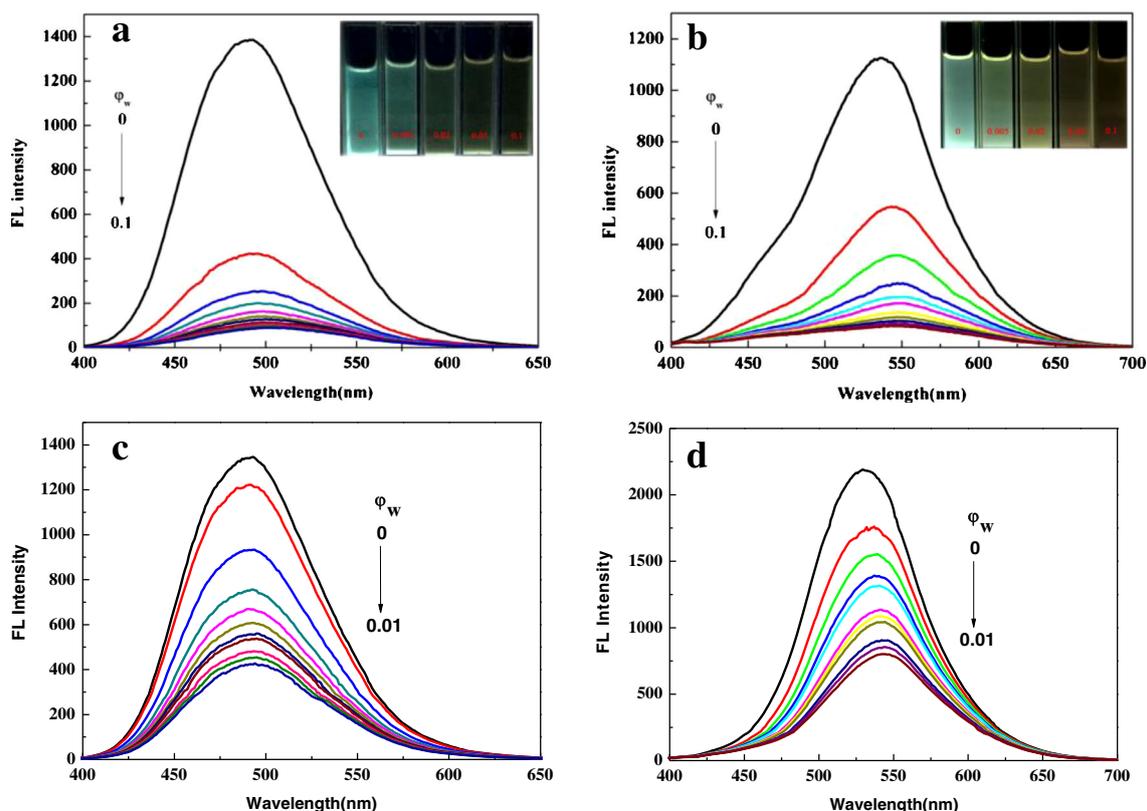
The similar behavior was observed in acetone. Figure 4 presents emission spectra and luminescence photographs of BOPIM-1 and BOPIM-2 in acetone, recorded for changing water concentration in solvent. From pure to acetone containing water, there were also obvious decreases of fluorescence intensity of BOPIMs, accompanied with red-shift in emissions and dimming in photos. The emission intensity drop

dramatically to about 30 % when  $\varphi_w=0.01$  for BOPIM-1, 48 % for BOPIM-2, respectively. Moreover, the fluorescence emission spectra of two BOPIMs with the addition of water in three other organic solvents: THF, MeCN, *iso*-propanol were investigated (shown in Fig.S2-Fig.S4). Similarly the presences of low level water in organic solvents affect significantly the emission intensity and wavelength except in *iso*-propanol. The emissions of two BOPIMs in *iso*-propanol were less obvious change with the water addition when  $\varphi_w$  below 0.01, complicating they were less sensitive of water in *iso*-propanol.

Fluorescent quenching was observed with increasing water content in various solvents, accompanied by the red shift of the emission, which was attributed to the formation of TICT

**Table 1** The fluorescence emission wavelength ( $\lambda_{em}$ , nm) changes in five organic solvents containing water ( $\varphi_w=0.1$ ), excitation at 365 nm

Solvents		Diox	THF	MeCN	Acetone	<i>iso</i> -propanol
BOPIM-1	Pure solvent	455	465	500	493	467
	Containing water	472	483	514	501	472
BOPIM-2	Pure solvent	495	462	548	536	547
	Containing water	543	502	555	543	546



**Fig. 4** Fluorescence emission spectra of (a) BOPIM-1 and (b) BOPIM-2 ( $5.0 \times 10^{-5}$  M) in acetone containing different amount of water (a, b:  $\varphi_w = 0-0.1$ ; c, d:  $\varphi_w = 0-0.01$ ); inset: a BOPIM-1 and b BOPIM-2 fluorescence

photographs in acetone with water contents ( $\varphi_w$ , from left to right: 0, 0.005, 0.02, 0.05, and 0.1)

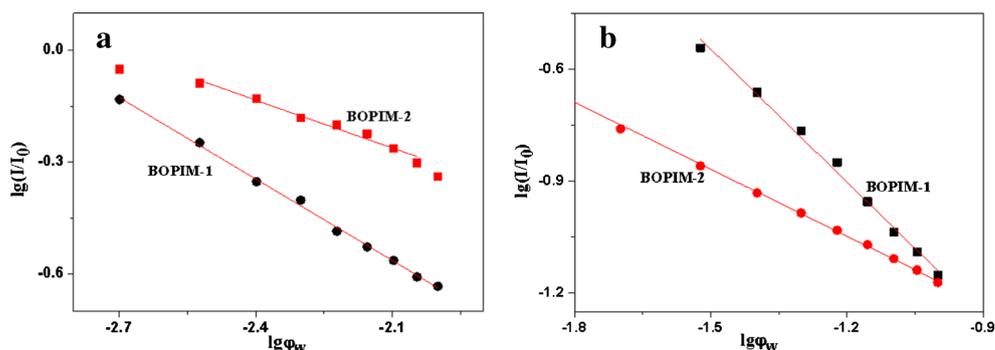
excitation of BOPIMs by hydrolysis. The introduction of water to these organic solvents result in the suppression of local emission and the formation of TICT state due to an non-fluorescent twisted structure by hydrolysis of BOPIMs. Addition of water into solvent results in an increase in the solvent polarity, which twists the luminogen conformation and moves the equilibrium from local to the TICT state, leading to a bathochromic shift in the emission with the dramatic decreasing intensity. It is indicated that two compounds are two very

good water-sensitive indicators, and suitable for constructing water sensors to monitor the concentration of water in organic solvents.

### BOPIMs Based Water Quantification

The fluorescence intensity of BOPIMs decreased dramatically with the addition of water in organic solvents even below  $\varphi_w$  0.01. For the purpose of establishing the quantitative

**Fig. 5** Calibration curves of  $\lg \frac{I}{I_0}$  against  $\lg \varphi_w$  for BOPIMs ( $5.0 \times 10^{-5}$  M) in water containing Diox. a  $\varphi_w = 0.001-0.01$ ; b  $\varphi_w = 0.01-0.1$



**Table 2** The calibration equations and correlation coefficients

Solvent	Fluorescence indicator	The range of $\varphi_w$	Calibration equation	$R^2$
Diox	BOPIM-1	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -2.095 - 0.7291 \lg \varphi_w$	0.9975
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -2.332 - 1.1901 \lg \varphi_w$	0.9931
	BOPIM-2	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -1.086 - 0.3961 \lg \varphi_w$	0.9840
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -1.770 - 0.6011 \lg \varphi_w$	0.9990
Acetone	BOPIM-1	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -1.431 - 0.4711 \lg \varphi_w$	0.9941
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -1.356 - 0.4671 \lg \varphi_w$	0.9767
	BOPIM-2	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -1.844 - 0.665 \lg \varphi_w$	0.9992
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -2.045 - 0.9221 \lg \varphi_w$	0.9937
THF	BOPIM-1	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -1.269 - 0.4091 \lg \varphi_w$	0.9847
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -1.904 - 0.6381 \lg \varphi_w$	0.9969
	BOPIM-2	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -0.450 - 0.1321 \lg \varphi_w$	0.9863
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -0.387 - 0.0951 \lg \varphi_w$	0.9804
MeCN	BOPIM-1	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -2.678 - 0.8321 \lg \varphi_w$	0.9847
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -2.639 - 0.8211 \lg \varphi_w$	0.9985
	BOPIM-2	$\varphi_w < 0.01$	$\lg \frac{I}{I_0} = -2.03 - 0.7061 \lg \varphi_w$	0.9859
		$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -1.818 - 0.6331 \lg \varphi_w$	0.9919
<i>iso</i> -propanol	BOPIM-1	$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -0.6045 - 0.3281 \lg \varphi_w$	0.9947
	BOPIM-2	$\varphi_w > 0.01$	$\lg \frac{I}{I_0} = -1.053 - 0.5451 \lg \varphi_w$	0.9798

relationship between the fluorescence intensity ( $I$ ) and water fraction in solvent ( $\varphi_w$ ), the graph of  $\lg \frac{I}{I_0}$  ( $I_0$ : the fluorescence intensity in pure solvent) as a function of  $\lg \varphi_w$  was obtained in the range of  $\varphi_w$  0.001~0.01, 0.01~0.1, respectively. As it can be seen from Fig. 5, for BOPIM-1 in Diox, the good linear relationship can be developed:  $\lg \frac{I}{I_0} = -2.095 - 0.7291 \lg \varphi_w$  ( $R^2=0.9975$ ) when  $\varphi_w$  below 0.01,  $\lg \frac{I}{I_0} = -2.332 - 1.1901 \lg \varphi_w$  ( $R^2=0.9931$ ) when  $\varphi_w$  higher than 0.01. Whereas the slope of linear for BOPIM-2 are much smaller than BOPIM-1 (Table 2), and the equation is obtained as  $\lg \frac{I}{I_0} = -1.086 - 0.3961 \lg \varphi_w$  ( $R^2=0.9840$ ) ( $\varphi_w < 0.01$ ),  $\lg \frac{I}{I_0} = -1.770 - 0.6011 \lg \varphi_w$  ( $R^2=0.9990$ ) ( $\varphi_w > 0.1$ ), respectively. The response curves in the other four different solvents showed a similar trend to that in Diox (Fig. S5-S8), and the equation and the relation values are summarized in Table 2. Many of the correlation coefficients ( $R^2$ ) reach up to 0.99, some even 0.999, thus these

calibration equations can serve as the quantitative basis for the determination of water in organic solvents. As a consequence, the quenching of the fluorescence intensity due to the presence of water in solvents was described by linear equation

**Table 3** Determination of water content in real organic solvent (Diox) using the proposed method

Indicator	Sample	Added $\varphi_w$	Measured $\varphi_w$	Recovery %
BOPIM-1	1	0.00210	0.00205	97.72
	2	0.0390	0.0367	94.00
	3	0.0780	0.0724	92.88
BOPIM-2	1	0.0260	0.0259	99.45
	2	0.0650	0.0595	91.49
	3	0.0780	0.0789	101.1

of  $\lg \frac{I}{I_0}$  vs.  $\lg \varphi_w$  as measured for the solution of the indicator in the organic solvent.

The foregoing procedure was applied to evaluate the values of water content in real solvents using the proposed two fluorescence indicators. Herein Diox without treatment was taken for example to discuss the measurement recovery in real solvent using standard addition method. The values of  $\varphi_w$  derived from calibration equation according to measured fluorescence intensity of BOPIMs, together with the recoveries in three samples can be seen in Table 3. The tests showed consistent results with the real water content in Diox samples, and the reasonable recoveries were obtained both for BOPIM-1 and BOPIM-2. The results revealed that the present method can workable in real organic solvent samples.

## Conclusions

It was found that two boron-fluorine derivatives with TICT characteristic acts as highly sensitive fluorescence sensors for the detection of a trace amount of water in organic solvents. Introduction of low level water to organic solvents, especially, for moderate polar solvents, resulted in obvious intensity decrease and bathochromic shift in fluorescence emission, which was attributed to the formation of TICT excitation of BOPIMs by hydrolysis. Besides, the observable luminescence changes were displayed in two fluorescence indicators. A quantification method to detect water content was developed, described by linear equations:  $\lg \frac{I}{I_0}$  vs.  $\lg \varphi_w$ . Real organic solvent sample are also tested to support this method, it proves that two proposed BOPIMs have good sensitivities and provide promising strategies for the detection of trace water content in organic solvents.

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