Supporting information

Substituent and solvent effects on the fluorescent and photochromic properties of 2-(2-pyridyl) imidazole containing diarylethene derivatives

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1. Lippert-Mataga equations

\[ \Delta v = \nu_{ab} - \nu_{fl} = \frac{2\Delta f (\mu_e - \mu_g)^2}{hca^3} + C \]  

(1)

\[ a = (3M/AN\pi d)^{1/3} \]  

(2)

\[ \Delta f = f - \frac{1}{2} f' = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{1}{2} \frac{n^2 - 1}{(2n^2 + 1)} \]  

(3)

Where, \( \nu_{ab} \) and \( \nu_{fl} \) are the wave numbers of the absorption and emission maxima, respectively, \( \mu_e \) and \( \mu_g \) is the excited state and ground state dipole moments of a solute, \( h \) is the Planck’s constant, \( c \) is the velocity of light in vacuum, \( a (\text{Å}) \) is Onsager radius of solute, which can be derived from the Avogadro number \( N \), molecular weight \( M \), and density \( d \) of solute. \( C \) is a constant. The solvent polarity parameter \( \Delta f \) is a function of the dielectric constant \( \varepsilon \) and the refractive index \( n \).
2. Absorption and fluorescence spectra

![Absorption and fluorescence spectra](image)

**Figure S1.** Absorption spectra (left, the insets show the reversible color changes between the open forms and photostationary states) and emission spectra ($\lambda_{ex} = 325$ nm, right) of L1–L5 (5×10$^{-5}$ mol/L) in CH$_2$Cl$_2$ upon irradiation with UV light.
**Figure S2.** Absorption spectra (left, the insets show the reversible color changes between the open forms and photostationary states) and emission spectra ($\lambda_{\text{ex}} = 325$ nm, right) of L3 ($5\times10^{-5}$ mol/L) in various solutions upon irradiation with UV light.
3. Fatigue resistance

**Figure S3.** Fatigue resistance of L3 ($5 \times 10^{-5}$ mol/L) was tested in degassed CH$_2$Cl$_2$ by alternatively irradiating with the UV ($\lambda = 302$ nm) and the visible light ($\lambda = 520$ nm) (open (○) and closed (●) form), monitored by the absorbance at 572 nm.

4. Solvent effect

**Figure S4.** Linear relationship between the Stokes shift ($\Delta\nu$) values of L3 in various solvents and the DN.

Electronic Supplementary Material (ESI) for RSC Advances
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5. Reference


6. Copies of $^1$H NMR

(1) 2-methylbenzo[b]thiophen-3-ylboronic acid (5)

(2) 1-(4-methoxyphenyl)-2-(2-pyridyl)imidazole (9)
(3) 1-(4-nitrophenyl)-2-(2-pyridyl)imidazole (11)

(4) 1-(4-methoxyphenyl)-4,5-dibromo-2-(2-pyridyl)imidazole (12)
(5) 1-phenyl-4,5-dibromo-2-(2-pyridyl)imidazole (13)

(6) 1-(4-nitrophenyl)-4,5-dibromo-2-(2-pyridyl)imidazole (14)
(7) 1-(4-methoxyphenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (L1)

(8) 1-phenyl-4,5-bis-[2-methylbenzo[b]thiophen-3-yl]-2-(2-pyridyl)imidazole (L2)
(9) 1-phenyl-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (L3)

(10) 1-phenyl-4,5-bis-[2,5-dimethyl-3-thienyl]-2-(2-pyridyl)imidazole (L4)
(11)
1-(4-nitrophenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (L5)

7. Copies of $^{13}$C NMR

(1) 1-(4-methoxyphenyl)-2-(2-pyridyl)imidazole (9)
(2) 1-(4-nitrophenyl)-2-(2-pyridyl)imidazole (11)

(3) 1-phenyl-4,5-dibromo-2-(2-pyridyl)imidazole (13)
(4) 1-(4-nitrophenyl)-4,5-dibromo-2-(2-pyridyl)imidazole (14)

(5) 1-(4-methoxyphenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (L1)
(6) 1-phenyl-4,5-bis-[2-methylbenzo[b]thiophen-3-yl]-2-(2-pyridyl)imidazole (L2)

(7) 1-phenyl-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (L3)
(8) 1-phenyl-4,5-bis-[2,5-dimethyl-3-thienyl]-2-(2-pyridyl)imidazole (L4)

(9) 1-(4-nitrophenyl)-4,5-bis-[5-chloro-2-methyl-3-thienyl]-2-(2-pyridyl)imidazole (L5)