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ORIGINAL PAPER

Structure and properties of 2-[(*E*)-2-(4-dipropylaminophenyl)-1-ethenyl]-1,3,3-trimethyl-3*H*-indolium chloride

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The structure of styryl dye, 2-[(*E*)-2-(4-dipropylaminophenyl)-1-ethenyl]-1,3,3-trimethyl-3*H*-indolium chloride (*I*), was investigated using methods such as UV-VIS, fluorescence spectroscopy, and NMR (^{1}H, ^{13}C, APT, HMQC, COSY) and also by examining its electrochemical properties. A study of the acid–base properties revealed the existence of three different forms of the dye. The mechanisms of protolysis and hydrolysis are discussed. The reagent exists in a reactive single-charged form I^+ over a wide range of acidity (pH 4–11). The optimum analytical wavelength of the single-charged form is 550 nm, where the molar absorptivity is 5.51×10^4 L mol^{-1} cm^{-1}. The values of the optimum analytical wavelength and molar absorptivity of the protolysed and hydrolysed forms are: λ_{max}(*I*-H^{2+}) = 380 nm, ε(*I*-H^{2+}) = 2.01×10^4 L mol^{-1} cm^{-1}; λ_{max}(*I*-OH) = 320 nm, ε(*I*-OH) = 1.12×10^4 L mol^{-1} cm^{-1}. A theoretical study of the spectral and chemical properties of *I* was carried out by performing quantum chemical calculations.

Keywords: 2-[(*E*)-2-(4-dipropylaminophenyl)-1-ethenyl]-1,3,3-trimethyl-3*H*-indolium chloride, structure, properties

Introduction

Styryl dyes belong to the group of polymethine dyes characterised by the presence of the conjugate chain —CH═CH—C_6H_4—. Styryl dyes are generally asymmetrical in structure; their solubility can increase and their optical, thermal, and electronic properties can change depending on the type of substituent present (Gawinecki & Trzebiatowska, 2000; Kormosh et al., 2002; Krieg et al., 2008).

Many papers have been published on the synthesis and investigation of the experimental and theoretical properties of various styryl dyes (Bricks et al., 2000; Vasilev et al., 2008; Li et al., 1998; Horiguchi et al., 2002; Rangnekar & Sonawane, 2000; Wang et al., 2009; Deligeorgiev et al., 2010; Fedyunyayeva et al., 2011; Kim et al., 2003; Wang et al., 2007). These dyes are commercially important for their applications as sensitisers in photography, optical and fluorescent materials, and for their use in various other fields, for example in dye-sensitised solar cells and dyes with nonlinear optical properties. In addition, the most important applications of these dyes are in cell biology and medicine (Krieg et al., 2008; Deligeorgiev et al., 2010; Balanda et al., 2007; Tokar et al., 2006; Kovalska et al., 2005).

Styryl dyes also have uses in analytical chemistry as reagents for the determination of inorganic and organic compounds. *N*,*N*-Dialkylamino-styryl dyes can also be used as specific and highly fluorescent substrates for peroxidase, hence they have possible applications in histochemistry and immunohistochemistry (Krieg et al., 2008). Styryl dyes are also used in analytical chemistry as amyloid sensors (Li et al., 2004) or for the determination of Ba^{2+} and Ca^{2+} cations (Mitewa et al., 1995). Spectrophotometric and SIA determinations of small amounts of nitrophenols and picric acid are based on the formation of ion associate (IA) with a

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