



Short communication

Solvatochromicity of 3-hydroxy-4-(1-(2,4-dihydroxyphenyl)-2-hydroxy-2,2-diphenylethylidene)cyclohexa-2,5-dienone for screening of solvents

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ABSTRACT

The quinonic compound 3-hydroxy-4-(1-(2,4-dihydroxyphenyl)-2-hydroxy-2,2-diphenylethylidene)cyclohexa-2,5-dienone (**1**) is synthesised by the reaction of benzil with 1,3-dihydroxybenzene in basic medium. Solution of this compound shows visibly distinct colour differences in different solvents. From the different absorption maxima of the compound in visible spectra it can be used as an excellent analytical reagent to screen different solvents.

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1. Introduction

The colour of quinonic compounds is decided by substituent attached to the quinone unit and also by the solvent used [1–6]. The quinonic compounds having extended conjugation through π -electron delocalisation show colour changes on change of pH of the medium [7,8]. We are pursuing studies on quinone methides [9,10] to understand their colour properties in confined medium. While pursuing such study we found that the compound 3-hydroxy-4-(1-(2,4-dihydroxyphenyl)-2-hydroxy-2,2-diphenylethylidene)cyclohexa-2,5-dienone (Fig. 1) to be exceptionally sensitive to change colour on dissolution in different solvents. In different solvents this compound shows optical absorbance maximum at well distinguishable wavelengths. In this article we present the colour properties of this compound.

2. Materials and methods

The UV–vis spectra were recorded on a Perkin-Elmer Lambda750 UV–vis spectrophotometer. For each UV–vis spectra measurement, a specified amount of the compound was dissolved in HPLC/spectroscopic grade solvent, taken in a quartz cuvette (3 ml) and the visible spectra were recorded. The transition energies of

the visible absorption peaks are calculated [11] using Eq. (1):

$$E_T(\text{kJ mol}^{-1}) = \frac{hcN}{\lambda} = 119,625 / (\lambda/\text{nm}) \quad (1)$$

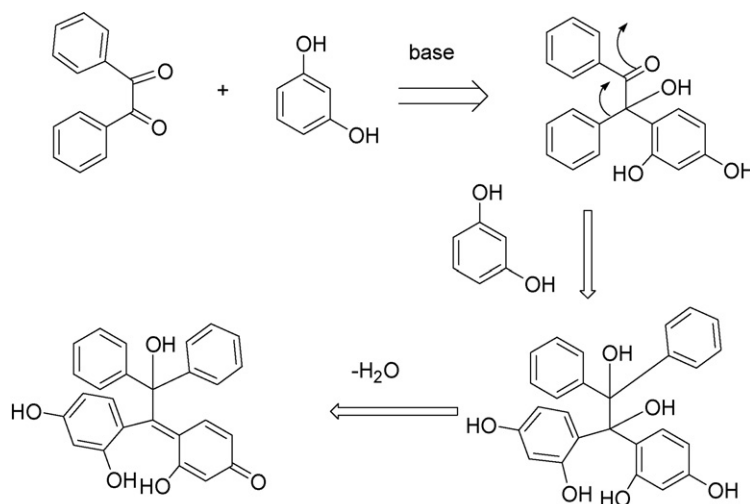
2.1. Synthesis

A solution of benzil (0.63 g, 3 mmol) and potassium hydroxide (0.17 g, 3 mmol) in water (2 ml) and ethanol (4 ml) was taken in a round bottom flask (100 ml). To this solution 1,3-dihydroxybenzene (0.33 g, 3 mmol) was added and the solution was placed on an oil bath at 80 °C for 6 h with constant stirring; the colour of the solution changed from dark blue to dark red. The reaction mixture was brought to room temperature and was extracted with ethylacetate (100 ml) and repeatedly washed with water. The ethylacetate extract was concentrated and the compound was separated using preparative TLC as red solid. Yield 55%.

2.2. Spectroscopic data

IR (cm^{-1} , KBr): 3428 (s), 3058 (w), 2926 (w), 1599 (m), 1557 (s), 1467 (w), 1434 (s), 1334 (m), 1210 (w), 1170 (m), 1108 (m), 1069 (w), 1026 (w), 929 (w), 900 (w), 844 (m), 711 (s), 679 (w). ^1H NMR (DMSO- d_6 , 400 MHz): 7.84 (1H, dm, $J=7.6$ Hz); 7.56 (1H, m); 7.37 (1H, d, $J=7.5$ Hz); 7.28 (3H, m); 6.67 (1H, dd, $J=7.8, 2$ Hz); 6.12 (1H, d, $J=7.5$ Hz); 6.01 (1H, s). ^{13}C NMR (DMSO- d_6 , 100 MHz): 180.9, 158.1, 139.2, 134.5, 130.2, 130.1, 129.8, 129.4, 129.1, 127.9, 124.2, 109.1, 103.9. LC–MS [M^+]: 414.9845.

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Scheme 1. A possible pathway for formation of I.

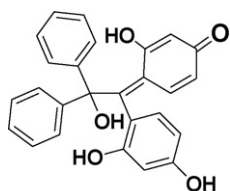
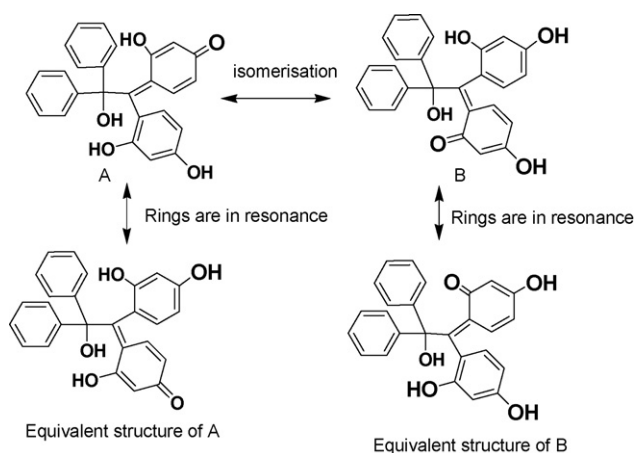


Fig. 1. The structure of 3-hydroxy-4-(1-(2,4-dihydroxyphenyl)-2-hydroxy-2,2-diphenylethylidene)cyclohexa-2,5-dienone (I).

3. Result and discussions

3.1. Synthesis and characterisation

The compound **I** was synthesised in basic medium by reacting 1,3-dihydroxybenzene with benzil. In this reaction the benzil reacts with 1,3-dihydroxybenzene which rearranges to give the desired product (**Scheme 1**). The phenyl migration depicted in the scheme is similar to the phenyl migration in conversion of benzil to benzilic acid in basic medium [12]. The compound is characterised from its spectroscopic properties such as ^1H NMR, ^{13}C NMR, IR and mass spectra. The mass spectra of the compound gave the desired m/e value. The ^1H NMR of the compound is highly solvent dependent and it is discussed under a separate sub-section.



Scheme 2. Two different types of keto forms of I.

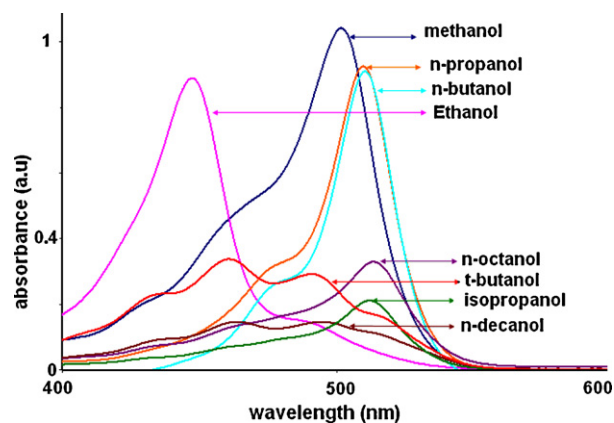


Fig. 2. Visible spectra of I (0.075 mol/dm³) in different alcohols.

3.2. Solvatochromicity

The compound **I** can adopt several keto-enol forms and among them two keto forms as shown in **Scheme 2** can play major role in determining the colour changes in different solvents. Depending on the formation of these forms in different solvents the π - π^* transition of the compound is affected. The π - π^* transition in visible spectra of **I** at equal concentration in different alcohols, namely,

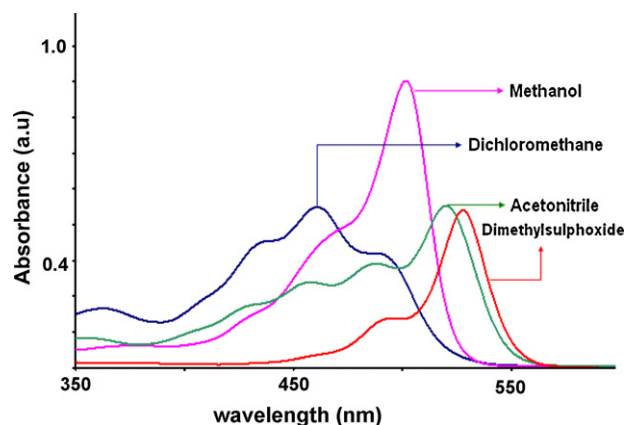


Fig. 3. Visible spectra of I (0.075 mol/dm³) in different solvents.

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