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Ground and excited state dipole moments of some flavones using solvatochromic methods: An experimental and theoretical study

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ABSTRACT

The absorption and fluorescence characteristics of biologically active flavone derivatives 6-Hydroxy-7,3′,4′,5′-tetramethoxyflavone (6HTMF) and 7-Hydroxy-6,3′,4′,5′-tetramethoxyflavone (7HTMF) are studied at room temperature (298 K) in solvents of different polarities. Excited state dipole moments of these compounds have been determined using the solvatochromic shift method based on the microscopic solvent polarity parameter E_T^N. Dipole moments in excited state were found to be higher than those in the ground state in both the molecules. A reasonable agreement has been observed between experimental and theoretically calculated dipole moments (using AM1 method). Slightly large value of ground and excited state dipole moments of 7HTMF than 6HTMF are in conformity with predicted electrostatic potential maps. Our results would be helpful in understanding use of these compounds as tunable dye lasers, optical brighteners and biosensors.

1. Introduction

In addition to their marked biological activities such as anti-inflammatory, anti-cancerous, and anti-allergic [1–4], flavones show promising photo physical and photochemical properties [5,6]. This class of compounds is widely used as dye lasers, indicators of biophysical processes and optical brighteners [7–9]. Flavones have also been used as fluorimetric reagents for determination of metal ions [10].

The excited state dipole moments of a molecule control the tunability range of their emission energy as a function of solvent polarity [11]. Several studies have been reported for determining ground and excited state dipole moments using solvatochromic shift methods [12–16]. Among the various techniques available [17] for determining the excited state dipole moment, the most popular is the one based on the Lippart-Matagen Equation. Other methods such as Stark splitting of rotational levels and Microwave conducting are also exploited in the same field [18–21].

In continuation of our earlier work [22–24] on the photo physical properties of novel natural products, we have investigated the effect of solvents on flavones and determined ground and excited state dipole moments for the compounds 6-Hydroxy-7,3′,4′,5′-tertramethoxyflavone (6HTMF) and 7-Hydroxy-7,3′,4′,5′-tertramethoxyflavone (7HTMF) (Fig. 1) experimentally, as well as theoretically. A fair agreement between experimentally and theoretically calculated dipole moment values has been observed. Our results can be helpful to understand use of these flavones as tunable dye lasers and biosensors etc.

2. Experimental and theoretical methods

The flavones used were synthesized according to the standard methods [25,26]. Their structures and purity were confirmed on the basis of their known melting points and ^{1}H NMR spectra. All the solvents used, such as, benzene, ethyl acetate, acetonitrile, ethanol, methanol and triple distilled water were of spectroscopic grade. The absorption and fluorescence spectra were measured on a Kontron UV-930 spectrophotometer and Jasco FP-770 spectrofluorimeter respectively.

2.1. Experimental determination of dipole moments

Two methods of solvatochromism have been employed in the present study.

Method 1