Synthesis of new fluorogenic dyes based on the solvatochromism of barbituric acid derivatives

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1. INTRODUCTION

Solvatochromic dyes can be used apply various field such as measuring the polarity of solvents and colorimetric sensor arrays for volatile organic compounds. Solvatochromic dyes are defined that when dissolved in different solvents, the absorption or emission spectra of the molecule were changed. Among other things, merocyanine dyes are known to apply solvatochromic because of their electronic structure. The merocyanine dyes have a push-pull system at the ground-state electronic structure. The resonance occurs between neutral and zwitterionic molecular structures. The barbituric acid can be used useful fragment in a solbatochromic dyes because barbiturate groups are strongly electron-withdrawing.

Also, they gain aromatic stabilization upon reduction. On the other hand, triphenylamine and carboazole are widely considered to be the rich-electron.

In our study on this subject, we synthesized two new solvatochromic dyes similar to merocyanine with barbituric acid, triphenylamine and carboazole. We investigated their absorbance and fluorescent emission spectroscopic behaviors in different solvents. We compare interesting color differences various solvents.

2. EXPERIMENT

2.1. Synthesis of 5-(4-(diphenylamino)benzylidene)-1,3 -dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (dye1)

A mixture of 1,3-dimethylpyrimidine-2,4,6(1H, 3H, 5H)-trione 1 (0.312g, 0.002mol) and 4-(diphenylamino) benzaldehyde 2 (0.546g, 0.002mol) and in acetic anhydride (5ml) was refluxed for 3h. The resulting cooled mixture was filtered and recrystalized in acetic acid to give 0.48g with 59% yield.

2.2. Synthesis of 5-(4-(9H-carbazol-9-yl)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione(dye2)

A mixture of 1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione 1 (0.312g, 0.002mol) and 4-(9H-carbazol-9-yl) benzaldehyde **3** (0.54g, 0.002mol) and in acetic anhydride (15ml) was refluxed for 3h. The resulting cooled mixture was filtered and recrystalized in acetic acid to give 0.46g with 57% yield.

3. RESULTS AND DISCUSSIONS

The emission spectra of dye 1 and dye2 was measured differently according to different solvents. Also, the emission spectra change of dye2 is clearer than the emission spectra change of dye1.

The dyes 1 and dye 2 have same acceptor group, similarly two different donor fragments. So, donor fragment of carbazole is better than donor fragment of triphenylamine. These features indicate a strongly allowed π - π * transition with charge-transfer characters.

4. CONCLUSTION

In this study, we synthesized two new solvatochromic merocyanine dyes based on barbituric acid. The dye 2 which was made with barbituric acid and cabazole fragment exhibited solvatochromic properties in various solvents.

5. REFERENCE

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