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Synthesis and characteristic of solvatochromic fluoresecent dyes : *donor- π- acceptor* structural design

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1. INTRODUCTION

Triphenylamine dyes are prominent and crucial class of synthetic π-conjugated materials and have captured much attention due to their promising potential functions for high technology applications named as functional dyes. Triphenylamine dyes can access a set of highly fluorescent π-conjugated, triphenylamines bearing a function linker at various positions on one phenyl ring is reported.

In this paper, we investigated the D-(π)-A system triphenylamine moieties using the cyclicvoltammetry and computational calculation method named by *Materials studio 4.3*.

2. EXPERIMENT

2.1 Measurements

Cyclicvoltammetry (CV) measurements used the 3-electrod system (glass carbon/Pt wire/reference electrode) in acetonitrile present of tetrabutlyammonium hexafluorophosphate electrolyte. Computational calculation method used the *Materials studio 4.3*. UV-Vis absorption spectra and fluorescent properties were recorded on Agilent 8453 spectrophotometer and Shimadzu RF-5301 spectrophotometer, respectively.

2.2 Preparation

1,3-indanedione (1.5 mmol) and 4-formyl -triphenylamine (1.5 mmol) were dissolved in n-butanol (30 mL) and refluxed for 2 hr. After cooling, red precipitate was collected, washed with ethanol, and dried. b and c were condensated using corresponding aldehyde.

3. RESULT AND DISCUSSION

Using the CV, we estimate the HOMO/LUMO levels of used compounds. Equation (1) shows the calculation method of HOMO and LUMO energy levels using the CV.

$$\text{HOMO (or LUMO) eV} = -4.8-(E_{onset\ or\ peak} - E_{1/2}(\text{Ferrocence})) \quad (1)$$

According to the equation (1), LUMO levels of compound a and b were -3.68eV and -3.70eV, respectively, compound c was poor solubility in the acetonitrile. The HOMO levels of a, b, and c were -5.17, -5.37, and -5.49eV, respectively. These values showed the compound a, b and c belongs to the D-(π)-A system. Computational calculation methods of these compounds were estimated by Dmol3. Computational calculation and CV data showed the three compounds electrochemical properties. CV data showed the HOMO/LUMO energy levels and computational calculation showed the electron distribution. As a result, intramolecular charge transfer (ICT) processes were suggested for all three dyes.

4. CONCLUSION

In conclusion, significant features, such as strong fluorescence in solution and solid state, solvent-reliant properties, unusually large Stokes shifts, lower LUMO and higher HOMO levels, were observed in the three dyes.

5. REFERENCES

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