

## Abstract

Three acceptor-donor (AD) molecular rotor compounds were synthesized and characterized in this work whereby dyads p-AD and m-AD and triad m-ADA contained BODIPY and Benzodithiophene (BDT) as electron acceptor and donor respectively. In all the compounds, the donor and acceptor moieties are electronically decoupled by a phenyl spacer, either through a para coupling or through a Meta coupling. Through spectroscopic studies, structure property relationships have been deduced in this work. Earlier, p-ADA was synthesized based on BODIPY dye as acceptor and BDT as electron donor decoupled with a para-phenyl spacer. The compound showed dual emission with efficient twisted intramolecular charge transfer (TICT) band at  $\sim 700$  nm with Stokes shift of  $\sim 194$  nm. Prominent fluorescence solvatochromism in solvents of increasing polarity was observed for p-ADA. Efficient aggregate induced emission and a reasonable charge carrier mobility of p-ADA in thin films of  $\sim 4 \times 10^{-4}$  cm<sup>2</sup>/Vs. However, meta regioisomeric triad m-ADA showed well-defined aggregation in solution evident from absorption and emission studies. On the other hand, the dyad counterparts of these two compounds p-AD and m-AD showed distinct photophysical characteristics whereby the dyad p-AD showed multiple emissions with TICT band at 660 nm characterized by a smaller Stokes shift of  $\sim 149$  nm and prominent solvatochromism. Notably, all compounds showed temperature tunable and viscosity dependent emission changes. The temperature dependence of emission intensities of p-AD and p-ADA render these molecules useful ratiometric sensors. On the other hand, viscosity dependence of fluorescence is indicative of their potential applications as viscosity sensors for biologically or material science relevant micro-environments. This study substantiates the fact that by subtle and minimal variations in the chemical structures, optical and electronic properties of such rotor molecules can be tuned to a great extent that have potential applications in biolabelling and sensing. Such multifunctional rotor molecules with readily tunable emission properties are potential temperature and viscosity sensors for bio(medical) and material applications.