World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:12, No:09, 2018

Photophysics and Torsional Dynamics of Thioflavin T in Deep Eutectic Solvents

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Abstract : Thioflavin-T (ThT) play a key role of an important biologically active fluorescent sensor for amyloid fibrils. ThT molecule has been developed a method to detect the analysis of different type of diseases such as neurodegenerative disorders, Alzheimer's, Parkinson's, and type II diabetes. ThT was used as a fluorescent marker to detect the formation of amyloid fibril. In the presence of amyloid fibril, ThT becomes highly fluorescent. ThT undergoes twisting motion around C-C bonds of the two adjacent benzothiazole and dimethylaniline aromatic rings, which is predominantly affected by the micro-viscosity of the local environment. The present study articulates photophysics and torsional dynamics of biologically active molecule ThT in the presence of deep-eutectic solvents (DESs). DESs are environment-friendly, low cost and biodegradable alternatives to the ionic liquids. DES resembles ionic liquids, but the constituents of a DES include a hydrogen bond donor and acceptor species, in addition to ions. Due to the presence of the H-bonding network within a DES, it exhibits structural heterogeneity. Herein, we have prepared two different DESs by mixing urea with choline chloride and N, N-diethyl ethanol ammonium chloride at ~ 340 K. It was reported that deep eutectic mixture of choline chloride with urea gave a liquid with a freezing point of 12°C. We have experimented by taking two different concentrations of ThT. It was observed that at higher concentration of ThT (50 µM) it forms aggregates in DES. The photophysics of ThT as a function of temperature have been explored by using steady-state, and picoseconds time-resolved fluorescence emission spectroscopic techniques. From the spectroscopic analysis, we have observed that with rising temperature the fluorescence quantum yields and lifetime values of ThT molecule gradually decreases; this is the cumulative effect of thermal quenching and increase in the rate of the torsional rate constant. The fluorescence quantum yield and fluorescence lifetime decay values were always higher for DES-II (urea & N, N-diethyl ethanol ammonium chloride) than those for DES-I (urea & choline chloride). This was mainly due to the presence of structural heterogeneity of the medium. This was further confirmed by comparison with the activation energy of viscous flow with the activation energy of non-radiative decay. ThT molecule in less viscous media undergoes a very fast twisting process and leads to deactivation from the photoexcited state. In this system, the torsional motion increases with increasing temperature. We have concluded that beside bulk viscosity of the media, structural heterogeneity of the medium play crucial role to guide the photophysics of ThT in DESs. The analysis of the experimental data was carried out in the temperature range 288 ≤ T = 333K. The present articulate is to obtain an insight into the DESs as media for studying various photophysical processes of amyloid fibrils sensing molecule of ThT.

Keywords : deep eutectic solvent, photophysics, Thioflavin T, the torsional rate constant
Conference Title : ICP 2018 : International Conference on Photochemistry
Conference Location : Paris, France
Conference Dates : September 20-21, 2018