

Abstract

This thesis presents the results of investigations into organic conjugated system stability in different kinds of conditions through optoelectronic characterization by UV-Vis and Photoluminescence spectrophotometers. The amalgamation of experimental methods characterization techniques used in this work exposes advantageous perceptions into the correlations between conjugated system stability in chlorinated and non-chlorinated solvents, and provides clues to utilize less toxic and environment friendly solvents. The stability of the conjugated materials utilize in OPV devices is an active area of research.

Optoelectronic properties of two kinds of conjugated materials, PTB7-Th which is from the generation of OPV donor polymers and O-IDTBR which is a non-fullerene acceptor molecule has been investigated. Various parameters which affect the stability of the conjugated materials have been employed and the resultant bathochromic and hypsochromic shifts have been recorded. The studies such as solvent effect, Stokes shift and binary blends were done on both the donor and acceptor molecules. The extensive studies like concentration effect, sunlight degradation in chlorinated and non-chlorinated solvents, thermal degradation in non-chlorinated solvent, binary solvent mixture effect in ten dilutions, stability of binary solvent mixture in sunlight, cold and dark environments, stability in chlorinated solvent by the addition of base and rate of degradation in distilled and without distilled solvents has been done on a conjugated donor polymer PTB7-Th.

The results of the studies revealed that the conjugated materials showed good solubility in both the chlorinated solvents (chloroform and chlorobenzene) and non-chlorinated solvents (toluene and xylene). According to the study of the concentration effect it has been noticed that high concentration makes the conjugated materials more stable. Their spectra showed a red shift at room temperature in all kinds of solvents with more pronounced aggregates peak as compared to the polymer solutions at low concentration. Similarly, the rate of sunlight degradation at low concentration is higher as compared to the high concentration solution. The chlorinated solvents degrade the polymer at a faster rate as compared to the non-chlorinated solvents. The polymer solution in chloroform degraded at low temperature even. So the chlorinated solvents do not only harm the environment but also affect the stability of the conjugated materials. The addition of base in chlorinated polymer solution reduces the rate of degradation. The

absorption and emission spectra showed a blue shift in the degradation of the polymer. The spectra revealed that the aggregates break first following the breakage of the polymer backbone. Toluene is the most suitable solvent regarding stability in sunlight. The order of the polymer stability in different solvents were toluene>xylene>chlorobenzene>chloroform. The chloroform degrades the conjugated material regardless of the purity of the solvent like even in distilled and without distilled solvent at the same rate. Concomitant with the drop in absorption intensity a blue shift in the spectra is observed. The studies from the binary solvent mixture solutions showed that methanol which is a poor solvent induce aggregates in the polymer solution with red shift. A noticeable drop in fluorescence emission spectra was observed in 70:30 (CH₃OH: MeOH) because of quenching. The sunlight degradation of the binary solvent mixture revealed that in 50:50 of chloroform and methanol the polymer does not breakdown and remains stable even after 8 hour exposure in sunlight. At low temperature all the dilution from 90:10 to 10:90 (CH₃OH: MeOH) showed a red shift with a more observed peak of J-aggregates. That means, high temperature breaks the aggregates while low temperature enhances aggregation. The study on binary blends of PTB7-Th: O-IDTBR showed that the charge transfer happened by quenching the donor peak and the peaks of blends similar to the acceptor peak. This phenomena is more prominent in film state as compared to the solutions.