Effect of triphenylamine as electron-donor evenly spaced in 2, 4, 6 and 8 thiophene units of the main chain: synthesis and properties

Sánchez C.O.

Schott E.

Zárate X.

MacLeod-Carey D.

Sobarzo P.

Gatica N.

Several poly(thiophene) derivatives containing triphenylamine (TPA) as electron-donor were synthesized by chemical homopolymerization in CHCl3 media using FeCl3 as oxidizing agent. Monomers containing TPA bonded by imine groups to terminal thiophene, bithiophene, terthiophene units allows polymerization to be performed in conditions similar to thiophene. TPA units are regularly spaced in 2, 4, 6 and 8 thiophenyl units in the main chain. TPA electron-donor effect on the polymers chains, as compared to poly(thiophene) was studied. Polymers, labeled as poly(TPA-Th), poly(TPA-biTh) and poly(TPA-Terth) were characterized by 1H-NMR, FT-IR and UV?visible spectroscopy, elemental analysis, thermal stability (TGA) intrinsic viscosity, differential scanning calorimetry (DSC) and electrochemically using cyclic voltammetry (CV). The characterizations are consistent with the proposed structures. The polymers exhibited different optical absorption. They exhibited low intrinsic viscosity, a different effective conjugation and high thermal stability. Moreover, the polymers displayed two redox processes with a redox potential lower than that of poly(thiophene). Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO) and optical band gap (Eg) were measured and the obtained values were compared with those of poly(thiophene). The effect of the presence of TPA units in the thiophenyl chains on HOMO, LUMO, band gap, redox potential and on TGA is reported. To complete the series, HOMO/LUMO levels and band gap of a polymer containing TPA with 8 thiophenyl units in the chain were determined using theoretical calculations. The results proved that, with respect to

poly(thiophene), it is possible to decrease HOMO and LUMO without changing the band gap, projecting itself as a potential polymer to be studied in organic photocells.