Title

Thiophene- and bithiophene-based ?-conjugated Schiff base oligomers containing binaphthalene moieties in the backbone. Properties and computational simulations

Abstract

New ?-conjugated Schiff base oligomers (o-AZdAN1Th and o-AZdAN2Th) based on a binaphthalene core and containing thiophene or bithiophene units in their backbone were synthesized from the reaction between [1,1?-binaphthalene]-4,4?-diamine with thiophene-2,5-dicarbaldehyde and [2,2?-bithiophene]-5,5?-dicarbaldehyde by a high-temperature polycondensation method. These new materials were slightly soluble in non-protic polar solvents, such as chloroform and dichloromethane. From GPC analysis of the CHCl3-soluble fraction, o-AZdAN1Th was found to be a tetramer, whereas o-AZdAN2Th was a trimer with 1.4 kDa and 1.3 kDa average molecular weight (Mn), respectively. Both samples exhibited high thermal stability with T5% values of 452 °C and 456 °C and relatively high Tg values of 346 °C and 384 °C, for o-AZdAN1Th and o-AZdAN2Th, respectively. The samples showed absorptions in the deep-blue (o-AZdAN1Th) and blue (o-AZdAN2Th) regions of the visible spectrum, and emission responses at 387 nm and 447 nm, respectively, with moderate Stokes shifts (77-95 nm). Their optical and electronic properties were similar to those described for thiophene-based materials, with optical bandgap values close to 2.4 eV. HOMO energy values of ?5.98 and ?5.95 eV and LUMO energy values of ?3.87 eV and ?3.84 eV were obtained for o-AZdAN1Th and o-AZdAN2Th, respectively. Theoretical DFT and TD-DFT calculations were used to compare the effect of increasing thiophene units along the backbone for the real and also theoretical o-AZdANxTh samples (x = 3 and 4 thiophene units). According to our study, these two new thiophene-based can be proposed for optoelectronic applications. © 2024 The Royal Society of Chemistry.

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Absorption spectroscopy; Amines; Dichloromethane; Electronic properties; Oligomers; Organic solvents; Supercomputers; Binaphthalenes; Bithiophenes; Computational simulation; Energy value; GPC analysis; High temperature polycondensation; Polar solvents; Property; Schiff base oligomer; Synthesised; Thiophene

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