Novel Schiff base self-condensed oligomers in complexation with metallic triflates of low-band gap properties

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Schiff base oligomers obtained by self-condensation from monomers containing simultaneously amino and aldehyde groups are rare in the literature. Novel conjugated oligomers were synthesized by self-condensation of 5-(4-aminophenyl) aryl-2-carboxaldehyde prepared in situ from the corresponding nitro homologous compounds. The oligomers were characterized by spectroscopic methods. Band gap and absorption effect on the oligomers in the presence and absence of metal triflates were surveyed. The oligomers presented good UV?Vis absorption and a 2.2 eV band gap. In the presence of metal triflates, a maximum absorption shift toward longer wavelengths took place. As a result of this, the band gap decreased to 1.8 eV. This value has been the lowest band gap reported for Schiff base oligomers and polymers. Some oligomers dissolved in m-cresol containing metal triflate have afforded blue solutions with maximum wavelength of 571 nm that decrease as triflate concentration increases. Furthermore, to give a better explanation on UV?Vis observed transitions, the oligomeric structure was simulated using time-dependent density functional theory (TD-DFT) calculations to see the involved orbitals in the UV?Vis transitions. The calculated band gap for the oligomer was in very good agreement with the experimental results. Furthermore, the TD-DFT calculations showed that the transitions were delocalized over the whole structure.

Low-band gap oligomers

Metallic triflates

Oligomers

Optical properties

Self-condensation

Complexation

Condensation

Density functional theory

Metals

Oligomers

Optical properties

Spectroscopic analysis

Homologous compounds

Low band gap

Oligomeric structure

Schiff base oligomer

Self-condensation

Spectroscopic method

Time dependent density functional theory

Triflates

Energy gap