Iran Polym J (2015) 24:911–918
DOI 10.1007/s13726-015-0379-3

ORIGINAL PAPER

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

Christian O. Sánchez[1] · Patricio Sobarzo[1] · Eduardo Schott[2] · Ximena Zarate[3] · Carlos Bustos[1]

Received: 4 February 2015 / Accepted: 7 July 2015 / Published online: 14 September 2015

Abstract 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.

Keywords Optical properties · Oligomers · Self-condensation · Metallic triflates · Low-band gap oligomers

✉ Christian O. Sánchez
christiansanchez@uach.cl

Eduardo Schott
maschotte@gmail.com

Ximena Zarate
jazminac@gmail.com

[1] Instituto de Ciencias Químicas, Facultad de Ciencias, Universidad Austral de Chile, Avda. Las Encinas 220, Campus Isla Teja, Valdivia, Chile

[2] Departamento de Química Inorgánica, Facultad de Química, Pontificia Universidad Católica de Chile, Avda. Vicuña Mackenna 4860, Santiago, Chile

[3] Instituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Avda. Pedro de Valdivia 641, Santiago, Chile

Introduction

Conjugated polymers such as Schiff base polymers, also known as poly(azomethines) or poly(imines), have been widely studied. Schiff base polymers containing imine groups (–CH=N–) in their backbone have been synthesized in a variety of structures because of their low solubility, excellent properties and wide application fields, such as selective membranes [1], magnetic properties [2], hole transport material [3], metallic complexes [2, 4], electrochromic properties [5], catalyst support [6, 7], electrical properties [8, 9], batteries [10] and optoelectronics [11, 12].

Conjugated Schiff base polymers are usually synthesized by the reaction between two comonomers: aromatic diamines and aromatic dialdehydes (or diketone) [13, 14]. Another approach consists in introducing an imine group into the monomers containing thiophene or pyrrol as terminal units and polymerization by oxidative condensation. In this type of reaction, the monomer reacts with oxidizing agents in an electrochemical cell on the surface of an inert electrode [15, 16].

Conjugated polymers based on monomers such as thiophene, furan and pyrrole have also been studied. These