PÔSTER - RESUMO - DISPOSITIVOS OPTOELETRÔNICOS

2 + 2 MAKES A POLYMER: CATALYSED HETEROATOMIC DIELS-ALDER REACTIONS TO MAKE NEW POLY(FULLERENE)S

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Over the past few years, fullerenes and their derivatives have constituted a pivotal class of materials for the development of organic photovoltaic devices (OPVs), owing to their remarkable versatility, particularly in the design of advanced compounds that exploit their high electron affinity and superior electron-accepting capability [1-3]. The practical application of pristine C60 is frequently limited by its low solubility in common organic solvents, as well as its pronounced tendency toward aggregation and crystallization [4]. These factors significantly deteriorate the morphology of the active layer and progressively impair device performance. In this context, numerous synthetic strategies have been developed to promote the chemical functionalization and reactivity of this carbon allotrope. Main-chain poly(fullerene)s (PFs) have emerged as a strategic alternative, integrating the outstanding electronic properties of fullerenes with the processability and film-forming characteristics of polymeric systems, thereby mitigating undesirable phase segregation. The most widely employed synthetic approaches for these materials typically rely on radical-based methodologies,

such as atom transfer radical addition polymerization (ATRP), as well as cycloaddition reactions including Diels–Alder and Prato chemistry [5-7].

In this work, an innovative synthetic route was proposed for the preparation of versatile poly(fullerene)s via the reaction of newly designed quinoline derivatives with C60 and PCBM. The selection of quinoline units as comonomers is grounded in their donor–p–acceptor (D–p–A) architecture, which is well recognized for promoting enhanced thermal stability and efficient p-conjugation. The polymerization reaction was catalyzed by dichloro[1,3-bis(diphenylphosphino)propane]nickel(II) ([Ni(dppp)Cl2]). The most notable feature of this synthetic methodology is its mechanistic pathway, proceeding through a [2+2] cycloaddition—an unprecedented route in the literature for the formation of fullerene-based polymers—thus distinguishing it from conventional strategies such as ATRAP or Diels–Alder reactions.

Structural characterization of the resulting copolymers was successfully performed using one- and two-dimensional Nuclear Magnetic Resonance (^{1}H and ^{13}C NMR, including 2D experiments), together with Gel Permeation Chromatography (GPC), which confirmed polymer chain growth and effective incorporation of the designed functional groups. Additionally, optoelectronic properties were investigated by cyclic voltammetry. The electrochemical data revealed a significant enhancement in the redox response of quinoline-containing systems compared to non-functionalized analogues, corroborating the beneficial impact of the D–p–A molecular architecture on electronic modulation. Accordingly, this study establishes not only an efficient and original protocol for the synthesis of poly(fullerene)s but also provides a promising framework for the incorporation of other conjugated molecules via catalytic coupling strategies, targeting next-generation high-performance organic electronic devices.

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Palavras-chave: quinoline derivatives; diels-alder reaction; polyfullerenes; opv; pcbm.