

Synthesis and Evaluation of Conjugated Poly(phenylacetylene) Derivatives As New Carbon Fiber Precursors

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Abstract

This paper systematically investigates a series of conjugated poly(phenylacetylene) derivatives containing various π -electrons conjugated side groups. The objective is to understand the side chain effect to the carbonization of this conjugated polymer system, which is essential in designing a new carbon fiber precursor to replace current polyacrylonitrile (PAN) precursor that is expensive and only offers ~50% C yield with many toxic gas by-products. The complex thermal conversion process and low carbonization efficiency are relative to the requirement of stabilization reaction in air (O_2) atmosphere and the subsequent ejection of O and N heteroatoms in the precursor structure during the carbonization reaction. The newly designed polymer system is based on pure hydrocarbon polymers (without any other heteroatom) with a fully π -electrons conjugated molecular structure along the backbone and side chains. The ideal conjugation structure shall facilitate stabilization reactions (i.e. cyclo-addition, crosslinking, etc.) in an inert atmosphere at low temperatures (below the polymer chain degradation temperature). The resulting larger polyaromatic moieties between the polymer chains allow the subsequent carbonization process under elevated temperatures to remove most of hydrogen (H) elements and promote ring fusion to transform the material into the hexagonal carbon (graphene) sheets with high C yields. As will be discussed, two poly(phenylacetylene) derivatives containing para-substituted acetylene (poly(PA-A)) and phenylacetylene (poly(PA-PA)) side chains show 90% and 80% C yields, respectively, in an one-step thermal conversion process under N_2 atmosphere. Poly(PA-A) almost reaches to the theoretical values with only the removal of H atoms in its structure during the whole thermal conversion process.