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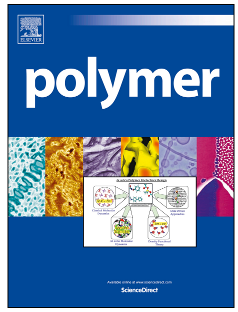

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Reaction Kinetics and Simulations of Ring-Opening Polymerization for the Synthesis of Polybutylene Terephthalate

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ABSTRACT: Cyclic polybutylene terephthalate (PBT) was polymerized with 2-ethylhexanoic acid tin(II) salt activated by 1-dodecanol in order to study the reaction mechanisms dominant in ring-opening polymerization (ROP) for polyester synthesis. Initiator-to-monomer content and temperatures were varied from 0.05% to 0.5% and 190^{o}C to 250^{o}C, respectively. The living-like character of ROP was confirmed by the characteristic effect of initiator content on cyclic oligomer conversion, along with the linear dependence of the number-average molecular weight upon conversion. The molecular weight distribution is mainly a function of the interplay between chain transfer and transesterification reactions. Since the PBT macrocycles appear in different sizes from 2 to 7 repeat units, each carbonyl group theoretically contributes to ring reactivity, where in this system both size-dependent and size-independent approaches to simulate propagation deliver appreciable results. The corresponding rate constants have been determined and, in contrast to other polymer systems, the proximity of these values to those of chain transfer and transesterification is significant.

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