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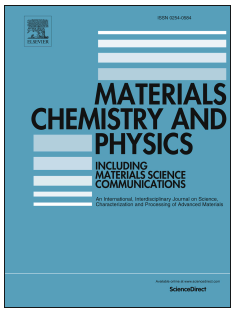

Styrene based copolymers for consistent reactivity ratio evaluation

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ACCEPTED MANUSCRIPT

Styrene based copolymers for consistent reactivity ratio evaluation

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ABSTRACT

The reactivity ratio parameters or *r*-parameters are the most important indicators for the characterization of copolymers. Consequently, over the last decades, a variety of methods have been developed to determine and predict the *r*-parameters. Among these, the prediction with the Alfrey-Price *Q,e*-scheme is one of the oldest and most commonly used techniques. The synthesis of 21 binary methacrylate-based copolymers with lauroyl peroxide as the initiator (radical starter) shows large deviations between the experimentally determined copolymerization parameters and those calculated with the *Q,e*-values taken from the established literature. Assuming an error tolerance of ± 0.05, only 20.6% of the *r*-parameters were predicted correctly. To address this problem, copolymerizations with styrene as the comonomer are performed to maintain comparable *Q,e*-values. It is found that structural similarities of the monomers favor correct prediction. Furthermore, the use of specific parameter sets can improve the prediction, resulting in the maximum of 42.3% correct findings.

INTRODUCTION

Copolymers are an important compound class in polymer science since they enable a wide range of functions that exceed those of the homopolymers.[1,2] However, even for the simplest binary copolymer five different copolymer types can be found. Examples of a homopolymer chain and various copolymer

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