Accepted Manuscript

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PII: S0254-0584(18)30084-1

DOI: 10.1016/j.matchemphys.2018.01.077

Reference: MAC 20349

To appear in: Materials Chemistry and Physics

Please cite this article as: Daniel Zaremba, Henning Menzel, Wolfgang Kowalsky, Hans-Hermann Johannes, Styrene based copolymers for consistent reactivity ratio evaluation, *Materials Chemistry and Physics* (2018), doi: 10.1016/j.matchemphys.2018.01.077

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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 \pm 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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