

NMR study of microstructure of copolymers of butyl acrylates with methyl methacrylate and *tert*-butyl methacrylate

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Acrylic polymers due to wide spectrum of properties including excellent stability, clarity, durability, UV stability and color retention are used to manufacture a variety of commercial products. They are used in optics and medicine and in an astounding variety of applications, mainly as paints and adhesives, but also in the textiles area. Acrylic polymers can be used in various forms from a very soft adhesive materials and fine powders, to rigid non-film forming products. Macroscopic properties of polymeric materials strongly depend on subtle differences in polymer chain, called polymer microstructure. During polymerization of acrylic monomers, an asymmetric carbon is formed in the main chain and relative configuration of consecutive asymmetric centers (tacticity) has considerable influence on macroscopic properties of the polymer formed. The method of analysis, which is crucial in the study of the structure and properties of macromolecular compounds is nuclear magnetic resonance spectroscopy (NMR). Apart from the typical analytical tasks like identification and determination of composition, NMR spectroscopy is so far the only tool that allows for precise observations of microstructural differences in polymer chains.

The PhD was devoted to the detailed analysis of uninvestigated so far acrylate–methacrylate copolymers obtained from methyl methacrylate, *tert*-butyl methacrylate and four possible butyl acrylates, as well as their respective homopolymers. These systems are very interesting due to their possible industrial applications, ranging from building (adhesives, paints, varnishes) and automotive to pharmaceutical industry (e.g., manufacture of extended-release drugs). In this study the carbonyl and the main-chain methylene carbon (β -CH₂) signals of ¹³C NMR spectra were used to determine distribution of configurational-compositional sequences. For the homopolymers the analysis was performed at the heptad and hexad level for carbonyl and methylene signal, respectively, while in the case of copolymers the distribution of stereosequences was determined for carbonyl signal at pentad level. The analysis was verified performing computer simulation of the NMR spectra applying Bernoulli and/or 1st order Markov statistics and incremental calculation of chemical shifts for individual configurational-compositional sequences.