Microstructures of Poly(Vinyl Acetate) Studied by Nuclear Magnetic Resonance Spectroscopy

Hongyang Yao

College of William & Mary, Department of Applied Science, 1997
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Advisor: William Starnes, Jr., Gottwald Professor of Chemistry

Abstract

Carbon-13 NMR spectroscopy was used to investigate the microstructures of poly(vinyl acetate) prepared by solution polymerization in benzene. A series of aromatic compounds was synthesized in order to model he structures formed via chain transfer to solvent. The peaks near 126.5 and 128.5 ppm in the spectra of the polymer samples were assigned to a 1-phenyl-(2n+1)-multi-acetoxyalkane (where n= 1, 2, 3, etc.) microstructure. The concentration of that structure obtained from NMR spectra was correlated with the concentration calculated from reported kinetic data.

Chain transfer to benzene was shown to occur by addition of the macroradical to benzene, followed by rearomatization involving loss of a hydrogen atom. No evidence was obtained for a transfer mechanism involving hydrogen abstraction from benzene, and the copolymerization of benzene with vinyl acetate also was shown to be absent. The transfer mechanism actually established accounts for the unexpectedly large transfer constant of benzene in vinyl acetate polymerization. General mechanisms are proposed for the solution polymerization of vinyl acetate in aromatic solvents.