YS-1

Studies of Allyl Alcohol Radical Polymerization by PFG-HMQC and HMBC NMR at 750 MHz

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The structures of poly(allyl alcohol) were characterized by one- and two-dimensional gradient enhanced heteronuclear multiple quantum coherence (gHMQC) and gradient enhanced heteronuclear multiple-bond connectivity (gHMBC) NMR spectroscopy. Main chain structures and chain-end structures were identified from the spectra. The polymerization of allyl alcohol can be described by degradative chain transfer to allyl alcohol monomers, which results in distinctive chain-ends as well as low molecular weight polymers. After the allylic hydrogen abstraction by initiator radicals, allyl radicals produce chain-ends with vinyl groups and aldehyde groups. The chain-ends were identified by the correlation peaks in gHMQC and gHMBC spectra.