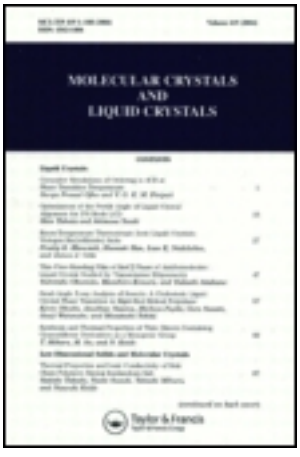

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Thermal Isomerization of Polyacetylene Films

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THERMAL ISOMERIZATION OF POLYACETYLENE FILMS

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Abstract. Isomerization of the as-formed (-78°C) cis-polyacetylene to the trans isomer is relevant to the electronic structure, the crystal structure and the electrical properties of this prototypical conductive polymer. We have studied the process using Fourier transform infrared (FTIR) and ^{13}C magic angle nuclear magnetic resonance (NMR) spectroscopies at temperatures between 80 and 110°C. The observed kinetics will be discussed in terms of three basic processes: a second order process which randomly converts cis-cis-cis (CCC) sequences to trans-cis-trans (TCT) sequences via a pair of biradicals, a fourth order process that converts CTCC sequences to TCTT sequences via four biradicals, and two fourth order processes which allow sequential migration along the chain. The correlation of observed electron spin resonance and x-ray results, among others, with these mechanisms will be shown.