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Scientific Session III

^{13}C Coupled Relaxation Study on Segmental Motions of *n*-Undecane in Solution

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Segmental motions involving methylene groups in carbon chain backbone of *n*-undecane in solution state have been investigated by 13C NMR coupled relaxation method. For sensitivity enhancement each 12C atom at the position 2, 3, 4, 5, 6, was selectively labeled by its isotope 13C. The sample was prepared by dissolving the 13C-labeled *n*-undecanes in CDCl3. Five pulse sequences designed to create various initial states were applied to the carbon and proton transitions of these *AX*2 spin systems, and partially relaxaed 13C spectra for several magnetization modes were obtained as a function of evolution time. Experiments were performed over the temperature range from 238 to 308 K at the interval of 10K. The data were interpreted based on the Redfield equation in terms of dipolar spectral densities which contain important dynamical information for the motions of C H bond in 13CH2 spin system in solution.

These spectral densities were analyzed on the basis of a motional model for the chain motions proposed previously by our laboratory and, as a result, some relevant motional parameters were obtained. These parameters reveal that the local segmental motions in *n*-undecane become more vigorous as we move from the center of molecule towards the terminal part of the chain. The rise of temperature is also found to intensify these segmental motions. Finally, we have compared our model with those proposed previously by others in order to help us grasp clearer picture of the segmental motions in hydrocarbon chain backbone.