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HARD SEGMENT GEOMETRY AND DYNAMICS OF MDI-BASED POLYURETHANE

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ABSTRACT

MDI-based polyurethanes consist of two molecular moieties, namely, MDI hard segment and the polyol soft segments. The properties of these polymers are assumed to be highly connected to the packing of hard and soft segments. In various studies it has been observed that response of these polymers to UV radiation is rather unusual with initially diminished peak at 356 nm that reappeared upon relaxation in fluorescence spectroscopy when irradiated with UV radiation. In searching for an explanation for this phenomenon, this study was focused on understanding the geometry and the dynamics of a model system that represents the hard segment of the MDI-based polymers. The geometry of the model system was initially optimized with AM1 level of theory. It is clearly seen in the optimized structure that the polymer molecule will have a v-shaped (bent) hard segment owing the SP^3 hybridization of the CH2 carbon that connects the phenyl moieties. Subsequently, this molecule was used to perform the conformational analysis. All possible conformations of the model system was auto-generated with molecular mechanics and the Boltzmann distribution of these conformers were obtained. The most probable conformation shows that the phenyl rings on the either side of the middle -CH2- group are in a relatively rigid conformation where it has very limited rotation around the CH2 – phenyl bond. This dihedral is confined to $\pm 30^0$ for each phenyl rotation. This result was confirmed by the single-chain molecular dynamics (MD) simulations in vacuum. The average value for this dihedral was found to be - 2.27 degrees as obtained from 10 ns MD simulation. As indicated above, the hard segment of the MDI-based polymers has a rigid v-shaped geometry. Based on the results obtained in this study, these primitive results indicate that the hard segment geometry is deviated from literature.

Keywords: MDI, Topology of MDI, Dynamics of MDI