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The local dynamics of polyetherimides: Conformational probes, IR Fourier transform spectra, and quantum-chemical calculations

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Abstract

The IR Fourier transform absorption spectra were used to study the rotational mobility of macromolecule fragments (local dynamics) of several vitreous polyetherimides by the method of conformational probes. The temperatures of the freezing of conformational equilibria of probes were determined. The IR spectra of diphenyl ether, 2,2-diphenylpropane, phthalimide, and N-phthalimide were studied; these molecules were used as models of fragments of monomeric units of polyetherimides. Quantum-chemical calculations of the energies and vibrational spectra of these molecules were performed by the B3LYP method with the 6-31G(d,p) basis set. The rotational mobility of benzene rings in the main chain of polyetherimide macromolecules was estimated, and the nature of secondary relaxation transitions was determined. The IR spectra of polyetherimides were interpreted. The rotational mobility of the CH3 and CF3 groups of polyetherimides was estimated from the temperature dependence of absorption band contours of these groups.

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