117.Title: Polarization and temperature dependent spectra of poly(3-hydroxyalkanoate)s measured at terahertz frequencies

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Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS
Volume:13
Issue:20
Pages: 9173-9179
Publication year: 2011
Document type:Journal article (JA)

Abstract: Temperature-dependent terahertz (THz) absorption spectra of poly(3-hydroxyalkanoate)s (PHAs) were measured by using a Fourier transform far-infrared (FT-FIR) spectrometer and a THz time-domain spectrometer over a temperature range of 10 K to 465 K with a liquid helium cryostat and a heating cell. Clear differences were observed between the spectra of crystalline and amorphous polyhydroxybutyrate (PHB), indicating that the absorption peaks observed in the THz spectra originated in the higher-order conformation of PHB. The polarization spectra of a stretched PHB sample were measured, and the direction of the vibrational transition moment was determined. The temperature dependences of the spectra reveal frequency shifts and broadening of the absorption peaks with temperature, suggesting large anharmonicity of the vibrational potential. The temperature shift behaviour is quite different in each transition. Some of the transitions show a blue shift, which cannot be explained by a simple anharmonic potential model. Frequency shifts of the peaks were mainly observed below 10 THz, which suggests a large anharmonicity of the vibrational potential at lower frequencies.