

Computational and quantum chemical study on high-frequency dielectric function of *tert*-butylmethyl ether in mid-infrared and near-infrared regions.

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Streszczenie

Complex dielectric function of *tert*-butylmethyl ether (TBME) was determined and analyzed in a broad spectral region covering mid-infrared (MIR) and near-infrared (NIR) regions (6500–560 cm⁻¹). Spectra of the complex electric permittivity and complex molecular polarizability have been derived from complex refractive index spectra. The molar vibrational polarization (P^{vib}) corresponding to individual modes has been estimated based on the data derived from fitting damped harmonic oscillator model to the experimental complex permittivity spectrum. Factors determining the dielectric functions due to vibrational resonance absorptions corresponding to fundamental and non-fundamental (overtones and combination modes) modes were taken into account. Direct comparison of contributions to total P^{vib} value stemming from corresponding fundamental and non-fundamental modes has been carried out and discussed for the first time. In order to identify overtones and binary combination modes, quantum chemical calculation of the vibrational spectrum of *tert*-butylmethyl ether was performed for MIR and NIR regions. Fully anharmonic approach by means of generalized second-order vibrational perturbation theory (GVPT2) was applied on DFT-B2PLYP/SNST level. An accurate reproduction of experimental data was achieved with subsequent assignment of fundamental and non-fundamental bands, which enabled detailed discussion of relations between dielectric contributions of fundamental and non-fundamental modes of *tert*-butylmethyl ether.

Słowa kluczowe

Dielectric function, Molar vibrational polarization, VPT2, Overtones and combination modes, Anharmonic vibrational analysis, NIR spectra, *tert*-Butylmethyl ether

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