



Thin film IR and computational studies of liquid di-n-butylether.

Autorzy

Krzysztof B. Beć

Jerzy P. Hawranek

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Streszczenie

The complex refractive index spectrum in the NIR and MIR range of liquid di-*n*-butylether (DNBE) was determined. Thin film recording technique was required to obtain quantitative transmission spectra in the MIR range. Raman spectrum was also collected. The experiment was supported by a conformer population analysis and anharmonic vibrational analysis, with the use of B2PLYP/N07D method.

Słowa kluczowe

neat liquid di-*n*-butylether, complex refractive index, thin film IR spectra, IR dispersion, anharmonic vibrational analysis

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