

## Vibrational analysis of liquid *n*-butylmethylether.

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### Streszczenie

The complex refractive index spectrum in the NIR and MIR range of liquid *n*-butylmethylether (NBME) was determined. Thin film recording technique was required to obtain quantitative transmission spectra in the MIR range. The experimental part was supported by a conformer population analysis and anharmonic vibrational analysis based on the B2PLYP/N07D method. The resulting population of 11 NBME conformers was analyzed and their calculated anharmonic vibrational spectra and calculated abundances (at 298 K) were used to obtain the resultant spectrum of *n*-butylmethylether. The band assignment procedure was based on the calculated potential energy distributions.

### Słowa kluczowe

Neat liquid *n*-butylmethylether, Complex refractive index, Thin film IR spectra, IR dispersion, Anharmonic vibrational analysis

### Adres publiczny

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### Strona internetowa wydawcy

<http://www.elsevier.com>