Vibrational analysis of neat liquid *tert*-butylmethylether.

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Rok wydania

2014

Czasopismo

Journal of Molecular Liquids

Numer woluminu

196

Strony

26-31

DOI

10.1016/j.molliq.2014.02.028

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Among aliphatic ethers, the most known is *tert*-butylmethylether (TBME), mainly for its significance in the fuel industry. It was the subject of numerous investigations, including industrial, environmental and medical studies. The literature however is lacking of any insightful infrared studies of TBME in neat liquid phase. In this work we determined the optical constants of TBME, from transmission studies in the IR range (11,700–560 cm^{-1}). The use of quantitative thin film recording techniques was essential due to the high absorption of neat liquids in the MIR range. Low temperature matrix investigation was also carried out, to elucidate details of the vibrational spectrum of TBME. The experiment was supported by an anharmonic vibrational analysis including the simulation of experimental spectrum, based on the B2PLYP/N07D level of theory. The chosen method delivered good results with a relatively modest computational cost.

Słowa kluczowe

IR dispersion, Complex refractive index, Neat liquid tert-butylmethylether (TBME), Thin film IR spectra, Low temperature matrix IR spectra, Anharmonic vibrational analysis, B2PLYP/N07D

Adres publiczny

http://dx.doi.org/10.1016/j.molliq.2014.02.028

Strona internetowa wydawcy

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