Optical constants of liquid pyrrole in the infrared.

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Streszczenie

The spectrum of the complex refractive index in the 12,500–500 cm^{-1} region was determined for liquid pyrrole from transmission studies. In the MIR region very thin layers with thicknesses of a few micrometers had to be used to obtain reliable data. FT-Raman spectra of the liquid are also reported. Identifications for numerous bands observed in the liquid phase were proposed basing on DFT and MP2 harmonic and anharmonic vibrational analyses. A short comparison of a few popular computational methods including B2PLYP functional with the aug-cc-pVTZ and N07D basis sets was performed.

Słowa kluczowe

Pyrrole, Thin film IR spectra, IR dispersion, anharmonic vibrational analysis

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