

Anharmonic interactions and Fermi resonance in the vibrational spectra of alcohols.

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The vibrational Raman spectra of liquid alcohols ($\text{CH}_3(\text{CH}_2)_n\text{OH}$, $n=0-3$) were studied experimentally at room temperature in a wide spectral range ($1000-4000\text{cm}^{-1}$). Special attention was paid to investigation of the high frequency region ($\geq 3000\text{cm}^{-1}$) with the OH-vibration. In addition, DFT calculations of the vibrational spectra were performed. The features of the spectra in the region of $\sim 3000\text{cm}^{-1}$ and the appearance of very broad bands were explained by Fermi resonance as well as very strong coupling between the low frequency vibrational modes and those related to hydrogen bond interactions.

Słowa kluczowe

Raman scattering, Alcohols, Vibrations, Anharmonic interactions, DFT calculations, Fermi resonance, Anharmonicity

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