Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism, and Raman Optical Activity

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Streszczenie

The aim of this paper is 2-fold. First, we want to report the extension of our virtual multifrequency spectrometer (VMS) to anharmonic intensities for Raman optical activity (ROA) with the full inclusion of first- and second-order resonances for both frequencies and intensities in the framework of the generalized second-order vibrational perturbation theory (GVPT2) for all kinds of vibrational spectroscopies. Then, from a more general point of view, we want to present and validate the performance of VMS for the parallel analysis of different vibrational spectra for medium-sized molecules (IR, Raman, VCD, ROA) including both mechanical and electric/magnetic anharmonicity. For the well-known methyloxirane benchmark, careful selection of density functional, basis set, and resonance thresholds permitted us to reach qualitative and quantitative agreement between experimental and computed band positions and shapes. Next, the whole series of halogenated azetidinones is analyzed, showing that it is now possible to interpret different spectra in terms of mass, electronegativity, polarizability, and hindrance variation between closely related substituents, chiral spectroscopies being particular effective in this connection.

Słowa kluczowe

Circular dichroism spectroscopy, Energy, Infrared light, Infrared spectroscopy, Scattering

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