Calculating the number of active modes of vibrations in BeCl2 molecule using Jmol and calculating density functional theory (DFT) in the simulated FTIR spectra obtained through Gaussian in Webmo

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Abstract

The study focuses on determining the number of vibrational modes in the $BeCl_2$ molecule using Jmol and correlating the results with the number of peaks observed in the simulated FTIR spectrum obtained through Gaussian calculations in Webmo.The vibrational modes of $BeCl_2$ are first analyzed theoretically using group theory and molecular symmetry to predict the expected normal modes.

Using Jmol, the vibrational motion of the molecule is visualized to confirm these modes. Subsequently, density functional theory (DFT) calculations are performed in Gaussian via the WebMO interface to generate a simulated FTIR spectrum, which provides a detailed vibrational analysis. The observed peaks in the FTIR spectrum are then compared with the theoretical predictions and Jmol visualizations to verify the computed vibrational modes. This study highlights the effectiveness of computational tools in vibrational spectroscopy and molecular structure analysis, demonstrating the relationship between theoretical vibrational modes and experimentally simulated spectra.

Keyword

Modes of vibrations, Jmol, Gaussian, Webmo, FTIR.