Calculating the number of modes of vibrations in CO_2 molecule using Jmol and correlating with number of peaks in the simulated FTIR spectra obtained through Gaussian in Webmo

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Abstract

This work aims at predicting the number of modes of vibrations in CO_2 molecule. The 3D structure of CO_2 molecule was drawn in the Jmol interface and energy minimization was done. The energy minimized 3D structure of CO_2 molecule was saved as **.mol** file. This **.mol** file was given as the source file to the Gaussian engine for generating the simulated FTIR spectra in the Webmo platform. Comparison of number of modes of vibrations calculated theoretically and the number of peaks obtained in simulated FTIR spectra was done. By comparing, it paves way to learn the method of interpreting the FTIR spectra.

Keyword

Modes of vibrations, Jmol, Gaussian, Webmo, FTIR