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Structure and Spectroscopic Studies of Aloe-emodin and Chrysophanol using Density Functional Theory and Experimental Methods*

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The experimental and theoretical spectra studies of Aloe-emodin and Chrysophanol are reported in this work. Experimentally the Fourier transform infrared, Raman, and UV-Visible spectra were recorded for Aloe-emodin and Chrysophanol. With the help of density functional theory and B3LYP, the functional triple zeta basis set def-TZVP was used to optimize structures and calculate the vibrational frequencies. It was found out that the conformations of Aloe-emodin and Chrysophanol with the double intramolecular hydrogen bonds between the OH and C=O groups were the most stable conformations among the different conformations obtained. The intramolecular hydrogen bonds increase the bond lengths of the respective O−H and C=O bonds which are involved to form the intra molecular hydrogen bonds. The calculated infrared frequencies of the most stable geometry of Aloe-emodin and Chrysophanol correlate well with their respective Fourier transform infrared spectra. The vibrational frequency analysis for both the molecules was done in detail for all the vibrational modes assigning the individual ring vibrations besides the different types of individual vibrations of specific bonds. The Fourier transform infrared and the Raman spectral bands attained from the experiments correlate well with the theoretical data.

Keywords: Aloe-emodin, Chrysophanol, density functional theory, infrared,Raman, UV-Vis spectra.

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