

A comparative study on the structural and spectroscopic properties of the chalcones (*E*)-1-(4-aminophenyl)-3-(4'-ethoxyphenyl)-prop-2-en-1-one and (*E*)-1-(aminophenyl)-3-(4'-methoxyphenyl)-prop-2-en-1-one

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Palavras Chave: Raman spectroscopy, Infrared spectroscopy, Chalcone.

Introduction

Chalcones form a molecular base of various chemical compounds. We can find them in the nature in plants, vegetables, and fruits or by synthesis. Its basic molecular formula is 1,3-diaryl-2-propan-1-one, found in the *trans* and *cis* forms, being the most thermodynamically stable the *trans* form. The enone system ($C\beta=C\alpha-C-C$) presents in the chalcones reacts with nucleophilic groups in the formation of heterocyclic derivatives, such as isoxazolines and pyrazolines. Chalcones and their derivatives have received a great deal of attention due mainly to their relatively simple molecular structures and the diversity of pharmacological activities which they exhibits, among them: anti-inflammatory, antimicrobial, and anti-tumor activity [1]. In this work, we carried out a comparative study of the structural and spectroscopic properties of the chalcones: (*E*)-1-(4-aminophenyl)-3-(4'-ethoxyphenyl)-prop-2-en-1-one (hereinafter referred to as PAAPEB) and (*E*)-1-(aminophenyl)-3-(4'-methoxyphenyl)-prop-2-en-1-one (hereinafter referred to as PAAPFB). The chalcones PAAPEB and PAAPFB were structurally characterized through Fourier transform Raman (FT-Raman) and Attenuated Total Reflection Fourier Transform Infrared (FTIR) spectroscopy at room temperature in the regions 130 cm^{-1} to 4000 cm^{-1} and 40 cm^{-1} to 4000 cm^{-1} , respectively. Vibrational wavenumber and wavevector have been predicted using the Density Functional Theory (DFT) calculations with the hybrid functional B3LYP, and the basis set 6-311 G(d,p).

Results and Discussions

Figure 1 shows the molecular structures of the chalcones PAAPFB and PAAPEB.

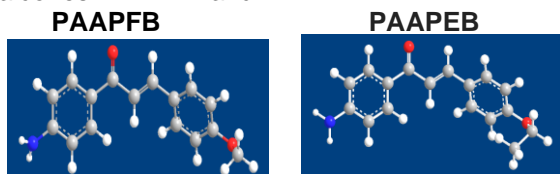


Figure 1. Molecular structures of the chalcones PAAPFB and PAAPEB.

Figure 2 shows the vibrational spectra of the chalcones PAAPEB and PAAPFB.

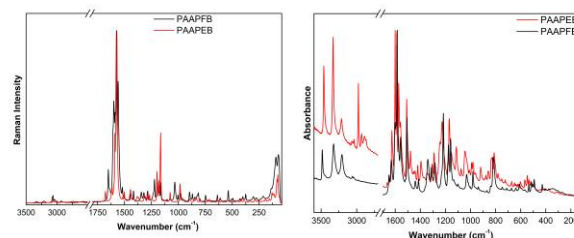


Figure 2. FT-Raman and FT-IR spectra of the chalcones PAAPEB and PAAPFB.

We observed significant differences in the vibrational spectra of the chalcones PAAPEB and PAAPFB. These differences are attributed to changes in the geometric parameters of these molecular structures, especially in torsion angles of the enone chain ($C\beta=C\alpha-C-C$), as well as those which are due to the vibrational modes of the characteristic bands associated with each one these chalcones.

Conclusions

We observed Raman and infrared bands identical and other presented difference in the intensities and wavenumbers. Also, we identified the characteristic bands of inherent groups of each of these chalcones. From the structural study, it was possible to observe changes especially in the geometric parameters of them.

Acknowledgments

We thank the CENAPAD-SP and the financial support from the FUNCAP, CAPES and the CNPq.

¹ C. L. ZHUANG; W. ZHANG; C.Q. SHENG; W.N. ZHANG; C.G. XING; Z.Y. MIAO. Chalcone: A Privileged Structure in Medicinal Chemistry. *Chemical Reviews*, v. 117, n. 12, p. 7762-7810, 2017.