# Vibrational Infrared Spectrum of Anacardic Acid

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## Introduction

The liquid from cashew nut (CNSL) has attracted considerable attention because has components with anti-tumor and antioxidant activity among others [1], in addition, its major component, anacardic acid (AA) [2], exhibits ant parasitic activity against the Chagas disease, which cause the inhibition of the enzyme GAPDH [3]. In our review not were found records of studies about structural, electronic, vibrational and optical properties of AA. The goal is to evaluate the vibrational properties of AA showing the results of measurements in infrared and to compare with theoretical calculations made by Density Functional Theory (DFT).

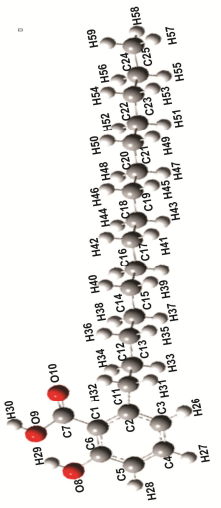


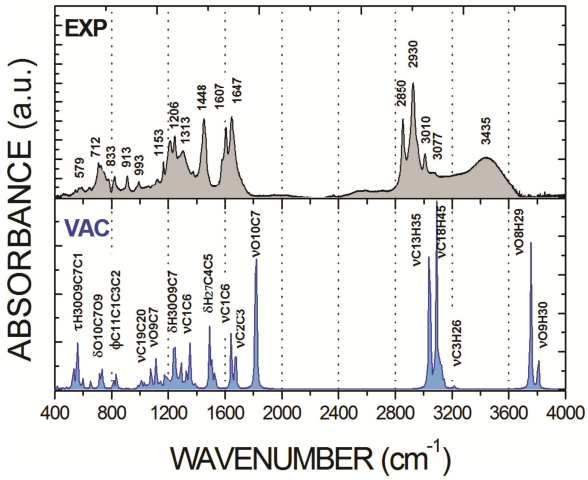
**Fig. 1.** Optimized AA

## Results and Discussion

The vibrational properties of AA was evaluated through of comparison between the experimental and theoretical spectra. The theoretical spectrum was calculated by DFT with functional m062x and basis 6-311+G(d,p) using Gaussian 09 software and the Veda software for the assignments. The conformer of least energy was obtained after scanning and optimization of geometry (Figure 1). The experimental spectrum was obtained through of measure of absorbance of compound liquid in KBr tablet in the region of 400 to 4000 $cm^{-1}$.

It can be observed in Figure 2 that the peak at 3435 $cm^{-1}$ in the experimental spectrum corresponds to assignments vO8H29 and vO9H30. The peaks in 1647 and 1607 $cm^{-1}$ corresponds to assignments vO10C7, vC2C3 and vC1C6. These modes are important because they play the functional part of molecule where occurs the formation of hydrogen bonds accountable for effects of interactions with enzymes such GAPDH.

**Figure 2.** Infrared spectra of AA: EXP) experimental; VAC) theoretical in vacuum




## Conclusion

The normal modes of AA in vacuum have good adequacy with experimental spectrum of compound. DFT calculation in vacuum was successful to attribute the main peak of the experimental spectrum obtained for the AA in KBr.

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