Vibrational analysis of Thymol in gaseous state

[1]Ferreira, L. G., [1]Paes, A. C., [1]Da Silva, K. J. R., [1]Da Silva, J. K. R., [2]Siqueira, M. R. S., [1]Paschoal. Jr., W.

[1]Universidade Federal do Pará; [2]Universidade Federal do Amapá

ABSTRACT

The use of antibiotics dates back decades and, although they have been replaced by artificial products, there has been a shift towards natural antibiotics promoted by the World Health Organization (WHO). Spice oils have been used for millennia, however in recent years attention has been drawn towards their antibiotic applications which are in line with WHO's objectives. Among them, there is Thymol, present in Amazonian plants and still poorly understood. The gaseous state simulations were performed using the Density Functional Theory (DFT), using the B3LYP / 6-311 ++ G (d, p) [1,2] computations. The initial geometries were based on the works of Gochev, Girova [3], and later optimized with the objective of obtaining the structure corresponding to a ground state of energy. Simulations of electronic transitions and vibrational spectra were performed using the Gaussian 09W package [4]. Analysis of the orbital and electron transitions reveals the absorption bands of the Thymol molecule. Analysis of the UV-vis spectrum shows that there is an accumulation of possible transitions in the range of 150 nm to 200 nm, the region corresponding to the ultraviolet region. The most frequent transitions are from the HOMO-1 orbitals to LUMO and HOMO-1 to LUMO + 1. The analysis of the activities in Infrared and Raman shows that this molecule has vibrations associated with modes of angular deformation outside the molecular plane and "breathing" modes, which are not active for analysis by Raman activity, since they are observed as noises. Thymol is important because of its potential as a natural antibiotic. Its presence in the Amazon forest promotes a conscious preservation of an element of Amazonian flora which also fits the overall objectives of sustainability. The results show that it has a stable structure in the gas phase, whose electronic and vibrational properties are presented as an initial step for future analysis, such as solid state.

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