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Combined Raman spectroscopy and first-principles calculation for essential oil of Lemongrass[1] ROZILAINE A.P.G. FARIA, NÁGELA F.M. PICANÇO, GLADíS S.D.L. CAMPO, Instituto Federal de Mato Grosso / IFMT, JORGE L.B. FARIA, Instituto de Física / UFMT, INSTITUTO FEDERAL DE MATO GROSSO / IFMT TEAM, INSTITUTO DE FíSICA / UFMT COLLABORATION — The essential oils have increased food's industry interest by the presence of antioxidant and antimicrobial. Many of them have antimicrobial and antioxidant, antibacterial and antifungal activities. But, due to the concentrations required to be added in the food matrix, the sensory quality of the food is changed. The production and composition of essential oil extracted from plants depend on the plant-environment interactions, the harvest season, phenophase and physiological state of the vegetal. *Cymbopogom citratus* (Lemongrass) has a good yield in essential oil with neral (citral A), geranial (citral B) and myrcene, reaching 90% of the oil composition. In our experimental work, the essential oil of lemongrass was obtained by hydrodistillation in Clevenger apparatus for 4 hours. The compound was further analyzed by Raman scattering in a spectrometer HR 800, with excitation at 633nm, in the range 80-3400 cm^{-1}. The spectrum obtained was compared with DFT calculations of molecules of the oil components. Our results show the vibrational signatures of the main functional groups and suggest a simple, but very useful, methodology to quantify the proportions of these components in the oil composition, showing good agreement with Raman data.

[1]CNPq/Capes/Fapemat

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