Vibrational and electronic spectral analysis of thymol an isomer of carvacrol isolated from Trachyspermum ammi seed: A combined experimental and theoretical study

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H I G H L I G H T S

- Isolation of Essential oil : Thymol (2-isopropyl-5-methylphenol)
- First comparative theoretical and experimental study on Thymol and Carvacrol
- The optimized geometrical parameters of Thymol and Carvacrol have been obtained by B3LYP/6-31 + G (d, p) method.
- Experimental spectra compared with theoretically simulated spectra of Thymol and an isomer Carvacrol.
- HOMO and LUMO .The Mulliken atomic charge distribution and thermo dynamical parameters were computed.
- The fundamental modes of vibrations have been made.