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VIBRATIONAL SPECTROSCOPY AND THEORETICAL STUDIES OF MOLECULAR STRUCTURE AND THE RELATED THERMODYNAMIC PROPERTIES OF INDOLE AT VARIOUS LEVELS

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Abstract

Molecular geometry, vibrational frequencies, and the related thermodynamic properties of indole at the ground state have been calculated by using ab initio/HF and DFT/B3LYP methods using various basis sets. The optimized geometrical parameters such as bond length and bond angles are calculated and they are found to be in good agreement with experimental values. Comparison of the obtained fundamental vibrational frequencies of indole are compared with the experimental values and it is shown that the result obtained by by DFT/B3LYP (6-311G++(d,p)) method, are in a close agreement with the experimental data due to higher basis set and the inclusion of electron correlation.

Keywords: Indole, vibrational frequencies, ab initio, DFT, basis sets.