Prediction study by ab initio / HF and DFT / B3LYP methods of modes Vibration molecular frequencies by IR spectroscopy with structure Architecture and substituting reactivity effect from microscopic scale of Thiohydantoin molecular to medicine

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Abstract—The Molecular geometry, vibrational frequencies, energy gaps, net charges, dipole moments and heats of formation for ThioHydantoin at the ground state, in present work, we have been calculated and performed by using the Molecular Mechanics, Quantum mechanics methods by different basis set in order to obtain optimized geometrical parameters are in good agreement with experimental values. Comparison of the obtained fundamental vibration frequencies of ThioHydantoin result by Density Functional Theory developed by Becke, Lee, Yang, and Parr method with simple regression, are in a close agreement with the experimental data. ab initio/ Hartree-Fock with three basis set was used to investigate the effects of a variety of substituants (methyl ,dimethyl, trimethyl ,and chloride ,dichloride ,trichloride) on the electronic properties of ThioHydantoin derivatives. Detailed vibrational wave number shifts and vibrational mode analyses were reported.

Keywords—*Thi**o**Hydantoin; Vibrational frequencies; Substituent effect; DFT; ab initio.*