Ab Initio Hartree-Fock and Density Functional Theory Study on Molecular Structures, Energies, and Vibrational Frequencies of 2-Amino-3-, 4-, and 5-Nitropyridine

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The molecular structures, vibrational frequencies, and corresponding vibrational assignments of 2-amino-3-, 4-, and 5-nitropyridine have been calculated by using ab initio Hartree-Fock (HF) and density functional theory (B3LYP) methods with 6-311++G(d,p) basis set level. The calculated vibrational frequencies and optimized geometric parameters (bond lengths and bond angles) were found to be in well agreement with the experimental data. The comparison of the observed and the calculated results showed that the scaled B3LYP method is superior to the scaled HF method for both the vibrational frequencies and the geometric parameters. For well fitting the calculated and the experimental frequencies we used scale factors obtained from the ratio of the frequency values of the strongest peaks in the calculated and the experimental spectra. These obtained scales seem to cause the better agreement of the gained vibrations to the experimental data.

Key words: Amino Nitropyridine; Vibrations; IR Spectra; Raman Spectra; HF; DFT.