

Vibrational Spectroscopic Investigation of Free and Coordinated 5-Aminoquinoline: The IR, Raman and DFT Studies

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Quinoline family compounds are of great interest in pharmacy and widely used as a parent compound to make drugs. In this study experimental IR and Raman spectra of 5-aminoquinoline (5-AQ) and its zinc halide complex $\{Zn(5-AQ)_2Cl_2\}$, together with the computational results of free AQ and its hydrogen bonded complex $\{H_2O-5AQ\}$ have been reported. For computational studies Gaussian 03 program package were used. The geometry of the free 5-AQ and 5-AQ interacting with H_2O through the ring nitrogen, were optimized using both ab initio HF and DFT methods at B3LYP/6-31++G(d,p) levels of theory. Harmonic and anharmonic vibrational frequencies and infrared intensities were calculated at the same level of theory. The Total Energy Distribution (TED) of the vibrational modes of the molecules was calculated with the Scaled Quantum Mechanics (SQM) method by using Parallel Quantum Mechanics Solutions (PQS) program and the fundamental vibrational modes were characterized by their total energy distribution. Experimental and theoretical results allowed us to determine the presence of intra and inter-molecular interactions and to discuss their strengths.