MOLECULAR STRUCTURE, VIBRATIONAL SPECTRA AND POTENTIAL ENERGY DISTRIBUTION OF PROTOPINE USING *AB INITIO* AND DENSITY FUNCTIONAL THEORY

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UDC 539.19

This work is devoted to theoretical study on molecular structure of protopine. The equilibrium geometry, harmonic vibrational frequencies and infrared intensities were calculated by *ab initio* Hartree–Fock and density functional B3LYP methods with the 6-31G(*d*) basis set and were interpreted in terms of potential energy distribution (PED) analysis. The internal coordinates were optimized repeatedly for many times to maximize the PED contributions. A detailed interpretation of the infrared spectra of protopine is reported. The calculations are in agreement with experiment. The thermodynamic functions of the title compound were also performed at HF/6-31G(*d*) and B3LYP/6-31G(*d*) level of theory. The FT-IR spectra of protopine were recorded in solid phase.

Keywords: FT-IR spectra, PED, protopine, molecular structure, vibrational spectra.