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Structural, Spectroscopic Investigation and Quantum Chemical Calculation studies on Methyl L-α aspartyl -L-Phenyl alaninate (Aspartame) for pharmaceutical Application

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Abstract : The Fourier transform infrared (FTIR-ATR) and FT-Raman spectra of Methyl L-α aspartyl -L-Phenyl alaninate have been recorded in the range of 4000-400cm^{-1} and 4000-50cm^{-1} respectively. A detailed interpretation of the vibrational spectra of this compound has been made based on the calculated potential energy distribution (PED). The equilibrium geometries, harmonic frequencies and infrared intensities calculated by density functional B3LYP method with the 6-31G(d,p) basis set. The vibrational frequencies were calculated by this methods and were compared with the experimental frequencies which yield good agreement between observed and calculated frequencies. The calculated Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies show that the charge transfer occurs in the molecule. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. The entropy of the title compound is also performed B3LYP/6-31G(d,p) levels of theory. The linear polarizability (α) and first order hyperpolarizability (β) values of the investigated molecules using DFT quantum chemicalcalculation was calculated. ^{13}C and ^{1}H nuclear magnetic resonance chemical shift of the molecule was calculated using gauge independent atomic orbit (GIAO) method. Molecular Electrostatic potential (MESP) was performed by the DFT method.

Keywords : FTIR, PED, HOMO, LUMO, Molecular DFT, Aspartame.

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