

Synthesis and Vibrational Spectroscopic Investigation of Methyl L-Proline Hydrochloride: A Computational Insight

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ABSTRACT In our present work, methyl L-proline hydrochloride has been synthesized from L-proline amino acid and characterized by Fourier transform infrared and Fourier transform Raman spectra via experimental and computational methods. Ab initio Hartree-Fock and density functional theory (B3LYP) calculations have been made for the structure, and atomic charge distributions were also predicted for the title compound by using the 6-311++G(d,p) basis set. Predicted vibrational frequencies have been assigned and compared with experimental Fourier transform infrared and Fourier transform Raman spectra. The thermodynamic properties such as heat capacity, enthalpy, entropy, and Gibbs energy have been calculated at different temperatures. The calculated highest occupied molecular orbital and lowest unoccupied molecular orbital energy show the charge transfer behavior within the molecule.

KEYWORDS density functional theory, Hartree-Fock, highest occupied molecular orbital, lowest unoccupied molecular orbital, methyl L-proline hydrochloride, synthesis, thermodynamic functions

INTRODUCTION

L-Proline is an amino acid, which has one secondary amine and a carboxylic acid functional group with a chiral center. It is not an essential amino acid because the human body can synthesize it. L-Proline is one DNA-encoded amino acid out of 20 amino acids. It is a five-member hetero ring system having one nitrogen and four carbon annular atoms, and this contributes to it having a rigid ring structure, which leads to its special characteristic features such as the bending template effect in peptide chains. The synthetic products of L-proline derivatives show significant biological activity and organo catalytic behavior. Especially, they are used in enantio-selective aldol, Mannich, and Michael addition reactions and in the synthesis of certain macrocyclic molecular systems.^[1–5]

L-Proline is the derivative of glutamine amino acid. It has a significant role in the human biological system. It contributes to the healthy functioning of the bone, muscles, skin, and immune system. A deficiency in this amino acid might lead an individual to have tears in tissues and very slow healing ability.

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