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Structural, vibrational and electronic properties of *cis* and *trans* conformers of 4-hydroxy-*l*-proline: a density functional approach

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Abstract. 4-hydroxy-*l*-proline is formed by hydroxylation of proline, an amino acid found in protein, whose inhibition results in hair problems in human, causing scurvy disease. We report a theoretical study on *cis* and *trans* conformers of 4-hydroxy-*l*-proline using first principle density functional approach at B3LYP/6-31+G(d,p) level. The equilibrium structures of both conformers are obtained to analyze their vibrational properties. The calculated vibrational modes are assigned and interpreted on the basis of potential energy distribution analysis. A good correlation has been obtained between calculated frequencies and corresponding experimental values from FTIR spectra. The electronic properties of both conformers are also calculated and discussed.

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Key words: 4-hydroxy-*l*-proline, *cis*-*trans* conformers, vibrational analysis, density functional theory

1 Introduction

4-hydroxyproline or 4-hydroxy-*l*-proline (4HLP) is a non native amino acid which differs from proline, a proteinogenic amino acid, by the presence of a hydroxyl (−OH) group attached to the gamma carbon. It was isolated from hydrolyzed gelatin by Hermann Emil in the beginning of 20th century. Although, it is not directly incorporated into proteins, it comprises about 4% of all amino acids found in animal tissue, an amount greater than

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many other translationally incorporated amino acids [1]. Furthermore, hydroxyproline is a major component of the protein collagen [2] which plays key roles in collagen stability [3], permitting the sharp twisting of the collagen helix [4]. For this reason, its content has been used as an indicator to determine collagen and/or gelatin amount. Moreover, hydroxyproline rich glycoproteins are also found in plant cell walls [5].

The pharmacological impact of this non-proteinogenic amino acid can never be ignored. Since, the hydroxylation of proline requires ascorbic acid i.e. vitamin C, the absence of vitamin C in humans inhibits the hydroxylation, consequently reducing the stability of collagen molecule and causing the hair problems i.e. scurvy. Apart from this, the increased serum and urine levels of hydroxyproline have also been demonstrated in Paget's disease [6]. Quantum chemical methods provide a lot of information about the system of biological interests that often complements with the experiment findings. Many chemical and/or biological properties are closely associated to the molecular structures or geometries. Different conformations of the same molecule may lead to different chemical properties. The aim of the present study includes detailed structural and vibrational analyses of two potential conformers of 4HLP, namely, *cis*-4HLP and *trans*-4HLP. Our literature survey reveals a recent study performed on *trans*-4HLP [7], however, there is no corresponding study on *cis*-4HLP to the best of our knowledge. Thus, the present study provides a comparative analysis of *cis* and *trans* conformers of 4HLP for the first time.

2 Computational methods

Our quantum chemical calculations are based density functional scheme as implemented in Gaussian 09 package [8]. Initial geometries of *cis*- and *trans*-4HLYP are fully optimized without any symmetry constraint in the potential energy surfaces (PESs) using gradient corrected hybrid functional B3LYP [9, 10] and 6-31+G(d,p) basis set. B3LYP is one of the most widely used functionals in case of medium size biomolecules and hence, employed successfully in a number of previous studies [7, 11-14]. Vibrational frequency calculations are repeated using optimized geometries at the same level of theory. All calculated frequencies are found to be real which ensure that the optimized geometries belong to true minima on respective PESs.

Normal modes of both conformers of 4HLP are interpreted and assigned in terms of potential energy distribution (PED) using Gar2ped program [15]. The calculated frequencies are uniformly scaled by a factor of 0.9648 [16] in order to compensate for anharmonicity of vibrations as well as electron correlations. The scaled frequencies are compared with corresponding experimental FTIR values. The FTIR spectra of *cis*-4HLP and *trans*-4HLP are adopted from literature, which are available from SDBS website [17].