# THE CONFORMATIONAL LANDSCAPE OF L-THREONINE: MATRIX ISOLATION INFRARED AND *AB-INITIO* STUDIES

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Amino acids, containing hydroxy side chains such as L-threonine and tyrosine play an important role in molecular recognition, such as in the docking of propofol, which is a commonly used anaesthetic. A rich conformational landscape of these amino acids makes them interesting candidates in the study of intra and intermolecular interactions. In this work, the conformational landscape of L-threonine was studied, as it can be expected to serve as a basis for understanding structure and functions of polypeptides and other biomolecules. The matrix isolation technique (MI) coupled with a high temperature effusive molecular beam (EMB) nozzle was used to trap conformers of amino acid, which were then characterized using FTIR spectroscopy. The usefulness of MI-EMB-FTIR spectroscopy is that it can trap structures corresponding to the local minima along with the global minimum and hence allows for a better exploration of the potential energy surface. A major challenge in conformational analysis of amino acids using matrix isolation FTIR arises from its non-volatile nature. A home built heating system which was mounted close to the cryotip, was used to evaporate the non-volatile amino acids. Our infrared spectra show that three conformations were trapped in the matrix. Experimental results were supported by *ab-initio* calculations performed using the CCSD(T), MP2 and M06-2X methods together with 6-311++G(d,p) and aug/cc-pVDZ basis sets. The side chains of the amino acids appeared to have an influence on the preferential stabilisation of a particular backbone structure of amino acids. Factors such as entropy, anomeric effect and intramolecular H-bonding were also found to play an important role in determining conformal preferences, which will be discussed.

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