Amino Acids at High Pressure

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The use of pressure to perform structural studies has been of important use to many areas of research, from Physics to Geochemistry. However, pressure studies have become a new notable tool in Chemistry and Biology to study the structure of small compounds. The main reason for this is the necessity of a better understanding of different processes, which happen even at extreme conditions of pressure, such as the existence of life in the deep ocean. Thus, small molecules may play important roles in these biological processes and therefore, a good knowledge of their structural features could be essential to explain how they happen.

In this work we are exploring the behaviour of amino acids structures at high pressure. Changes in pressure have been known to induce conformational changes in small molecules. We are trying to extend this research to the larger amino acids.

We have been working, principally, with L-glutamine, L-asparagine monohydrate, L- glutamic acid and L-aspartic acid. It was found that by applying pressure the cell parameters were reduced but no structural rearrangement was found up to pressures of 50-60 kbar. *Ab initio* computational studies were then performed to establish a possible relationship between the energetics of the hydrogen bonding with their compressibility.

Keywords: high-pressure crystallography, amino acids, *ab initio* calculations