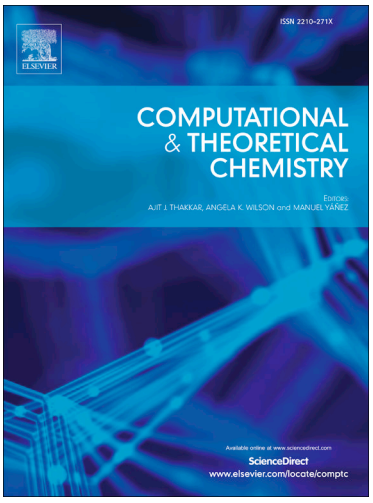

A density functional theory investigation of the fragmentation mechanism of deprotonated asparagine

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A density functional theory investigation of the fragmentation mechanism of deprotonated asparagine

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Abstract In this study, the fragmentation mechanism of deprotonated asparagine (Asn) was investigated in detail using density functional theory at the BH*and*HLYP/6-311++G(2df,2pd) level of theory. The H_2O-, NH_3- and CO_2-loss fragmentation reaction profiles constructed by the relative Gibbs free energies of the located stationary points were used to analyze the preferred dissociation pathways and the structures of the resulting molecular ion products. Furthermore, we also examined the temperature dependence of the thermodynamics and kinetics of key dissociation reactions, which provided further insight into the dominant fragmentation channel and the corresponding product distribution under different experimental dissociation energies. This study offered a computational support for building the fragmentation model of deprotonated amino acids.

Keywords: deprotonated asparagine, fragmentation reaction, theoretical computation, product distribution, density functional theory

1. Introduction

Asparagine (Asn), as one of the common amino acids in most plants, is not only a building block of proteins [1] but also plays an important role in the transportation and storage of nitrogen [2-5] and nitrogenous metabolism [6,7] of plants. Asn is one of the non-essential amino acids in the human body [8,9]; however, it has great significance in the synthesis of proteins [10,11]. In addition, Asn can also be used in