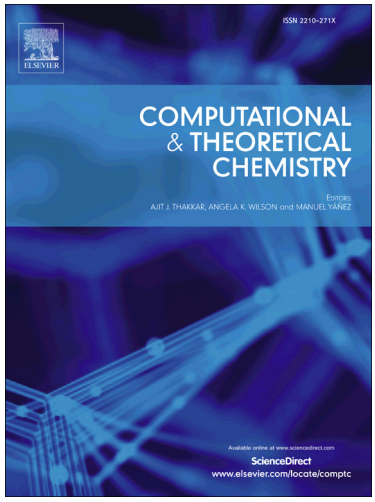

Theoretical study of fragmentation pathways and product distribution of deprotonated aspartic acid

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Theoretical study of fragmentation pathways and product distribution of deprotonated aspartic acid

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Abstract In this study, the fragmentation processes of deprotonated aspartic acid to eliminate CO_2, NH_3, and H_2O were investigated by a quantum-mechanism computation at the B3LYP/6-311++G(2df,2pd) and MP2/6-31+G(d,p) levels of theory. By constructing the fragmentation reaction potential energy profile using the Gibbs free energies and enthalpies of the located stationary points, we explored both the preferred dissociation pathways and the product distribution. Furthermore, the thermal energy correction to key stationary points was computed to evaluate the temperature dependences of the dominant reaction channels and product distribution. Additionally, the similarities and differences between the present theoretical investigation and available experiment were discussed in detail.

Keywords Deprotonated aspartic acid; Fragmentation; Theoretical computation; Dissociation; Potential energy profile

1. Introduction

Aspartic acid (Asp) is one of the α-amino acids [1,2] and includes D- and L-enantiomorphs [3]. D- and L-Asp are important precursors or intermediates in the syntheses of other amino acids [4] and medicines [5], and polymerized L-Asp has often been used as key reactants in chemistry [6], materials science [7], and biomedicine [8], among other research areas.