

# Fragmentations of hydroxymethyl radical cation: An ab initio Study

麥富德

F.-D. Mai;C.-C. Yu;H.-F. Lu;F.-Y. Li;S. H. Lin

摘要.

## Abstract

The probable fragmentation channels of hydroxymethyl radical cation were studied through the H and H<sub>2</sub>-abstraction and C-O bond breaking reactions including their related isomerization reactions. The energy barriers for hydroxymethyl cation undergoing isomerization reactions are generally higher than those undergoing the concerted 1,2-elimination reactions to generate CHO<sup>+</sup> and H<sub>2</sub>. The fragmentation reaction to form CHO<sup>+</sup> and H<sub>2</sub> through the 1,2-elimination pathways is the major fragmentation channel for hydroxymethyl cation, consistent with the experimental observation. H abstraction from the hydroxyl group of CH<sub>2</sub>OH<sup>+</sup> is more difficult than that from the methylene group. The feasible path to lose H is to generate CHOH<sub>2</sub><sup>+</sup> through hydrogen transfer reaction as the first step and then to undergo H-elimination to generate trans-CHOH<sup>+</sup>. Among all the reactions found in this study, the OH-elimination to generate CH<sub>2</sub><sup>+</sup> has the highest energy barrier. Our calculation results indicate that the major signals contributed from the related species of hydroxymethyl cation found in the mass spectrum should be m/e 29, m/e 30.