Measurement of fragment ions from adenine molecules in fast heavy-ion collisions

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We have investigated the fragmentation of adenine molecules induced by 0.7-MeV and 1.2-MeV C^+ collisions. In this work, we report the time-of-flight mass spectra of positive and negative ion species produced from adenine molecules. Various kinds of fragment ions, such as $C_4H_4N_4^+$ and $C_3H_3N_3^+$, are identified. We compare the mass spectra obtained for the different incident energies.

1. Introduction

Heavy ion radiotherapy is nowadays widely recognized as one of the effective methods for cancer treatment. This method involves the fragmentation of biomolecules induced by fast heavy-ion collisions. To improve its safety and efficiency, it is essential to obtain the fundamental data about the fragmentation processes in detail to understand the underlying mechanisms of DNA damage. So far, we have been studying the reaction processes of isolated gas-phase molecules in fast heavy-ion collisions. Recently, we observed that negative fragment ions are produced from various polyatomic molecules, including water, ethanol, and glycine molecules [1] [2]. In this work, we focus on nucleobases, especially adenine molecules (Fig. 1). We performed the coincidence measurements of positive and negative fragment ions.

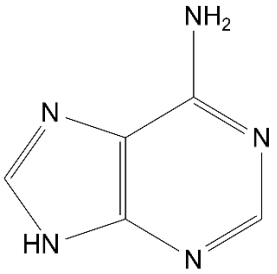

Fig. 1 Adenine molecule

2. Experiment

The experiment was performed using a 1.7 MV Cockcroft-Walton tandem accelerator facility at the Quantum Science and Engineering Center, Kyoto University. Fig. 2 shows a schematic of the experimental setup. 0.7-MeV or 1.2-MeV C^+ ion beams were obtained from the accelerator and charge-purified by the magnetic charge selector just before entering the collision chamber. Then, they collided with the gas-phase target of adenine molecules. Produced positive and negative ions were extracted by electrostatic fields in the opposite directions each other and perpendicular to the incident beam axis. Product ions were detected with microchannel plate detectors (MCPs). The background signals owing to secondary electrons were suppressed by applying a weak static magnetic field on the drift tube for negative ions. The

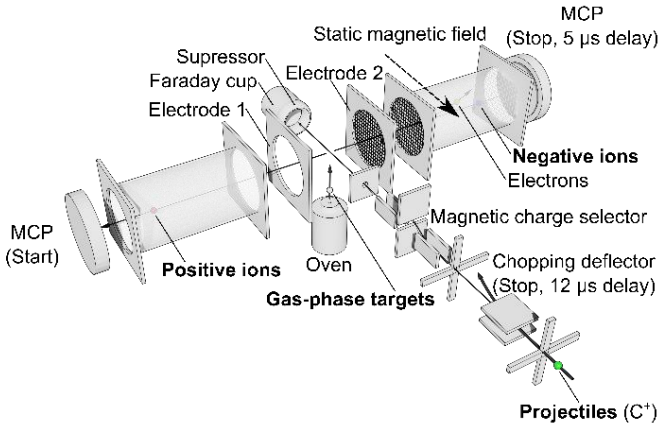

Fig. 2 Experimental setup

gas-phase adenine target was prepared by heating adenine powder in the oven to a temperature of 433 K. Mass-to-charge ratios of the all positive and negative product ions were analyzed independently by the time-of-flight (TOF) mass spectrometry.

3. Results and Discussion

The TOF mass spectra of positive ions from gas-phase adenine molecules are shown in Fig. 3. In both 0.7 and 1.2-MeV C^+ collisions, $C_4H_4N_4^+$ and $C_3H_3N_3^+$ were observed. These ions are produced as a result of the separation of some HCN from parent ions $C_5H_5N_5^+$. This phenomenon was reported in some previous works [3] [4]. In addition, $C_4H_3N_3^+$ and $C_3H_2N_2^+$ are observed. They might be produced by desorption of NH from $C_4H_4N_4^+$ and $C_3H_3N_3^+$. The peak with m/q = 28 is assigned to fragment ions of N_2^+ and CH_2N^+. Besides, C_2N^+ and $C_2HN_2^+$ were also detected. Note that the spectra have some peaks of the product ions heavier than adenine molecules, such as ions with m/q = 149, 185, and 211. They might be contamination caused by some impurities in the collision chamber. In contrast to the spectra of positive ions, only limited number of ion species were detected, such as C^-, C_2^-, and CN^- in the negative mass spectra (although not shown here). This characteristic feature is consistent with other molecules obtained in our previous glycine studies [2]. This indicates that the dissociation processes are basically common in adenine and glycine molecules. In this energy range, we could not observe a large difference in the mass distributions depending on the incident energy.

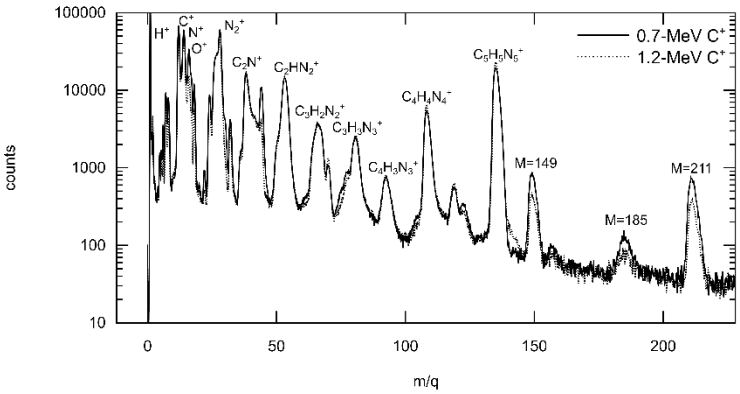

Fig. 3 The TOF mass spectra of positive ions produced by 0.7-MeV C^+ (solid line) and 1.2-MeV C^+ (dotted line). The representative ions are indicated at each conspicuous peak.

4. Summary

We have performed the coincidence measurements between the positive and negative product ions from adenine molecules in collision with fast heavy ions. In the TOF mass spectra of positive ions, $C_4H_4N_4^+$ and $C_3H_3N_3^+$ were detected. This indicates that loss of some HCN was the significant process in the dissociation of adenine. Many other kinds of fragment positive ions were observed. We could not find a notable difference in mass spectra depending on the projectile energy in this energy range.

References

[1] M. Isobe, Graduation Thesis, Kyoto Univ., 2018.
[2] M. Isobe, Master Thesis, Kyoto Univ., 2020.
[3] J. M. Rice , G. O. Dudek, J Am Chem Soc. 89(11) 2719-2725, 1967.
[4] A. Tatematsu, T. Goto , S. Matsuura, Nippon Kagaku Kaishi 87(1) 71-74, 1966.