TIME-OF-FLIGHT PROFILES OF SINGLY CHARGED FULLERENE-LIKE FRAGMENT IONS PRODUCED IN FAST He^{2+}-C_{60} COLLISION

Yoichi Nakai*, Tadashi Kambara and Yasunori Yamazaki
RIKEN (The Institute of Physical and Chemical Research)
Wako, Saitama 351-0198

Akio Itoh
Department of Nuclear Engineering, Kyoto University
Kyoto 606-8501

Hidetsugu Tsuchida
Department of Physics, Nara Women's University
Nara 630-8506

A number of studies of C_{60} fragmentation have been performed with various excitation probes.[1-8] The mass distribution of product ions strongly depends on the energy deposition into C_{60}. In low-energy deposition events in the collisions with electrons, photons, surfaces and so on, it is believed that an excited C_{60} ion emits neutral C_2 clusters in a few micro seconds or a longer time scale after excitation.[2-8] The time-of-flight (TOF) peak profile for each product ion contains information on fragmentation mechanism, such as the kinetic energy release, reaction rate and so on. We have developed a high-resolution TOF mass spectrometer to obtain information on the fragmentation mechanism. Using this spectrometer, we have measured TOF peak profiles in the mass range from C_{50}^+ to C_{58}^+ in the collision with 10MeV He^{2+}. We compare them with simulations of sequential C_2 emission based on the Rice-Ramsperger-Klein-Marcus (RRKM) formalism. It is shown that the experimental results support high activation energies and a very loose transition state, as discussed in ref. 8 and 9.

Each experimental TOF peak of fullerene-like fragment ions is asymmetric as shown in Fig. 1. The peaks of fullerene-like fragment ions are skewed to the longer TOF side. This asymmetry becomes more obvious with heavier fragment ions. It is note that the asymmetric shapes do not arise from a mixture of C_{60} with a different number of ^{13}C because the peak widths of fragment ions are much wider than those of C_{60} ions. The thermal motion of C_{60} is not the cause of the asymmetric peak, either. Roughly, the peak intensities of C_{60-2n}^+ (n=1 to 5) exponentially decrease with n. This is similar to other studies of fullerene-like fragment ion production.

We simulated the TOF spectrum by sequential C_2 emission using two sets of transition states and activation energies. In Fig. 1, we show the simulated TOF spectra. For each set of transition state and activation energies, we determined the internal energy distribution of parent C_{60}^+ ions by assuming the simple exponential functional form so as to reproduce the peak intensity ratios from C_{50}^+ to C_{58}^+. When the conventional transition state and activation energies, 7.1eV for C_{60}^+, are used, the simulated TOF spectrum does not agree with the experimental TOF spectrum, as shown Fig. 1-a. However, when a very loose transition state

*FAX: +81-48-462-4644, e-mail: nakaiy@postman.riken.go.jp

and high activation energy[8,9] (9.5eV for C_{60}^{+}) are used, the simulated result agrees with the experimental spectrum fairly well, as shown in Fig. 1-b. Our results support high activation energies and a very loose transition state and indicate that the dominant production process of singly charged fullerene-like fragment ions is the sequential C_2 emission in the collision of C_{60} with fast He^{2+} ion.

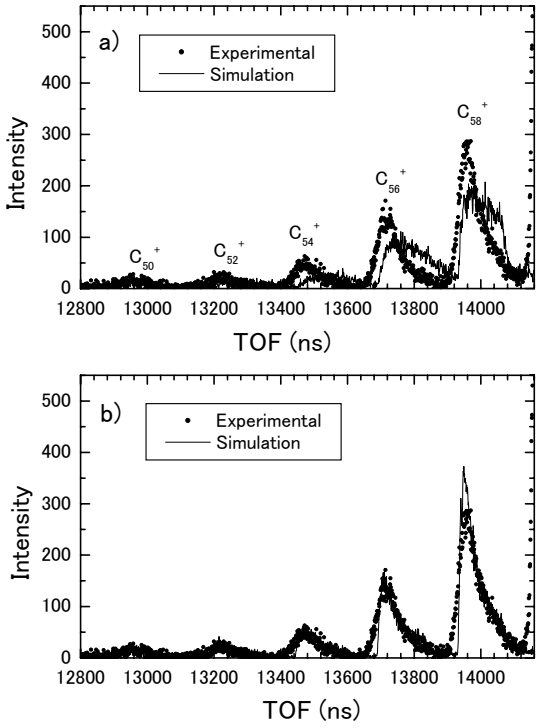

Fig. 1. Comparison of the experimental TOF spectrum with simulation results. Solid circles correspond to experimental results. Solid lines correspond to the simulations. See text for the difference between (a) and (b)

1) Y. Nakai *et.al*., J. Phys.B: At. Mol. Opt. Phys., **30**, 3049 (1997).
2) M. Foltin *et al*., J. Chem. Phys., **107** 6246 (1997).
3) P. Weis *et al*., J. Chem. Phys., **104** 6246 (1996).
4) R. Wörgötter *et al.*, J. Chem. Phys., **101** 8674 (1994).
5) M. Foltin *et al.*, J. Chem. Phys., **98** 9624 (1993).
6) R. K. Yoo *et al.*, J. Chem. Phys., **96** 911 (1992).
7) J. Laskin *et al.*, Chem. Phys. Lett., **242** 249 (1995).
8) J. Laskin *et al*., Int. J. Mass Spectrom., **177** L9 (1998)
9) C. Lifshitz, Int. J. Mass Spectrom., **198** 1 (2000)