GEC17-2017-000388

Abstract for an Invited Paper
for the GEC17 Meeting of
the American Physical Society

Fragmentation dynamics of simple molecules by electron collision

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The dissociation of multi-charged molecule is of great importance in various fields, such as plasma physics and planetary atmospheric chemistry. Most of the multi-charged molecules are in transient states that always dissociate through various pathways, which contain valuable information of the potential energy surfaces of the molecular ions. Recently, the three-body fragmentation dynamics of multi-charged CO_2, OCS, CS_2 molecules have been studied by electron collision using momentum imaging technique in my group. Nonsequential and sequential fragmentation dynamics of CO_2^{3+} has been investigated by electron collision at an impact energy of 500 eV. The dissociation mechanisms are clearly distinguished by combined use of the Dalitz plot together with momentum correlation spectra. The angular distributions and kinetic-energy releases (KERs) of different fragmentation processes are obtained. By analyzing KERs together with the help of potential-energy curves exploration at the multi-reference configuration interaction level, we conclude that the sequential fragmentation occurs in the ground state and the first two low-lying electronic excited states of the CO_2^{3+} ion. Fragmentation dynamics of CO_2^{4+} are also analyzed and the distributions of momentum correlation angles between ionic fragments and the KERs are obtained. Based on the Coulomb explosion model, the bond angle and the bond length of CO_2^{4+} before fragmentation are reconstructed. The results agree quite well with the geometry parameters of neutral CO_2 molecule. We also investigated the fragmentation dynamics of OCS^{q+} and CS_2^{q+} (q = 2, 3, 4) induced by electron collision at an impact energy of 500 eV using the momentum imaging technique. Various dissociation channels are analyzed in details. Recently, we have performed molecular dynamics simulation of the ground state of CO_2^{3+}. The evolution of the molecular bond breakage in time range of 0-200 fs is investigated. The results will be presented in the talk.