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Charge transfer and fragmentation in C$_{60}^+$ + C$_{6}^+$ collisions


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Synopsis

We have evaluated charge transfer and fragmentation cross sections in C$_{60}^+$+C$_{6}^+$ collisions. The collision has been studied using a semi-classical model in which the electronic degrees of freedom are quantum mechanically treated. For the fragmentation we have used statistical mechanics based methods. Competition between evaporation and fission (C$_2$ vs C$_2^+$ emission) has been studied as a function of the charge of the parent C$_{60}^+$ and the energy deposited in the collision.

Collisions of highly charged ions with C$_{60}$ have been intensively studied for more than one decade (see e.g. [1,2]). In these collisions, several C$_{60}$ electrons may be ionized and transferred to the charged projectile, thus leading to the formation of multiply charged C$_{60}^{q+}$ fullerenes. Experimental results have shown that the remaining charged fullerenes produced in the collision undergo fragmentation by emitting one or several fragments. The electronic processes (electron capture, ionization and excitation) are much faster than fragmentation. Thus, fragmentation can be considered as a post-collisional process in which the energy deposited by the collision in C$_{60}$ is transferred to the nuclear (dissociative) degrees of freedom.

We have evaluated charge transfer, excitation and fragmentation cross-sections in collisions of C$_{60}$ fullerenes with C$_{6}^+$ ions. The collision is studied using a fully quantum mechanical description of the relevant electronic degrees of freedom in the framework of the independent electron model. We have used the density functional theory (DFT) to describe the electronic structure of C$_{60}$, within the jellium approximation. The collision velocities considered in this work are much smaller than the orbital velocities of the fullerene electrons. Thus, we have solved the semi-classical time-dependent Schrödinger equation by expanding the one-electron wave functions in a basis of Born-Oppenheimer molecular states: “molecular close-coupling” formalism in which the only nuclear degree of freedom included is the relative distance between the fullerene and the ion. From the calculated one-electron amplitudes, inclusive many-electron transition probabilities have been obtained. The energy deposited in the remaining C$_{60}^{q+}$ fullerene, E$_{dep}$, has been also evaluated. This is a key quantity that relates the collision process with the ensuing fragmentation. From E$_{dep}$ we have evaluated the fragmentation rate constants ($k$) within the statistical theory of Weisskopf. The basic ingredients (geometry, frequencies, etc) needed to evaluate $k$ have been taken from ab initio DFT calculations [3]. A set of coupled equation are then integrated on time to obtain the probability of intact C$_{60}^{q+}$ and the fragments at a given excitation energy. In particular, competition between emission of C$_2$ and C$_2^+$ (evaporation vs fission) has been studied as a function of the energy deposit and the charge of the C$_{60}^{q+}$ fullerene. All these methods have been previously used with success to describe collisions of ions with metal clusters [4], fullerenes [5] and small carbon clusters [6]. Results on charge transfer cross-sections, energy deposited and fragmentation processes will be presented during the conference. We will compare our theoretical predictions with available experimental measurements.

References


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