Absolute charge transfer and fragmentation cross sections in He$^{2+} + C_{60}$ collisions

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Abstract. We present a set of theoretical methods to study the different processes taking place in ion-fullerene collisions. In particular, we focus on charge transfer, excitation and fragmentation processes. These methods have been successfully applied to the case of He$^{2+} + C_{60}$ collisions. We have found that single and double charge transfer cross sections are of the same order of magnitude in the velocity range studied (impact energy $\sim 0.1 - 10$ keV). Fragmentation of $C_{60}^+$ into $C_{58}^+ + C_2$ is observed only with large excitation energies and/or if one waits long enough (detecting the fragments at large distances from the collision). The agreement between our predictions and the experimental results supports the validity of the methods presented.

1. Introduction

Since the discover of the $C_{60}$ fullerene$^1$ a huge number of works has been carried out in the field of $C_{60}$ collisions. Ionization and fragmentation have been observed in $C_{60}$ bombarded by fast atoms, ions, electrons and laser pulses. An exhaustive compilation of experimental and theoretical work in this area has been reviewed in Refs. [2–5]. In the particular case of collisions with (highly) charged ions, several electrons may be ionized or transferred to the charged projectile leading to the formation of multiply charged $C_{60}^{q+}$ fullerenes (see e.g. [6–15]). Although $C_{60}^{q+}$ fullerenes have been detected with $q$ up to 12 [16], we have theoretically predicted that $C_{60}^{14+}$ might be observable [17]. However, as $C_{60}^{q+}$ ions are usually produced in excited states, they can undergo fragmentation. The complex fragmentation patterns of excited highly charged $C_{60}^{q+}$ fullerenes extremely depend on the initial charge state $q$, and on its excitation energy $E^*$ (see e.g. [9, 14, 18]). Variations in these quantities ($q$ and $E^*$) lead to different decay channels: successive emission of neutral $C_2$, fragmentation of one or more light charged clusters and
fragmentation in several singly charged fragments with small mass:

\[ C_{60}^{q+*} \rightarrow C_{58}^q + C_2 \]  \hspace{1cm} (1)

\[ C_{60}^{(q-r)+} \rightarrow C_{60-m}^r + C_m^+ \]  \hspace{1cm} (2)

\[ C_m^+ + C_n^+ + C_p^+ + \ldots \]  \hspace{1cm} (3)

These three processes are respectively known as sequential evaporation (1), asymmetric fission (2) and multifragmentation (3).

In this work we consider the collision of \(^4\text{He}^{2+}\) ions with \(C_{60}\) fullerenes in the region of impact energies 0.1-10 keV, in which charge transfer is the dominant process and the resulting neutral, singly and doubly charged \(C_{60}\) fullerene preferentially decays by emission of neutral \(C_2\) molecules [9, 15, 19]. At these impact energies, all electronic processes (electron capture, ionization and excitation) are much faster than fragmentation [20]. Thus, fragmentation can be considered as a post-collisional process in which the energy deposited in the \(C_{60}^{q+}\) by the collision is transferred to the nuclear (dissociative) degrees of freedom. Therefore, the mass spectrum associated with charge transfer in ion-\(C_{60}\) collisions is determined by the charge transfer cross sections \(\sigma_{CT}\) and the collision energy deposit \(E_{dep}\). The former determines the proportion of the different \(C_{60}^{q+}\) ions produced in the collision and the latter the ensuing fragmentation. Both quantities are not easy to determine either theoretically or experimentally. This is due to the large number of active electrons and nuclear degrees of freedom involved, which implies, from the experimental point of view, the detection in coincidence of many particles and makes fully quantum dynamical theoretical approaches unfeasible.

Experimentally, absolute cross sections have been measured for \(H^+ + C_{60}\) at very high impact energies [21] (see also [18]), where charge transfer is no longer the dominant process. Absolute values of \(\sigma_{CT}\) in the low impact-energy region, needed to provide a reference for future measurements, have been recently presented in \(\text{He}^{2+}+C_{60}\) collisions at the impact energies between 0.1 and 250 keV [22]. Additionally, Chen et al. [15] have been able to measure \(E_{dep}\) in low energy \(H^+ + C_{60}\) collisions by analyzing in coincidence the kinetic energy loss of the scattered \(H^-\) anion and the time of flight of the recoil \(C_{60}^{2+}\) ion. This provides a direct measure of the energy deposit following double capture without additional modelling.

In this paper we present a complete set of computational methods to describe the processes that take place in fullerene–ion collisions: charge transfer, excitation and fragmentation. The methodologies presented are applied to the study of \(\text{He}^{2+} + C_{60}\) collisions and have been compared with recent experimental measurements [15, 22]. The agreement between our predictions and the experimental results supports the validity of the methods presented.

2. Theoretical methods

Within the impact velocity range considered in this work (\(E_{col} \sim 0.1–10\) keV) the collision time (\(\tau_{col} \sim 10^{-14}\) s) is much shorter than the cluster vibrational period (\(\tau_v \sim 10^{-12}\) s). Therefore, the only relevant degree of freedom during the collision is the relative distance between the fullerene and the ion. In addition, the electron-phonon coupling, which is responsible for the cluster fragmentation, has a characteristic lifetime of \(\tau_{el} \sim 10^{-13}–10^{-12}\) s. Thus, we consider that the electronic excitation energy deposited during the collision will be relaxed into vibrational degrees of freedom well after the collision, leading to the fragmentation of the cluster. In summary, the different time scales of these processes, allow us to evaluate the fragmentation separately from the collision, \(\text{i.e.}\) as a post-collisional process. The energy deposited in the collision is the quantity that relates both processes. In this section we briefly present the theoretical methods employed to evaluate the collision dynamics, charge transfer cross sections, energy deposit and fragmentation of the excited fullerenes.
2.1. Collision dynamics

We have followed the methodology presented in reference [23] to describe the electronic structure of the C\textsubscript{60} fullerene. It consists in using an extension of the spherical jellium model of Puska and Nieminen[24]. Then, we apply the Kohn-Sham formulation of the density-functional theory to describe the electronic density of the cluster in terms of single-particle orbitals. From these orbitals we obtain the corresponding one-electron potentials using the local-density approximation with exchange-correlation and self-interaction correction (LDAXC-SIC). The orbital-dependent potentials obtained with this method exhibit the correct asymptotic coulomb behavior \((-1/r)\), which is crucial in this work because charge transfer and excitation occur mainly at large distances.

The orbitals and the potentials are then used in the dynamical simulations of the collision. In particular, the molecular approach for ion-atom collisional problems at low energies has been used. In collisions where many electrons are active, this approximation enables us to describe multi-electron processes such as transfer-excitation or multi-excitation of the target. The \(N_e\)-body problem is solved within the independent electron model (IEM) and the inclusive probability method introduced by Lüdde and Dreizler [25]. A full quantum-mechanical description in the IEM is possible because each active electron moves in the field produced by two potentials: the potential for the \(\text{He}^{2+}\) projectile and the calculated (LDAXC-SIC) potential of the fullerene. In the range of impact energies covered by the present work, the collision velocities are always smaller than the velocity of one electron in any orbital. This fact justifies the use of the molecular approximation for the description of the ion-atom (ion-cluster) collision. For further details in the collision treatment see [26, 27].

2.2. Charge transfer cross section

Charge transfer cross sections have been evaluated using the inclusive probability method [25], which consists in calculating the probability \(P_{f_1 \cdots f_q}\) of finding \(q\) of the \(N_e\) electrons in the sub-configuration \((f_1 \cdots f_q)\) while the remaining \(N_e - q\) electrons occupy any other states after the collision. This probability is given by the \((q \times q)\) determinant:

\[
P_{f_1 \cdots f_q} = \det(\gamma_{nn'}); \quad n, n' = 1, \ldots, q; \quad q < N_e,
\]

where \(\gamma_{nn'}\) is the one-particle density matrix \((\gamma_{nn'} = \langle f_n | \hat{\rho} | f_{n'} \rangle)\). The inclusive probability of finding \(q\) occupancies and \(L - q\) holes, \(P_{f_{q+1} \cdots f_L}\), can be written in terms of the probabilities (4) related only to occupancies [25]. We have successfully used this procedure in previous works to study charge transfer in metal cluster – atom/ion collisions[20, 26–28].

In order to determine the charge transfer cross section \(\sigma_{CT}\) we have first evaluated, for each impact parameter \(b\), \(P(\text{He}^+)\) and \(P(\text{He}^0)\), which are the probabilities of producing \(\text{He}^+\) and \(\text{He}^0\) irrespective of the fate of all the other electrons. Finally, the charge transfer cross section is evaluated by integration of the corresponding probability over the impact parameter:

\[
\sigma_{CT} = \int_{R_C}^{\infty} b P_{CT}(b) db
\]

where \(P_{CT} = P(\text{He}^+)\) for the single-capture cross section and \(P(\text{He}^0)\) for the double-capture cross section (see [23, 26] for details); \(R_C\) is the fullerene radius.

2.3. Energy deposit

As mentioned above, when the collision is over, the excited fullerenes can transfer their electronic excess of energy to the internal modes through electron-phonon coupling. If the excess of energy is larger than the lowest dissociation energy, it may induce fragmentation of the cluster. In
order to analyze this possibility in the C$_{60}^+$, we have evaluated first the energy deposit at a given impact energy. We define the average electronic excitation energy associated with P(He$^+$) as:

$$E_{C_{60}^+}^*(b) = \sum_{ij} \Delta \epsilon_{ij} P_j^i(b)$$

(6)

where $\Delta \epsilon_{ij} = \epsilon_j - \epsilon_i$. $\epsilon_j$ and $\epsilon_i$ are the electron energies of the $j^{th}$ and $i^{th}$ orbitals of C$_{60}^+$; and $P_j^i(b)$ is the probability of finding an electron in the $j^{th}$ excited orbital and simultaneously a hole in the $i^{th}$ orbital of the C$_{60}^+$ fullerene.

2.4. Fragmentation of excited clusters

The fragmentation of the exited clusters has been evaluated from the calculation of the excitation energy assuming a sequential C$_2$ evaporation mechanism:

$$C_{60}^+ \rightarrow C_{58}^+ + C_2 \rightarrow C_{56}^+ + C_2 \rightarrow C_{54}^+ + C_2 \rightarrow \cdots$$

(7)

The fragmentation rate constants in each step ($C_n^+ \rightarrow C_{n-2}^+ + C_2$) have been computed by using the microscopic and microcanonical statistical theory of Weisskopf as implemented in Ref. [29]:

$$k_W^{frag} = \omega \int_0^{E^* - D} \frac{\rho_{n-2}(E^* - D - e)}{\rho_n(E^*)} de,$$

(8)

where $\omega$ is a frequency factor, $D$ is the dissociation energy of the process $C_n^+ \rightarrow C_{n-2}^+ + C_2$, $\rho_n(e)$ is the density of states of a C$_n^+$ cluster at the energy $e$ and $E^*$ is the excitation energy:

$$E^* = E_0^* + E_{dep}$$

(9)

$E_0^*$ is the initial vibrational energy of the C$_n$ cluster before the collision (due to the temperature) and $E_{dep}$ is the electronic excitation energy deposited in the collision, equation (6). We compare our results with those obtained if one uses a simpler description of the fragmentation rates given by the Arrhenius equation:

$$k_A^{frag} = A \exp \left( \frac{-D}{k_B T_e} \right),$$

(10)

The pre-exponential factor $A$ has been taken from [30] and the definition of the emission temperature $T_e$ has been taken from [31, 32].

The input data that both models need (mainly dissociation energies and vibrational frequencies) have been taken from Density Functional Theory calculations[33, 34]. After the evaluation of the fragmentation rate constants, a set of coupled equations are integrated on time to obtain the probability of intact C$_{60}^+$ and the fragments (C$_{58}^+$, C$_{56}^+$, C$_{54}^+$, ...) at a given excitation energy.

3. Results

Preliminary results obtained with a reduced basis of molecular states have been reported in [23]. In the present work, a much larger basis has been used, which ensures a reasonable convergence up to an impact energy of $\sim 10$ keV. This is important in order to account for ionization processes occurring at the higher impact energies. The calculated cross sections for He$^+$ and He$^0$ formation are shown in Fig.1 together with recent measurements[22]. They are in reasonable agreement in the region where they overlap. Both theory and experiment predict that He$^+$ and He$^0$ cross sections are comparable in magnitude for a wide range of impact energies and comparable to the geometrical cross section ($\sim 56 \times 10^{-16}$ cm$^2$).
Figure 1. Cross sections for production of He$^+$ and He$^0$. Full lines: present theoretical results; full symbols: experimental results of Rentenier et al. [22]; opened symbols: experimental results of Afrosimov et al. [35, 36] normalized as explained in [22].

Fig. 2a shows the variation of the relevant molecular orbitals of the (C$_{60}$-He)$^{2+}$ system with $R$ (the cluster ion distance) and Fig. 2b the calculated energy deposit, $E_{\text{dep}}$, as a function of impact parameter, $b$, for C$^+_n$ ions produced at an impact energy of 0.1 and 10 keV. As can be seen, the energy deposit is important even at large $b$ values, which is the consequence of electron transfer from the inner $\pi$ orbitals of C$_{60}$ (mainly the $p$, $d$ and $f$ ones) to the empty He$^+(n=2)$ orbitals at $R < 25$ a.u. (see Fig. 2a). Thus, charge transfer already occurs when the projectile is far away from C$_{60}$ (the radius of the latter is $R_C \sim 8$ a.u.). Since charge transfer creates one or several holes in the inner $\pi$ orbitals of C$_{60}$, the resulting charged fullerene will lie in an excited state. The presence of a hole in these inner $\pi$ orbitals implies an excitation energy of the order of 0.3-0.4 a.u. (i.e., $\sim 8$-11 eV, see Fig. 2a). This is the dominant process at $b > 17$ a.u. (see Fig. 2b). At smaller $b$ values, $E_{\text{dep}}$ is significantly larger, implying that electron capture is accompanied by the simultaneous excitation or ionization of other $\pi$ electrons as, e.g., in transfer-ionization processes. Transfer-ionization is expected to be negligible at very low impact energy; thus, the difference between the energy deposit at 0.1 and 10 keV is mostly due to that process (see Fig. 2b). Therefore, the calculated $E_{\text{dep}}$ at higher impact energies not only describes excitation of C$_{60}^+$ but also of C$_{60}^{q+}$ ($q \geq 2$) formed in transfer-ionization. In other words, only at low impact energies, the energy deposited in C$_{60}^+$ is close to the calculated $E_{\text{dep}}$ ($\sim 40$ eV at 0.1 keV); at 10 keV, it is approximately half of the calculated $E_{\text{dep}}$ [22].

Figure 2. (a) Correlation diagram for the relevant molecular orbitals of (C$_{60}$-He)$^{2+}$ denoted by their character at infinite separation. Full lines: occupied orbitals at the beginning of the collision; dashed lines: orbitals dissociating into He$^+$ ones; dotted lines: orbitals dissociating into empty C$_{60}$ ones. (b) Collision energy deposit in C$_{60}^+$ as a function of impact parameter at 0.1 keV (brown) and 10 keV (black). Dashed line: average value at 0.1 keV. Notice that $(b^2 = R^2 + v^2t^2)$, where $v$ is impact velocity and $t$ is time.
Fig. 2b shows that at impact energy of 10 keV, $E_{\text{dep}}$ is larger than the energy required to evaporate a single C$_2$ unit from C$_{60}^+$ (which is 10.6 eV [37]). However, the experiment shows that, at this impact energy, almost no C$_{58}^+$ is observed [22]. A similar apparent contradiction has been observed in Ref. [15]. To understand this behavior, we have calculated the probability of producing C$_{60}^+$ and C$_n^+$ fragments ($n = 58, 56, 54$ and $n < 54$) as a function of the time of flight TOF within the Weisskopf model. For simplicity, in these calculations, we have used the average energy deposit $< E_{\text{dep}} >$ at an impact energy of 10 keV ($\sim 70$ eV). Fig. 3 shows that fragmentation of C$_{60}^+$ into C$_{58}^+$ + C$_2$ is a very slow process at the chosen impact energy: it takes longer than the available TOF (which is $\sim 3.5 \mu$s). As the impact energy increases a monotonous enhancement of C$_{58}^+$ production is observed. At larger TOF smaller fragments might be detected.

For the case of doubly charged species, we compare in Fig. 4 our results with the experimental measurements by Chen et al. [15]. In the left panels we present the probability of producing intact C$_{60}^{2+}$ and C$_n^{2+}$ fragments ($n = 58, 56, 54$ and $n < 54$) as a function of the excitation energy computed within the Weisskopf and the Arrhenius approaches using the experimental TOF ($\tau \sim 3.5 \mu$s). In the right panels we show the experimental results of Chen et al. [15, 38] together with the theoretical results obtained after the convolution with the energy distribution function shown in dashed lines in the left panels. We have successfully applied a similar strategy for describing the fragmentation of small carbon cluster [29, 39]. The energy deposit distribution is represented by a gaussian function with a full width at half maximum (FWHM) of 18 eV to mimic the experimental results. The maximum of the curve has been displaced to populate $\sim 10\%$ the C$_{58}^{2+}$ fragmentation channels (as in the experiment). A shift in the energy between the models and the experiment is observed. This could be the result of using a very high preexponential factor in the Arrhenius formulation. Other possible explanation is the internal energy due to the temperature that the C$_{60}$ fullerene present before the collision. In the simulations we have not taken into account this energy; i.e., $E_0^* = 0$ in equation (9). Other deexcitation pathways such as radiative cooling have not been taken into account and they might influence the rate constants. The main feature of both experimental and theoretical results is that the C$_{60}^{2+}$ is the dominant cluster, being the C$_n^{2+}$ species much more unlikely. It would be of great interest to have experimental results with a larger energy deposit, and therefore a larger probability of detection of the smaller fragments, to check the validity of the methodology proposed and other statistical methods [29, 40].

4. Conclusions
In this paper we have presented theoretical calculations of charge transfer cross sections in He$^{2+} + C_{60}$ collisions at low impact energies. We have compared our results with the recent experimental measurements of Rentenier et al. [22]. The experimental and theoretical cross sections have been found to be in reasonable agreement with each other, which reinforces
Figure 4. Probability of intact $C_{60}^{2+}$ and $C_{n}^{2+}$ fragments ($n = 58$, 56, 54 and $n < 54$) as a function of the excitation energy computed within the Weisskopf (a) and the Arrhenius (b) approximations using the experimental TOF ($\tau \sim 3.5 \mu$s). Energy distribution function (dashed line) has been used to convolute the results in (a) and (b) to obtain (d) and (e) respectively. In (c) the experimental results of Chen et al. are shown [15, 38].

the quantitative value of our predictions and the validity of our theoretical modelling. The theoretical methods employed explain the various charge transfer mechanisms and provide the energy deposit that eventually leads to fragmentation. We have found that the cross sections for the formation of $He^+$ and $He^0$ are comparable in magnitude, which cannot be explained by the sole contribution of pure single and double electron capture but also by contribution of transfer-ionization processes that are important even at low impact energies. The experimental results of [22] show that multifragmentation is only important at impact energies larger than 40 keV; at lower energies, sequential $C_2$ evaporation is the dominant process. To understand these results, an analysis of the fragmentation patterns has been carried out by using different theoretical models. We have also applied the fragmentation models to compare with the recent experimental measurements of Chen et al.[15, 38].

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