Multiple ionization and fragmentation of fullerene dimers by highly charged ion impact

H Zettergren 1,2, H T Schmidt 1, P Reinhed 1, N Haag 1, D Fisher 1, Z Berényi 1, H Cederquist 1, J Jensen 3, P Hvelplund 4, S Tomita 5, B Manil 6, J Rangama 6, and B A Huber 6

1 Physics Department, Stockholm University, AlbaNova University Center, SE-106 91 Stockholm, Sweden
2 Departamento de Química, C-9, Universidad Autónoma de Madrid, 28049-Madrid, Spain
3 Division of Ion Physics, Ångström Laboratory, Uppsala University, Box 534, SE-75121 Uppsala, Sweden
4 Department of Physics and Astronomy, University of Aarhus, DK-8000, Aarhus C, Denmark
5 Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305-0006, Japan
6 Centre Interdisciplinaire de Recherches Ions Lasers (CIRIL), rue Claude Bloch, BP 5133, F-14070 Caen Cedex 05, France

Abstract. We have studied the stabilities of multiply charged van der Waals dimers in slow \( \text{Xe}^{30+} + [\text{C}_{60}]^2 + [\text{C}_{70}]^2 \rightarrow \text{Xe}^{(38-s)+} + [\text{C}_{60}]^{(r-s)+} + [\text{C}_{70}]^{(r-s)+} + (r-s)e^- \) electron-transfer collisions \((v=0.4\ \text{a.u. and } r\leq 7)\). The relative ionization cross sections display even-odd variations as functions of \( r \) for \([\text{C}_{60}]^2\), \([\text{C}_{60}\text{C}_{70}]^2\), and \([\text{C}_{70}]^2\). This is in clear contrast to the typical smooth decreasing behavior of the cross sections for multiple ionization of fullerene monomers, which can be explained within the framework of the classical over-the-barrier model. In addition, we report the branching ratios and the kinetic energy releases for the dominant fragmentation processes that yield intact fullerenes. The experimental results are discussed in view of a simple electrostatic model for dimer ionization and recent results from high level density functional theory calculations.

1. Introduction
Multiple ionization and fragmentation of isolated fullerene monomers (\( \text{C}_{60} \) and \( \text{C}_{70} \)) have been studied extensively during the past decades in collisions with e.g. fast or slow atomic ions, photons or electrons [1,2]. There have also been studies of clusters of fullerenes using different ionizing agents [3–9]. In one such study it was revealed that there is a high charge communication between the monomer constituents in charged clusters of fullerenes when ionized by highly charged ion impact [8], as concluded from the absence of multiply charged \( \text{C}_{60} \) in the fragmentation products of multiply charged clusters. This clearly contrasts to the charge localization effect observed in a similar study of multiply charged Ar\(_n\) clusters [10], where it was concluded that the highly charged projectile only captures electrons from one (or a few) Ar-atoms in the clusters. Thus these collisions events may to some extent be regarded as ion-atom collision(s) in terms of sequential ionization through electron transfer processes, as there is no communication between neighboring Ar-atoms in the cluster. In the case of clusters of fullerenes, however, the collision scenario is only ion-fullerene like if the timescale for the charge communication is longer than the collision time.

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The simplest fullerene aggregates (i.e. fullerene dimers) serve as an excellent model system for studying the inherent properties and interactions between neighboring fullerenes in more complex fullerene materials. Here, we have used slow highly charged ions to multiply ionize fullerene dimers in $\text{Xe}^{30+} + [\text{C}_{60}]_2, [\text{C}_{60}\text{C}_{70}], [\text{C}_{70}]_2 \rightarrow \text{Xe}^{(30-s)+} + [\text{C}_{60}]^{r+}_2, [\text{C}_{60}]^{(r-s)}_2 - \text{e}^-$ collisions at 600 keV ($v=0.4$ a.u.). The paper is organized as follows. In Sec. 2 we describe the multi-coincidence technique used to register the subsequent fragmentation processes and the method to extract the relative cross sections for producing $[\text{C}_{60}]^{r+}_2, [\text{C}_{60}\text{C}_{70}]^{r+}_2, [\text{C}_{70}]^{r+}_2$ as functions of $r$. This method also gives information on the branching ratios and kinetic energy releases for the dominant dimer fragmentation processes. The experimental results are presented in Sec. 3, where a simple electrostatic model framework and results from density functional theory (DFT) calculations [11] are used to interpret these results and to discuss charge localization and delocalization effects in the collision process.

2. Experimental method

The experiments were performed at CIRIL (Centre Interdisciplinaire de Recherche Ions Lasers) in Caen, France. The $[\text{C}_{60}]_2, [\text{C}_{60}\text{C}_{70}], [\text{C}_{70}]_2$ dimers (and larger clusters of fullerenes) are created in a cluster-aggregation source. Fullerene powder is sublimated in a small oven typically kept at 550-600 °C. A jet of (C_{60} and C_{70}) monomers exit an aperture in the oven and pass through a region filled with He gas at a pressure of ~1 mbar and a temperature of ~80 K (the region is cooled by liquid nitrogen). There, the monomers are cooled in collisions with cold
He atoms and may then start to form van der Waals dimers (and larger clusters). A mixture of monomers, dimers, and larger clusters of fullerenes are guided by the He atoms out of the aggregation source through a 2 mm nozzle and travel through regions of differential pumping toward the interaction region. In this region, the cluster beam crosses with a projectile beam of highly charged ions produced from an ECR (Electron Cyclotron Resonance) ion source. The two beams are perpendicular both to each other and to the axis of the linear time-of-flight (TOF) spectrometer, as shown schematically in the left part of Fig. 1.

Ionized fullerene species (monomers, dimers, clusters, and fragments) created in collisions with the highly charged ions are extracted by an electric field into the TOF spectrometer and detected (cf. left part of Fig. 1). The projectile beam and the extraction field are pulsed in such a way that the extraction field is switched on 500 ns after the projectile pulse has left the interaction region (typical pulse lengths and repetition rates are 10 µs and 2 kHz respectively). Simultaneously with the switching of the extraction field, a start signal is sent to a multi-hit time-to-digital converter (TDC). After the extraction region the ions travel in a field free region of approximately one meter before they are accelerated toward a conversion plate held at a voltage of -25 kV. The secondary electrons emitted from the conversion plate are guided (by means of a weak magnetic field) onto a micro-channel-plate (MCP) detector, which sends a stop signal to the TDC. There may be several stop signals for each start signal. The time difference(s) between the start signal and the stop signal(s) is then used to distinguish between ions of different mass-to-charge (m/q) ratios. The electron shower from the conversion plate assures that for every ion there will be a stop signal. The high detection efficiency together with the multi-stop TDC make it possible to investigate the correlation between two or more charged fragments that originate from the same collision event.

The right part of Fig. 1 shows the two-stop correlation data, where the projections above and on the right hand side of the correlation map correspond to the time-of-flight spectrum for the first (t₁) and second hits (t₂), respectively. There are enhanced intensities for (t₁,t₂) events corresponding to correlations between pairs of monomers such as e.g. \(\text{[C}_{60}\left[C_{r}^{1+}\right]\rightarrow\text{C}_{60}^{1+}+\text{C}_{r}^{1+}\) and \(\text{C}_{2}^{2+},\text{C}_{2}^{2+}\). These originate from the fragmentation of \(\text{[C}_{60}\left[C_{r}^{2+}\right],\text{[C}_{60}\left[C_{r}^{3+}\right],\text{and [C}_{60}\left[C_{r}^{4+}\right] dimers into two intact (charged) fullerenes. The relative ionization cross sections can thus be extracted by adding these events for \(\text{[C}_{60}\left[C_{r}^{2+}\right]+\text{C}_{60}^{1+}\text{C}_{r}^{1+}\rightarrow\text{C}_{60}^{1+}+\text{C}_{r}^{1+}\) and \(\text{[C}_{60}\left[C_{r}^{3+}\right]+\text{C}_{60}^{1+}\text{C}_{r}^{1+}\rightarrow\text{C}_{60}^{1+}+\text{C}_{r}^{1+}\) (r≤7) fragmentation channels.

The reason for this is that fragmentation of the individual fullerene ions are found to be negligible processes. Furthermore, there are strong indications that only neutral and singly charged dimers are stable on the experimental time scales as we do not see dimers in higher charge states in the one-stop spectrum. This is supported by the results from the present model (see below).

The data analysis is straightforward for \(\text{[C}_{60}\left[C_{r}^{1+}\right]\rightarrow\text{C}_{60}^{1+}+\text{C}_{r}^{1+}\text{C}_{60}^{1+}\text{C}_{r}^{1+}\text{C}_{60}^{1+}\text{C}_{r}^{1+}\) events with r=r1/2=r2/2 are necessary as two ions arriving close in time may be falsely registered as one-stop events. This is illustrated in the insets in the right part of Fig. 1. For \(\text{[C}_{60}\left[C_{r}^{1+}\right]\) the t₁ and t₂ distributions are well-separated in time, while the two distributions overlap for \(\text{[C}_{60}\left[C_{r}^{2+}\right])\) events. In order to extract (dead time corrected) relative ionization cross sections for the \(\text{[C}_{60}\left[C_{r}^{2+}\right]\) dimers, we carried out a number of simulations using the SIMION package [12] in which we assumed different values of the kinetic energy releases \(E_{KER}\) for the fragmentation processes that yield intact fullerenes. In these simulations, we randomly generated the start positions and dimer orientations at the moment of dissociation, and each distribution were convoluted with the experimental response function (as given by the corresponding one-stop distribution shown as dashed curves in the insets in the right part of Fig. 1).

In Fig. 2a we show comparisons of simulated and experimental (t₂-t₁) distributions for \(\text{[C}_{60}\left[C_{r}^{2+}\right]→\text{C}_{60}^{1+}+\text{C}_{r}^{1+}\) for three different values of \(E_{KER}\) and a common dead time of 45 ± 12 ns. In order to determine the best fits we minimized the reduced chi-squared function \(\chi^2\) as a
Figure 2. a) Experimental $E_{KER}$-values (data points) and simulated ones (solid curves) for three different simulated values of $E_{KER}$ in the dissociation process $[C_{60}]^{2+} \rightarrow C_{60}^+ + C_{60}^+$. b) A quadratic fit of $\chi^2$ as a function of $E_{KER}$ with the $\chi^2$-values from the fits shown in a) indicated (I-III).

Figure 3. Left: Relative ionization cross sections for $[C_{60}]^{r+}_2$ (squares), $[C_{60}C_{70}]^{r+}_2$ (circles), and $[C_{70}]^{r+}_2$ (triangles, normalized to $[C_{60}]^{3+}_2$). A clear even-odd effect as a function of $r$ is seen in all three dimer systems. Right: Relative ionization cross sections for $C_{70}^{r+}$. No even-odd effects are observed.

function of $E_{KER}$. In Fig. 2b we show a quadratic fit of $\chi^2$ as a function of $E_{KER}$, showing that $E_{KER} = 0.44$ eV has the lowest $\chi^2$-value and thus corresponds to the experimental value for $[C_{60}]^{2+}$. For $[C_{60}]^{4+}$ and $[C_{60}]^{6+}$, the corresponding simulations giving the best fits were consistent with the same dead time as for $[C_{60}]^{2+}$ (45 ± 12 ns). In all three cases, about 25% of the dimer events are not registered as separate events and thus the relative ionization cross sections for $r=2, 4$, and 6 have to be corrected accordingly. Note that no dead time corrections are necessary for the odd charged $[C_{60}]^{r+}_2$ or for even or odd charge states of $[C_{60}C_{70}]^{r+}_2$.

However, we also carried out simulations for odd charged $[C_{60}]^{r+}_2$ in order to extract the kinetic energy releases for all charge states of these systems.
3. Experimental results and discussions

The left part of Fig. 3 shows the relative ionization cross sections for \([C_{60}]^{2+}\), \([C_{60}C_{70}]^{+}\), and \([C_{70}]^{+}\) as functions of charge states \((r)\). There are clear even-odd variations well beyond the statistical uncertainties in the cross sections for all three systems. A sharp drop in the cross section can be seen when going from a dimer in an even charge state to the next odd charge state \(r+1\). In contrast, the differences in cross sections leading to dimers in charge states \(r\) \((r\ \text{odd})\) and \(r+1\ \text{(}r+1\ \text{even) are small}.\) These oscillatory behaviors are not observed in the sequences of ionization cross sections for fullerene monomers \(C_{r}^{+}\) or \(C_{r}^{+}\) (cf. the right part of Fig. 3).

The branching ratios shown in Tab. 1 give a clue for understanding the markedly different behavior between the monomer and dimer cross sections. These show that there is a strong propensity for the charge on the dimer system to be shared as equal as possible between the fullerences when the dissociation occurs. In a break up of a dimer in an even charge state, the fullerene fragments will in the majority of the cases have the same charge state \((r=1=r_2=r/2)\), while a break up of a dimer in an odd charge state will lead to fullerene charges \(r=1=r_2+1\). When a \([C_{60}C_{70}]-\text{dimer in an odd charge state breaks up, the } C_{r_2}^{+}\ \text{fullerene will in most cases carry away more charge such that we often have } r_1=r_2+1\).

These results strongly indicate that the charge may move between the two fullerences as the collision geometry most often is such that the projectile is closer to one of the fullerene monomers throughout the collision. This is consistent with the observed high charge communication in clusters of fullerences [8]. In addition, the charge communication appears to occur on a time-scale faster than the time between sequential electron transfers as otherwise the collision scenario would resemble that from a monomer target (ion-fullerene like collisions). One would thus expect a smooth decreasing dimer ionization cross sections rather than the even-odd effects displayed in the left part of Fig. 3.

We use an electrostatic model to aid the interpretation of the experimental results and give

### Table 1. Branching ratios for the different dissociation channels. In the break up of a dimer the charge will to a large extent be shared as equally as possible between the fragment monomers.

| Dimer Dissociation channel | BR(%) | Dimer Dissociation channel | BR(%) |
|---------------------------|-------|---------------------------|-------|
| \([C_{60}]^{2+}\)        | C\(_{60}^{+}\) + C\(_{60}^{+}\) | 100 | \([C_{60}C_{70}]^{2+}\) | C\(_{60}^{+}\) + C\(_{70}^{+}\) | 100 |
| \([C_{60}]^{3+}\)        | C\(_{60}^{+}\) + C\(_{60}^{+}\) | 100 | \([C_{60}C_{70}]^{3+}\) | C\(_{70}^{+}\) + C\(_{70}^{+}\) | \(\approx 87\) |
| \([C_{60}]^{4+}\)        | \(C_{60}^{2+}\) + \(C_{60}^{2+}\) | \(\approx 95\) | \([C_{60}C_{70}]^{4+}\) | \(C_{70}^{2+}\) + \(C_{70}^{2+}\) | \(\approx 84\) |
| \([C_{60}]^{5+}\)        | \(C_{60}^{3+}\) + \(C_{60}^{3+}\) | \(\approx 5\) | \([C_{60}C_{70}]^{5+}\) | \(C_{70}^{3+}\) + \(C_{70}^{3+}\) | \(\approx 13\) |
| \([C_{60}]^{6+}\)        | \(C_{60}^{4+}\) + \(C_{60}^{4+}\) | \(\approx 6\) | \([C_{60}C_{70}]^{6+}\) | \(C_{70}^{4+}\) + \(C_{70}^{4+}\) | \(\approx 2\) |
| \([C_{60}]^{7+}\)        | \(C_{60}^{5+}\) + \(C_{60}^{5+}\) | \(\approx 4\) | \([C_{60}C_{70}]^{7+}\) | \(C_{70}^{5+}\) + \(C_{70}^{5+}\) | \(\approx 9\) |
| \([C_{60}]^{8+}\)        | \(C_{60}^{6+}\) + \(C_{60}^{6+}\) | \(\approx 9\) | \([C_{60}C_{70}]^{8+}\) | \(C_{70}^{6+}\) + \(C_{70}^{6+}\) | \(\approx 18\) |
| \([C_{60}]^{9+}\)        | \(C_{60}^{7+}\) + \(C_{60}^{7+}\) | \(\approx 10\) | \([C_{60}C_{70}]^{9+}\) | \(C_{70}^{7+}\) + \(C_{70}^{7+}\) | \(\approx 4\) |
Figure 4. a) The model potential energy curves for $[C_{60}]_{2}^{r+}$ (r=0-3). The dotted curves display the pure Coulomb energy for the corresponding system. b) The model and experimental kinetic energy releases in the fragmentation of $[C_{60}]_{2}^{r+}$→$C_{r1}^{+}+C_{r2}^{+}$ as functions of charge (r=r1+r2=2-7). c) The monomer (open squares) and model dimer ionization energies (solid squares).

a qualitative explanation for the even-odd effects in the ionization cross sections. In this model, the Girifalco potential [13] is used for describing the neutral $[C_{60}]_{2}$ system. For the charged system, the mutual electrostatic interactions between two metal spheres [14] is superimposed on the neutral interactions. The metal sphere radius (a) is the only model parameter needed for extracting the interaction energies as functions of center-center distance between the monomer constituents [14–16]. Here, we use a=8.37 $a_0$ from a linear fit to the sequence of ionization energies for $C_{60}$ calculated by means of high level density functional theory [17], which follows the same behavior as the classical expression for a metal sphere [14]. On the basis of the experimental results, we further assume that the charge is always equally divided or differ by one unit of charge on the monomer constituents. The model potential energy curves for $[C_{60}]_{2}^{r+}$ (r=0-3) are shown in Fig. 4a, where the asymptotic limits are given by the differences in monomer ionization energies used for extracting the metal sphere radius [17]. The binding energies for the neutral (0.277 eV) and the singly charged (0.362 eV) dimer systems are in agreement with the experimental results [7], 0.275±0.080 eV and 0.372±0.080 eV, respectively. The binding
distances for these systems (\( \sim 19 \text{ a}_0 \)) lie well inside the classical over the barrier distances for the \( C_{60}^{q+} - C_{60} \) system (\( q \geq 1 \)). This is consistent with the high charge mobility observed in the experiments as electrons are classical allowed to be transferred between the two monomers as soon the system is singly charged.

For \( r = 2 \), the model gives a very shallow (thermodynamical unstable) minimum of \( \sim 0.05 \text{ eV} \), suggesting that the doubly charged dimers are unstable on the experimental timescales (order of \( \mu \text{s} \)). For \( r \geq 3 \) the Coulomb repulsion clearly dominates the mutual interactions and these systems will thus promptly decay. This is consistent with the experimental results as there are no signs of multiply charged dimers in the one-stop spectra. The potential energy curves for \( r \geq 2 \) give the model kinetic energy releases (\( E_{KER} \)) for the dominant fragmentation processes that yield intact fullerenes. These are shown in Fig. 4b together with the corresponding experimental results from the simulations described above. In addition, we show the results from recent high level density functional theory (DFT) calculations of \( [C_{60}]_2^{r+} \) [11], where the dimer geometry was set to two neutral monomers from Ref. [17] separated by 18.9 \text{ a}_0 \) (i.e. a static geometry was used for all charge states). The DFT and simple model kinetic energy releases are similar, while the experimental values are significantly lower. The deviations from the experimental results increase with increasing charge state, indicating that there are important internal excitations during the fragmentation processes. Similar observations have recently been reported in grazing collisions between fullerene ions and metal surfaces [18], where the internal excitations of neutralized fullerenes were found to increase with increasing normal energy (in the range 3-10 \text{ eV}).

The potential energy curves in Fig. 4a also give the vertical dimer ionization energies (IE’s), which are shown in Fig. 4c together with the monomer ionization energies [17] and the DFT results for dimers [11]. There are clear even-odd variation from a linear dependence for the model dimer values, which qualitatively explain the even-odd effects in the relative ionization cross sections (cf. left part of Fig. 3). The reason for this is that the collision scenarios are often such that the projectile captures electrons from one of the monomers. When the first electron is captured, the fast charge communication within the dimer system allows for the monomer closest to the projectile to become neutralized once again during the collision. As a consequence, the ionization energy for the singly charged dimer is only slightly higher than for the neutral system (due to presence of the singly charged monomer furthest away from the projectile). Thus the second electron may be transferred at nearly the same distance as the first electron. Similar arguments can be made for all steps in the ionization ladder, which thus give drops in the ionization cross sections for all odd charge states. It should be noted that the even-odd behaviour of the model values may be reproduced by DFT calculations of the ionization energies of a charged monomer (\( C_{60}^{r+} \)) in the electrostatic field of a point charge (\( r \) or \( r+1 \)) located at 18.9 \text{ a}_0 \) from the center of the fullerene cage [11], which thus to some extent support the results from the present electrostatic model.

In contrast to the electrostatic model, the DFT calculations for the full dimer system show that the global minima for the odd charge systems correspond to a completely delocalized charge [11]. As a consequence, the sequence of DFT dimer ionization energies shown in Fig. 4c follow a linear dependence, which would lead to a smooth decreasing ionization cross section as function of charge similar to the behavior for a monomer target. This suggests that the present experiment do not probe the adiabatic ionization energies. Instead it appears to be a dynamical effect that gives rise to the even-odd effects observed in the experiments, which to some extent is included in the simple electrostatic model approach.

4. Summary and Conclusions
We have studied the ionization and fragmentation of van der Waals fullerene dimers by multiply charged ion impact. Time-of-flight multistop correlation technique was used to measure the kinetic energy releases in the binary fission processes \( [C_{60}]_2^{r+} \rightarrow C_{60}^{r+} + C_{60}^{r+} (r=2-7) \) and the
relative ionization cross sections for production of $[C_{60}]^{2+}$, $[C_{60}C_{70}]^{r+}$, and $[C_{70}]^{2+}$. The experimental results were rationalized within the framework of a classical electrostatic model based on the Girifalco potential and the interaction energies between two metal spheres. These results were compared with recent DFT calculations [11].

The simple model and the previously reported experimental activation energies ($[C_{60}]^{r+} \rightarrow C_{60} + C_{60}$) of the neutral ($r=0$) and the singly charged ($r=1$) dimers [7] were found to be in good agreement. For the multiply charged species ($r \geq 1$), the DFT and model kinetic energy releases were found to be similar, while the differences compared to the experimental results increase with increasing dimer charge state. This suggests that a substantial amount of the energy released in the fragmentation goes to internal heating of the fullerene cages, which is consistent with recent experimental results from grazing collisions between fullerene ions and a metal surface [18].

The relative dimer ionization cross sections display even-odd variation as a function of the charge state, in sharp contrast to the smooth decreasing cross sections for multiply ionization of monomers. This may be explained within the framework of the simple electrostatic model, which rely on the experimental findings that the charge is shared as equally as possible between the two $C_{60}$ constituents and the assumption that the charge communication is faster than the time between sequential electron transfers. However, in an adiabatic picture, the dimer ionization energies display no such variations as the charge for the odd charge systems is completely delocalized according to the DFT calculations [11]. Thus, theoretical approaches taking the dynamical picture into account (timescales and collision geometries) are needed in order to further investigate these intriguing aspects of charge localization and delocalization time scales on fullerene van der Waals dimers.

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