PHYSICAL REVIEW A **95**, 012704 (2017)

Absolute cross sections for ethylene-dication production by electron impact

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(Received 31 October 2016; published 19 January 2017)

This work reports absolute cross-section measurements for the production of ethylene dications by electron impact, with the energy ranging between 25 and 800 eV. Separation of the entangled $C_2H_4^{2+}$ and CH_2^+ fragments with the same mass-to-charge ratio, in the time-of-flight spectrum, is properly carried out using the DETOF technique. This separation shows that stable $C_2H_4^{2+}$ can be produced either by two primary vacancies or by a single primary vacancy in an inner valence shell, with its subsequent de-excitation through Auger-like decay. Our findings show that the latter process can be an important player in dication formation, prevailing in the case of ethylene at projectile energies above 500 eV.

DOI: 10.1103/PhysRevA.95.012704

I. INTRODUCTION

The physics and physical chemistry regarding molecular dications have been the subject of many studies of their production, stability, and subsequent fragmentation [1–7]. Processes leading to singly charged final states can only lead to fragmentation into singly charged and neutral moieties; meanwhile, the possibility of dications dissociating into fragments with a high kinetic energy due to Coulombic repulsion [8–10], leading to kinetic energy releases of the order of tens of electron volts, may ascribe them a key role in the chemistry of energized media [11]. Therefore, in processes governing both atmospheric and cometary reactions, and molecular formation and breakup in plasma environments, dication formation is likely to be an important factor. Their presence in planetary atmospheres has been predicted by many authors and the kinetic energy release resulting from their fragmentation can lead to a local increase in the atmospheric temperature, which in turn is directly connected to planetary escape [1,12,13].

On the other hand, the mechanisms that govern dication production and stability remain elusive. A previous work regarding the oxygen molecule's dication production [14] by electron impact hinted that its most probable channel would be not a direct double-ionization process, but a single-vacancy production at an inner-valence molecular orbital, followed by Auger-like de-excitation. This process is the predominant decay route for core orbital ionization, but recently it was observed, both theoretically and experimentally, that it is present in inner valence shell ionization of both atoms (e.g., Ne [15–17]) and molecules (e.g., O_2 [14] and water [18,19]). These facts raise the question of the relevance of such single- and double-primary-vacancy production processes for the production of molecular dications—and whether their stability may be related to them. Particularly, if single-vacancy production plays a significant part in dication formation, this leads to a different understanding of the role dications play in the ionization yields at high projectile velocities. Indeed, the cross section for direct double ionization decreases more rapidly than single-ionization processes with an increase in the projectile's impact velocity. If the dication can be formed via a single-vacancy production followed by the removal of a second electron by a postcollisional relaxation, then it should retain the same ratio to the parent molecule's monocation, even for high-velocity impact. Thus, an investigation of the pathways that lead to the dication formation of relevant molecules in energized media is important to provide a more accurate description of their physical chemistry.

Small hydrocarbon compounds, for example, have been found to be present in many astrophysical environments, including the interstellar medium and planetary (including Titan's) atmospheres [20–24], where they are constantly bombarded by photons, electrons, and heavier particles. Studies show that molecular dications should be present in both the interstellar medium and Earth's atmosphere, although they have not been detected yet [12,13,25,26]. On the other hand, they are also constantly produced and fragmented in tokamaks and other plasma fusion devices, and the subsequent reactions they induce are obviously intrinsically linked to the kinetic energy of the produced fragments [27–29]. Therefore, deeper knowledge of the stability, formation, and dissociation mechanisms governing hydrocarbon dications is crucial in order to understand both the inventory of astrophysical media and the consequences of the interaction of plasmas and carbon fiber parts present in plasma fusion experiments, and many studies of their properties have been undertaken, both experimentally and theoretically [30–33].

Among these molecules, ethylene (or ethene), besides its essential role in vegetal life origin and development and its applications in the food industry [34], is the simplest hydrocarbon with a double bond and serves as a benchmark for comparison against more complex organic compounds, regarding both kinetic energy release and dication formation. Ethylene structure [35], as well as its ionization and fragmentation by electron [27,36–39] and photon [40–43] impact, has been considerably studied over the years. Moreover, it has been observed that cyclic organic molecules have a tendency to release ethylene- and acetylene-like charged and neutral fragments, C_2H_n, in breakup processes following irradiation [44,45].

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However, even though information on the cross section for the production of ethylene dication, for the reasons stated above, is needed to attempt a full description of its physical-chemical properties in energized media, so far there are no data on electron or heavy-particle impact. For photon irradiation, recent studies have been able to shed some light on its branching ratios at specific photon energies [42,43]. This lack of measurements is linked to the difficulty in separating, in time-of-flight (TOF) spectrometers, fragments with the same mass-to-charge ratio (m/q) in symmetric molecules, such as ethylene (namely, the dication $C_2H_4^{2+}$ and the fragment CH_2^+, with $m/q = 14$). Throughout the years, attempts to circumvent this kind of problem have involved the use of diatomic heteroisotopic molecules (e.g., $^{14}N\,^{15}N$ and $^{16}O\,^{17}O$ instead of the abundant $^{14}N_2$ and $^{16}O_2$, respectively) in order to separate the dication peak from the molecular fragments' peaks due to their same mass-to-charge ratios in the TOF spectra [46–48]. It is much harder to perform the same trick with hydrocarbons, since the many hydrogen atoms present in these molecules make it considerably more difficult to establish their respective proportions.

Nevertheless, the DETOF (delayed extraction time-of-flight) technique [14,29,49–51] has recently been established as a tool to measure the cross sections of different energy distributions of charged ions and molecular fragments produced in a collision. Hence it is possible to separate dication contributions for the TOF peak from a molecular fragment with the same mass-to-charge ratio, as has already been performed for both nitrogen and oxygen molecules' dication production by electron impact [14,50].

In this work, we present data for the absolute cross sections for ethylene-dication production by 25- to 800-eV electron impact. The mechanisms that can lead to a doubly ionized parent ion are also identified, in terms of single- and double-vacancy production by the incident electron, and it is seen that both processes contribute to the dication formation. This information provides new insight not only into the different processes that can produce a metastable doubly ionized molecule but also into the relevance of this interaction channel for higher energy impact, since the cross section for a single ionization followed by a postcollisional Auger-like de-excitation does not decrease with an increase in the impact energy, as much as a direct double-ionization process.

II. EXPERIMENTAL SETUP

The experimental setup used in this work consists of an electron gun coupled to a gas cell and a double-focusing TOF spectrometer. The details have been thoroughly described previously [52,53], and therefore it is presented here briefly.

An electron gun, operating here in the 25- to 800-eV energy range, produces a stream of 50-ns electron-beam pulses at a frequency of 20 kHz. The electrons interact with the target molecules inside a gas cell, kept at 2×10^{-4} Torr to guarantee a single-collisional regime, and are guided to the TOF drift tube by means of a 100-ns pulsed electrostatic extraction field of 21 V/mm across the collection region, which works as the start signal for the TOF acquisition electronics. The TOF drift tube, 476 mm long, has two focusing elements, namely, a 6.0-mm conical collimator at its entrance and an Einzel-like lens placed at one-third of its length, in order to attain a higher resolution in the TOF spectra [52]. The ions and charged fragments produced and guided through the TOF tube in this process are then collected by a microchannel plate (MCP) detector and fed to a standard acquisition electronics and are time-resolved by a FAST-COM [54] time-to-digital converter analyzer. The electron beam is collected by a Faraday cup and the gas cell pressure is measured with an absolute capacitive manometer. Thus, by knowing the number of incident electrons, the number of scattering centers of the gas target, the dimensions of the interaction region, and the efficiency of the spectrometer, absolute ionization and fragmentation cross sections can be obtained. The procedure to determine the absolute efficiency of the spectrometer has been described in detail elsewhere [52].

The pulsing of both the electron gun and the extraction field is synchronized with an adjustable time delay. The DETOF technique consists of gradually increasing this time delay between the two pulses beyond a minimum delay time t_0 after the passing of the electrons, allowing the ions and charged molecular fragments produced in the collision a free-flight time t. If this time t is long enough, the fastest fragments may leave the collection region and will not be guided through the collimator into the TOF drift tube when the extraction field is turned on. Thus, this progressive increase in the time delay plays the role of a velocity selector, in which only the slower fragments are collected. Since $C_2H_4^{2+}$ acquires no kinetic energy in the fragmentation process, the ion of interest retains a Maxwell-Boltzmann energy distribution throughout the collision process, while the fragment with the same m/q, CH_2^+, gains kinetic energy due to momentum conservation at the molecule's breakup. Since the ethylene dication supports long metastable lifetimes [42,55], this allows its disentanglement from the molecular fragment CH_2^+. The experimental data for different time delays at 100-eV electron impact energy, in terms of the ratio between the number of collected ions for a delay time t and the minimum delay time t_0 of 300 ns, are presented in Fig. 1.

It can be seen that the $m/q = 14$ group can be described by three energy distributions: (i) Maxwell-Boltzmann (MB), accounting for fragments with only thermal energy—in this case, the ethylene dication ($C_2H_4^{2+}$); (ii) exponential (Expo), which can be associated with fragments with only suprathermal kinetic energies—here, CH_2^+ with an average kinetic energy of 0.04 eV; and (iii) Gaussian ($G_{0.8}$), centered at a kinetic energy of 0.8 eV, corresponding to more energetic CH_2^+ fragments, due to repulsive states of the molecule leading to its fragmentation. It is important to stress that all three of these distributions are necessary in order to account for the behavior of the experimental data as a function of the time delay. For all measured energies, the adjustment curve of the experimental data, being the sum of these three distributions, kept an $R^2 > 0.99$, and their uncertainties were determined using the criterion of keeping $R^2 > 0.97$.

It should be noted that there is also a contribution coming from a Gaussian distribution centered above 5.0 eV, which is likely coming from the $C_2H_4^{2+} \rightarrow CH_2^+ + CH_2^+$ pathway, but the vast majority of its ions are lost before the minimum time delay of t_0 to be properly quantified by the DETOF technique and, thus, are not presented here, although the CH_2^+ cross-

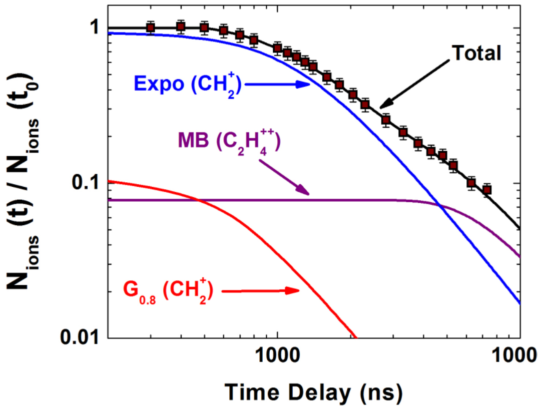

FIG. 1. Number of collisional products with an m/q ratio of 14 (CH_2^+ and $C_2H_4^{2+}$) for different time delays, normalized to their respective number at the minimum delay time of 300 ns. The black line (total) represents the sum of all the distributions present in order to accomplish the best possible fit, using the DETOF technique. The purple line (MB) corresponds to the Maxwell-Boltzmann distribution, which accounts for the $C_2H_4^{2+}$. The remaining distributions, Expo (blue line) and $G_{0.8}$ (red line), represent different energy distributions of the CH_2^+ fragment.

section data are corrected for its contribution. Further analysis of CH_2^+ and other ethylene fragments will be addressed in a future work, since the focus here is to describe the behavior of the ethylene-dication production.

III. RESULTS AND DISCUSSION

First, absolute cross sections for both the parent ion molecule and the moieties with $m/q = 14$ were obtained and compared to the measurements of Tian and Vidal [38]. These data are displayed in Fig. 2, and it can be seen that the agreement is remarkable over the entire measured energy range. It is worthwhile to mention that no contributions from molecular oxygen were observed in the TOF spectra. Since molecular nitrogen and ethylene have the same mass, the absence of oxygen indicates that no air contaminants were present in the experimental system, and hence it can be assumed that the peak with $m/q = 28$ corresponds solely to the singly ionized ethylene molecule.

The absolute cross sections values are also listed in Table I, where the $m/q = 14$ group is already separated into its two constituents, $C_2H_4^{2+}$ and CH_2^+, for the different electron impact energies. No previous measurements of absolute cross sections for ethylene-dication production have been reported, to the authors' knowledge.

It can be seen from the behavior of the cross sections for high impact energies that both singly and doubly charged species follow a very similar tendency, with the same slope. In order to further analyze this, the ratio between the doubly and the singly ionized parent molecules as a function of the impact energy is presented in Fig. 3. It is clear that this ratio reaches a constant value for electron energies above 500 eV. This indicates that in this higher energy regime there is a predominance of single-vacancy production, leading to a doubly ionized molecule via a subsequent de-excitation, since the expected tendency for a double-vacancy production process is for it to decrease more rapidly with an increase in the impact energy than single-vacancy ones. The latter feature appears also clearly from the maximum at ∼100 eV up to ∼500 eV, which decreases following an approximately $1/E$ dependency typical of double-vacancy production for that ratio (where E is the electron impact energy).

As stated above, this kind of postcollisional relaxation is an important mechanism of the multiple ionization of atoms [15,56,57] and molecules [58]. In the latter case, Auger-like decay of inner valence orbitals has been identified (in water, pyrimidine, and pyridazine, for example) as one of the main

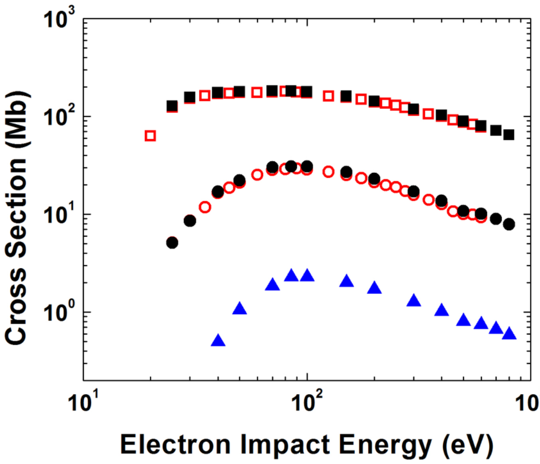

FIG. 2. Absolute cross sections for the production of $C_2H_4^+$ (squares), species with $m/q = 14$, comprising both $C_2H_4^{2+}$ and CH_2^+ (circles), and the disentangled $C_2H_4^{2+}$ (blue triangles) as a function of the electron impact energy. Filled black or blue symbols, this work; open red symbols, Tian and Vidal [38]. The $m/q = 14$ group is presented as a whole in order to compare it with the data of Tian and Vidal, being the sum of the cross sections of the three energy distributions presented in Fig. 1, whose relative weights are a function of the electron impact energy.

TABLE I. Absolute cross sections for $C_2H_4^+$, CH_2^+, and $C_2H_4^{2+}$, for the measured electron impact energies (in Mb). Uncertainties are estimated to be less than 10% for $C_2H_4^{2+}$ and 4% for CH_2^+ and $C_2H_4^+$.

E (eV)	$C_2H_4^+$	CH_2^+	$C_2H_4^{2+}$
25	128	5.50	
30	157	8.89	
40	175	17.0	0.495
50	179	21.4	1.06
70	182	29.0	1.84
85	181	28.9	2.28
100	178	29.0	2.29
150	161	26.1	2.01
200	143	21.7	1.70
300	118	16.1	1.26
400	103	13.2	1.02
500	89.1	10.6	0.801
600	79.8	9.61	0.746
700	71.6	8.45	0.664
800	64.6	7.31	0.584

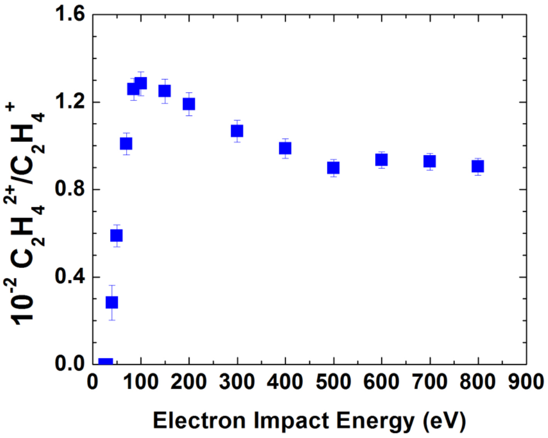

FIG. 3. Ratio between double- and single-ionization cross sections for the unfragmented parent molecule as a function of the electron impact energy. It can be seen that there is a peaked structure centered at 100-eV impact energy and that the ratio behavior tends to a constant value for higher impact energies, which indicates that an Auger-like single-vacancy process contributes to the ethylene-dication formation. Error bars indicate calculated uncertainties below 11% for 40 eV, 8% for 50 eV, and up to 6% for the remaining electron impact energies.

pathways leading to molecular fragmentation into two charged moieties at high impact velocities, for both electron and proton impact [58]. The present measurements show that this postcollisional relaxation is also able to leave some molecules in a stable dication state. This finding suggests that both direct double ionization and Auger-like decay, although very different two-vacancy production mechanisms, can lead to the same final molecular states, resulting in a stable $C_2H_4^{2+}$.

Previous measurements of Auger-like de-excitation leading to doubly ionized states in O_2, Ne, and H_2O [14–19] presented a dependency between the ratio of doubly to singly charged parent ions and the projectile velocity, which indicated Auger processes coming from inner valence shell ionization, since its characteristic features were present for impact energies below their *K*-shell ionization thresholds. In the present case, on the other hand, the inflection point shown in Fig. 3 is at a higher impact energy than the ionization threshold of the carbon's *K* shell. In order to verify the role of the *K* shell in the ethylene-dication formation, the ratio (R) between the ethylene dication and its parent ion cross sections is represented by the function $R \sim A/E + B\sigma_K/\sigma_{C_2H_4^+}$, where the first term corresponds to the dependence on the projectile energy of the ratio between double- and single-vacancy production, and the second term represents the contribution from *K*-shell ionization, being the ratio between the combined two carbons' *K*-shell ionization cross section [59] and the measured parent ion cross section. Using $A = 2.368$, in order to normalize it to the ratio in Fig. 3 at 200-eV impact energy, and $B = 0.6$, a very good agreement with the measured ratio is obtained for impact energies above 300 eV. This means that Auger decay from the *K* shell can indeed be a likely candidate for the production of stable ethylene dication at high impact velocities. This rough estimate suggests that about 60% of the *K*-shell Auger decays end as stable ethylene dication.

Previous works were not able to provide such clear evidence that both direct and postcollisional relaxation processes contribute to a stable dication formation. Indeed, as mentioned, there are indications that Auger-like decay could be the dominant process for molecular oxygen dication formation by swift electron impact [14]. In those measurements, however, the range of the electron impact energy was limited to a maximum value of 400 eV, and therefore the asymptotic behavior and the postcollisional relaxation were not as clear as presented here for ethylene. This does not seem to be the case for the nitrogen molecule [50], where the continuous decrease in the ratio relative to the parent molecular ion related to direct double ionization appears to be the prominent feature. Again, due to the impact energy limit of 400 eV, this result for nitrogen dication is not conclusive. What can be conclusively inferred from these three cases is that the relative contributions from two-step and postcollisional relaxation for dication formation can vary significantly from molecule to molecule.

The wide impact energy range investigated here allows observation of the single-vacancy production predominance above 500 eV. Indeed, this clearly shows that the dication production cannot be dismissed as negligible even for higher impact energies, since it retains the same proportional relation to the parent ion yield (~0.9%). Meanwhile, in the low and intermediate electron impact energy region (from 25 to 500 eV), a combination of both processes—single-vacancy production followed by postcollisional ionization and direct double-impact ionization—is present and contributes to the dication production cross section.

IV. CONCLUSION

Absolute cross sections for the dication production of ethylene (C_2H_4; also known as ethene) by electron impact have been reported; this was accomplished using the DETOF technique in order to separate $C_2H_4^{2+}$ and CH_2^+, which have the same mass-to-charge ratio.

The range of electron impact energies investigated in this work (25–800 eV) allowed the observation that, for higher impact energies, the ratio between ethylene dication and its parent ion tends to a constant value. This leads to the conclusion not only that $C_2H_4^{2+}$ results from direct double-impact ionization, but also that a significant contribution comes from single-vacancy production processes. Auger-like de-excitation is shown here to be a key factor in the production of ethylene dication, through the carbons' *K*-shell ionization, and it becomes the dominant process for high impact energies (above ~500 eV). An important consequence of this finding is that the doubly ionized molecule retains a nonnegligible yield throughout the range of possible impact energies. Since at our highest measured impact energy the collision time is within the attosecond time scale and the Auger decay is within the femtosecond time scale, this result can be considered postcollisional relaxation, thus, it depends only on the site of the electron's removal and should also be valid, although with different cross-section values, for photon and heavy-particle impact. Thus, in ethylene-containing atmospheres, ethylene dications not only should be present, but can be an important factor in the physical chemistry description of environments subjected to energetic particles.

ACKNOWLEDGMENTS

The authors would like to acknowledge the Brazilian funding agencies CNPq, CAPES, and FAPERJ.

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