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Branching ratios for the dissociative recombination of hydrocarbon ions III: the cases of $C_3H_n{}^+$ ($n = 1$–8)

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Abstract

Branching ratios for C–C bond scission during the dissociative recombination of hydrocarbon ions $C_3H_n{}^+$ have been measured using the storage ring technique. It is found that the channel leading to the scission of one of the carbon–carbon bonds is always possible but is particularly important for $n = 1$ and $n = 6$–8.

Keywords: Dissociative recombination; Isomers; Branching ratios; Hydrocarbon ions

1. Introduction

The dissociative recombination of hydrocarbon ions is of great importance in astrophysics [1–4], combustion [5,6] and industrial plasmas [7,8]. In recent experiments [9,10] (papers I and II) branching ratios for the dissociative recombination of $C_4H_n{}^+$ ions ($n = 1$–9) with low-energy electrons have been measured experimentally. In the present paper, we report on further measurements in which the branching ratios for the dissociative recombination of $C_3H_n{}^+$ ($n = 1$–8) ions have been determined.

2. Experimental method

The experiment was performed using the electron–ion merged beams technique at the heavy-ion storage ring ASTRID at the University of Aarhus, Denmark. The ions under study were produced from *n*-butane in a Nielsen electron impact source, accelerated to 150 keV and injected into the storage ring (shown in Fig. 1).

In ASTRID, the ions are accelerated to 2.5 MeV and this process takes about 4 s to accomplish. An electron beam of known energy, formed in the electron cooler assembly is merged with and de-merged from the ions in the storage ring using the dipole magnets B and C shown in the figure. The field of these magnets is rather weak and has little effect on the fast heavy-ion beam. The electron beam, can be turned on and off by removing the bias from a grid in front of the cathode. The electron velocity is tuned to be essentially identical to that of the ions so that a very low center-of-mass collision energy can be achieved.

Neutrals, formed in the straight section between magnets A and D (Fig. 1) pass un-deflected through magnet D and are detected by a surface-barrier detector located at a distance of 6 m from the exit of the electron cooler magnet C. There are two sources for these neutrals. One involves interaction of the stored ion beam with the background gas in the storage ring which is maintained at a pressure of about 10^{-11} Torr. The other source is interaction of the ions with the electron beam. For low center-of-mass collision energies, this interaction is only due to dissociative recombination. When molecular ions undergo dissociation in a stor-

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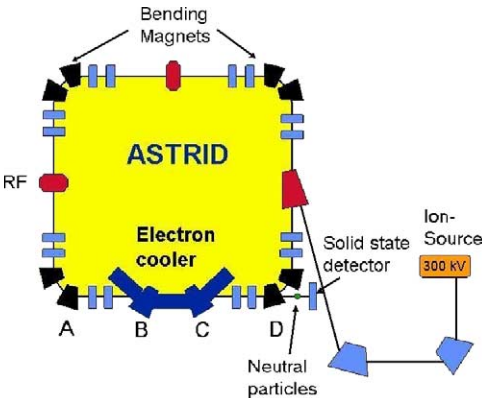

Fig. 1. Layout of ASTRID storage ring showing beam injection, electron cooler and neutral particles detection system. Magnets are labeled A–D.

age ring, the resulting fragments carry away with them kinetic energies that are distributed according to the fragment mass since they continue their passage through the machine with essentially the same velocity as the primary ion. (Velocity changes due to the release of dissociation energy are small compared with the primary ion velocity and for the purposes of the present discussion can be neglected.) The surface barrier detector is energy sensitive and so is capable of distinguishing between fragments that arrive individually with differing masses.

Fig. 2 shows the pulse height spectra for products arising from C_3H^+ ions, accumulated with the electrons on and off. The three peaks correspond to molecular fragments with 1, 2 or 3 carbon atoms. In fact these peaks are made up of sub-peaks due to fragments with differing numbers of hydrogen atoms but the resolution is insufficient to distinguish between them. There should also be peaks due to released hydrogen atoms and molecules but these lie low in energy and fall into the electronic noise of the detector that is removed using a discriminator. We are thus unable to determine by direct means, the number of hydrogen atoms that are distributed between the fragments. We can, however, observe the scission of C–C bonds.

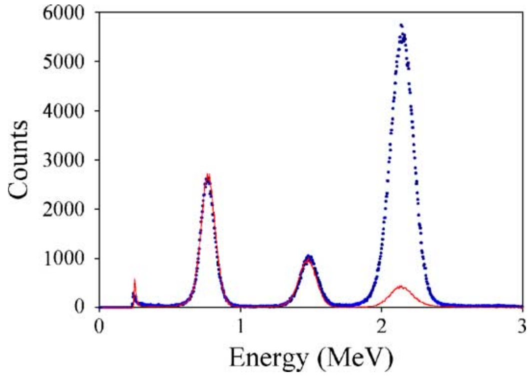

Fig. 2. Pulse height spectrum for neutral products arising from C_3H^+ ions due to electron–ion and background gas collisions (electron beam on dotted curve). With the electron beam off (continuous curve), only the latter are present. The abscissa is calibrated in terms of the energies of the arriving particles. The small peak on the left is part of the electron noise of the detector, truncated by using a pulse discriminator.

In the absence of the electron beam, the peaks (I–III) in the neutral particle spectrum arise from background gas reactions such as:

$$C_3{}^+ + X \rightarrow C_2{}^+ + C + X \tag{1a}$$

$$C_3{}^+ + X \rightarrow C_2 + C^+ + X \tag{1b}$$

$$C_3{}^+ + X \rightarrow C_3 + X^+ \tag{1c}$$

where X is a background gas molecule and we have ignored the hydrogen atoms. The ionic species are deflected away by the dipole magnet D and so do not reach the detector.

When the electron beam is on, in addition to these background reactions, the following recombination processes occur:

$$e^- + C_3{}^+ \rightarrow C_3 \tag{2a}$$

$$e^- + C_3{}^+ \rightarrow C_2 + C \tag{2b}$$

$$e^- + C_3{}^+ \rightarrow C + C + C \tag{2c}$$

Since the recombination fragments are all neutral, they arrive simultaneously at the detector, appear as if they were a single full-energy particle and accumulate in Peak III.

In order to distinguish between ion–background gas processes and ion–electron processes, the electron beam is chopped electrostatically and measurements of the neutrals are performed when the electrons are on and when they are off. Neutrals due to recombination are thus determined by subtracting the two measured count rates.

2.1. Branching ratio measurement

The goal of the present experiment is to determine the branching ratios, i.e., the relative proportions of the three possible recombination channels (2a–c) that give rise to products having different combinations of carbon atoms. By limiting the probability of all the particles reaching the detector by placing a mesh grid with a known transmission T in front its entrance window [11], one is able to distinguish between the various recombination channels since the probability of one atom or molecule reaching the detector is T, for two atoms or molecules it is T^2 etc and $T < 1$. When not all particles from a given recombination event arrive at the detector, those that do will therefore, fall into lower energy channels since not all the energy is deposited. We can analyze the contributions from each of the recombination channels that fall into peaks I–III but one must take into account not only the probability of a particle passing through the grid and being detected but the probability for a particle to be stopped by the grid and thus fail to be detected, and the number of ways that a given situation can occur. Thus, the number particles in peaks I–III being N_{I}, N_{II} and N_{III} is given by:

$$N_1 = T(1-T)N_{2b} + 3T(1-T)^2 N_{2c}$$

$$N_2 = T(1-T)N_{2b} + 3T^2(1-T)N_{2c}$$

$$N_3 = TN_{2a} + T^2N_{2b} + T^3N_{2c}$$

where N_{2a}, N_{2b} and N_{2c} are the fractions of the total number of recombinations that yield channels 2a–c, respectively. This method has been used previously in a large number of branching ratio measurements with hydrocarbon molecular ions at ASTRID [9,10,12] and also at CRYRING at the Manne Siegbahn Laboratory in Sweden [13–18].

A series of equations was presented in [9] that allowed for corrections due to light fragments missing the detector. For all the measurements described here, it was verified that in fact there were no such losses. This was done by examining the measured counts without a grid in front of the detector and verifying that the only difference between the (electrons-on) and (electrons-off) count rates, occurred in the third peak.

The actual measurement was performed using two separate grids with measured [19] transmission values $T_1 = 0.675$ and $T_2 = 0.235$ known to an accuracy of ±0.5%. The values of $N_{\mathrm{I-III}}$, used as input into the probability equations were determined from the difference in measured pulse height spectra (Electrons on minus electrons off) by fitting the resulting individual peaks using a Levenberg–Marquart non-linear fitting method [20] assuming that they are formed from a set of Gaussian peaks. (A given peak, arising from the recombination of an ion $C_3H_n{}^+$ will consist of contributions from C_mH_p fragments where m is the peak number and $p \leq n$). The pulse height analyzer has an associated live-time that is a function of the input count rate, and since this is different during the electrons-on and electrons-off cycles, a correction must be made for this by multiplying the electrons-on count rate by the ratio of the (electrons-off)/(electrons on) live-times. A typical value for this factor is 0.95. It is also possible that a high peak can be contaminated by pulses destined for a low peak due to two such pulses arriving at the same time. This effect is known as pulse pile-up and care was taken to avoid this.

A χ^2-based error analysis method taking account of statistical counting errors and errors due to the fitting procedures, pulse pile-ups and live-time corrections is applied to the data and the results of this, along with the branching ratio measurements are presented in the following.

Table 1
Branching fractions for the dissociative recombination of $C_3H_n{}^+$ ions

Species	C_3 (%)	$C_2 + C$ (%)
C_3H^+	66.2 ± 1.5	33.8 ± 1.7
$C_3H_2{}^+$	87.5 ± 1.7	12.5 ± 2.1
$C_3H_3{}^+$	90.7 ± 1.1	9.3 ± 0.5
$C_3H_4{}^+$	89.7 ± 2.5	10.3 ± 1.2
$C_3H_5{}^+$	86.7 ± 4.0	13.3 ± 2.6
$C_3H_6{}^+$	69.3 ± 1.6	30.7 ± 1.3
$C_3H_7{}^+$	66.8 ± 2.3	33.2 ± 2.3
$C_3H_8{}^+$	67.9 ± 2.9	32.1 ± 2.8

3. Results and discussion

Due to the long storage time of the ions before recombination, we make the assumption that if different isomeric forms are initially created, they have time to relax to the lowest lying forms. If different stable isomers exist, however, that are separated by isomerization barriers, our population of $C_3H_n{}^+$ ions will remain not well defined. The possible isomeric forms of $C_3H_n{}^+$ ions will be discussed separately for each ion. Channels energetically open for dissociative recombination were determined by the use of thermochemical data, provided unless otherwise noted, by refs. [21,22].

The branching fractions measured for $C_3H_n{}^+$ ions with "n" ranging from 1 to 8 are listed in Table 1. The estimated errors in these measurements, determined using the procedure discussed above are shown.

For all $C_3H_n{}^+$ ions presented in the Table 1, the branching ratio for the third channel (2c) leading to three carbon containing fragments was found to be negligible. It is seen that the dissociation recombination of $C_3H_2{}^+$, $C_3H_3{}^+$, $C_3H_4{}^+$ and $C_3H_5{}^+$ ions goes mainly to the C_3 channel, the $C_2 + C$ channel contributing between 9 and 13% to the total. C_3H^+, $C_3H_6{}^+$, $C_3H_7{}^+$ and $C_3H_8{}^+$ recombine in a common way but differently compared to the first group of ions. The most probable channel here is C_3 accounting for between 66 and 70% and around 30% goes to the $C_2 + C$ channel. For all ions, the loss of a hydrogen atom or molecule without C–C bond breaking is possible and will yield a C_3 product.

3.1. C_3H^+

The more stable form of the propynylidene cation, C_3H^+, is the linear form shown in Fig. 3a and its heat of formation is 383 kcal/mol [23,24].

The next highest linear structure is the bent form (Fig. 3b) that lies 52.7 kcal/mol higher [24]. Ikuta [25] has found that a cyclic isomer (Fig. 3c) of C_3H^+ also exists and this lies 17 kcal/mol above the lowest linear isomer. Nothing in known about eventual isomerization barriers between the

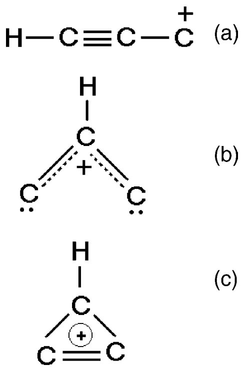

Fig. 3. Isomeric forms of C_3H^+.

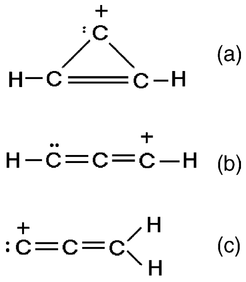

Fig. 4. Isomeric forms of $C_3H_2^+$.

three isomers, but it seems reasonable to assume that the bent form will relax to the straight linear one. Our C_3H^+ ions could consist therefore, of a mixture of linear (Fig. 3a) and cyclic (Fig. 3c) isomers. The experiment shows that 66.2% of dissociative recombinations of C_3H^+ go to the C_3 channel, 33.8% go to the $C_2 + C$ channel. According to thermochemical data [26], either one C–C bond (simple or multiple) or the C–H bond can be broken during recombination. Channels $C_2 + C$ and C_3 are open for the linear form, but only the C_3 channel is open for the cyclic form. The observed high percentage of recombinations that lead to a C–C breakage might be an argument for saying that the linear form dominates in the ring but this statement should be taken with caution.

3.2. $C_3H_2^+$

$C_3H_2^+$ can exist in both a cyclic (Fig. 4a, cyclopropelinydene cation) and in a linear (Fig. 4b, propandienylidene cation) form. Both of the corresponding neutral radicals have been observed in the interstellar medium [27,28] the former being the first cyclic molecule to be observed in space.

Experimental [29] and theoretical [30] studies show that the lowest energy isomer for the ion is the cyclic structure with the linear isomer lying only 6 kcal/mol higher in energy. It is thus possible that our beam contains both forms though other experimental studies [31,32] have shown that the linear form is dominant. The heat of formation of the linear form ΔH_f ($C_3H_2^+$) has been calculated to be 332 ± 5 kcal/mol. A third possible isomeric form $HCCCH^+$ has the structure shown in Fig. 4c and is predicted to lie about 46 kcal/mol higher than C–$C_3H_2^+$ [30].

The experiment shows that 87.5% of dissociative recombinations of $C_3H_2^+$ go to the C_3 channel, 12.5% go to the $C_2 + C$ channel. Kinetic energy release calculations for this ion indicate that the third channel $C + C + C$ is closed which is consistent with our observations. Pulse height spectra of neutral products arising from $C_3H_2^+$ with Grid 2 in front of the detector are presented in Fig. 5.

3.3. $C_3H_3^+$

Abouelaziz et al. [33] have reported an experimental value for the 300 K rate coefficient for dissociative recombination of $C_3H_3^+$ of $7 \pm 2 \times 10^{-7}$ cm^3/s, measured using a Flowing Afterglow Langmuir Probe–Mass Spectrometer (FALP-MS) apparatus while Graham and Goodings [34] found a value for the rate coefficient of 1×10^{-7} cm^3/s at 2000 K in a flame sampling experiment.

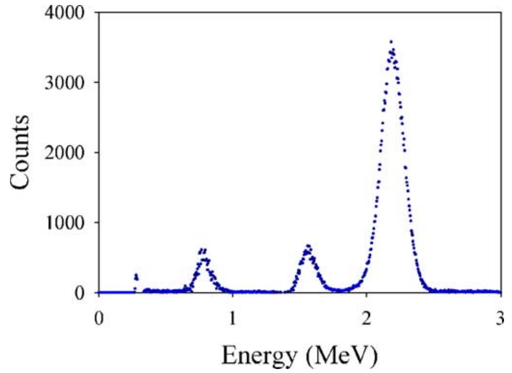

Fig. 5. Pulse height spectrum of neutral products arising from the recombination of $C_3H_2^+$ ions with electrons. Spectrum taken with a 23.5% transmission grid in front of the detector.

$C_3H_3^+$ is an ion that is found ubiquitously in hydrocarbon plasmas and is the dominant ion in fuel rich flames. It is known to exist in two possible low-energy forms; the cyclic cyclopropenyl form (Fig. 6a) and the linear propargyl form (Fig. 6b).

Calculations and experiments [24,35–37] show that the cyclopropenyl ion is the lowest energy form of $C_3H_3^+$ and that the propargyl cation lies about 25 kcal/mol higher in energy. The heat of formation of the cyclic ion has been calculated [35] and measured [37] to be 256 kcal/mol while that for the linear form is 282 kcal/mol. Experimental studies of Lossing [37] indicate that the linear form is much less stable than the cyclic form but ICR work [38,39] showed that the propargyl cation could survive at low pressure. In the present study, where no collision occur after ion mass selection, it can be assumed that we are dealing with both isomers.

Talbi [40] has studied the excited states responsible for the recombination of both cyclic and linear $C_3H_3^+$ and found that while there is an optimal curve crossing for the former that can explain the high observed rate coefficients, the linear ion has a curve crossing that lies above the minimum

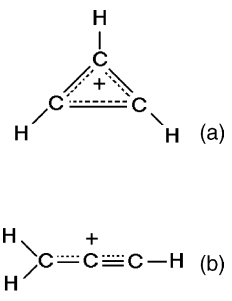

Fig. 6. The cyclopropenyl (a) and propargyl (b) isomers of $C_3H_3^+$.

of the ion ground state and so would be expected to display a considerably slower rate (D. Talbi, personal communication, 2003). The measured branching ratios are thus mainly related to the recombination of the cyclic ion.

We find that the most probable channel for the recombination of $C_3H_3{}^+$ is the C_3 channel accounting for 90.7% of the total. This channel corresponds to the loss of a single hydrogen atom or to the loss of a H_2 molecule from the cyclic ion. The linear ion, if recombining, can also lose two separate H atoms. The $C_2 + C$ channel is not negligible, and accounts either for a unique C–C bond break in the linear ion, or for ring opening of the cyclic ion. In this case, two C–C bonds must be broken, or considerable rearrangement must occur prior to splitting.

The $C_4H_5{}^+$ ion has a rather similar structure to cyclopropenyl, having a three carbon ring but with the hydrogen atom replaced by a methyl group. In recent measurements [9,10] of the dissociative recombination of that ion, we found that the channel involving ring breakage and subsequent rearrangement ($C_2 + C_2$) accounted for 40% of the total recombinations while the channel that would have involved merely throwing off the methyl group accounted for just 10%. We look forward to theoretical analysis of these processes in order to shed some light on what is a most interesting phenomenon.

3.4. $C_3H_4{}^+$

Structural isomerization of allene and propyne (Fig. 7a and b) has been extensively studied experimentally [41,42] and appears to proceed through a common intermediate (Fig. 7c) below the level of dissociation [41]. Allene is 13.8 kcal/mol more stable than propyne but isomerization barriers allow them to co-exist in amounts depending upon the experimental conditions. We thus make the assumption that both forms exist in the ring.

When a molecular ion recombines, the energy available for bond breaking is the ionization energy of the corresponding neutral. In the case of allene, this energy is 10.3 eV, which is enough to break a double C=C bond. Thus, besides the usual dissociation channel that involves the loss of H atoms, both ions could contribute to the $C_2 + C$ channel. Experimentally, however, it is found that the C_3 channel accounts for 90% of all recombinations while the $C_2 + C$ channel accounts for just 10%.

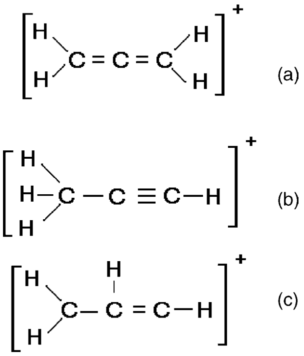

Fig. 7. (a) Allene, (b) propyne, and (c) common intermediate form.

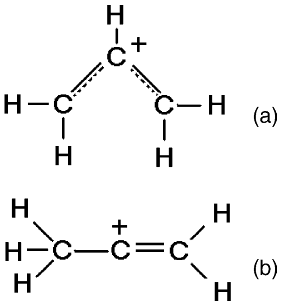

Fig. 8. The allyl and 2-propenyl isomers of $C_3H_5{}^+$.

3.5. $C_3H_5{}^+$

Many studies both theoretical and experimental have reported on $C_3H_5{}^+$ [43]. Six possible structures have been identified theoretically [43] but only two of them, the allyl and 2-propenyl cations have also been seen experimentally [44–46] and are truly minima on the potential energy surface.

The allyl cation is the most stable isomer and its heat of formation is 226 kcal/mol. The 2-propenyl cation is 8 kcal/mol higher in energy but is separated from its lower energy isomer by a 26 kcal barrier [41]. If both are found in the storage ring, they are likely to survive as distinct isomers (Fig. 8).

Experimentally, we find that in the recombination process, the C_3 channel is dominant (86.7%) though the $C_2 + C$ channel (13.3%) is significant. This is not unexpected given these isomeric structures.

3.6. $C_3H_6{}^+$

Four isomeric $C_3H_6{}^+$ ions have been postulated to exist in the gas-phase, namely the propene radical cation, the cyclopropane radical cation, the trimethylene distonic ion and the dimethylcarbene radical cation [47] (Fig. 9). It is unclear, however, whether the cyclopropane radical cation and the trimethylene distonic ion are distinct entities [48].

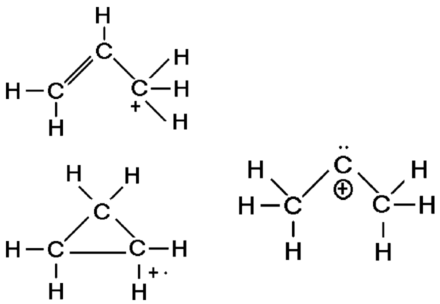

Fig. 9. Propene, cyclopropane and dimethylcarbene radical cations.

The global minimum on the potential energy surface is the propene radical [48] with the cyclopropane radical cation lying 9 ± 1 kcal/mol higher [48,49]. Isomerization of the latter into propene is, however, prevented by an activation barrier [50] whose height has been calculated to be about 25 kcal/mol [48,49]. The dimethyl carbene ion lies 20 kcal higher in energy than the propene, and is separated from it by a barrier of 8.4 kcal [51]. It has been produced in the gas-phase using 2,2,4,4,-tetramethyl-1,3-cyclobutanedione as precursor, and is therefore not expected to be produced from *n*-butane, as in our experiment Fig. 9.

It has been demonstrated that when produced from electron impact of propane or propene, only the linear form of the ion is produced [52–54]. Conversely, only the cyclic form is produced by electron impact of cyclopropane [47]. One can, however, notice that the formed ions retain the molecular structure of their precursors, so that in our experiment, only propene should be present.

We find that 69.3% of recombinations yield C_3 products while the C_2+C channel yields 30.7%. The latter is certainly an expected result if as expected, the propene isomer is dominant. The $C+C+C$ channel is found to be closed, also as expected.

The pulse height spectra obtained (in the presence of a grid) with this ion are presented in Fig. 10. The fact that the C_2+C channel is much stronger than for the smaller cations in this series is clearly evident from this figure.

3.7. $C_3H_7^+$

The dissociative recombination of $C_3H_7^+$ has been measured experimentally using the storage ring method at CRYRING in Stockholm [18]. The detector used in that study had a much higher energy resolution than ours and so they were able to identify the different channels leading to hydrogen atom and hydrogen molecule loss.

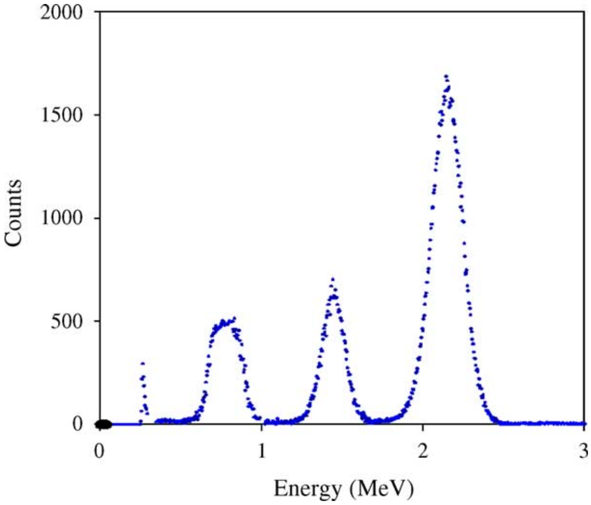

Fig. 10. Pulse height spectrum of neutral products arising from the recombination of $C_3H_6^+$ ions with electrons. Spectrum taken with a 23.5% transmission grid in front of the detector.

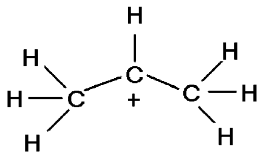

Fig. 11. The iso-propyl isomer of $C_3H_7^+$.

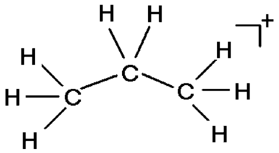

Fig. 12. The propane cation.

Ehlerding et al. [18] have discussed the isomeric state of the ions present in the storage ring and have concluded that due to rapid isomerizations, the ion that was studied had the iso-propyl structure (Fig. 11).

Our results concerning branching ratios are in close agreement with those of the CRYRING group. We find a branching ratio toward $C_2 + C$ of 33%, while they find 37 ± 3%.

3.8. $C_3H_8^+$

The structure of the propane cation, $C_3H_8^+$ is shown in Fig. 12. The channel leading to C+C+C products is formally open according to thermodynamic arguments but in fact we find that its contribution is negligible. Like the previous two ions, the $C_2 + C$ channel is large, accounting for 32% of all dissociations.

4. Conclusion

From observation of the various ions, it can be correlated that when a carbon is attached to another carbon, via a single bond, then ejection of that carbon atom is an important recombination channel. This occurs for C_3H^+, $C_3H_6^+$, $C_3H_7^+$, and $C_3H_8^+$. For the other ions studied here, the fact that the isomer is cyclic or that it contains only multiple bonds seems to be the factor that limits the importance of this channel though it is non-negligible in all cases. The channels that involve the breaking of two carbon–carbon bonds are found to be negligible throughout. Dissociative recombination is a very complex process, however, and to discuss breakup routes simply in terms of isomeric form may be altogether too much of a simplification. This has been seen for the cases of C_4H^+ and $C_4H_5^+$ [9,10]. Theoretical analysis of these processes should prove to be a very interesting endeavor.

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