

Hydrogen migration and C–C bond breaking in 1,3-butadiene in intense laser fields studied by coincidence momentum imaging

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ARTICLE INFO

Article history:

Received 23 September 2009

In final form 3 November 2009

Available online 6 November 2009

ABSTRACT

Two-body dissociation processes of $\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2^{2+}$ induced by an intense laser field were investigated by the coincidence momentum imaging method. Four dissociation pathways, $\text{C}_4\text{H}_6^{2+} \rightarrow \text{CH}_2^+ + \text{C}_3\text{H}_4^+$, $\text{C}_4\text{H}_6^{2+} \rightarrow \text{CH}_3^+ + \text{C}_3\text{H}_3^+$, $\text{C}_4\text{H}_6^{2+} \rightarrow \text{C}_2\text{H}_3^+ + \text{C}_2\text{H}_3^+$ and $\text{C}_4\text{H}_6^{2+} \rightarrow \text{C}_2\text{H}_2^+ + \text{C}_2\text{H}_4^+$, were identified. The existence of the second and fourth pathways can be regarded as evidences of the chemical bond rearrangement processes associated with hydrogen migration in the intense laser field. It was found that the hydrogen atom bonded originally to one of the two central carbon atoms migrates preferentially to its neighboring terminal carbon atom site.

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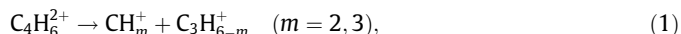
1. Introduction

During the last several years, ultrafast hydrogen migration processes within a molecule in intense laser fields have been investigated extensively, not only because of the findings that hydrogen atoms (or protons) move extremely rapidly within a molecule, but also their potential applicability for controlling chemical bond breaking processes [1–9]. The hydrogen migration process, in which hydrogen atom(s) or proton(s) migrate from one site to another within a molecule, can induce large scale deformation of molecular skeletal structure and rearrangement of chemical bonds [10–12]. Such processes induced by intense laser fields have been demonstrated so far in various hydrocarbon molecules. For example, in the case of methanol (CH_3OH), the observation of singly charged OH_2^+ , OH_3^+ , and CH_4^+ , generated through two-body Coulomb explosion of $\text{CH}_3\text{OH}^{2+}$, confirmed that hydrogen atom(s) or proton(s) migrate between the methyl group and the hydroxyl group induced by an intense laser field ($\sim 10^{14} \text{ W/cm}^2$, $\sim 800 \text{ nm}$, $\sim 60 \text{ fs}$) [13].

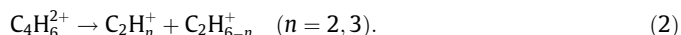
In the present study, we investigate hydrogen migration processes in 1,3-butadiene ($\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$) induced by an ultra-short intense laser field by detecting singly charged fragment ions generated through two-body fragmentation processes of doubly charged 1,3-butadiene using the coincidence momentum imaging (CMI) method [1]. The simple conjugated diene, 1,3-butadiene, is one of the simplest hydrocarbon molecules containing both single and double C–C bonds and could offer a possibility of studying

the effect of the changes in the bond-order associated with the migration of hydrogen atoms (and/or protons).

By the CMI method all the fragment ions originating from the dissociation of a single parent ion can be detected in coincidence, so that the decomposition pathways can be identified uniquely. Two types of two-body fragmentation pathways from the doubly charged parent ion were unambiguously identified: (i) two pathways in which one of the two side C–C bonds is broken,



and (ii) two pathways in which the central C–C bond is broken,



The existence of the $m = 3$ and $n = 2$ pathways proves that a hydrogen atom (or a proton) migrates prior to the C–C bond breaking. From the relative yields of the four fragmentation pathways and the distributions of the momentum vectors of the singly charged fragment ions, we discuss the fragmentation processes of doubly charged 1,3-butadiene molecules induced by an intense laser field.

2. Experiment

The experiments were carried out both at The University of Tokyo and Vienna University of Technology. The experimental apparatus used in Tokyo has been described elsewhere in detail [12,14]. Briefly, a Ti:Sapphire chirped pulse amplification (CPA) laser system (Pulsar 5000, Amplitude Technologies) was used to generate laser pulses with a duration of $\sim 40 \text{ fs}$, a repetition rate of 5 kHz, and a center wavelength of $\sim 795 \text{ nm}$. The laser pulses

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were focused by a quartz lens ($f = 15$ cm) into an ultrahigh-vacuum chamber with a background pressure of $\sim 5.3 \times 10^{-9}$ Pa. The laser field intensity was $\sim 2.2 \times 10^{14}$ W/cm² at the focal spot. The sample gas (1,3-butadiene) was introduced into the ultrahigh-vacuum chamber by a skimmer (0.20 mm $\varnothing$) to form an effusive molecular beam. The laser and the molecular beams crossed at right angles, and the ions generated at the laser focal spot were projected onto a position-sensitive detector (PSD) with delay-line readout by three equally spaced parallel-plate electrodes in the velocity mapping configuration. The voltages applied to the repeller and the accelerator plates were adjusted to be $U_{\text{rep}} = 1000$ V and $U_{\text{acc}} = 700$ V, respectively. In order to secure the coincidence conditions, the number of events of detecting positively charged fragment ions per laser shot was kept to be ~ 0.55 events/pulse by keeping the pressure in the vacuum chamber at $\sim 1.7 \times 10^{-8}$ Pa. The laser polarization direction was set to be parallel to the detector plane.

The experiment in Vienna was performed using cold target recoil ion momentum spectroscopy (COLTRIMS) [15]. Ti:Sapphire laser pulses with a pulse duration of ~ 28 fs and a center wavelength of ~ 795 nm at a repetition rate of 5 kHz were focused onto a supersonic gas jet of 1,3-butadiene molecules by a spherical mirror with a focal length of 60 mm in an ultra-high vacuum chamber at a background pressure of $\sim 1.5 \times 10^{-8}$ Pa. Ions and electrons created in the focus, located at the radial center of the spectrometer, were guided by a 9.5 V/cm uniform electric and 8 G magnetic field towards two multi-hit capable position and time sensitive detectors with delay-line anode for position readout. The length of the spectrometer was 5.7 cm for positively charged ions and 44.5 cm for electrons. The polarization direction of the laser pulses was set to be along the spectrometer axis. The temporal and spatial detector resolutions were approximately equal to those in the experiment in Tokyo. The event rates of detecting ions and electrons were set to 0.2 and 0.6 events/pulse, respectively, by tuning the target-gas backing pressure and the nozzle position. The pulse energy was adjusted to yield a pulse peak intensity of $\sim 1.5 \times 10^{14}$ W/cm² on target by measuring the proton spectrum of molecular hydrogen, H₂, dissociation [16]. In the present study, we do not use the data recorded by the detector for electrons. The coincidence momentum data recorded in Tokyo and Vienna are consistent with each other within experimental uncertainties.

3. Results and discussion

3.1. Identification of the four bond-breaking pathways

The time-of-flight (TOF) mass spectrum of the ion species generated from C₄H₆ in the intense laser field is shown in Fig. 1. The sharp peaks marked with an asterisk originate from residual gases in the vacuum chamber. As can be seen in this figure, H_i⁺ ($i = 1, 2$), C²⁺, CH_i⁺ ($i = 0-3$), C₂H_i⁺ ($i = 0-4$), C₄H₆²⁺, C₃H_i⁺ ($i = 0-5$), and C₄H_i⁺ ($i = 0-6$) are observed. The two peaks at $m/z = 18$ and 44 marked with an asterisk are ascribable to H₂O⁺ originating from the residual water vapor in the chamber, and to C₃H₈⁺ from the contamination of the 1,3-butadiene sample, respectively.

In the present study, we focus on the fragment ions that originate from the two-body fragmentation processes of doubly charged parent ions, C₄H₆²⁺. Two-body fragmentation processes can be identified as thin distributions along curved lines in the two-dimensional coincidence map, Fig. 2, where the two dominant fragmentation pathways that correspond to $m = 3$ and $n = 3$ are clearly visible.

In Fig. 3a–d, the two-dimensional coincidence momentum imaging maps of the fragment ions CH₂⁺, CH₃⁺, C₂H₃⁺, and C₂H₂⁺ recorded in coincidence with C₃H₄⁺, C₃H₃⁺, C₂H₃⁺ and C₂H₄⁺, respec-

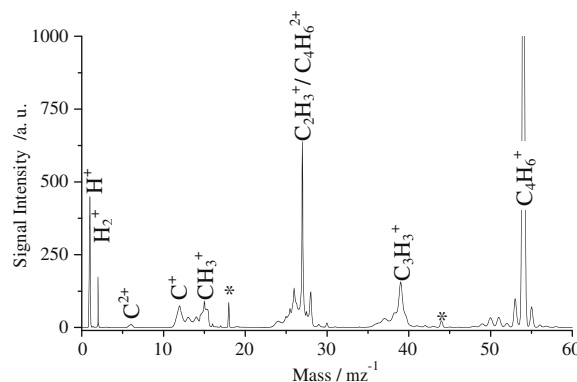
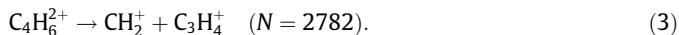


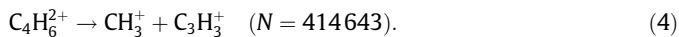
Fig. 1. Time-of-flight mass spectrum of 1,3-butadiene in an intense laser field (~ 40 fs, 2.2×10^{14} W/cm²) recorded in Tokyo.

tively, are shown as thin slices of the momentum sphere. The four CMI maps correspond to the following four two-body fragmentation pathways:

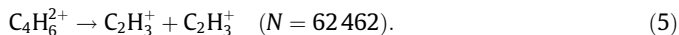
Breaking at the side C–C bond without hydrogen migration



Breaking at the side C–C bond with hydrogen migration



Breaking at the central C–C bond without hydrogen migration



Breaking at the central C–C bond with hydrogen migration

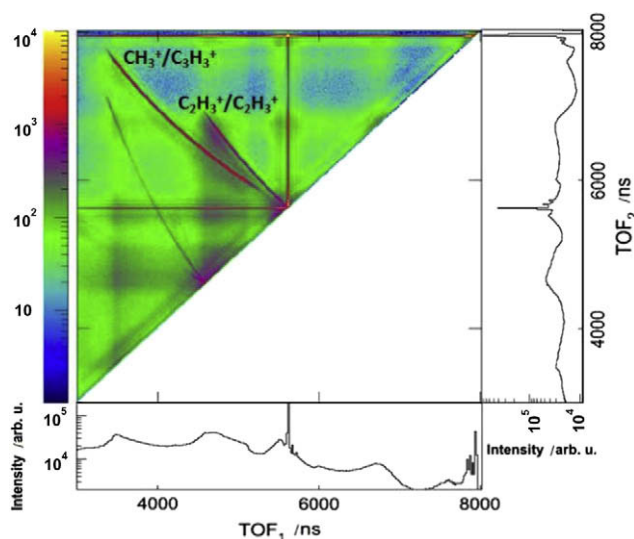
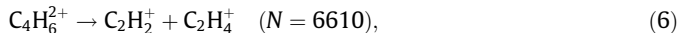


Fig. 2. Two-particle coincidence time-of-flight map (center) and two one-dimensional TOF mass spectra (right and bottom) of the fragment ions generated from 1,3-butadiene by an intense laser field (~ 28 fs, 1.5×10^{14} W/cm²) recorded in Vienna. Only the flight time range relevant for the fragmentation channels considered in this work is shown. A two-particle decomposition process is represented as a curved line because the TOF is a non-linear function of the momentum. The two strongest curved lines correspond to the fragmentation pathways (4) and (5), as marked in the figure. The horizontal and vertical lines at ~ 5600 ns and ~ 7900 ns represent singly and doubly charged 1,3-butadiene parent ions, which appear in the one-dimensional TOF spectra as the corresponding narrow peaks.

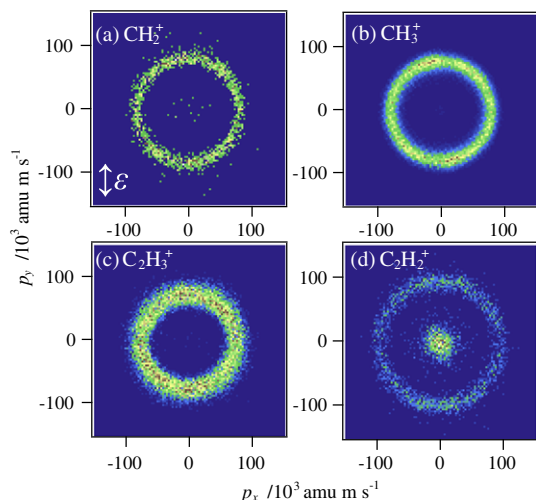


Fig. 3. Slices of the three-dimensional coincidence momentum sphere of the fragment ions generated through the four fragmentation pathways from $C_4H_6^{2+}$ observed in Tokyo. The slices are presented in the p_x – p_y plane, which is parallel to the detector plane. The direction p_z is perpendicular to the detector plane and parallel to the spectrometer axis. The laser polarization direction (ϵ) was set to be parallel to the p_y axis as indicated by the arrow. In the respective pathways, the momentum map of only one of the two fragment ions is shown; (a) CH_2^+ ($|p_z| < 50 \times 10^3 \text{ amu m s}^{-1}$), (b) CH_3^+ ($|p_z| < 50 \times 10^3 \text{ amu m s}^{-1}$), (c) $C_2H_3^+$ ($70 \times 10^3 < |p_z| < 80 \times 10^3 \text{ amu m s}^{-1}$), and (d) $C_2H_2^+$ ($|p_z| < 50 \times 10^3 \text{ amu m s}^{-1}$). The signals appearing in the central parts originate from false coincidence events.

where N represents the number of the coincidence events of the corresponding pathway. The four different processes are illustrated in Fig. 4. It can be seen that the number of $N = 414\,643$ for the pathway (4) is much larger than the number of $N = 2782$ for the pathway (3), representing that the pathway (4) accompanied by the hydrogen migration dominates the side C–C bond breaking, while the number of $N = 62\,462$ for the pathway (5) is much larger than the number of $N = 6610$ for the pathway (6), representing the pathway (5) without hydrogen migration dominates the central C–C bond breaking. This indicates that the hydrogen migration may lead to a change in the bond energies of the central C–C and the side C–C bonds within the parent molecule.

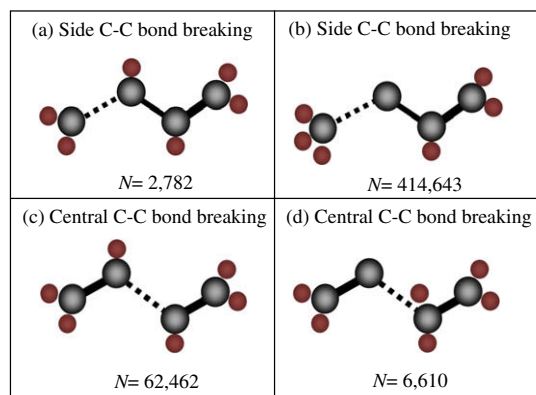


Fig. 4. Schematic diagrams of the four fragmentation channels of doubly charged 1,3-butadiene in an intense laser field, where N represents the number of the coincidence events. The number of $N = 6610$ is overestimated because of false coincidence events recorded for the pathway (6) as shown in the central part of Fig. 3d, and the number, $N = 62\,462$, obtained for the pathway (5) is underestimated because of the dead-time of the detector for two consecutive fragments with small momentum components p_z around zero that arrive within a short period.

In addition to the four two-body fragmentation pathways above, the three kind of two-body fragmentation pathways, in which one or more C–H bonds are broken to produce $H_n^+ + C_4H_{4-n}^+$ ($n = 1$ –3), were identified in coincidence.

3.2. Effect of the hydrogen migration on the C–C bond breaking

It can also be noted in Fig. 4b and d that for the two pathways (4) and (6) associated with the hydrogen migration, the number of the coincidence events obtained for the pathway (4), $N = 414\,643$, is almost two orders of magnitude larger than the number for the pathway (6), $N = 6610$. When the hydrogen atom located at one of the two central carbon positions moves to its neighboring terminal carbon atom site, the precursor species $CH_3^+ \cdots C_3H_3^+$ is formed, leading to the decomposition via the pathway (4). On the other hand, when the hydrogen atom bound to one of the two central carbon atoms moves to its neighboring central carbon position, the precursor species $C_2H_2^+ \cdots C_2H_4^+$ is formed, leading to the decomposition via the pathway (6). The significantly larger yield of the pathway (4) as compared to that of the pathway (6) indicates that the hydrogen atom bound to one of the two central carbon atoms moves preferentially to its neighboring terminal carbon atom site rather than to the other central carbon atom site in the course of the double ionization in the intense laser field.

As shown in Figs. 4a and c, for the two C–C bond-breaking pathways (3) and (5) without hydrogen migration, the number of the coincident events obtained for the pathways (3) is $N = 2782$, which is only 4.4% of the number, $N = 62\,462$, for the pathway (5). This shows that the central C–C bond of the parent 1,3-butadiene molecule is broken with a higher probability than the side C–C bonds, suggesting that the single bonded nature of the central C–C bond and the double-bonded nature of the two side C–C bonds of neutral 1,3-butadiene still remain in the doubly charged stage generated by the interaction with the intense laser field of 1.5 – $2 \times 10^{14} \text{ W/cm}^2$.

3.3. Theoretical confirmation of the C–C bond breaking and hydrogen migration

In order to confirm theoretically how efficiently the hydrogen migration proceeds and how the C–C bond dissociation energies vary depending on the position of the migrating hydrogen atom within the doubly charged parent molecule, we performed quantum chemical calculations using GAUSSIAN 03 program [17]. By the density functional theory (UB3LYP) with the 6-31G(d,p) basis set, the stable geometrical structures and the electronic energies of doubly charged 1,3-butadiene and its stable isomers were obtained by the GRRM 1.0 program developed by Ohno and Maeda [18–20]. The most stable equilibrium geometrical structure was found to be $[CH_3-C-CH-CH_2]^{2+}$, in which a hydrogen atom has migrated to the terminal carbon site from the neighboring central carbon atom, and its electronic energy was calculated to be -155.1182 hartree. The second lowest equilibrium geometrical structure was $[CH_2-CH-CH-CH_2]^{2+}$, in which all hydrogen atoms stay at the same carbon sites as in the neutral electronic ground state, and the electronic energy was calculated to be -155.1158 hartree. The electronic energy at the transition state between the two lowest equilibrium geometrical structures was calculated to be -155.1057 hartree. These calculations show that $[CH_2-CH-CH-CH_2]^{2+}$ can be transformed into $[CH_3-C-CH-CH_2]^{2+}$, which is lower in energy by -0.066 eV , via the transition state whose energy is higher only by 0.275 eV . The results of the calculations are depicted in Fig. 5. The very low barrier height is consistent with the observation that the yield of the pathway (4) that originates from the migrated form, $[CH_3-C-CH-CH_2]^{2+}$, is the largest among the four decomposition pathways.

The theoretical dissociation energy from $[\text{CH}_3\text{-C-CH-CH}_2]^{2+}$ into CH_3^+ and C_3H_3^+ was found to be lower by ~ 0.8 eV than that from $[\text{CH}_2\text{-CH-CH-CH}_2]^{2+}$ into C_2H_3^+ and C_2H_3^+ . This result also supports the observation that the yield of the pathway (4) (Fig. 4b) is almost one order of magnitude larger than that of the pathway (5) (Fig. 4c).

3.4. The momentum vector distributions of the fragment ions for the four pathways

From the CMI maps shown in Fig. 3 it becomes evident that all the four fragmentation pathways show almost isotropic distributions. The angular distributions, $I(\theta)$, of the fragment ions obtained from the corresponding coincidence momentum imaging maps can be characterized by the expectation values of the squared cosine defined as

$$\langle \cos^2 \theta \rangle = \frac{\int I(\theta) \cos^2 \theta \sin \theta d\theta}{\int I(\theta) \sin \theta d\theta}, \quad (7)$$

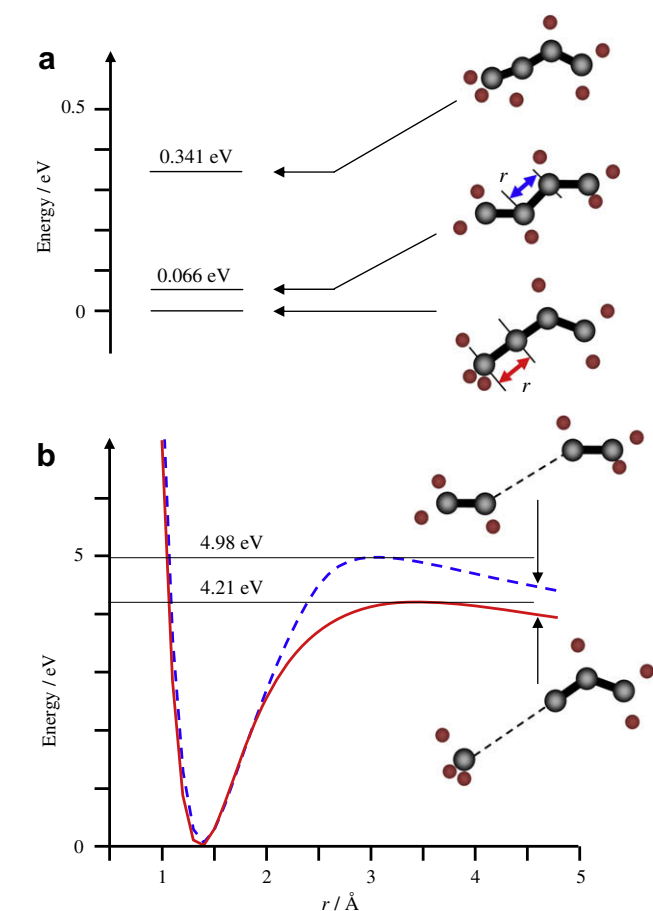


Fig. 5. (a) The geometrical structures and the relative energies of the two lowest-lying equilibrium geometries and the transition state connecting the two isomers of $\text{C}_4\text{H}_6^{2+}$ obtained from the theoretical calculations. The transition state of the hydrogen migration reaction connecting the two isomers, $[\text{CH}_2\text{-CH-CH-CH}_2]^{2+}$ and $[\text{CH}_3\text{-C-CH-CH}_2]^{2+}$, is located only 0.341 eV above the hydrogen-migrated isomer $[\text{CH}_3\text{-C-CH-CH}_2]^{2+}$, having the lowest energy. The C-C chemical bond to be stretched to draw the potential energy curves in (b) is denoted as ' r ' in both of the two isomers. (b) Calculated potential energy curves of the two isomers of $\text{C}_4\text{H}_6^{2+}$ as a function of the internuclear distance r shown in (a). The activation energy, that is, the height of the potential barrier for the decomposition reaction, $[\text{CH}_3\text{-C-CH-CH}_2]^{2+} \rightarrow \text{CH}_3^+ + [\text{C-CH-CH}_2]^+$, 4.21 eV, is lower by 0.77 eV than the following decomposition reaction, $[\text{CH}_2\text{-CH-CH-CH}_2]^{2+} \rightarrow [\text{CH}_2\text{-CH}]^+ + [\text{CH-CH}_2]^+$. When r is increased in the calculations for both of the isomers, the geometrical parameters other than r are assumed to take the same values as in the equilibrium geometry.

where θ is the ejection angle of the fragment ions with respect to the laser polarization direction. For an isotropic distribution, $\langle \cos^2 \theta \rangle$ takes the value of 1/3. The $\langle \cos^2 \theta \rangle$ values for the pathways (3)–(6) were calculated using all the accumulated coincidence events for the respective pathways to be $\langle \cos^2 \theta \rangle = 0.37, 0.39, 0.39$, and 0.38, showing almost isotropic distributions for all the four pathways.

The small $\langle \cos^2 \theta \rangle$ values can be ascribed to (i) the non-linear flexible skeletal C–C–C structure from which the fragment ions CH_n^+ , C_2H_n^+ and C_3H_n^+ can be ejected into the broad range of angles with respect to the laser polarization direction and/or (ii) to the overall rotational motion of the possibly long-lived parent molecules that are generated by the intense laser field [1]. The doubly charged parent ions, $\text{C}_4\text{H}_6^{2+}$, can be seen in Fig. 1, indicating that those ions can be prepared in the quasi-bound well of the low-lying electronic states of $\text{C}_4\text{H}_6^{2+}$, so that the lifetime is sufficiently long for surviving during the period of time when they are accelerated in the TOF spectrometer. On the other hand, the doubly charged species decomposing into a pair of the fragment ion species through the processes (3)–(6) are considered to be prepared in the vibrationally highly excited states of the low-lying electronic states or in the dissociative electronic states [12,13]. For confirming the origin of the isotropic distributions experimentally, it will be necessary to perform pump-and-probe measurements to measure the lifetime of the doubly charged precursor states.

From the three-dimensional momentum distributions of the fragment ions, the distributions of the released kinetic energy, E_{kin} , for the four pathways were obtained, where E_{kin} is the sum of the kinetic energies of a coincidence-pair of fragment ions. It was found that the peak energy of the distribution is $E_{\text{kin}} \sim 3.4$ eV and the full width at half maximum $\Gamma \sim 0.7$ eV for both pathways (3) and (4), respectively, in which one of the side C–C bonds is broken. The corresponding energies and widths for the pathways (5) and (6), in which the central C–C bond is broken, were determined to be $E_{\text{kin}} \sim 4.3$ eV and $\Gamma \sim 1.2$ eV, respectively. The observations suggest that the shape of the Coulomb-type repulsive potential for the C–C bond breaking in doubly charged 1,3-butadiene is not influenced much by the position of the migrating hydrogen atom.

4. Summary

Two-body decomposition processes of doubly charged 1,3-butadiene prepared by intense laser fields were investigated by using the coincidence momentum imaging method. A total of four fragmentation pathways via breaking of a C–C bond were uniquely identified: two pathways without hydrogen migration, i.e., $\text{C}_4\text{H}_6^{2+} \rightarrow \text{C}_2\text{H}_3^+ + \text{C}_2\text{H}_3^+$ and $\text{C}_4\text{H}_6^{2+} \rightarrow \text{CH}_2^+ + \text{C}_3\text{H}_4^+$, and two pathways with migration of one hydrogen atom, i.e., $\text{C}_4\text{H}_6^{2+} \rightarrow \text{CH}_3^+ + \text{C}_3\text{H}_3^+$ and $\text{C}_4\text{H}_6^{2+} \rightarrow \text{C}_2\text{H}_2^+ + \text{C}_2\text{H}_4^+$. Among them $\text{C}_4\text{H}_6^{2+} \rightarrow \text{CH}_3^+ + \text{C}_3\text{H}_3^+$ was found to be most abundant, indicating that the migration of a hydrogen atom from one of the two central carbon atom sites to the neighboring terminal carbon site occurs efficiently and weakens the side C–C bond. This observation was supported by the quantum chemical calculations.

Acknowledgements

The present research was supported by two grants from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan (Grant-in-Aid for Specially Promoted Research on Ultrafast Hydrogen Migration (#19002006), and Grant-in-Aid for Global COE Program for Chemistry Innovation), by one grant from JSPS Bilateral Japan–Austria Joint Research Project (#09035011-000061), and by two grants of the Austrian Science Fund, FWF (Special Research Program ADLIS, Project No. 19, and EURYI award U33-N16).

References

- [1] A. Hishikawa, H. Hasegawa, K. Yamanouchi, J. Electron Spectrosc. Relat. Phenom. 141 (2004) 195.
- [2] Y. Furukawa, K. Hoshina, K. Yamanouchi, H. Nakano, Chem. Phys. Lett. 414 (2005) 117.
- [3] A.S. Alnaser et al., J. Phys. B 39 (2006) S485.
- [4] T. Okino et al., J. Phys. B 39 (2006) S515.
- [5] H.L. Xu, T. Okino, K. Yamanouchi, J. Chem. Phys. 131 (2009) 151102.
- [6] R. Itakura, P. Liu, Y. Furukawa, T. Okino, K. Yamanouchi, H. Nakano, J. Chem. Phys. 127 (2007) 104306.
- [7] A. Hishikawa, A. Matsuda, E.J. Takahashi, M. Fushitani, J. Chem. Phys. 128 (2008) 084302.
- [8] K. Hoshina, Y. Furukawa, T. Okino, K. Yamanouchi, J. Chem. Phys. 129 (2008) 104302.
- [9] A.M. Mebel, A.D. Bandrauk, J. Chem. Phys. 129 (2008) 224311.
- [10] M. Katoh, C. Djerassi, J. Am. Chem. Soc. 92 (1970) 731.
- [11] R. Thissen, J. Delwiche, J.M. Robbe, D. Duflot, J.P. Flament, J.H.D. Eland, J. Chem. Phys. 99 (1993) 6590.
- [12] H. Xu, T. Okino, K. Yamanouchi, Chem. Phys. Lett. 469 (2009) 255.
- [13] T. Okino et al., Chem. Phys. Lett. 423 (2006) 220.
- [14] H. Hasegawa, A. Hishikawa, K. Yamanouchi, Chem. Phys. Lett. 349 (2001) 57.
- [15] J. Ullrich, R. Moshhammer, A. Dorn, R. Dörner, L.P.H. Schmidt, H. Schmidt-Böcking, Rep. Prog. Phys. 66 (2003) 1463.
- [16] A.S. Alnaser et al., Phys. Rev. A 70 (2004) 023413.
- [17] M.J. Frisch et al., GAUSSIAN 03, Revision C.02, Gaussian, Inc., Wallingford CT, 2004.
- [18] K. Ohno, S. Maeda, Chem. Phys. Lett. 384 (2004) 277.
- [19] S. Maeda, K. Ohno, J. Phys. Chem. A 109 (2005) 5742.
- [20] K. Ohno, S. Maeda, J. Phys. Chem. A 110 (2006) 8933.