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Three-Body Photodissociation of Thionyl Chloride

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The ultrafast photodissociation dynamics of thionyl chloride after excitation with a 235 nm pump pulse has been studied using a femtosecond time-resolved mass spectroscopy. The observed parent transient suggests that the excited states initiated by 235 nm are very short-lived, that is, approximately 166 fs. Not only a stepwise three-body dissociation pathway but also a concerted three-body dissociation pathway is observed.

Key words: Photodissociation, Thionyl chloride, Three-body, Time-resolved study

I. INTRODUCTION

Molecular dissociation is of significance in the chemistry of non-equilibrium environments. Most photo-initiated dissociation processes in the lower layers of the Earth's atmosphere are two-body dissociation processes. Usually, dynamics of the two-body dissociation processes can be obtained through relatively straightforward experimental methods [1, 2]. However, in combustion, as well as in the stratosphere, interstellar space, and other lower-density environments, high-energy processes can readily induce a three-body dissociation of neutral molecules. Unfortunately, owing to the challenges in predicting the involved complex nonadiabatic dynamics and in observing multiple dissociation products simultaneously, the investigation of three-body dissociation has been proven to be a hard stone for theoreticians as well as experimentalists [3, 4]. So far, three-body dissociation processes have been rarely explored, mainly because of the difficulty in getting a complete picture of these complex decay processes.

Conventional photofragment translational spectroscopy (PTS) [5] has been used to investigate the three-body dissociation dynamics [6]. Coincidence spectroscopy, which has been developed recently, can detect all fragments coincidentally [7] and is considered to be useful for investigating three-body dissociation process. However, such a technique is the most suitable for dissociative photoionization and dissociative photodetachment processes. In addition, coincidence spectroscopy constitutes a substantial experimental challenge. Femtosecond (fs) time-resolved spectroscopy [8, 9] is also considered as a very useful technique, which provides an alternate means to investigate the

three-body dissociation processes by monitoring the time evolution of the initial state, products and even intermediate.

Numerous molecular systems became objects for the study of three-body photodissociation dynamics [10–14]. Among them, acetone [15, 16] is probably the best-studied molecule. Triazine [17], tetrazine [18], dimethyl sulfoxide [19, 20], and phosgene [21] are other interesting systems that have also attracted extensive attention. Thionyl chloride (SOCl₂) is also an interesting system that possesses many interesting aspects [22]. Since the stepwise, synchronous concerted, or asynchronous concerted reactions are important processes in physics, biology, and chemistry, there has been a long history of debate to determine the dissociation is a stepwise or concerted for almost all of these molecules. It is also a hot topic for chemical dynamics to differentiate between the concerted and stepwise processes.

SOCl₂ [23] is a C_s point group non-planar molecule with a ¹A' ground state. The absorption spectrum is broad and extends into the spectral range where ultraviolet laser radiation can be easy to reach. The distinct shoulder at 40000 cm⁻¹ (250 nm) and the pronounced absorption maximum above 50000 cm⁻¹ (below 200 nm) are assigned to overlapping electronic transitions: the n_S→σ_{S-Cl}^{*} and n_S→π_{S-O}^{*} transitions from a non-bonding lone pair electron on the sulfur atom to the anti-bonding molecular orbitals of the S–Cl or the S–O bond. There have been several experimental studies on the photodissociation of SOCl₂. With ultraviolet laser excitation, the two equivalent C–S bonds probably break, producing the fragments of Cl+SO+Cl. Like other molecular systems undergoing three-body dissociation, there has been a long history of controversy about whether the dissociation is stepwise or concerted. The photodissociation of SOCl₂ has previously been studied experimentally for the photolysis wavelengths of 248, 235, and 193 nm. At 248 nm, PTS study [24] suggested that the two-

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body dissociation channel ($\text{SOCl}_2+h\nu\rightarrow\text{SOCl}+\text{Cl}$) becomes the main channel and the molecular elimination channel ($\text{SOCl}_2+h\nu\rightarrow\text{SO}+\text{Cl}_2$) contributes only insignificantly to the dissociation process [25]; however, no contribution of the three-body dissociation channel ($\text{SOCl}_2+h\nu\rightarrow\text{SO}+2\text{Cl}$) has been observed at this wavelength. These results agree well with the conclusions obtained by using microwave spectroscopy and laser-induced fluorescence (LIF) at the same wavelength [26]. At 193 nm, however, the dissociation dynamics was remarkably different, a concerted three-body decay has been found to be the main dissociation channel by a PTS study [27]. At 235 nm, a state-selective photofragment imaging experiment was carried out and showed bimodal kinetic energy distributions with a large contribution from the slow ground state Cl ($^2\text{P}_{3/2}$) fragments. This result hinted a competition between the two-body dissociation channel and the three-body one [28]. A one-dimensional resonance enhanced multi-photon/time-of-flight technique (REMPI/TOF) has also been used to study the photodissociation dynamics of thionyl chloride at 235 nm [25]. This study also observed the competition between the three-body and two-body dissociation channels, and indicated that the three-body decay was the most probably sequential. Three-dimensional (3D) imaging has been used to monitor the photofragments of SOCl_2 with a dissociation wavelength of 235 nm, which suggests that three-body decay channel was a sequential or asynchronously concerted decay [29].

Unlike the other molecules that experience three-body dissociation, the photodissociation process of SOCl_2 has not been inquired with femtosecond time-resolved spectroscopy. To date, there has not been a general conclusion regarding the mechanistic photodissociation of SOCl_2 . These notable gaps in the knowledge warrant intensive study using the femtosecond time-resolved method to get a clear picture of the photodissociation of SOCl_2 . To our knowledge, this is a first femtosecond time-resolved study on the three-body dissociation of SOCl_2 . Femtosecond time-resolved mass spectroscopy is used in our study. And, in order to investigate the competition between the concerted and stepwise three-body dissociation processes under identical energy conditions, the pump wavelength is fixed at 235 nm. The photodissociation processes of SOCl_2 , subsequent to excitation by the absorption of a 235 nm photon, have been directly observed in real time. Of particular note, the distinction between the concerted and stepwise processes and the confirmation of the time scales for the three body dissociation processes are very important.

II. EXPERIMENTS

The experimental setup has been described in detail elsewhere [30]. Briefly, the setup consisted of a pulsed

molecular beam combined with a time-of-flight (TOF) mass spectrometer and a Ti:Sapphire regenerative-amplified laser system (4.5 mJ, 1 kHz, 800 nm) (Coherent Inc.). The output light was split into two parts. One part was used to pump an optical parametric amplifier (OPA; Coherent Inc. TOPAS-C) to produce a pump pulse at 235 nm. Another fundamental output laser beam was converted to the probe pulse at 400 nm by a BBO (0.2-mm thickness) crystal. The probe pulse tracked the relaxation processes of SOCl_2 . Polarization vectors of the pump and probe lasers were aligned parallelly to each other and also set parallelly to the face of the detector. The pump-probe delay time was accurately controlled by a computer-controlled linear translation stage (PI, M-126.CG1). The two pulses were collinearly combined by a dichroic mirror then fused by a silica lens of $f=400$ mm on the thionyl chloride molecules. The employed apparatus [31], which consisted of a molecular-beam source chamber and an ionization-flight detection chamber, was similar to the apparatus designed by Eppink and Parker [32]. The liquid sample (SOCl_2 , 99.9% purity) 5% in helium buffer gas at a background pressure of 2 atm was prepared at room temperature and was expanded through a pulsed valve to create a pulsed molecular beam. The generated molecular beam was further collimated by a skimmer in a source chamber and introduced into the ionization-flight detection chamber, where it was crossed perpendicularly with the pump and probe pulses. The photoelectrons thus produced were accelerated by electrostatic lens system parallel to the molecular beam, and then projected onto a dual microchannel plate backed by a phosphor screen. The signal from the phosphor screen was monitored by a photomultiplier tube in order to obtain the total photoelectron and ion intensities. A multilayer μ -metal tube was used for a field-free region (360 mm) of the TOF spectrometer in order to avoid disturbance of the stray field.

III. RESULTS AND DISCUSSION

FIG. 1 shows the two color time-of-flight mass spectra recorded with the pump-probe configuration at $\Delta t=0$ (time-overlap). The peaks of the parent ion and fragment ions were observed in the spectrum. The peaks shown at m/z of 109, 82, 48, 32, and 28 corresponded to the SOCl_2^+ parent ion, SOCl^+ , SO^+ , Cl^+ and S^+ fragment ions, respectively. As shown in the mass spectra, not only the parent ion SOCl_2^+ , but also many fragment ions were observed. Furthermore, the SO^+ and SOCl^+ fragment ions were the dominant signals in the mass spectra. The mass spectra indicated that the parent ion probably underwent a photoinduced fragmentation process.

FIG. 2, FIG. 3, and FIG. 4 show the recorded time-resolved mass spectra ion signals of SOCl_2^+ , SOCl^+ , SO^+ and Cl^+ as a function of the pump-probe delay

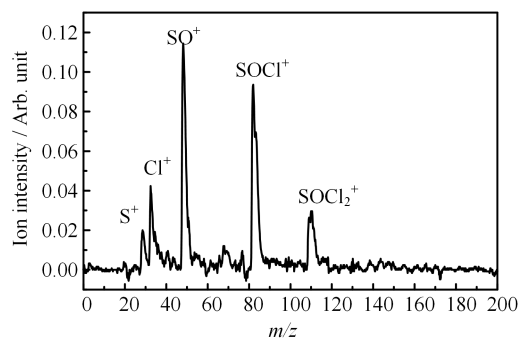


FIG. 1 Two color mass spectra (at time overlap) of thionyl chloride at 235 and 400 nm.

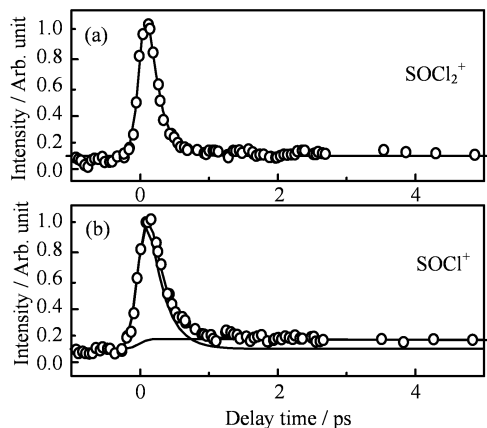


FIG. 2 Time-resolved SOCl_2^+ and SOCl^+ transients at a 235 nm pump and 400 nm probe. Experimental data are indicated by circles, whereas the fitting results are shown with solid lines.

time, respectively. Experimental data are indicated by circles, whereas the fitting results are shown with solid lines. The maximum pump-probe signal was more than 10 times larger than the one-color signals. The positive delay times in the time profiles meant that the pump laser (235 nm) arrived before the probe laser (400 nm), in turn, the negative delay times meant that the pump laser (235 nm) arrived after the probe laser (400 nm). At the small pump-probe delay time, the parent and all fragment ions time profiles show strongly enhanced pump-probe signals; after a pump-probe delay time of approximately 300 fs, the enhanced pump-probe signal disappeared quickly especially for the parent ion, although weaker enhanced signals remained for at least 20 ps for the fragment ions SO^+ and Cl^+ . The signal of the S^+ fragment ion was too weak to extract the time-resolved ion signal. Since the experimental results obtained in our study reveal the time evolution of the initial state, intermediate (SOCl), and final products (SO , Cl) for the three-body dissociation of SOCl_2 at 235 nm, the different signal profiles of the parent and fragment ions indicated a different decay behavior of the fragment ions compared with the parent ion.

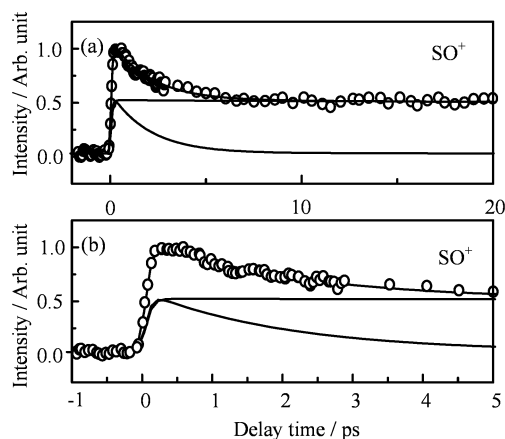


FIG. 3 Time-resolved SO^+ transients at 235 nm pump and 400 nm probe (a) from -2 ps to 20 ps and (b) -1 ps to 5 ps, Experimental data are indicated by circles, whereas the fitting results are shown with solid lines.

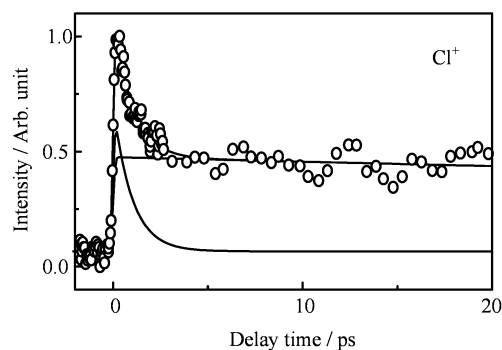


FIG. 4 Time-resolved Cl^+ transients at 235 nm pump and 400 nm probe, Experimental data are indicated by circles, the fitting results are shown with solid lines.

FIG. 2(a) shows that the parent ion signal of SOCl_2^+ decayed in a few hundred femtoseconds after the initial instantaneous rise. The parent ion signal could be fitted by an exponential decay function of 166 fs convoluted with the instrument response function of a Gaussian. Since the time resolved parent ion intensity reflected the excitation and decay processes of the excited states of SOCl_2 , it was acceptable to assign a lifetime constant of 166 fs to the decay dynamics of the initially excited states. Roth *et al.* [33] observed that the photodissociation of SOCl_2 at 235 nm proceeded through two potential-energy surfaces A'' and A' . According to their previous study, the femtosecond pump laser at 235 nm launched a nuclear wave packet on the $3A''$ and $3A'$ surfaces. The repulsive nature of the $3A''$ and $3A'$ states also suggested that the dissociation dynamics may occur rapidly. Thus, the parent time profile observed in our study immediately suggested that the excited states ($3A''$ and $3A'$ states) excited by 235 nm are very short-lived, that is, approximately 166 fs. This conclusion also agrees with the fact that the absorption spectrum in

the $3A''$ and $3A'$ states region was broad and diffuse.

The decay profiles of intermediate SOCl^+ (FIG. 2(b)) were fitted to two decay components with lifetimes of 230 fs and 8.7 ps convoluted with the instrument response function of a Gaussian. These two components indicated that there were two different channels for the production of the SOCl^+ ions. First, we consider the the fast decay time component of 230 fs. This component had a similar trend to the parent SOCl_2^+ ion time profile. It was reasonable to assign this component to the dissociation of the SOCl_2^+ ions after the pump-probe ionization. The parent molecule populated on the $3A''$ and $3A'$ excited states could be ionized to form the parent ion by absorbing the 400 nm probe light. Then dissociation occurred in the parent ion, which generated the fragment ions of SOCl^+ and Cl^+ . The long-time component suggested that a fraction of the SOCl was long-lived. We proposed that the second component of 8.7 ps could be attributed to a stepwise dissociation process. Dissociation could occur on the $3A''$ or $3A'$ surface of SOCl_2 and the neutral fragment SOCl could be easily ionized by absorbing probe photons to form the long lifetime fragment ions of SOCl^+ . Since the SOCl^+ transients reflected the temporal evolution of the SOCl intermediate, the 8.7 ps component was consistent with the decay of hot SOCl produced in the stepwise pathway. This assignment was in agreement with the previous studies, which suggested that the photodissociation of SOCl_2 at 235 nm underwent a stepwise dissociation process and produced the fragment of Cl with quite high quantum yield [34, 35].

The fitting results of the time-resolved SO^+ signals are shown in FIG. 3. The fitting was consistent with our experimental data. The time resolved SO^+ transients could be well-fitted to one rise component of $t_{\text{rise}}=63$ fs and one decay component of $t_{\text{decay}}=2.7$ ps convoluted with the instrument response function. The fast rise time of 63 fs obtained by fitting the SO^+ transients indicated that there was a very fast channel which can produce SO^+ . First, we considered that ion dynamics may be responsible for the femtosecond time scale appearance of SO^+ . Hence, the 63 fs time constant was shorter than that we obtained from the parent ion time profile, so we propose that ion dynamics were not responsible for the 63 fs constant. Another two possible mechanisms, including the molecular elimination channel and concerted three-body photodissociation channel, were considered to account for the 63 fs constant. The molecular elimination channel has been observed in the previous studies [36, 37]. Usually, molecular elimination channel occurs in the ground state with a very high barrier. Therefore, molecular elimination channel is estimated to arise very slowly. Moreover, as far as we know molecular elimination channel has not been observed in previous PTS experiments with more universal detection methods for the photodissociation of SOCl_2 at 235 nm excitation [24]. Therefore, we excluded the possibility of a molecular elimination chan-

nel responsible for the nearly instantaneous rise component of 63 fs. The other possible mechanism for the instantaneous rise component 63 fs was concerted three-body dissociation. This channel involves instantaneous breaking of the two equivalent Cl–S bonds which may be broken by a concerted fashion or in rapid succession within approximately 63 fs. If the initially excited dissociation state surface involved is repulsive along the two-bond dissociation coordinate, the two Cl–S bonds can break instantaneously by a concerted fashion or a rapid succession. In the previous study it was also suggested that concerted three-body dissociation is an important channel for 235 nm excitation [29]. Thus, a concerted three-body dissociation, which involved the almost simultaneous breaking of two Cl–S bonds, was probably responsible for the fast rise of the fragment ion SO^+ in 63 fs. However, it is necessary to explain here that our observation in this study does not distinguish whether the concerted three-body dissociation is a synchronous concerted or asynchronous concerted mechanism. The bond breaking may occur in an asymmetric fashion. It is possible that the dissociating intermediate SO–Cl , is under the influence of the leaving counter fragment Cl, and hence the dynamics of the entire dissociating complex, Cl–SO–Cl , is governed by the three-body potential.

To account for the decay component $t_{\text{decay}}=2.7$ ps, two possible mechanisms were considered. The first was the molecular elimination channel, which we considered above for the fast rise time of 63 fs. As mentioned above, molecular elimination channels were estimated to arise quite slowly. Unfortunately, molecular elimination channel has not been observed in previous PTS experiments with more universal detection methods for the photodissociation of SOCl_2 at 235 nm excitation [24]. We therefore ignored this channel. The second possible mechanism was a cascaded dissociation of hot SOCl produced in the stepwise pathway. However, the time constant was 8.7 ps for the stepwise three-body dissociation pathways, as discussed earlier by the temporal evolution of the SOCl intermediate. The time constant (2.7 ps) was slightly shorter than the value (8.7 ps) obtained from the temporal evolution of SOCl . With regard to the time constant $t_{\text{decay}}=2.7$ ps, a possible explanation was that both the stepwise pathway and ion dynamics possibly contributed to this time constant. This assignment was consistent with FIG. 5, which indicated that the ion dynamics were observed in this study.

The fitting results of the time-resolved Cl^+ signals are shown in FIG. 4. The fitting was consistent with our experimental data. The ion intensity of the Cl fragment could be well-fitted to a biexponential decay function ($t_{\text{decay}}=977$ fs and $t_{\text{decay}}=200.3$ ps) convoluted with the instrument response function. The Cl transients revealed that there were at least two major Cl product components: a “medium Cl component” that decayed in approximately 977 fs and a “slow Cl com-

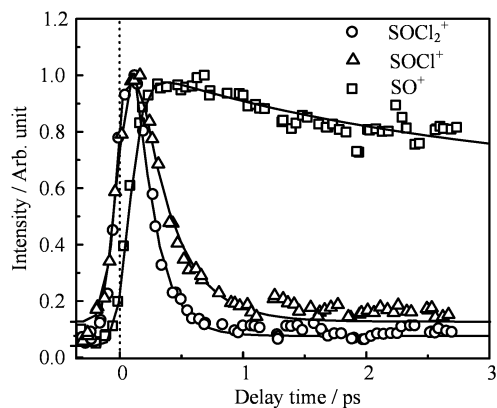


FIG. 5 Time resolved parent ion SOCl_2^+ and fragments ion SOCl^+ and SO^+ intensity.

ponent” that decayed much slower in approximately 200.3 ps. The primary Cl–S direct dissociation process, secondary Cl–S dissociation by stepwise process, and ion dynamics processes all produce Cl^+ ions. Hence, there were a lot of possible processes that could produce the Cl photofragment. Since these are probably very complex dynamic processes, it was difficult to resolve the possible processes only by a curve-fitting of the Cl ion signal. The two components were possibly a combination of the lifetimes of these possible processes.

FIG. 5 shows the time-resolved ion intensity of the parent ion SOCl_2^+ and its fragments SOCl^+ and SO^+ . The most important feature of FIG. 5 was the time shift between the SOCl^+ and SO^+ transients, where the time shift was 125 fs. The lines correspond to the fits of an exponential decay convoluted with a Gaussian that described the instrument response function. Time zero was defined as the pump-probe delay time corresponding to the instantaneous rise of the exponential decay function used to fit the corresponding parent ion transient. We propose that the time shift of ion intensity observed were a reflection of the ion dynamics on the SOCl^+ surface. It is possible if the excited state of SOCl^+ was repulsive or was crossed by a dissociative state in the first few eV. In this case, the excited state underwent a fast dissociation to generate the observed ionic fragment SO^+ . Unfortunately, no time shifts were observed between the parent ion SOCl_2^+ and the fragment ion SOCl^+ intensity, although we even observed SOCl^+ signals from the photodissociation of the SOCl_2 ion. The fs pump laser excited SOCl_2 to an excited state in the spectral region at approximately 235 nm. The initially excited state prepared by 235 nm continues to absorb at least two probe photons of 400 nm to ionize. Since pump probe total energy 11.47 eV was 1.2 eV above the SOCl_2 adiabatic ionization potential (IP) of 10.27 eV. However, it may be possible that the excited state of SOCl_2^+ was repulsive and underwent a very fast dissociation and the fast ion dissociation process was not observed with our experimental resolution.

IV. CONCLUSION

Ultrafast photodissociation of thionyl chloride initiated by the pump pulses of 235 nm has been directly followed with the probe pulses of 400 nm. Upon absorbing one photon of 235 nm, the thionyl chloride molecule were excited to the $3A''$ and $3A'$ states, which decay in 166 fs. In particular, the competition between the concerted three-body dissociation process and the stepwise one has been monitored. The concerted three-body dissociation is determined to approximately 63 fs, whereas the stepwise one was measured to be 8.7 ps. In addition, an ion dissociation process is also observed on the SOCl^+ ion surface after 125 fs. This work demonstrates that the femtosecond time-resolved mass spectroscopy is useful for unraveling complex dissociation reactions.

V. ACKNOWLEDGMENTS

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