II  Beiträge aus den Forschungsgruppen

• Interactions of Oriented Molecules

Effects of Molecular Orientation in Coulomb Explosion of Molecules Induced by Fast Ion Impact

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Abstract

We give an overview of our recent results on multiple ionization and dissociation of simple molecules by fast ions. The coincident measurement of correlated fragment-ion momenta yields information on the dissociation dynamics of highly charged molecular ions. For diatomic molecules the dependence of the cross sections on the alignment of the molecular axis with respect to the projectile beam axis is determined. The results are compared with model calculations.
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I. Introduction

The ion impact-induced multiple ionization and fragmentation of molecules, which is often referred to as a “Coulomb explosion”, is a process of fundamental importance in various areas of science ranging from the physics and chemistry of upper planetary atmospheres to the understanding of radiation damage to biological tissue. In contrast to studies of the molecular break-up by impact of electrons and photons the ion

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impact-induced fragmentation has yet received comparatively little attention. Experiments in which all fragment ions emitted after a particular collision are detected in coincidence provide valuable information about the charge state and potential energy surfaces of the intermediate multiply-charged molecular ion and about the excitation and fragmentation dynamics. Most work so far has concentrated on the observation of individual reaction products without further attention to the correlated behavior of the remaining fragments [1]. Exceptions can be found in dissociation studies of some diatomic molecules where the correlation of both fragments has been studied in detail (see, e.g., refs. [2, 3]) and in the “Coulomb explosion” studies of fast molecular ions penetrating thin foils [4]. This latter work is of particular interest since it allows a kinematically complete study of molecular fragmentation. The molecule under study is passed at high velocities through a thin foil where the outer electrons are stripped off. The fragments from the ensuing Coulomb explosion are detected in a position- and time-sensitive device; thereby the momentum vectors of correlated fragments can be derived. As powerful as it may be, this technique is in practice only applicable to molecular ions with kinetic energies of at least several MeV, and the data analysis is complicated by the complex interactions in the foil.

In collisions of fast ions with molecules the generated molecular ions and their fragments have fairly low energies in the eV region. A typical experiment employs, after the dissociation, an acceleration of the charged reaction products and their detection in a time-of-flight (TOF) spectrometer. In the works to be discussed here we use a time- and position-sensitive detector to establish correlations between low-energy fragments from a particular molecular break-up. It has been shown that coincident measurements with a position- and time-sensitive multiparticle detector provide a complete three-dimensional image of the break-up process for each individual event [5]. In the simplest case of diatomic molecules this means that the dissociation of the highly ionized molecular ions can be studied for a definite orientation of the interatomic axis. One of the advantages of the chosen experimental set-up is thus the possibility to study orientation effects for multiple ionization and fragmentation of molecules.

II. Experimental set-up

Figure 1 shows the principle of the experiment. Collimated beams of H+, He+, O++, and O7+ projectiles interact with a molecular gas target.

H+ and He+ ions were produced at the ion accelerator in Bielefeld; highly charged O7+ ions were provided by the electron cyclotron resonance ion source (ECRIS) of the KVI in Groningen. The slow ions and electrons generated in the collision process are separated by a weak homogeneous electric field perpendicular to the incident ion beam. Electrons are detected in a channeltron (CEM) at one side of the interaction region; positive ions are accelerated towards the position- and time-sensitive multi-particle detector [6] at the other side. The ions pass a field-free time-of-flight region before they hit the detector which is based on micro-channel-plates in combination with an etched crossed-wire structure consisting of independent “wires” in x- and y-direction. The first electron registered in the channeltron serves as a start pulse for the coincidence electronics which mainly consists of a specially developed time-to-digital conversion (TDC) system. Thereby, for each positive fragment the position \((x_i, y_i)\) on the detector and the time-of-flight \(t_i\) relative to the start electron are recorded.

The present set-up allows the simultaneous measurement of all reaction channels resulting in at least one electron and one or more posi-
tive fragments. Thus relative cross sections for the production of selected ions (as $\text{H}_2\text{O}^+$, $\text{H}^+$, or $\text{O}^+$ in collisions with $\text{H}_2\text{O}$) and special processes (like $\text{H}_2\text{O} \rightarrow \text{H}^+ + \text{OH}^+$ and $\text{H}_2\text{O} \rightarrow \text{H}_2^+ + \text{H}^+ + \text{O}^+$) can be obtained [5]; furthermore, if all fragments of a particular break-up process are detected information about the fragmentation dynamics as well as the molecular structure can be derived. Moreover, a study of angular correlations between fragments provides the possibility to investigate orientation effects in the molecular fragmentation. In the following we will concentrate on the two latter applications.

**III. Coulomb fragmentation of $\text{N}_2$**

**A. Kinetic energy spectra**

We studied the multiple ionization and fragmentation of $\text{N}_2$ in collisions with 50-350 kV $\text{H}^+$ and $\text{He}^+$ ions [7]. Besides $\text{N}_2^+$ and $\text{N}_2^{2+}$ we observed $\text{N}^+$, $\text{N}^{2+}$, and $\text{N}^{3+}$ as reaction products. The relative cross sections (especially those for $\text{N}_2^+$) show that for $\text{He}^+$-projectile the influence of electron capture is noticeable up to the energies of 200 keV; in collisions with $\text{H}^+$ it is of minor importance. Among the various reaction channels we concentrate on those leading to coincident pairs of $\text{N}$-ions; these are widely called "Coulomb explosions". For the simplest case the following classification holds:

\[
\begin{align*}
\text{X}^{q+} + \text{N}_2 & \rightarrow \text{X}^{(q-1)+} + \text{N}^+ + \text{N}^+ + 2e \quad \text{double ionization} \\
& \rightarrow \text{X}^{(q-2)+} + \text{N}^+ + \text{N}^+ \quad \text{capture and ionization} \\
& \rightarrow \text{X}^{(q-2)+} + \text{N}^+ + \text{N}^+ \quad \text{double capture}
\end{align*}
\]

Due to the missing start electron only the first and second process are observed. Similar relations hold for the more general case $\text{N}_2 \rightarrow \text{N}^{p+} + \text{N}^{q+}$. The coincidence map in Fig. 2 gives an overview on the two-particle events detected in collisions of 200 keV $\text{He}^+$ with $\text{N}_2$. Due to the internal crossed wire structure of the detector the coincident particles are ordered by their position on the detector; the practically symmetric appearance of the map is caused by the detector symmetry. The processes leading to $\text{N}^+ + \text{N}^+$, $\text{N}^{2+} + \text{N}^+$, $\text{N}^{2+} + \text{N}^{2+}$, $\text{N}^{3+} + \text{N}^+$, and $\text{N}^{3+} + \text{N}^{2+}$ are clearly separated. In case of the fourfold ionization the symmetric charge distribution $\text{N}^{2+} + \text{N}^{2+}$ by far dominates over the asymmetric one in $\text{N}^{3+} + \text{N}^+$.

Fig. 2. Coincidence map of correlated two-fragment events from collisions of 200 keV $\text{He}^+$ on $\text{N}_2$. $T_L$ and $T_R$ are the flight times of the fragments which hit the detector at the right- and leftmost position.

The positions $(x_i, y_i)$ of the correlated fragments and their flight-times $t_i$ are measured for each individual event which allows an absolute determination of the kinetic energy release by the use of classical mechanics [6]. Figure 3 shows the derived energy spectra for the most abundant reaction channels in collisions with 200 keV $\text{He}^+$. These data may be compared to the pure Coulomb explosion (CE) model: in the collision process several valence electrons are removed from the molecule during an interaction time which is short in comparison to the characteristic rotation and vibration periods of the molecule. In this case the
fragmentation dynamics is governed by the strong mutual repulsion of the generated fragment ions, and one might compute the kinetic energy release under the assumption of Coulomb forces between point charges. The dashed lines in Fig. 3 show the energy spectra predicted by this model; their width is mainly caused by the width of the \( \text{N}_2 \) vibration ground-state wavefunction. In contrast to the Coulomb explosion of \( \text{H}_2 \) and \( \text{D}_2 \), which is well described by the CE-model [3, 6], the agreement is comparatively poor in the case of \( \text{N}_2 \). Whereas in case of \( \text{H}_2 \) and \( \text{D}_2 \) only one potential curve describes the final \( \text{H}^+ + \text{H}^+ \) products, there are in general many states of \( (\text{N}_2)^{(p+q)^+} \) which finally result in \( \text{N}^p^+ + \text{N}^q^+ \) fragments with different characteristic energies. This is consistent with the work of Edwards and Wood [8] who studied the reaction \( \text{N}_2^2^+ \rightarrow \text{N}^+ + \text{N}^+ \) in collisions with 1 MeV \( \text{He}^+ \) using a pair of electrostatic analyzers. They postulated three dissociative states of \( \text{N}_2^2^+ \) with characteristic energy releases of 7.8, 10.2, and 14.8 eV to explain their data. In most cases the CE-model overestimates the kinetic energy release. Furthermore, the shape of the energy spectrum shows a distinct dependence on the projectile type which is inconsistent with a point charge CE-model.

Fig. 3. Total kinetic energy distribution of coincident fragment ions from collisions of 200 keV \( \text{He}^+ \) on \( \text{N}_2 \). Dashed lines are the predictions of a point charge Coulomb-explosion model.

**B. Orientation effects in multiple ionization**

In the past decade, significant experimental and theoretical efforts have been devoted to studies of possible molecular orientation effects in fast ion-molecule collisions. Based on the ideas from the pioneering work by Tuan and Gerjuoy [9], the influence of the molecular axis alignment on the electron capture to the projectile ion and on the related processes of transfer ionization and transfer excitation was theoretically studied (see [10] and references therein). For these processes the alignment dependence has been interpreted as an interference effect in electron capture from the two centers of the molecule. When the diatomic molecule is oriented perpendicular to the beam there is a minimum phase difference between the amplitudes describing the scattering of the two centers, resulting in constructive interference. When the angle between the interatomic axis and the beam decreases the phase difference increases and the constructive interference diminishes. Therefore, if charge transfer contributes significantly to the ionization, one can expect predominant ionization of molecules oriented perpendicular to the beam. A strong alignment effect as predicted by theory was later confirmed experimentally in \( \text{O}^n^+ \) transfer ionization collisions with \( \text{D}_2 \) [11, 12]. However, in this experiment as well as in proton collisions with \( \text{H}_2 \) [13, 14] no alignment dependence was revealed in double ionization and ionization-excitation. This result was supported by calculations in the first Born approximation (cited in [15]) which showed that pure ionization of \( \text{H}_2 \) by proton impact shows relatively little (typically 20 \%) alignment dependence. For heavier molecules, a noticeable orientation effect was measured in the double ionization of CO molecules by 96 MeV Ar ions [16]; here also more ionization events were registered when the CO axis was perpendicular to the beam axis.

Very recently another orientation effect was considered theoretically [17] in direct multiple ionization of diatomic molecules by ion impact. Using a very simple two-atom picture and an independent electron model, a significant suppression of the multiple ionization cross section for the perpendicular orientation was predicted as compared to the parallel one, due to the purely geometrical effect of the non-isotropic electron density distribution. To the best of our knowledge, so far there has been only one attempt to measure the alignment dependence of multiple ionization in ion-molecule collisions [18]. The analysis of recoil \( \text{N}^q^+ \) (\( q=1-5 \)) ions, produced by 19 MeV \( \text{F}^{2+} \) beam on an \( \text{N}_2 \) target, revealed that the production of the highest recoil charge states (4 and 5) preferred
molecular alignment along the beam axis. This qualitative result corroborates the above theoretical prediction. However, a quantitative analysis of the data was not performed because of experimental complications.

In our experiment [19] we measured the angular distributions of highly charged molecular fragments in collisions of 100-300 keV He\(^+\) ions with N\(_2\) molecules. The dissociation of a multiply charged diatomic molecular ion results in fragment ions which emerge in opposite directions. In principle, the direction of the molecular axis at the instant of fragmentation could be derived from the velocity vector of one fragment alone if the position of the collision were accurately known. However, since the finite size of the gas target would limit the achievable angular resolution, we utilize the ability of our system to detect both fragment ions in coincidence. In this case a *kinematically complete* image of the molecular break-up can be derived for each individual event; thus, the precise knowledge of the start position is no longer needed and momentum conservation may be used for a consistency check. In the data analysis the direction of the molecular axis was derived from the measured positions and times for each electron-ion-ion coincidence.

Figure 4 shows the measured intensity as a function of the angle θ between the molecular axis and the projectile beam. We present the results for the projectile energy of 200 keV which are representative of similar results obtained for other energies in the interval 100-300 keV. The main contributions to the double ionization of N\(_2\) consist of the symmetric Coulomb fragmentation \((N_2)^{2+} \rightarrow N^+ + N^+\) and the production of (meta-)stable N\(_2^2+\) ions. Only in the case of fragmentation is the orientation of the molecular axis experimentally accessible. The alignment dependence for the triply ionized \((N_2)^{3+}\) was derived from the angular distributions for the reaction \((N_2)^{3+} \rightarrow N^2+ + N^+\); in the case of \((N_2)^{4+}\) there are contributions from the channels \((N_2)^{4+} \rightarrow N^2+ + N^2+\) (≈ 85%) and \((N_2)^{4+} \rightarrow N^3+ + N^+\) (≈ 15%). Fivefold ionized N\(_2\) mainly fragments into N\(_2^3+\) + N\(_2^2+\). The experimental data are presented as histograms of \(dN/d\theta\) versus θ with equally spaced angular bins. When the ionization cross section is independent of the orientation of the molecule, the number of dissociation events with angles between θ and θ + dθ is proportional to sin θ. Our experimental data clearly indicate – at least for four- and fivefold ionization – significant deviations from the sine distribution, i.e. significant alignment effects. The alignment dependence for the highest degree of ionization shows a pronounced minimum at the perpendicular orientation in qualitative agreement with the prediction of the simple geometrical model by Wohrer and Watson [17].

Fig. 4. Alignment dependence for the multiple ionization of N\(_2\) molecules in collisions with 200 keV He\(^+\) ions. Histograms show the experimental results, dashed curves are the theoretical results of the SED-LDA model, and dotted curves show the sine distribution. All of the curves are normalized to have the same area as the experimental histograms, and θ is the angle between the ion beam direction and the molecular axis.
In order to quantitatively interpret the experimental results, an extended version of the statistical energy deposition model (SED) was developed [20, 21]. Based on the original ideas of Russel and Meli [22] and Cocke [23] the SED model implies that the probability of removing an electrons from a system containing N correlated electrons is proportional to the phase-space volume available in a particular ionization state. This probability is directly related to the deposited energy and the ionization potentials of the various levels. It is assumed that the electrons are removed slowly in comparison with the collision time and rapidly in comparison with the nuclear motion in the molecule, a condition which is commonly expected to be fulfilled in the processes discussed. Therefore, multiple ionization is considered for a fixed-in-space molecule.

The deposited energy, i.e. the energy transferred to the electrons of the target, is equal (with negative sign) to the electronic energy loss of the projectile. We treat the energy deposition as a stochastic quantity fluctuating with respect to collision events. A distribution of deposited energies is characterized by its first (mean energy loss) and second (energy straggling) moments. We calculated the mean energy loss and the energy straggling using the well-known local electron density approximation (LDA) of Lindhard and Scharff [24], which has been successfully used for a description of energy loss in ion-atom and ion-molecule collisions. In this approximation every elementary volume of the target molecule is considered as a free electron gas with the density equal to the electronic density, \( \rho (r) \). Then the mean energy loss and energy straggling of a charged particle moving along a straight-line trajectory through the molecule can be calculated using the relevant expressions derived for the electron gas [25, 26] The electronic density of the \( \text{N}_2 \) molecule was calculated in the Hartree-Fock approximation using the MOLPRO computer program [27 28]. A full description of the developed version of the SED model with the energy deposition calculated in the LDA is given elsewhere [20, 21].

The multiple ionization cross sections calculated within the SED-LDA model for \( \text{He}^+ \) ion collisions with \( \text{N}_2 \) molecules at the ion energy of 200 keV are shown in Fig. 5 as a function of the alignment angle. For convenience of comparison the calculated cross sections are divided by the cross section values at \( 0^\circ \). The results presented in Fig. 5 agree qualitatively with those obtained from the simplified model [17]. At small degree of ionization the variation of the cross section with the alignment angle is weak with slight increase at perpendicular orientation of the molecule relative to the beam direction. When several electrons are removed the cross sections have a pronounced minimum at the perpendicular orientation which becomes deeper for higher degrees of ionization.

The origin of this strong orientation effect is the anisotropy of the electron density distribution [17] and the related anisotropy of the energy deposition along a trajectory. For a given ion trajectory the transferred energy and therefore the multiple ionization probability depends crucially on the molecular alignment. In order to remove several electrons large energy deposition is needed. When a diatomic molecule is aligned with the beam the probability of a large energy deposition is greater than for a perpendicular orientation because the projected electron density sampled by the projectile is larger for trajectories close to the molecular axis. More pronounced alignment effects are expected with increasing degree of ionization since for those a larger energy transfer is required.
The calculated cross sections (multiplied by \( \sin \theta \)) are compared with the experimental data in Fig. 4. For higher degrees of ionization \((n = 3-5)\) the theory describes the experimental alignment dependence well. It is interesting that for double ionization of \( \text{N}_2 \) the experimental distribution is peaked at \( 90^\circ \) much more strongly than predicted by theory. One can speculate that this enhancement may be explained by the contribution of transfer ionization, which is not included explicitly in our model. Our estimations show that the interference effect [10] can be very large at least for the dominant electron capture to the 2s, 2p levels of \( \text{He} \). Therefore, the observed maximum at \( 90^\circ \) in the angular distribution for double ionization (and possibly some excess cross section for triple and 4-fold ionization) can probably be explained by the interference effect in the transfer ionization channel. More theoretical work is necessary to clarify this situation.

IV. Complete fragmentation of \( \text{H}_2\text{O} \)

A. Angular distributions of fragments

As an example of a triatomic molecule we discuss the ion-induced ionization and fragmentation of water molecules where we concentrate on the complete Coulomb fragmentations of the following type:

\[
\text{X}^+ + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}^{(q+2)+} + \text{X}^{(p-c)+} + (q + 2 - c) \text{e}^- \\
\rightarrow \text{H}^+ + \text{H}^+ + \text{O}^{q+}
\]

Experimentally these reactions are established as fourfold coincidences between an electron and three positive fragment ions which limits the sensitivity to those cases where at most \( c = q + 1 \) electrons are transferred to the projectile. In collisions with \( \text{H}^+ \) and \( \text{He}^+ \) we observed processes with \( q \leq 2 \) [5]; in collisions with \( \text{O}^{6+} \) and \( \text{O}^{7+} \) even reactions with \( q = 5 \) occurred [29]. In this case the conditions for a kinematically complete description are fulfilled and the fragmentation dynamics may be analyzed in terms of three independent parameters which are derived from the measured velocity vectors. A convenient parameter set consists of the kinetic energy release and two angles in velocity space [5]: the angle \( \theta \), between the two \( \text{O}^{q+}-\text{H}^+ \) relative velocities \( v_{\text{OH}} \), and the angle \( \chi \) between the \( \text{H}^+-\text{H}^+ \) relative velocity \( v_{\text{HH}} \) and the velocity of the \( \text{O}^{q+} \)-ion \( v_0 \).

An important problem concerning the dynamics of multi-fragmentation is the question whether the involved bonds break simultaneously or in a stepwise fashion. In case of \( \text{H}_2\text{O} \) the angle \( \chi \) may be used as an indicator for the time-scale of the molecular break-up: a break-up of both \( \text{OH} \)-bonds in a time short compared to the rotation and vibration periods of the system leads to a strong angular correlation between the corresponding velocities which shows up as a narrow peak in the \( \cos \chi \)-distribution. In case of a two-step process the ‘intact’ \( \text{O}^{(q+1)+} \) subsystem may rotate around its center of mass and the correlation would be lost resulting in a uniform \( \cos \chi \) distribution. In all collision systems studied so far the measured \( \chi \)-spectra are compatible with the assumption of a practically simultaneous bond-breaking in the \( \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{H}^+ + \text{O}^{q+} \) fragmentation [5, 7, 29].

Figure 6 shows measured \( \chi \) spectra for 100 keV \( \text{He}^+ \) and 126 keV \( \text{O}^{7+} \) impact together with a Monte-Carlo simulation of a simultaneous fragmentation into \( \text{H}^+ + \text{H}^+ + \text{O}^q \) based on the MCSCF-calculations described below. The widths of experimental and calculated curves are in reasonable agreement indicating a practically simultaneous bond-breaking in the \( \text{H}_2\text{O}^{3+} \rightarrow \text{H}^+ + \text{H}^+ + \text{O}^q \) fragmentation. A more detailed analysis of the simulation shows that the width of the \( \cos \chi \) distribution is different for each of the considered molecular states (see below) of the intermediate \( \text{H}_2\text{O}^{3+} \) ion; thus, the remaining small deviations may be attributed to neglected states or different transition strengths. The same holds in case of all observed \( \text{H}_2\text{O}^{(q+2)+} \rightarrow \text{H}^+ + \text{H}^+ + \text{O}^{q+} \) processes \( q = 1,2 \) for \( \text{H}^+ \) and \( \text{He}^+ \) impact and \( q = 1 \ldots 5 \) for \( \text{O}^{6+} \) and \( \text{O}^{7+} \) impact at the collision energies studied.

B. Kinetic energy spectra

A simultaneous break-up into positive fragment ions suggests the application of the simple Coulomb explosion model: as a first approximation the kinetic energies and emission angles may be computed by assuming Coulomb forces acting between point charges. In this picture (at least for the short collision times under consideration) the result of the calculation is independent from the details of the ionization process. Figure 7 shows the result of a simulation based on this model in comparison to the measured kinetic energy release in collisions of 250 keV \( \text{He}^+ \) and 92.4 keV \( \text{O}^{6+} \) with \( \text{H}_2\text{O} \). Similar to the \( \text{N}_2 \)-results the CE-model again overestimates the energy release; the width of the distribution caused by
the initial distribution of the ions as given by the H$_2$O vibrational groundstate is smaller than the experimental spectra. Furthermore, the experimental data clearly depend on the projectile type. Several competing processes which all result in three positive fragment ions must be involved to explain this behavior.

To account for the most dominant reaction channels we used the MOLPRO code [27, 28] for an ab initio multi-configuration self-consistent field computation (MCSCF) of the lowest molecular states of the intermediate (H$_2$O)$^{(q+2)+}$ ions. In case of (H$_2$O)$^{3+}$ the nine calculated potential surfaces correspond to the lowest states of the O$^+$-ion having a fully occupied 2$s$-orbital and three electrons in the 2$p$-orbitals. For each of these potential surfaces the resulting total kinetic energy and angular distributions were calculated by Monte-Carlo techniques assuming a Franck-Condon transition from the H$_2$O ground state to the particular dissociating (H$_2$O)$^{(q+2)+}$ state. The derived energy and angular distributions show a distinct dependence on the occupation of the (H$_2$O)$^{(q+2)+}$ orbitals. The position of the maximum of each distribution is marked in Fig. 7. Note that most of these states result in energies which are lower than the energy predicted by the CE-model. A major problem for a quantitative comparison with the experimental data are the unknown transition strengths for the individual states. Since a multi-parameter fit to the data gave ambiguous results we assumed a transition strength proportional to $1/E_i^2$ (with $E_i$ the excitation energy of the corresponding
intermediate H₂O³⁺ state), a scaling behavior which is well known, e.g., in inner shell ionization. Of course a more detailed calculation would be highly desirable. Figure 7 shows the weighted sum of the nine energy distributions convoluted with the response function of the detector. A comparison of the measured energy spectra to the MCSF-prediction shows reasonable agreement. The best agreement is achieved in collisions with highly charged ions: according to the classical over-barrier model excited states are expected to be less important in such “gentle” collisions which is in agreement with the experimental finding.

Conclusion

We have demonstrated that the study of multiple ionization and fragmentation of small molecules by fast ion impact in kinematically complete experiments yields a wealth of information on the dissociation dynamics of highly charged molecular ions. The measured energy distributions of fragments and their directional correlations provide a good test of theoretical models describing the process. In particular, the measured kinetic energy release shows that the often used point-charge Coulomb explosion model is insufficient for a detailed explanation of the data. Apparently the particular electronic states of the intermediate molecular ion play an important role in the dissociation dynamics. The strong orientation effect in multiple ionization of diatomic molecules, observed in our experiments, confirms earlier expectations based on simple geometrical considerations. The developed extended energy deposition model is in good agreement with the observed experimental angular distribution.

Acknowledgements

This work has been supported by the Center for Interdisciplinary Research of Bielefeld University in the research group “Interaction of Oriented Molecules” and in part by the Deutsche Forschungsgemeinschaft (DFG). N.M.K. is grateful to the Center for Interdisciplinary Research of Bielefeld University for its hospitality. We are indebted to Dr. K. Stark and Dr. V.N. Kondratyev for useful discussions and help with the calculations.

References

[27] MOLPRO is an ab initio program written by H.J. Werner and P.J. Knowles with contributions from J. Almlöf, R. Amos, S. Elbert, K. Hampel, W. Meyer, K. Peterson, R. Pitzer, and A. Stone.
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We give an overview of our recent results on multiple ionization and dissociation of simple molecules by fast ions. The coincident measurement of correlated fragment-ion momenta yields information on the dissociation dynamics of highly charged molecular ions. For diatomic molecules the dependence of the cross sections on the alignment of the molecular axis with respect to the projectile beam axis is determined. The results are compared with model calculations.

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I. Introduction

The ion impact-induced multiple ionization and fragmentation of molecules, which is often referred to as a “Coulomb explosion”, is a process of fundamental importance in various areas of science ranging from the physics and chemistry of upper planetary atmospheres to the understanding of radiation damage to biological tissue. In contrast to studies of the molecular break-up by impact of electrons and photons the ion

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