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Femtosecond Laser Induced Ionization/Dissociation of Polyatomic Molecules

TMR Large-Scale Facilities Access Programme

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Femtosecond Laser Induced Ionization/Dissociation of Polyatomic Molecules

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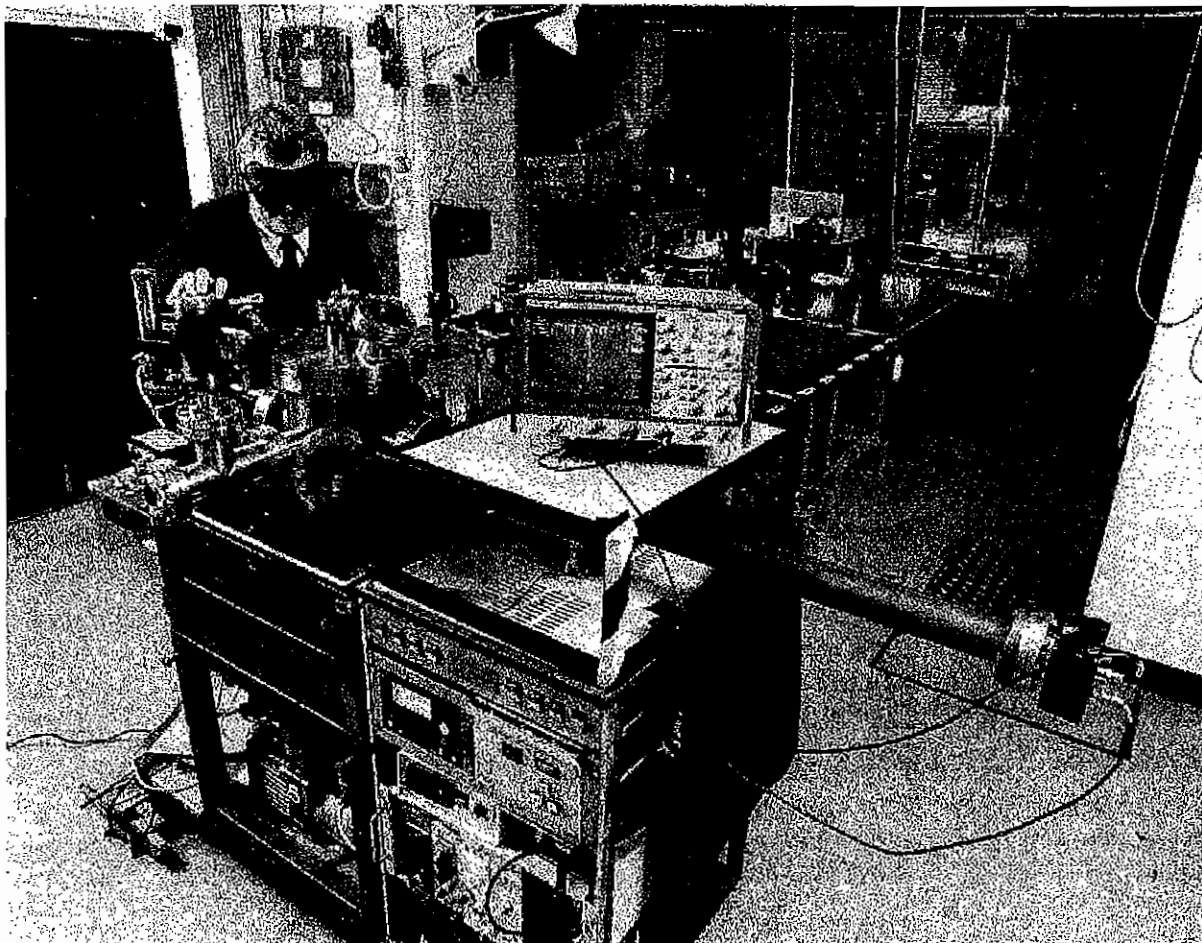
SUMMARY

This report describes the experiment entitled 'Femtosecond Laser Induced Ionization/Dissociation of Bimolecules; carried out at the Central Laser Facility (CLF) from the 6th April to the 4th May 1998. The experiment, funded by the Framework IV Large-Scale Facilities Access Scheme, was proposed by Dr C Kosmidis, Department of Physics, University of Ioannina, Greece and carried out by visiting researchers from the Department. They were supported by researchers from the Department of Physics and Astronomy, University of Glasgow and the Central Laser Facility, Rutherford Appleton Laboratory.

Results Summary

- The Ionisation /Dissociation of a number of polyatomic molecules have been carried out using femtosecond laser pulses at both 390 and 780nm.
- It would appear that at intensities about 10^{15} Wcm⁻² the molecules do not dissociate to any degree but behave more like atoms.
- This phenomenon which we have called femtosecond laser mass spectrometry (FLMS) has enormous potential as an ultra-sensitive molecular analytical procedure. We hope to apply this technique to the detection of biomolecules which is likely to be a burgeoning area in the next few years.
- As the intensity is raised to 10^{16} Wcm⁻² the molecules explode with a coulomb explosion. This was carried out for a number of molecules but it was shown that for CS₂ that the molecules explodes in directions associated with the polarisation of the laser beam.

The CLF makes beam time at its facilities available to European Researchers with funding from DG-XII, CEC under the Large-Scale Facilities Access Scheme. For further information contact Dr. Chris Edwards at the CLF. Tel: (0)1235 445582, e-mail: c.b.edwards@rl.ac.uk



Dr. Ken Ledingham of the University of Glasgow pictured adjusting the Time of Flight mass spectrometer (TOF) equipment.

Femtosecond Laser Induced Ionization/Dissociation of Polyatomic Molecules

INTRODUCTION

It is well known that stepwise multiphoton ionisation and fragmentation of polyatomic molecules like benzene can yield exclusively parent ions at 10^7 Wcm^{-2} using nanosecond laser pulses in the UV (soft ionization). As the intensity is increased to about 10^9 Wcm^{-2} , dissociation increases dramatically until low mass fragments dominate the spectrum with the parent peak often being missing entirely^{1 - 3)}. This process is called ladder switching fragmentation. For ladder switching to occur, fragmentation and subsequent photon absorption from the excited state neutral or parent ion must occur within the laser pulse width. On the other hand if the laser pulse is extremely short then the ladder climbing mechanism should dominate. It has been shown⁴⁾ that dissociation can largely be suppressed using intense (normally IR) laser beams up to 10^{14} Wcm^{-2} with the parent ion often being the strongest peak. This has also been observed recently for aromatic molecules using intense near-infrared radiation^{5, 6)}.

The multiple ionisation of molecules in intense laser fields has become one of the most active areas of current study in atomic and molecular physics. In particular using picosecond and femtosecond lasers with intensities in the range $10^{14-16} \text{ Wcm}^{-2}$, the electric fields generated are no longer small compared to the binding molecular fields of the valence electrons and hence new physical effects are expected. For example for the irradiation of small molecules in intense laser fields, doubly charged parent ions can be detected and higher charged parent ions are present as transient species^{7 - 12)}. A special feature of this intense laser field ionization is multielectron ionization followed by dissociation through coulomb explosion of charged fragments¹³⁾.

Although the understanding of the interaction of intense laser beams with polyatomic molecules is at a preliminary stage⁶⁾, many laboratories are now showing considerable interest. The object of the present work is to demonstrate that a number of polyatomic molecules irradiated by intense laser beams with short laser pulses $<90 \text{ fs}$ and in the

wavelength range 750-790 nm produce multiply charged parent ions and do not fragment appreciably to produce light particles. This was noticed without comment by Cornaggia ⁸⁾ for C₃H₄ and has recently been demonstrated by Smith et al ¹⁴⁾ for benzaldehyde. In this sense the molecules behave more like atoms.

Studies of the angular distributions of CS₂ at intensities on the order of 10¹²-10¹⁴ W/cm² have been previously undertaken ^{15, 16)} with pulse widths of 35 ps, and it was now sought to extend this for intensities of the order 10¹⁵-10¹⁶ W/cm² using pulse widths of 50-100 fs. Sanderson et al ¹⁸⁾ have also recently studied the alignment and bending of CO₂ molecules by intense femtosecond laser pulses at 60 fs and 750 nm. They measured the angular distributions of the CO₂ fragment ions.

Experimental set-up

In the experiments described in this report the details of the apparatus have been described in a number of previous papers ^{14, 18-20)} dealing with one of the applications of this technology, namely femtosecond laser mass spectrometry (FLMS). Suffice it to say that a time of flight mass spectrometer (TOF) was used with unit mass resolution up to 100D. Gases were introduced effusively to the vacuum chamber at pressures up to 10⁻⁵ torr. A laser beam was focussed with a 100 mm mirror into the sensitive volume of the TOF to irradiate the molecular samples.

The TOF system (figure 1) is a conventional linear system, the field-free length being 1.2 m, and an Einzel lens fitted to increase ion extraction. Ions are detected by an electron multiplier connected to a LeCroy 9304 digital oscilloscope.

The laser system used is based on a Spectra Physics Ti:S oscillator pumped by an argon ion laser ²¹⁾. It produces 50 fs pulses at 790 nm, and energy/pulse of 2 mJ, after being stretched, amplified in a 7 mm long Ti:S rod (Crystal Physics), which is pumped by a Nd:YAG (Spectra Physics) laser, before being re-compressed to 50 fs. The repetition rate was 10 Hz. Pulse widths for 750 nm were 50 fs, whilst that for 375 nm were 90 fs.

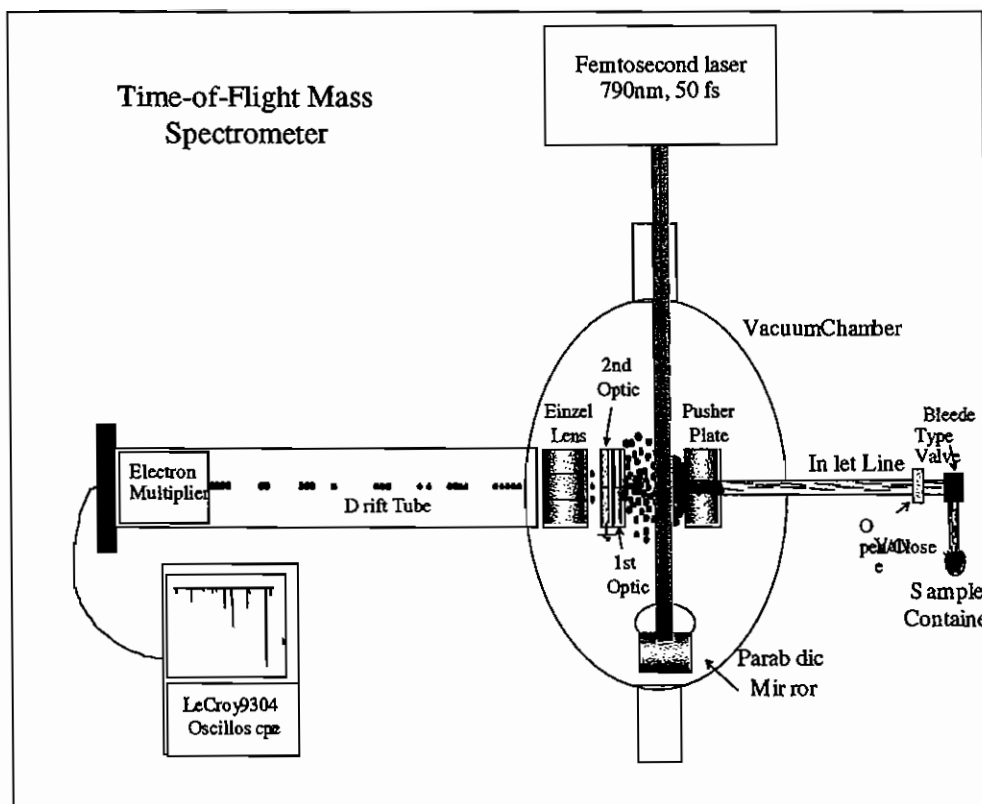


Figure 1. TOF system with effusive gas sample and focused with a mirror to the centre of the ion optics.

1. Investigation of Polyatomic Molecules in Intense Infrared Laser Beams

Figure 2a shows a typical mass spectrum of deuterated benzene (C_6H_5D) with a purity of 98%. The irradiation conditions were $2 \times 10^{15} \text{ Wcm}^{-2}$ at 50 fs and at 790 nm. From previous work done in our laboratory on benzene⁴ at high laser intensities, it was noticed that a strong peak appeared at mass 39 which could be due to the symmetric fragmentation of the parent to $C_3H_3^+$ or the doubly ionised parent mass. With deuterated benzene such an ambiguity was eliminated.

It can be seen that the parent ion mass (79) is by far the strongest peak in the spectrum. The two expanded areas (b,c) correspond to the 3^+ and 2^+ charged parent ion peaks. The 2^+ peak at $m/z=39.5$ is the second strongest peak in the spectrum. This graph has been presented in logarithmic form to show clearly the small peaks between $m/z=36-40$ on either side of the main peak. The 3^+ parent molecule produces an unambiguous peak at $m/z=26.3$. There were impurity peaks at 18(H_2O), 28(N_2) and 32(O_2) but these caused no confusion. To the

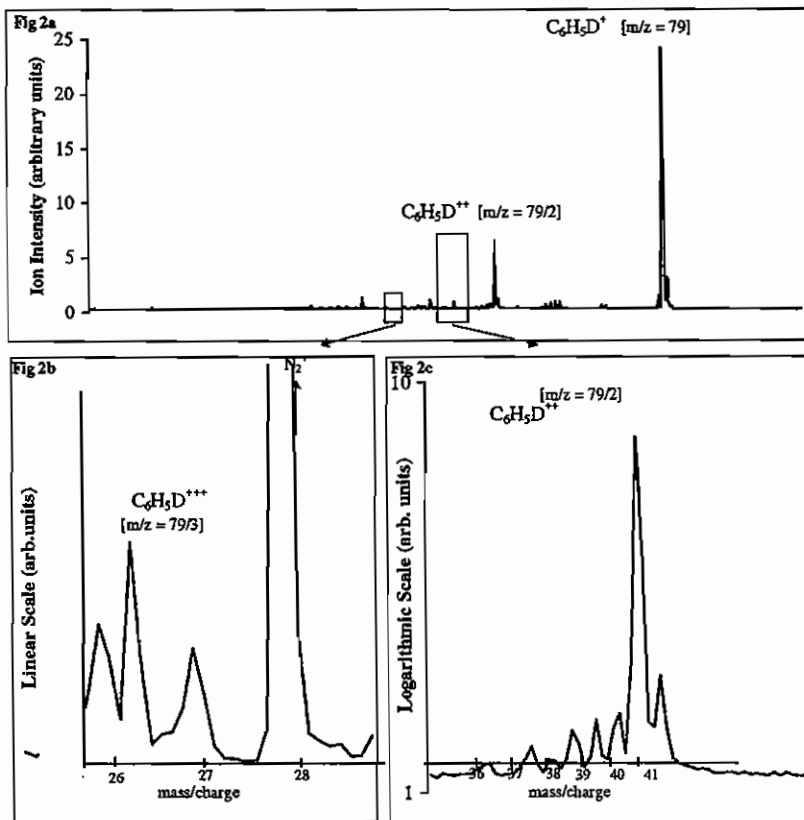


Figure 2. The mass spectrum of deuterated benzene with expanded areas around the 2^+ and 3^+ parent ion. The laser intensity is $2 \times 10^{15} \text{ Wcm}^{-2}$ with a pulse width of 50 fs and a wavelength of 790 nm.

knowledge of the authors, this is the first time that highly ionised parent masses have been observed for medium mass molecules following intense laser irradiation.

It is worth pointing out that the appearance potentials of the 2^+ and 3^+ deuterated benzene are respectively 26 and 44 eV²²⁾ and that the appearance potential for C^+ in the fragmentation of benzene using a UV ns laser is also about 26 eV¹⁾. The fact that the 2^+ parent ion peak was at least an order of magnitude larger than the carbon ion suggests that the normal fragmentation routes for ns irradiation were being bypassed in the fs irradiations. To return to the double ionised spectrum in figure 1c, the small peaks on either side of the main peak also deserve comment. First of all there are two half mass peaks at 37.5 and 38.5. These correspond to $C_6H_3^{2+}$ and $C_6H_3D^{2+}$ respectively and the peak at mass 40 is due principally to the ion $C_5^{13}CH_5D^{2+}$. This also has the correct carbon isotope ratio for a molecule which contains six carbon atoms (7%). Thus the peaks at mass 38 and 39 are also likely to have a substantial doubly

ionised component. The envelope of doubly ionised peaks every half mass corresponding to the parent molecule (M) and a number of (M-nH) satellites seems to be characteristic of polyatomic hydrocarbon molecules when irradiated in the infrared at the high laser intensities $10^{14-15} \text{ W cm}^{-2}$ and the other hydrocarbon molecules presented in this paper all show this doubly ionised cation group. This can always be distinguished from fragments by the small half mass peak at $(M-13)^{13}\text{C}^{2+}$ which must have the correct isotopic ratio. There was little evidence of multiply charged carbon atoms which is characteristic of coulomb explosion for lighter molecules ¹³).

The intensities of the 1^+ , 2^+ and 3^+ parent peaks as well as some of the larger fragments from deuterated benzene are shown as a function of laser intensity in figure 3 at 790 nm and 50 fs pulse width. It would appear that the C_4H_5 and C_5H_4 ion peaks follow the intensity dependence of the parent ion while the 2^+ and 3^+ parent ion peaks have a stronger laser intensity dependence.

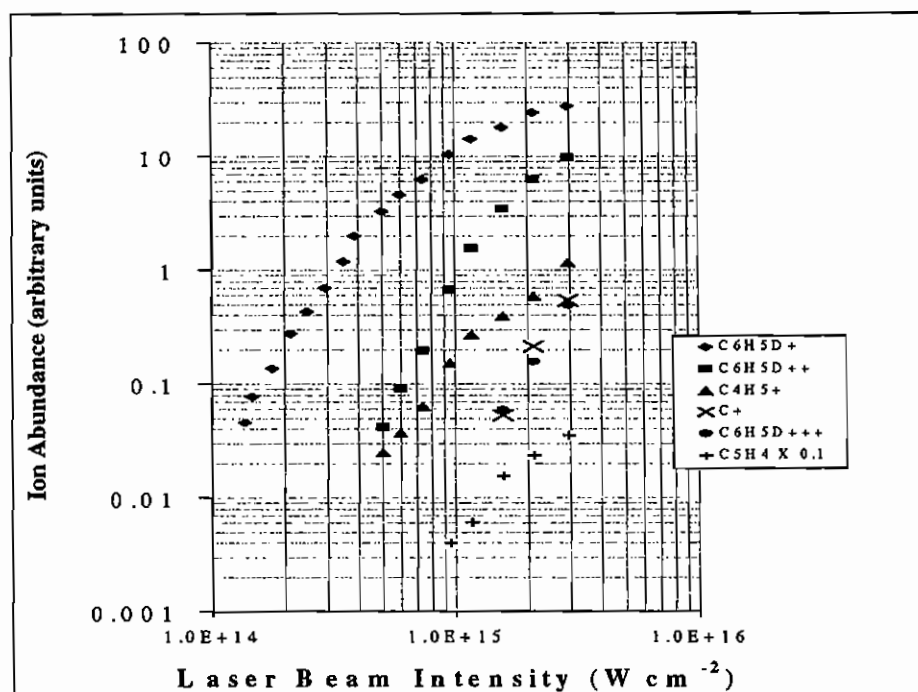


Figure 3. The ion abundances of a number of fragments and multiple charged species from deuterated benzene as a function of laser intensity under the laser conditions mentioned in figure 1. The gradients of the 2^+ and 3^+ ion curves are steeper than the others.

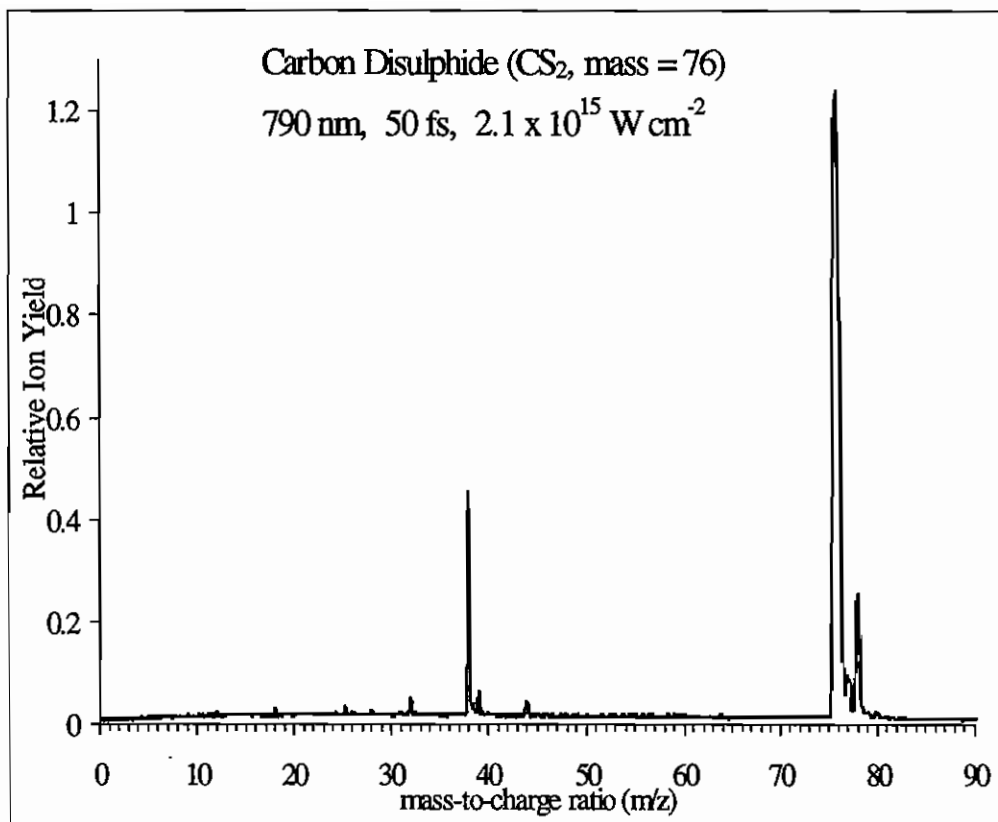


Figure 4. The mass spectrum of the linear molecule CS₂ with the single, double and triple ionised peaks visible. The laser conditions are similar to those described in figure 1.

It can be seen in the inset diagram that the ratio of the 1⁺ to 2⁺ charged peaks is a strong function of the laser intensity. The value at 10¹⁵ Wcm⁻² is close to the 1⁺ to 2⁺ ion ratio for atomic Xenon at similar laser intensities which was carried out under identical experimental conditions to the molecular work.

Figure 4 shows the mass spectrum of the linear molecule CS₂ at a laser intensity of 10¹⁵ Wcm⁻² for 790 nm and 50 fs. The appearance potentials of CS₂²⁺ and CS₂³⁺ are 27.5 and 53.6 eV respectively ²³⁾. This spectrum looks very similar to that of deuterated benzene with the 1⁺ and 2⁺ peaks being by far the strongest components and also an unambiguous CS₂³⁺ signature being visible. Any other fragmentation is very small. There was however evidence for coulomb explosion in this molecule since small peaks of multiply charged C and S were present.

Finally in figure 5 the mass spectra of a number of different molecules are shown at various intensities in the IR for pulse widths less than 90 fs. For all the molecules presented here, the

1^+ and 2^+ ion peaks are the dominant entities and any other fragmentation is small. The spectrum for Xenon is also presented. A general theme from the present work seems to be emerging. For laser intensities in the infrared at intensities in the range 5×10^{13} - 10^{15} Wcm^{-2} the fragmentation for the molecules described in this paper is small. Multiply charged ions are evident up to 3^+ and for the hydrocarbon molecules, an envelope of 2^+ ions of (M-nH) entities is visible. Exceptionally the 3^+ ion for toluene was not seen. The characteristic envelope of 2^+ ions for the hydrocarbon molecules had intensity thresholds $> 5 \times 10^{13}$ Wcm^{-2} . The low degree of fragmentation observed in the present work is in agreement with the studies of DeWitt *et al* on aromatic molecules. These authors did not observe multiple charging in their spectra and this is also in accord with the present work since their maximum laser intensity was about 4×10^{13} Wcm^{-2} , marginally lower than the thresholds mentioned above.

Conclusions

Under the intense laser irradiation reported in this letter, the polyatomic molecules which have been studied, show remarkable stability and electronic dynamics similar to that in atoms. Clearly ladder switching fragmentation of the type reported for ns pulses¹⁻³⁾ is not taking place to any great degree.

The simplest model of the molecular behaviour in the strong IR laser fields observed in the present experiment is as follows. The molecules reach the 1^+ ion level by multiphoton processes during the rise time of the pulse. They then absorb more photons sequentially and reach the 2^+ and 3^+ levels either by tunnelling ionization or by barrier suppression¹³⁾. This was the sequential mechanism proposed by Lambropoulos²⁴⁾ for multiple ionization of atoms by intense pulsed lasers. His calculations showed that multiply charged ions are only produced for laser intensities approaching 10^{14} Wcm^{-2} . For sequential ionization, a charge state can be produced only after the previous charge state begins to volume saturate²⁵⁾. This would certainly describe the data in figure 3 where the onset of the 2^+ signal coincides with the flattening off of the parent ion intensity. It is thought that much of the intensity of the single ionization peak comes from the lower intensity wings of the laser beam.

Coulomb explosion ionization is a possible mechanism for CS_2 since the multiply charged atoms of C and S are observed although at low intensities. No similar evidence for coulomb

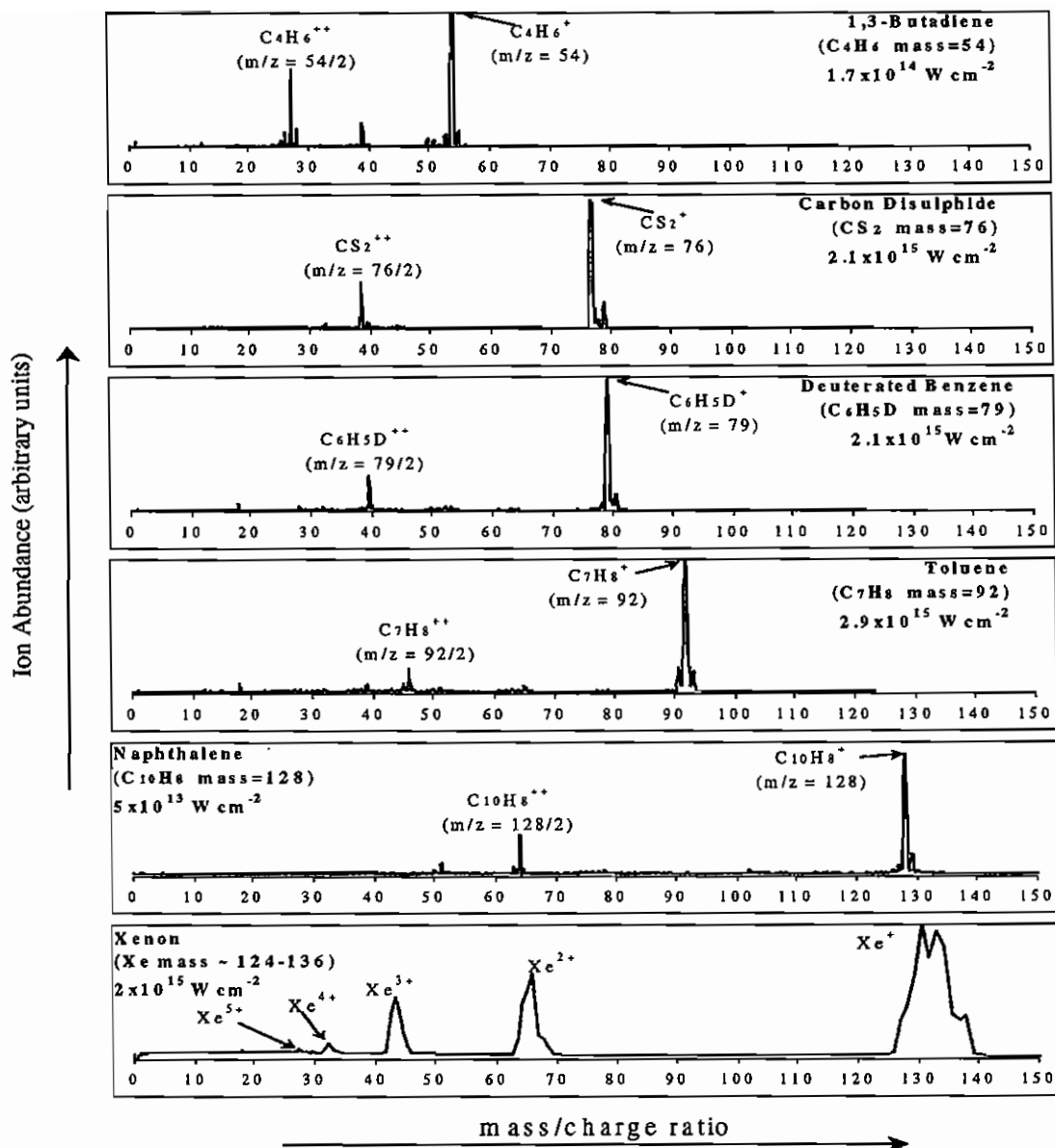


Figure 5. Mass spectra of polyatomic molecules. Laser conditions $5 \times 10^{13} \text{ W cm}^{-2}$ to $2 \times 10^{15} \text{ W cm}^{-2}$. The wavelength range is 750 -790 nm , pulse width 50-90 fs. This is compared with the Xe spectrum taken at the same intensity. The 1^+ and 2^+ charged parent peaks are the principle entities and any fragmentation is very small. This behaviour is similar to that of the inert atoms.

explosion is evident for the hydrocarbon molecules studied here. However an envelope of 2^+ cations is observed for these molecules and this shedding of hydrogen atoms at the 2^+ level or a mixture of charged and uncharged hydrogen atoms from the 3^+ level is a striking characteristic of this intensity regime.

Conventional coulomb explosion is unlikely to explain the present observations. For light molecules, multiply charged ions which lead to coulomb explosion are only transient

species ¹³⁾ while in the present work, the 2⁺ and 3⁺ parent ions have lifetimes at least of the order of the flight time in the TOF (about tens of μ secs). Any dissociation, particularly the shedding of hydrogen atoms, seems to be a rather gentle process similar to ordinary photodissociation after excitation to a predissociating electronic state. Newton has claimed that multiple ionisation is favoured for molecules which have sufficient numbers of nonbonding or delocalised electrons ²³⁾.

2. Dissociative Ionization and Angular Distributions of CS₂ using ultra intense laser beams

A typical mass spectrum of CS₂ at 375nm is shown, (figure 6). It can be seen that there is considerable fragmentation, as the parent ion is not the dominant peak, even at these short pulse widths (fragmentation was pronounced at ns time-scales, but reduced for fs studies ²⁶⁾). It was noted that the intensities are not the same for horizontal and vertical polarization, a consequence of the molecular alignment. The S⁺ peak is the most pronounced in both polarisations. It is also possible that post dissociative ionization could occur for some fragments, although it may be a weak process given the short pulse durations.

The dominant peaks for the horizontal case are: CS₂⁺, CS⁺, S²⁺, and C⁺, all of approximately equal intensity. There are also S³⁺ and S⁴⁺ peaks present. Other dominant peaks in the vertical spectra are: C⁺, CS₂⁺, and CS⁺, in decreasing order and a significant C²⁺ peak, as well as a S²⁺, CS²⁺, S³⁺, and a tentative CS₂³⁺ peak. The different sulphur isotopes are present with the correct isotopic abundances. For both polarizations, at 375 nm, it has been observed that there is a sizeable S₂⁺ peak occurring at m/z=64. This may come about, by transitions to states with bent geometrical configurations, (which cannot be as easily accessed at 750 nm).

Typical mass spectra for 750 nm, relative to that for 375 nm, have less pronounced fragmentation. The parent ion is dominant for both polarization orientations. The strongest fragment ions present in the vertical case are: CS⁺, CS₂²⁺, S⁺, and C⁺ ions. There are also smaller CS²⁺, S²⁺, and C²⁺ ion peaks. In the horizontal spectra, there are: CS⁺, CS₂²⁺, S⁺, S²⁺, and C⁺ primary fragment ions, with smaller CS²⁺, S³⁺, and C²⁺ ions present.

CS₂ is believed to be linear under 750 nm irradiation, due to the near absence of any peak at $m/z = 64$, i.e., S₂⁺. This moiety is thought to be produced when CS₂ has a bent structure, and thus the 2 peripheral S-atoms are sufficiently close to bond with each other, and break from the C-atom. The lack of the S₂⁺ ion is consistent with the idea that no bent geometrical states of the CS₂ molecule, or its ion, can be excited above 532 nm, and also the observation of Mathur et al. ³⁾, who noticed that no S₂⁺ ions were produced when irradiated by 532 nm, 35 ps pulses.

Angular distributions for S²⁺, and C²⁺ are presented, (figures 7-8). It has been seen that all fragments are anisotropic, even the C-atom at 790 nm, where an isotropic distribution would be expected from this 'stationary' central atom. The C-distributions are, however, perpendicular to the polarization-vector, for 395 and 790 nm. Bhardwaj et al. ²⁷⁾, when considering bent triatomics such as NO₂, explain the perpendicular NO distribution by the directional components of the induced dipole moment of NO₂, whose parallel component is bigger than the orthogonal component, even for small fields, produced in the rising-edge of the pulse. In linear triatomics the fragments should all align along the field direction. The CS and the CS₂ distributions are essentially isotropic.

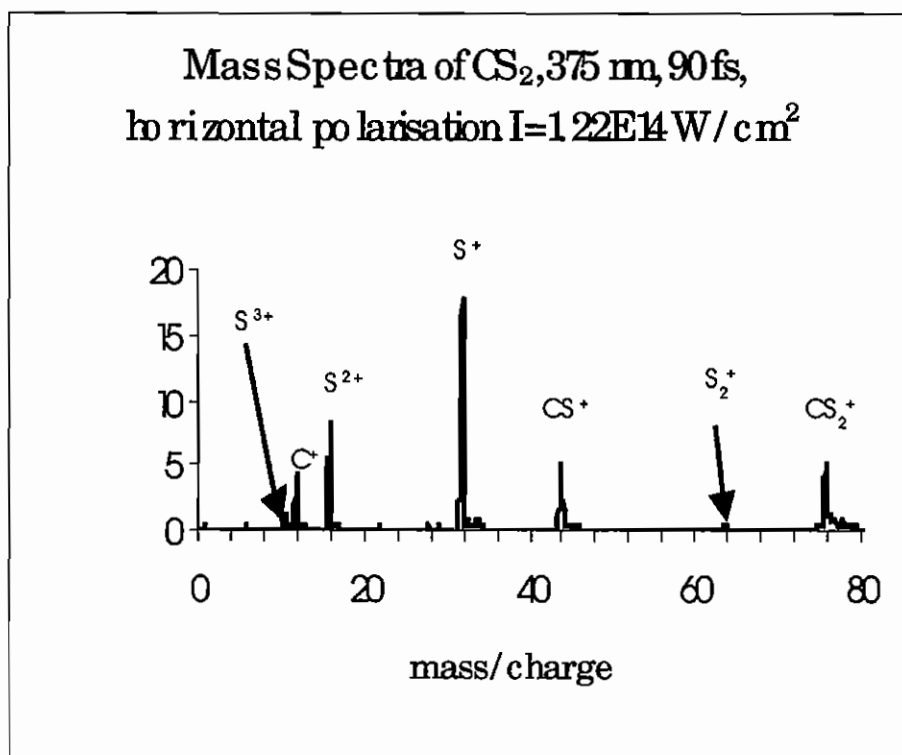


Figure 6. Mass spectra at 375 nm showing a number of multiply charged S ions. The fragmentation at 750 nm is considerably reduced

Since the majority of carbon ions can be detected at angles orthogonal to the axis of polarization, this presents a way of distinguishing the fragments coming from the explosive dissociative ionization of CS₂.

Finally, angular distributions were carried out for up to C³⁺ and S⁵⁺, possible with the higher intensities used. It was noticed that they were narrower for each successive charge-state, illustrating that the degree of alignment is stronger, as the electric field needed to produce the higher charge states will cause more of an alignment, and also due to the higher polarization value of the ions. The results are at variance with earlier distributions of CS₂ ions obtained by Kumar et al, using 35 ps¹⁵⁾ and this discrepancy is at present being studied extensively.

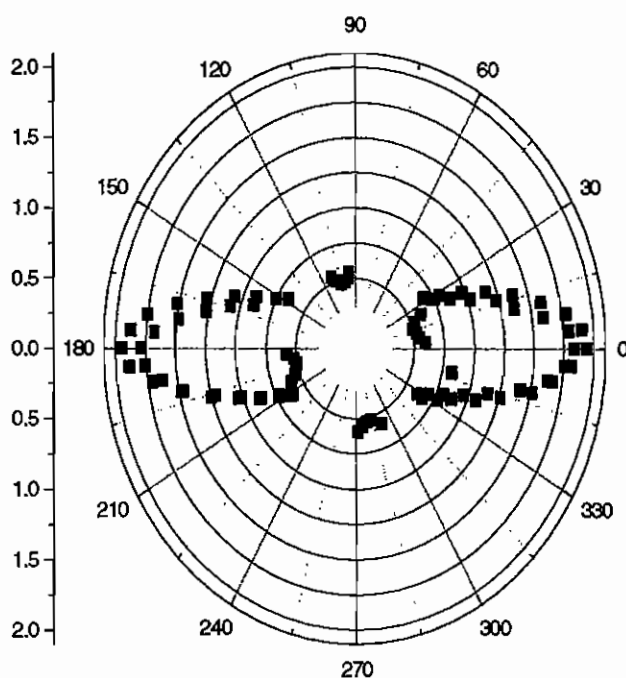


Figure 7. S²⁺ Distribution and all other Sⁿ⁺ distributions are similar.
The angular distributions of all the S ions are directed along the direction of polarisation of the laser.

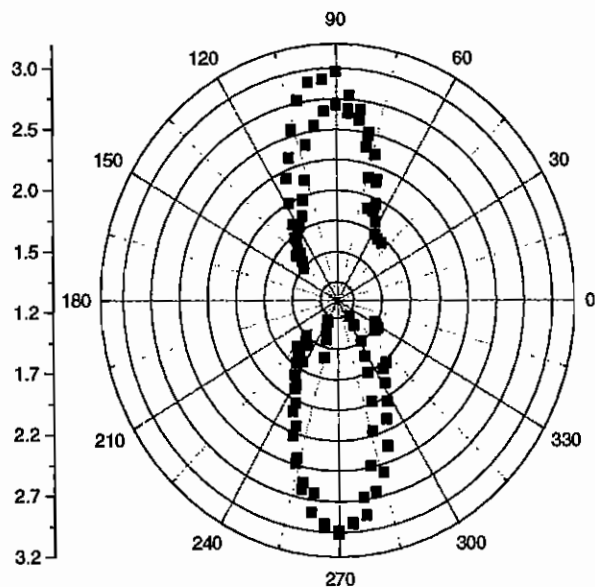


Figure 8. C^{2+} Distribution and all other C^{n+} distributions. It can be seen that the carbon ions unlike S ions, are distributed in a direction at right angles to the laser polarisation.

Conclusions

The results herein support the view that one charge-state starts when the previous one has saturated. Increasing the laser intensity merely increases the volume of production of an ion. Angular distributions were worked out by varying the polarization direction. It is noted that higher charge state ions have narrower distributions, as expected, and the results indicate alignment of the molecule. Finally, mass spectra were obtained at 375/395 nm and 750/790 nm, and fragmentation was found to be relatively increased at the shorter wavelength. This has also been observed for C_7H_6O ²⁸⁾, and C_4H_6 ²⁹⁾.

Production of the S_2^+ ion, indicative of exciting the parent to states with a bent geometrical structure, was also increased at 375 nm. For certain conditions at 790 nm, it was found that the ionization behaved very atomic-like, i.e., little fragmentation and multiple-charged parent ions³⁰⁾. This phenomenon has also been observed for both CH_3I , and 1-3 Butadiene²⁹⁾.

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