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Advances and challenges in electron–molecule scattering physics—A Report of the 14th International Symposium on Electron–Molecule Collisions and Swarms

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Abstract
A report is presented of the 13th International Symposium on Electron–Molecule Collisions Physics (Instituto de Fisica, Unicamp, Campinas, Brazil, 27–30 July 2005). This workshop covered low-energy electron interactions with atoms, molecules and condensed matter systems. Several important aspects of this symposium were to bring together theory and experimental advances in this field for gaseous targets as well as showcasing the increasing diversity of electron–molecule collision applications in condensed matter and biological applications. A summary session was held wherein were discussed aspects of the future of the field, including the development of new theoretical and experimental capabilities.

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1. Introduction

This international electron–molecule workshop is traditionally held in conjunction with the biennial International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC). ICPEAC XXIV was held for the first time in South America in Rosario, Argentina. Consequently, the 2005 conference was held in South America, Brazil in the beautiful campus of the Universidade Estadual of Campinas, with Professor Marco A P Lima as the organizing Chair [1]. This conference has a long history of common interest with both electron and positron (lepton) physics, but the Campinas meeting was the first to be held in parallel with the co-located ICPEAC satellite on Low-energy Positron and Positronium Physics (Positron-05). The electron–molecule workshop had 20 invited talks, lively outdoor (!) poster sessions and 70 registered participants. A slightly smaller number of participants were registered for Positron-05, with whom the workshop shared a programme of five plenary lectures. The workshop ended with a panel discussion on opportunities and challenges in electron–molecule scattering chaired by V McKoy (Caltech).

Topics covered at the Workshop included elastic electron-scattering, vibrational excitation (VE) of molecules by slow electrons, inelastic electron scattering from molecules, electron-attachment with molecules; new developments in electron scattering theory, experiments and facilities were also discussed. A keen topic of discussion was the selective dissociative electron attachment (DEA) to large molecules, which is of great interest because it has important ramifications for the breakup of biological molecules such as DNA and for the use of polyatomic gases in plasma processing. The CAMOP contributions by the type of processes investigated are addressed below, remembering that it is important to understand electron scattering processes from small (diatomic, triatomic) molecules before such

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processes in polyatomics such as amino acids, sugars, DNA and other biologically relevant compounds can be fully and accurately understood. We first address progress in experimental and theoretical methods, which are needed to produce accurate data (cross-sections and rates) for electron scattering processes.

2. Experimental methods

New experimental methods of significance included:

(1) The use of the magnetic angle changer (MAC) developed by the Manchester group [2, 3] and applied recently for elastic scattering from N_2 by Allan [4] for and from NO, CO_2, CH_4 and H_2O, reported at this meeting by S J Buckman (from the Australian National University, ANU) [5].

(2) The laser-trapped source of He(2^3S) metastables signifies an important application of optical molasses to the production of dense targets of excited metastable atoms [6], likely to be used to generate excited molecular targets in the future. The production of high resolution (sub-meV) electron beams, using a laser photoionization electron source on potassium were reported by H Hotop (Kaiserslautern) [7, 8]. These were used to investigate the low-energy electron attachment to molecular targets.

(3) The COLd Target Recoil Ion Momentum Spectroscopy (COLTRIMS) [9] method is also an important development which will be applied to electron impact fragmentation–ionization of molecules. Here, a contributed paper was given by A Dorn (Max-Planck Institut fur Kernphysik, Heidelberg, Germany, at CAMOP 2005, Campinas, Brazil (see [1])) and co-workers on a new apparatus developed using a pulsed electron beam and detectors with central bores to allow the passage of the primary electron beam.

(4) An innovative moveable target source method has been developed to enable the accurate removal of backgrounds in electron-gas target scattering experiments for both discrete features and continuum features [10]. This has been applied towards differential cross-section (DCS) measurements of electron impact excitation of molecular nitrogen [11].

(5) Finally, the development of a time-of-flight electron scattering experiment based on the work of Le Clair *et al* [12] was reported by Buckman (Atomic and Molecular Physics Laboratories, Australian National University, Canberra 0200, Australia, at CAMOP 2005, Campinas, Brazil (see [1])). In this instrument, the effect of focusing fields is reduced since no field gradients are used to determine the electron energies. Hence, the detection efficiency of scattered electrons is independent of their kinetic energy. This would allow for the measurement of very accurate differential (in energy and angle) scattering cross-sections. The new apparatus will be a significant improvement over that of Le Clair *et al* [12] since the source of electrons will be an energy-selected beam with a resolution of a few 10 s of meV, compared to the earlier unselected electron beam which had a 0.5–0.7 eV resolution. Also, the new apparatus will be moveable in angle and consequently map very low-energy differential cross-sections for electron attachment to molecules, and be able to make significant contributions to quantitative differential cross-section measurements.

3. Theoretical methods

A number of new theoretical approaches were described:

P Kolorenc (Charles University Prague) presented a method using a Feshbach–Fano *R*-matrix approach. The method [13] allows the calculation of the discrete state and the coupling for solution of resonance nuclear dynamics in diatomics. The strategy presented yields an efficient and computationally simple way of Feshbach–Fano partitioning the Hilbert space into the resonance and background components. Results for DEA to Cl_2 molecules and VE by electron impact were shown to be in good agreement with experiments [14].

C S Trevisan (University of California Davis) presented vibrationally resolved cross-sections for the open shell molecule, NO, and its isoelectronic neutral radical CF [15]. For these systems, they followed the successful strategy applied to the resonant process in e^-–CO_2 scattering based on the local (boomerang) and nonlocal potential models inputted with scattering data obtained with the Complex Kohn Method. J Tennyson (University College London) described the new Molecular *R*-Matrix with PseudoStates (MRMPS) method [16, 17] which extends low-energy techniques into the intermediate energy regime. MRMPS calculations can thus give *ab initio* near-threshold electron impact ionization cross-sections and treat processes such as electron impact electronic excitation above the ionization threshold. C Winstead (Caltech) presented a highly computationally scalable implementation of the Schwinger Multichannel Method and associated calculations on elastic e^-–C_2H_4 scattering [18] at the static-exchange-plus-polarization level and elastic scattering at the static exchange level for e^-–uracil scattering.

These three methods, *R*-Matrix, Complex Kohn, and the Schwinger Multichannel, under development since the early 1980 s, give computational strategies capable of dealing with electronic excitation of molecules by electron impact. They all work based on the following common steps: (i) define the target description using either a Hartree–Fock approximation or configuration-interaction technique. For this step, they all need to establish a single particle basis set (Cartesian Gaussian Functions or Slater type of orbitals) and obtain a good description of the ground and electronic excited states, besides good polarizabilities of the target; (ii) define the level of the multichannel coupling that will be taken into account. Usually, the molecular spectra is so dense that a judicious choice is necessary to define which states will be considered in the calculation (only calculations near to the lowest thresholds can take into account all open channels generated by a particular single particle basis set); (iii) define the single particle scattering basis set that combined with the electronic open and closed channel eigenfunctions will form the configuration space that will be used to solve the scattering problem. Each method employs a different formalism for solving the Schrödinger equation with the proper scattering boundary conditions, but they are all equivalent. Unfortunately, as discussed in the panel section of the meeting, theoretical agreement among applications of these methods for electronic excitation cross-sections by electron impact, even for simple systems like H_2, remains rare [19]. So, although good theoretical progress was evident at the conference, there remains a clear need for benchmark calculations which consider different levels of multichannel coupling.

4. Electron scattering from diatomic targets

Targets such as H_2, CO, NO, N_2, O_2 are of significance due to their role in atmospheric and astrophysical applications. Theoretical and experimental studies of electron scattering from N_2 were presented for elastic and VE at very low energies between 0.8 and 5 eV for all scattering angles, see figure 1. This is the first measurement of inelastic electron–molecule scattering using the MAC [4] to yield direct energy loss spectra, which yielded detailed results for angular distributions at low-energy elastic scattering. The results show good agreement with the earlier results of Sun *et al* [20] and reasonable agreement with the distributed spherical Gaussian calculations of Feng *et al* [21] for elastic scattering at low energies. However, for inelastic VE, the theory differs with the experiment for scattering angles below 60° even at low incident energies. The low incident electron energies provided by this work probes a very important regime of electron scattering, where resonances play an important role.

Additional electron impact excitation differential cross-sections for the A $^3\Sigma_u^+$, $B^3\Pi_g$, W $^3\Delta_u$, B′ $^3\Sigma_u^-$, a′ $^1\Sigma_u^-$, a $^1\Pi_g$, w $^1\Delta_u$ and C $^3\Pi_u$ states of N_2 were measured by Khakoo *et al* [11] for a large range of incident electron energies and scattering angles. Comparison of the earlier measurements of Cartwright *et al* [22] and Brunger and Teubner [23] showed mixed results. While the recent measurements in [11] used most recent time-of-flight cross-sections from [12], applied the moveable source method [10] and checks on the use of reliable Franck–Condon factors in the unfolding routine were made, this disagreement is to some extent surprising. Excellent qualitative agreement with the results of Zetner and Trajmar[4] [24] at 15 eV provides a positive affirmation of the recent measurements. Comparison of the *R*-Matrix calculations of Gillan *et al* [25] shows poor agreement and illustrates a general difficulty in performing reliable calculations of electron impact excitation differential cross-sections. These transitions play a significant role in atmospheric dynamics and because of the abundance of N_2 in the terrestrial atmosphere, it is important to understand these excitations from a theoretical viewpoint. For a comprehensive recent review of electron scattering from diatomic targets and small polyatomic targets, see [26].

The theoretical work on electron scattering from NO and the isoelectronic CF radical was discussed by Trevisan *et al* [27]. Reliable *ab initio* calculations are difficult at low-energy where the negative ion resonances dominate and require careful treatment of both the electron and nuclear dynamics. Trevisan *et al* [27] employed a nonlocal treatment of the nuclear dynamics, to remedy the principal deficiencies of the more usual local complex potential model. The resulting low-energy cross-sections are dominated by shape resonance contributions associated with the $^3\Sigma^-$, $^1\Delta$ and, to a lesser extent, $^3\Sigma^+$ states of NO and display pronounced, overlapping boomerang structures that give irregularly shaped VE cross-sections. Although agreement between experiments [28, 29] needs some improvement, in this difficult regime, the theory coupled with the experimental data sheds considerable light on the symmetry of the resonance structures and also on the shapes of the parent anion of the resonances, see figure 2. Similar structures to NO were found for CF, but the calculations require improvements for NO before the CF results can be validated.

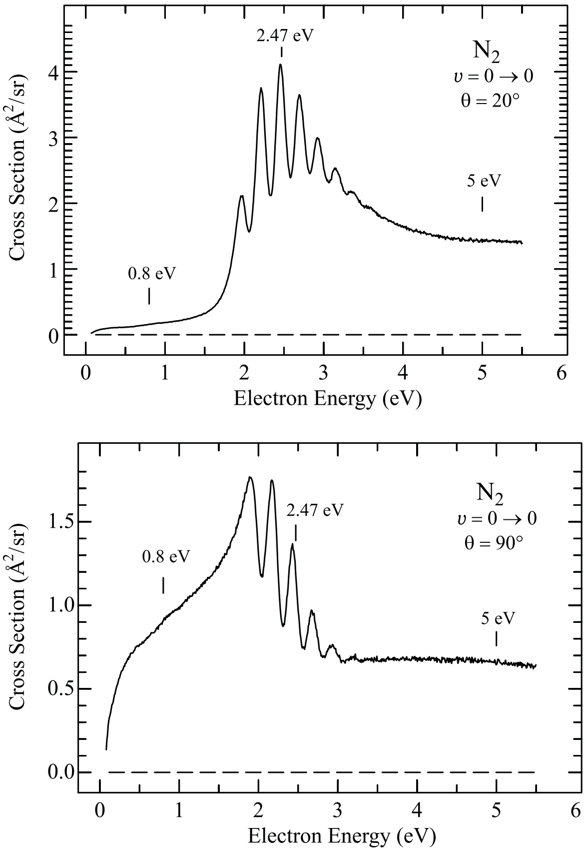

Figure 1. Rotationally summed differential scattering cross-section for elastic electron scattering from N_2 (Allan [4]) taken at scattering angles of 20° and 90° plotted as a function of incident electron energy.

5. Electron scattering from polyatomic targets

There has been a surge in this field recently owing to the pioneering work of Sanche [30] regarding the electron-driven damage in biomolecules. Previously it was thought that x-rays were directly responsible for breakup of DNA in tissue. The work of Sanche showed that the x-rays produced slow secondary electrons which through DEA to the tissue DNA were responsible for breakup of the DNA and hence an important process in radiobiology. However, before the x-ray photoionized secondary electrons can attach to the DNA, other scattering processes (elastic, inelastic, etc)

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[4] Data tabulated in [26].

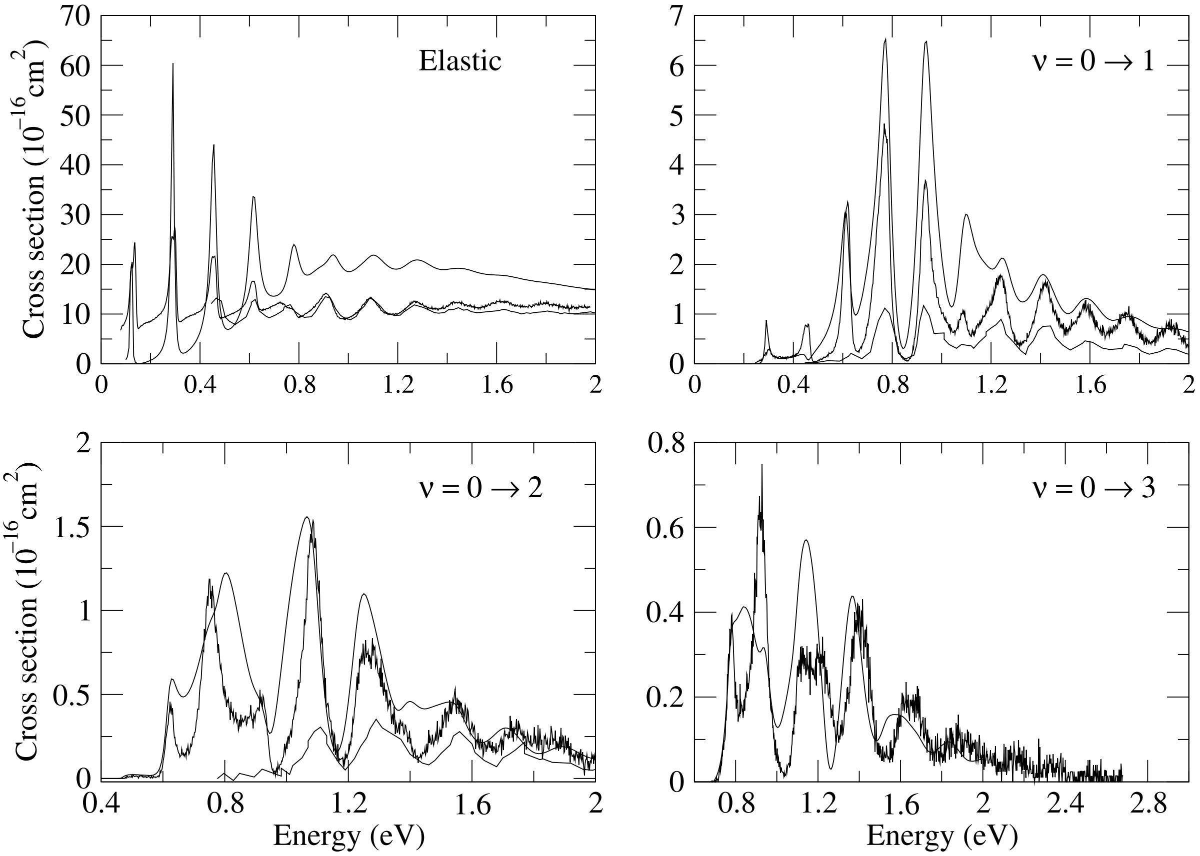

Figure 2. Comparison of theory and experiment electron-NO: elastic and VE cross-sections. Solid dark curves: calculations of Trevisan *et al* [27]; solid grey curves: measurements of Allan multiplied by 4π [28]; dashed curves: measurements of Jelisavcic *et al* [29].

take place which moderate these x-ray photoelectrons. In an effort to understand these processes via modelling, reliable theoretical models of electron scattering from polyatomic targets must be available. In turn, these theoretical models require experimental data to check them.

6. Electron scattering from small polyatomics

The most important triatomic molecule is H_2O, due to its biological and atmospheric significance. Elastic scattering from H_2O was recently measured by Cho *et al* [31] at nine energies between 4 and 50 eV for scattering angles from 10° to 180°. This experiment used the MAC in conjunction with a new spectrometer developed at Chungnam National University in Korea. These results are very well reproduced by *R*-Matrix calculations [32], which in turn suggest that there are still problems moving from measured differential cross-sections to integral cross-sections for highly dipolar molecules such as water. A recent review of electron-water scattering data is provided by Itikawa and Mason [33]. Recent Schwinger multi-channel with pseudo-potentials calculations performed by Varella *et al* [34] have been extended for other species such as H_2S, H_2Se and H_2Te.

A resurgence of interest in DEA, due in large part to the identification of low-energy DEA as an important damage mechanism in biological systems [30], has highlighted the need for better theory and a deeper understanding of the dynamics in polyatomic systems. Recent work on DEA to water molecules [35], the first *ab initio* treatment to study this process for a polyatomic molecule in full dimensionality, has established the feasibility of attacking the problem for triatomics from first principles. Furthermore it has pointed to the fundamentally polyatomic nature of the dissociation dynamics that cannot be explained by simple one-dimensional models. DEA in water proceeds through Feshbach resonances: the lowest such anion surfaces [35] as well as the associated dissociation dynamics [36] have been well characterized. The topology of the higher anion surfaces have been analysed [35] and a complete study of DEA on this benchmark system that includes wave-packet dynamics on all three low-energy Feshbach resonance surfaces is given in [36].

Another small polyatomic series that have been investigated are the hydrocarbons and halocarbons, such as CH_3F, CH_2F_2, CHF_3, CF_4, C_2H_4, C_2F_4 and C_2F_6, because of their importance for plasma etching. These studies were undertaken by the Caltech group in collaboration with Campinas and also by the Sao Carlos group [37, 38]. Most recently, an experimental study on electron–C_2F_6 collisions was undertaken by Iga *et al* [37] at intermediate and high energies (30–500 eV). Whereas excellent agreement is obtained between the experimental data in this work, the experimental results are in poorer agreement when compared to the less-elaborate independent-atom model (IAM) with a Yukawa potential. Similar experimental work on CHF_3, but at a lower energy of 20 eV, shows very good agreement with the theoretical results of Varella *et al* [39] obtained using a Schwinger multi-channel method with the Born-closure

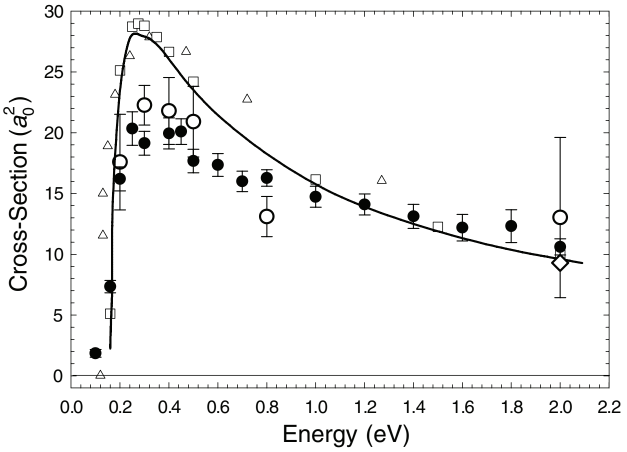

Figure 3. Integral electron-impact VE of the υ_3 vibrational mode of CF_4 from [44]: ○, current data; △results of [45] scaled by a factor of 0.7 as suggested in [44]; ●, positron-impact results shown for comparison; —— results of an analytic, Born-dipole approximation calculation for the cross-section using infrared measurements to fix the dipole; □, result of a local interaction potential calculation for electron impact [44].

procedure; these calculations are also in excellent agreement with earlier experimental differential cross-sections.

For C_2H_4, Panajotovic *et al* [40] took a significant body of experimental data for incident energies from 1 up to 20 eV. This work combines two measurements: DCSs of the Sophia University group and those of the ANU/Flinders group. In general, there is good agreement between the experiments, but some disagreements still remain even at 20 eV. More recent experimental DCS (100–500 eV, scattering angles up to 130°) and theoretical Schwinger Iterative Variational calculations (10–500 eV) by Brescansin *et al* [41] show excellent agreement at high energies, but do not solve the (small) disagreements at lower energies. Recently, Winstead *et al* [42] and Trevisan *et al* [43] revisited low-energy, from 0.5 to 10 eV, scattering from C_2H_2. They still observe small but important disagreements with the experimental data of [40]. The effect of nuclear motion is included in these theories but not at the level discussed for smaller systems above. We note that whereas Trevisan *et al* [43] obtain good agreement with the DCSs of the Sophia University group given in [40], they do not observe good agreement with the ANU/Flinders DCSs. The work of Winstead *et al* [42] elucidates the key components of symmetry that contribute to elastic scattering cross-sections, and the Ramsauer minimum in the ^2A_g earlier reported in the Kohn calculations.

Comparative measurements of slow electron and positron collisions with polyatomics was performed by the UC San Diego group who studied the excitation of the υ_3 vibrational mode of CF_4 [44]. Their data given in figure 3 show the first direct integral measurement of this electron impact cross-section. The strong similarity in both types of cross-sections is unusual, and the fact that the Born approximation works so well for this system for both electrons and positrons suggests that the scattering is dominated by the long-range electrostatic (polarization) potential (charge transfer from the C atom to the F atoms) during the vibrational υ_3 stretch mode.

Recent measurements of total cross-sections were reported by C Makochekanwa (Kyushu University) for positrons and electrons on c–C_4F_8 as well as for n-Hexane C_6H_{14} and c-Hexane C_6H_{12} using a time-of-flight total scattering apparatus [46]. These total cross-sections do not elucidate separated effects and are difficult to unravel except for extreme cases. However, such comparative data using both positrons and electrons are important in determining both common interactions (e.g. polarization) as well as differences such as positronium formation, electron exchange, etc.

High resolution experimental DEA investigations of important chlorine containing molecules have recently been explored by the Kaiserslautern group [8]. In one of their recent experiments, they measured the (relative) DEA cross-section for CF_3I, over the incident range 0.5–500 meV and used four variants of the laser photoelectron attachment method from earlier work with Cl_2 [14]. Their relative cross-sections for I^- formation were normalized to the recommended thermal DEA rate coefficient at $T = 300$ K and thus a new absolute DEA cross-section was obtained over the 0.5–500 meV range. Their *R*-Matrix model, which is fitted to the experimental cross-section, was in turn used to determine DEA from the individual vibrational levels. For the case of CF_3I, it was found that the DEA cross-section for $\upsilon = 4$ is about a factor of four higher than $\upsilon = 0$ at the higher (400 meV) energies of this experiment. So far, cross-sections have been reported for the molecules CF_3I [8], SF_6 [47] and CF_3Br [48]. In the case of SF_6, a downward cusp structure was observed in the cross-section for SF_5^- formation at the onset of VE of the symmetric stretch mode υ_1 up to $\upsilon_1 = 10$. This demonstrates that there is substantial inter-channel coupling of the primary attachment process with VE and indicating that both the SF_5^- ions and the long-lived SF_6^- ions result from the same intermediate SF_6^- state formed by intramolecular vibrational redistribution.

Recent work on the DEA of radical polyatomic molecules S_2O and S_2O_2 [49] was presented by T A Field (Queen's University of Belfast). They bombarded the after-discharge region of a microwave discharge of a mixture of SO_2 and He with electrons from a trochoidal monochromator, and detected the anions using a time-of-flight mass spectrometer. The experiment again monitored the yield of S^-, SO^-, S_2O^-, as a function of incident electron energy. The assignment of these DEA resonances from their parent molecule was determined qualitatively by comparing the spectra of these anions taken at three different inlet pressures of the discharge on and off conditions. Cross-sections for these DEA processes are estimated from referencing their intensities to the DEA intensities of SO_2 (reference molecule). More work is required to quantify the DEA of these radicals because such species are prevalent in discharges used in chemical plasma processing.

7. Electron scattering from large polyatomics

DEA spectra for a host of hydroxyl containing molecules, including methanol, phenol, diethyamine, tetramethylhydrazine, piperazine, pyrrole, and dimethylaniline were observed by Skalicky and Allan [50]. Their DEA spectra of these molecules, see figure 4, follow the familiar shape with incident electron energy, i.e. a low-energy yield produced by a shape resonance resulting from the capture of the scattering electron. The distortion of the original molecular frame by the

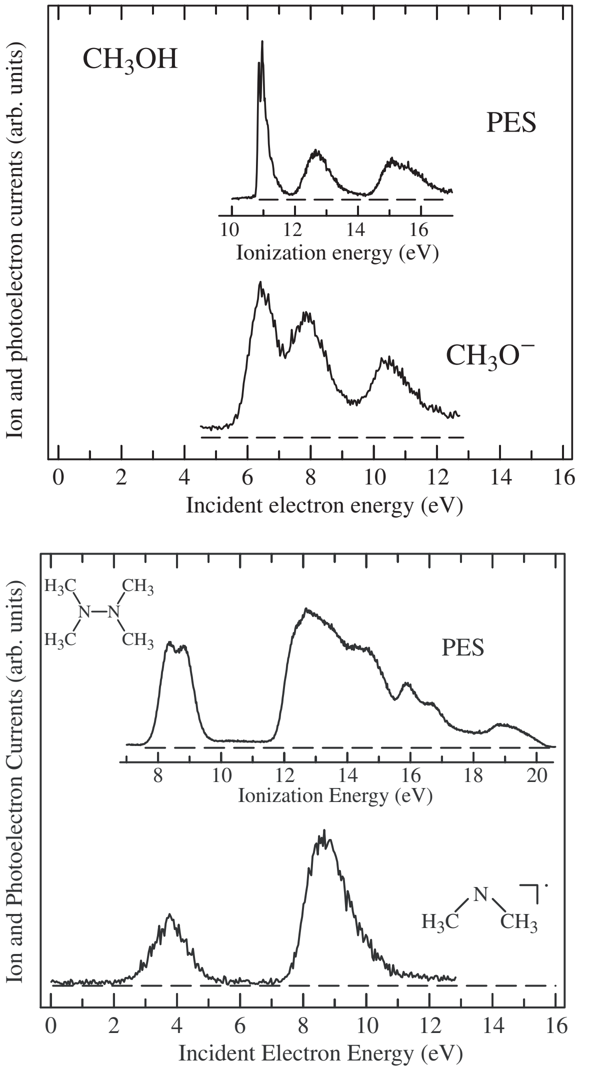

Figure 4. Photoelectron spectrum for methanol and for tetramethylhydrazine shifted by ≈4.5 eV for methanol and ≈4.6 eV for tetramethylhydrazine (these shifts are computed from the difference between the first ionization energy and the energy of the lowest DEA band of the molecule to identify the ionic core state) and the DEA spectrum in methanol and tetramethylhydrazine [50].

negative ion formation results in a fast autodetachment or stabilization of the negative charge due to this distortion. This stabilization can then either cause a scrambling of the atoms to give unexpected results or a simple selective bond breakup. Note that in figure 4, for tetramethylhydrazine in the higher-lying photo-electron spectrum above 14 eV, there are no corresponding DEA bands [50]. These are due to Rydberg orbitals based on the grandparent state. We also note that the widths of these resonances are directly related to the lifetime for autodetachment or decay by bond-breakup of this resonance.

We now concentrate on the dominant area of electron–polyatomic molecule, i.e. the area of bond-selective breakup, due to DEA. This work was initially conducted on thin films bearing DNA double strands and super-coiled DNA strands. The yield of H^-, O^- and OH^- from DEA processes indicates bond-selective breakup of the DNA either at a hydroxyl bond or an H bond or an oxide bond. Information is obtained by examining the yield of anions as a function of incident electron energy. A very recent and comprehensive review of this field is given by Sanche [30] to which the reader is urged to refer to. Representative data for these experiments are summarized in figure 5. Note that the amorphous form of H_2O (ice) yields a DEA curve which is too low to be associated with DEA to the structural water in DNA. Figure 5 also associates the production of H^- from the nucleic bases to be very dominant and important. The H^- yield for thymine is representative of the other nucleic acid bases cytosine, adenine and guanine. Sanche [30] also noted that the yield of OH^- and O^- is similar to the H^- yield and inferred that the O^- was produced from temporary electron localization on the DNA backbone phosphate group [30]. The OH^- desorption yield function resembles that of the O^- yield, but has a considerably lower intensity. This result suggests a two step process: formation of O^- via DEA to the phosphate group followed by (so-called) reactive scattering of the O^- ion with the nearby deoxyribose unit [30].

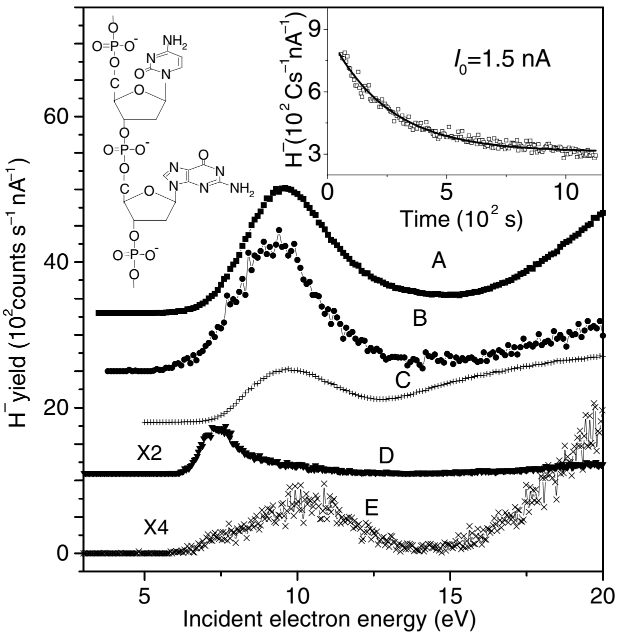

Figure 5. The H^- yield function from thin films of: (A) double stranded linear DNA, 40 base-pairs, (B) supercoiled plasmid DNA, (C) thymine, (D) ice and (E) a deoxyribose analogue. The zero-count baseline of curves A–D has been displaced for clarity. Part of a single DNA strand is shown in the left corner at the top. The dependence of the magnitude of the H^- signal on time of exposure to the electron beam is shown in the inset. From [51].

The inset in figure 5 shows the degradation of the H- signal with time, indicating the breakdown of the DNA with exposure to the electron beam. Clearly, much of the activity is due to electrons in the energy range of 5–15 eV. As reported by P Scheier (Innsbruck), this work has been affirmed by DEA studies with gas phase pyramidine, thymine and uracil [52]. The DEA cross-sections tend to be significant (e.g. peaking at about a few times 10^{-17} m^2).

A theoretical framework has been proposed to describe [53, 54] low-energy electron scattering from such large biomolecules, having a helical topology. The problem was decoupled into two parts: first the electron interacts with the entire molecule and then the new wavefunctions, defined by the atomic arrangement within the molecule, interact at a specific site of the molecule (e.g., a basic subunit). This choice was dictated by the important contribution to the scattering cross-sections arising from both resonances and electron diffraction at low energies; i.e. electron attachment requires the localization of the electron on a small subunit of the biomolecule and an electron of energy typically 5–15 eV has a wavelength that is of the order of molecular and intermolecular distances and is thus initially delocalized. In other words, the incident electron is first likely to undergo multiple intersite scattering before interacting at a specific site, where it can be captured in a resonant state. The simple model proposed consists of molecular subunits (i.e., bases, sugars and phosphates) immersed in an optical potential, which is constant between R-matrix shells, a working hypothesis used in the cross-section calculations for simple molecules [53] and in the theory of low-energy electron diffraction in solids [54]. The model was applied to scattering from the bases within DNA, which were represented by pseudomolecular units made of scattering centres.

F A Gianturco (Rome) and co-workers performed quantum dynamics calculations for the scattering of low-energy electrons from uracyl [55, 56] and glycine [57]. The scattering equations were formulated within a symmetry-adapted, single-centre expansion of both continuum and bound electrons, with the interaction forces obtained from a combination of *ab initio* calculations and non-empirical modelling of exchange plus correlation effects. Several open-channel shape resonances were obtained. For uracyl, they predicted three resonances of π^* symmetry at energies of 2.3, 3.5 and 6.5 eV and two resonances of σ^* symmetry at 0.01 and 10.7 eV [57]. However, as these structures are complicated, much theoretical refinement will be required before the overall process of fragmentation for different base structures and sugar-backbones and the couplings between them will be well understood.

8. Conclusions

The renewed activity regarding electron scattering from molecules on a large number of fronts was highlighted at the conference. The very wide interests of the participants, which is reflected in the large number of applications of electron–molecule collisions, means that this work will have a direct impact on other fields. This field has its foundations in physics and physical chemistry, but it is beginning to impact biological systems at a very basic, yet detailed level.

As a result of the range of the topics addressed, Professor Vince McKoy (Caltech) chaired a panel session on 'Opportunities and challenges in low-energy electron–molecule scattering'. The goal of this session was to stimulate dialogue on the challenges and opportunities in experimental and computational studies of low-energy electron–molecule collisions in the light of the progress and developments that were reported on at the meeting. Participants were asked to address the following questions:

(a) What have been the major advances in measurements, theory, and computations over the last 5–10 years?
(b) What are the major barriers to progress today in studies of electron collisions with molecules?
(c) What are the most interesting opportunities and challenges in the field today?

After a lively discussion lasting several hours and covering a variety of issues, some novel and some long-familiar, a clear consensus on the opportunities and challenges in the field over the next few years emerged. A summary of these, in no specific order of significance, follows:

1. Experimental and theoretical studies of electron collisions with polyatomic molecules, including biomolecules such as the bases and other moieties of DNA. The measurement of absolute cross-sections and rates is a particularly significant challenge here. On the computational side, the scaling of such calculations with molecular size would seem to make it essential to develop strategies that would allow us to exploit computers of the largest scale in such applications. The development of methods with inherently lower scaling with molecular size would also be highly desirable. There may be lessons to be learned here from recent progress in the development of molecular electronic structure methods with reduced scaling.
2. Experimental and computational studies of electronic excitation of small and large molecules at near-threshold energies. Robust benchmark measurements of these cross-sections would provide a challenge for related computational studies exploring the role of closed and open channels in these cross-sections.
3. Experimental and computational studies of collisions of low-energy electrons with molecular radicals, particularly those of interest in atmospheric and plasma modelling.
4. Seeking and exploiting international collaborations. Beyond their immediate scientific benefits, these collaborations often provide opportunities to influence national funding agencies.

Acknowledgments

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