Schedule

Time table	Wednesday, July 27	Thursday, July 28		Friday, July 29		Saturday, July 30	
08:20 - 08:30 h		Opening Remarks		-		-	
08:30 - 09:30 h		S. J. Buckman		M. Charlton		F. A. Gianturco	
09:30 - 10:00 h		Coffee Break		Coffee Break		Coffee Break	
10:00 - 10:30 h		P. Kolorenč	C. Y. Ho	L. G. Ferreira	G. P. Karwasz	C. Winstead	J. A. Young
10:30 - 11:00 h		A. Wolf	G. F. Gribakin	C. S. Trevisan	W. E. Kaupilla	R. Johnsen	R. J. Bunker
11:00 - 11:30 h		A. F. Borghesani	E. A. G. Armour	T. A. Field	S. Jonsell	Panel Session on Opportunities and Challenges	M. Bromley
11:30 - 12:00 h		N. J. Mason	A. S. Ghosh	C. Makochekanwa	D. B. Cassidy		Panel Session on Opportunities and Challenges
12:00 - 12:30 h		M. Radmilović	R. O. Barrachina	P. Scheier	F. Arretche		
12:30 - 14:00 h		Special Lunch		Lunch		Closing Remarks and Lunch	
14:00 - 14:30 h		K. Morgenstern	S. Armitage	M. A. Khakoo	Y. Nagashima	Additional information 1) Please, wear your badge at all times in order to help interaction between the two communities. 2) You have registered in only one conference, but free transit is allowed between sessions. 3) All meals are included in your registration fee and you will receive tickets related to them. Regular meals will be at a nearby restaurant and includes soft drink and dessert. 4) Buses to (from) Comfort Suites and Sleep Inn hotels will be provided at specific times. CPV is at walking distance of the conference site.	
14:30 - 15:00 h		Y. Sakai	C. Arcidiacono	M. Takahashi	L. V. Jorgensen		
15:00 - 15:30 h	Registration and Welcome Reception	L. A. Viehland	H. R. J. Walters	J. Tennyson	N. Oshima		
15:30 - 16:00 h		J. de Urquijo	J. P. Marler	T. Sommerfeld	H. Saito		
16:00 - 16:30 h		Coffee Break		Coffee Break			
16:30 - 17:30 h		G. Gabrielse		H. Hotop			
17:30 - 19:00 h		Poster Session		Poster Session			
19:00 - 20:00 h		Dinner and IOC Meeting		Conference Dinner			
20:00 - 21:00 h							
20:30 - 22:00 h							

International Symposium on Electron-Molecule Collisions and Swarms

27-30 July 2005
Campinas, SP, Brazil

Editors:
Sergio d'A. Sanchez
Romarly F. da Costa
Marco A. P. Lima

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Preface

It is with great honor that the Local Organizing Committee welcomes the participants of the 14th International Symposium on Electron-Molecule Collisions and Swarms in Campinas, Brazil - a satellite meeting of the XXIV International Conference on Photonic, Electronic and Atomic Collisions, in Rosario, Argentina.

This is the first time the EMS Symposium is held in South America and we sincerely hope this will stimulate the development of the field in the whole Continent, as indicated by the record number of contributed papers from South American countries.

This meeting, with its 28-year tradition, is also held for the first time in conjunction with the International Workshop on Low Energy Positron and Positronium Physics. There is an overlap between these two fields, with some of the researchers working on both areas, and this shall provide a profitable interchange for both communities.

Finally, we would like to acknowledge the help from the International Organizing Committee, the support provided by the Brazilian Physical Society in many ways, and those who willingly helped making this Symposium feasible.

Marco A. P. Lima, Chair
Local Organizing Committee
of the 14th International Symposium
on Electron-Molecule Collisions and Swarms

July, 2005

Conference General Information

1. Conference Site

"The University of Campinas was established in 1966, as a public university funded by the State of São Paulo. Its mission is to provide education and training, qualifying our students to play a key role in the process of social development. Unicamp seeks to contribute in the solution of social problems, through education, research and also through services to the community.

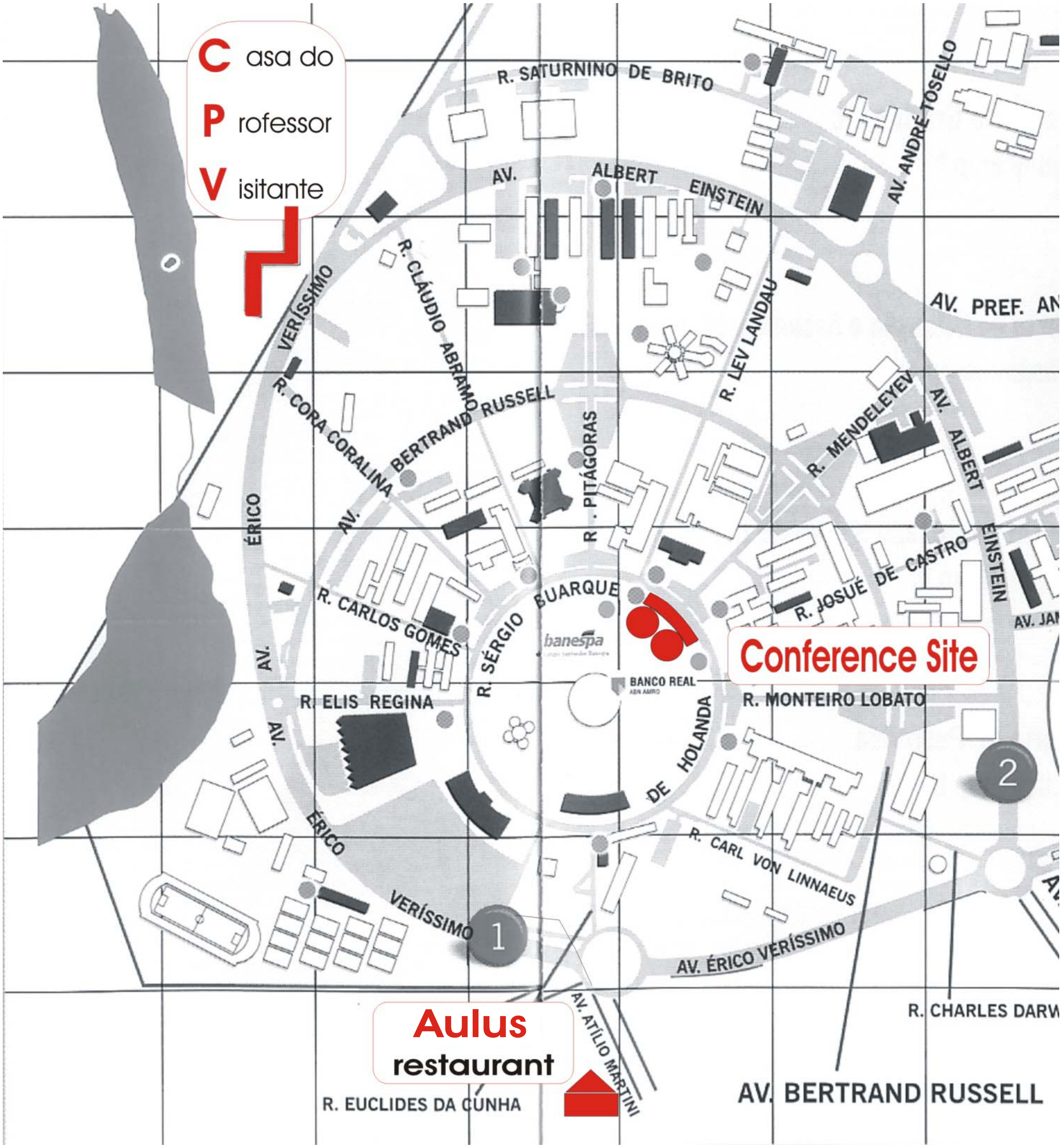
A healthy balance between research and teaching, pure and applied science has made Unicamp one of the most distinguished Brazilian academic Institutions. Unicamp receives undergraduate and graduate students from all over Brazil and also from abroad.

In Europe and even in the American Continent, the history of the oldest universities spans over centuries, while in Brazil it can still be counted in decades. Furthermore, if the history of the Brazilian university is recent, that of the State University of Campinas (Unicamp) is even more. Unicamp had its campus officially opened on October 5th 1966. Few years later it was already recognized as one of the leading Brazilian and Latin American institutions of higher education, conducting advanced research and tackling important social issues. Today, Unicamp can be considered as a fully consolidated university.

Unicamp combines its youth with a strong experience in producing new knowledge in virtually all areas. In effect, today, the University concentrates 15% of the total scientific production in this country and approximately 10% of the graduate courses. The result is its capability to maintain areas of scientific and technological compatibility with the main research centers in the world, through numerous international cooperation agreements. Unicamp is an autonomous autarchy of the São Paulo State. Financial resources are obtained mainly from the state government. Funding is also provided by national and international research funding agencies. Students do not pay tuition fee, since the University is financed by state funds", (from UNICAMP webpage)

The meeting will take place at Ciclo Básico I, a building specially designed to accommodate basic-level undergraduate classes, taken by most of Unicamp students. The classrooms are connected to high speed internet and have the necessary infrastructure for the EMS-05 meeting. A Campus map indicating the most important sites of the Symposium is shown below.

Map of Campus



2. Meals

The registration fee includes all the meals served during the Conference, and tickets will be provided for all participants. We request that you always bring the tickets to the restaurants, and also that you wear your badge at all time.

The Welcome Reception will be held at the Ciclo Básico I from 18:00 – 21:00 h July, 27.

A Special Lunch will be served on Thursday at Coxilha Grill, a famous “all you can eat” barbecue restaurant in Campinas. It offers a rich salad bar and about 26 different kinds of meat. The tickets will also include beer, mineral water, soft drinks, juices and dessert (ice cream).

Regular meals will be served at Aulus restaurant, located just outside the Campus (see the map). The tickets include the main dish, a soft drink and a dessert. Aulus is a self-service restaurant, so you are invited to help yourself. They have a large selection of salads, cold dishes, hot dishes, typical Brazilian juices and desserts.

The Conference Dinner will take place at Alphaville Club with typical Brazilian dishes (mainly fish and seafood, but there will be an alternative menu for vegetarians), provided by Idalvo’s, another very popular restaurant in Campinas.

The Farewell Lunch will be held at CPV. Nothing could be better to close the Symposium than the most famous Brazilian dish: feijoada, prepared with black beans, rice and pork.

Tickets will be provided to accompanying persons for the Welcome Reception and Conference dinner, and will be sold at the Conference desk for the other meals.

3. Ground Transportation

If you are staying at Comfort Suites or Sleep Inn, the Conference will provide ground transportation from/to these hotels to the Conference Site at scheduled times. On Wednesday, buses will take you to your hotel after the Welcome Reception at 21:00 h. On Thursday, Friday and Saturday buses will depart from the hotels at 08:00 h, and on Thursday they will leave Unicamp at 21:00 h. Those staying at Casa do professor Visitante (CPV), may walk to the Conference site (about five minutes).

Ground transportation will also be arranged for all participants for the Special Lunch and the Conference Dinner.

In the last day of the Conference, please leave your luggage at the hotel after checking-out. A bus to Guarulhos International airport will leave CPV after the Farewell Lunch at 15:30.

4. Poster Prize

We have the pleasure to announce that there will be a selection for the best poster of the meeting. The prize, in the amount of US$ 175.00, was donated by Ione Iga, Lee Mu-Tao, Luiz E. Machado, Luiz G. Ferreira, Luiz M. Brescansin, Marco A. P. Lima, and Romarly F. da Costa. The donors have requested that their posters as well as those of their co-workers should not be considered for election.

You will receive a voting ticket at the registration desk upon arrival. We will also have, at the same location, a place to cast your vote after making your decision (votes must be deposited by July 30th, Saturday, 10:00hs).

The result will be announced at the closing remarks just after the last session of the Conference.

5. Internet

Computers will be available at the Conference desk for participants to access the Internet.

6. Important Information on Campinas and Brazil

Electric power - In Campinas, the voltage is 110 V - 60 cycles, unless indicated otherwise, though most of the hotels have sockets for both 110 and 220 V.

Business Hours - Most stores open from 09:00 h to 18:00 pm on weekdays, and from 09:00 h to 13:00 h on Saturdays. Some malls are open up to 22:00 h on weekdays and on Sundays afternoon. Bank branches open from 10:00 h to 16:00 h, only on weekdays.

Car rental - As previously stated, ground transportation will be provided by the conference, but car rentals, with or without drivers, are available at all major international airports.

Taxis - There are a lot of taxis in Campinas and they may be called at the hotel desk. Most of the taxi drivers, however, do not speak any other language than Portuguese.

Tipping - A 10% tip is already included in the bill of most restaurants. If not included, the general rule is to give a 10% tip. Taxi drivers do not expect tips.

Scientific Program of the International Symposium on Electron-Molecule Collisions and Swarms

All sessions are in Ciclo Básico I – room CB01

Wednesday, July 27

15:00 – 21:00

Registration

18:00 – 21:00

Welcome Reception

Thursday, July 28

08:20 – 08:30

Opening Remarks

08:30 – 09:30
Plenary Lecture A – Chair: Franco A. Gianturco

Stephen J. Buckman, The Australian National University, Australia
Benchmark studies of electron (positron)–molecule (atom) scattering

09:30 – 10:00
Coffee Break

Session A – Chair: William McConkey

10:00 – 10:30

Přemysl Kolorenč, Charles University in Prague, Czech Republic
Use of Feshbach-Fano R-matrix approach to the calculation of the discrete state and the coupling for solution of resonance nuclear dynamics in diatomics.

10:30 – 11:00

Andreas Wolf, Max-Planck Institute for Nuclear Physics, Germany
Low-energy electron collisions of molecular ions in ion storage rings

11:00 – 11:30

Armando F. Borghesani, University of Padua, Italy
Electron transport in dense gases and more

11:30 – 12:00

Nigel J. Mason, The Open University, UK
Electron and positron induced chemistry; New methods for studying chemical dynamics

12:00 – 12:30

Marija Radmilović, Institute of Physics, Serbia and Montenegro
Modeling of rf and dc breakdown

12:30 – 14:00
Special Lunch

Session B – Chair: Zoran Lj. Petrović

14:00 – 14:30

Karina Morgenstern, Universitaet Hannover, Germany
STM investigation of single molecule surface processes

14:30 – 15:00

Yosuke Sakai, Hokkaido University, Japan
Electron swarms and cross section data

15:00 – 15:30

Larry A. Viehland, Chatham College, USA
Current status of ion swarms

15:30 – 16:00

Jaime de Urquijo, Centro de Ciencias Físicas, UNAM, Mexico
Transport coefficients of ions and electrons in pure gases and mixtures: Recent measurements and calculations

16:00 – 16:30
Coffee Break

16:30 – 17:30
Plenary Lecture B – Chair: Edward A. G. Armour

Gerald Gabrielse, Harvard University, USA
Positron quantum cyclotron and antihydrogen

17:30 – 19:00
Poster Session

19:00 – 21:00
Dinner and IOC Meeting

Friday, July 29

08:30 – 09:30
Plenary Lecture C – Chair: Cláudio L. Cesar

Michael Charlton, University of Wales Swansea, UK
Progress with cold antihydrogen

09:30 – 10:00
Coffee Break

Session C – Chair: Jiří Horáček

10:00 – 10:30

Luiz G. Ferreira, Universidade Estadual de Campinas, Brazil
A geometrical optics model for electron scattering by molecules

10:30 – 11:00

Cynthia S. Trevisan, University of California, Davis, USA
Electron scattering by molecular radicals (NO, CF)

11:00 – 11:30

Thomas A. Field, Queen's University, UK
Electron interaction with radicals; experimental observation of dissociative electron attachment to S_2O and S_2O_2

11:30 – 12:00

Casten Makochekanwa, Kyushu University and Sophia University, Japan
Electron and positron collisions with molecules

12:00 – 12:30

Paul Scheier, Institut fuer Ionenphysik, Austria
The use of isotope and site labeling for the identification of DEA peaks in biomolecules

12:30 – 14:00
Lunch

Session D – Chair: Lee Mu-Tao

14:00 – 14:30

Murtadha A. Khakoo, California State University, USA
Low energy electron impact excitation of simple diatomic molecules – H_2 and N_2

14:30 – 15:00

Masahiko Takahashi, Tohoku University, Japan
Probing electron momentum densities of molecular orbitals using new multichannel (e,2e) spectrometers

15:00 – 15:30

Jonathan Tennyson, University College London, UK
R-matrix calculations of electron-molecule collisions at low and intermediate energies

15:30 – 16:00

Thomas Sommerfeld, University of Pittsburgh, USA
Electrons attached by long-range forces: Quadrupole bound anions

16:00 – 16:30
Coffee Break

16:30 – 17:30
Plenary Lecture D – Chair: Ann E. Orel

Hartmut Hotop, Universität Kaiserslautern, Germany
High resolution studies of dissociative electron attachment to molecules

17:30 – 19:00
Poster Session

19:00 – 22:00
Conference Dinner

Saturday, July 30

08:30 – 09:30
Plenary Lecture E – Chair: Hiroshi Tanaka

Franco A. Gianturco, The University of Rome "*La Sapienza*", Italy
Modelling dynamical processes in molecular gases induced by low-energy positrons

09:30 – 10:00
Coffee Break

Session E – Chair: Jimena D. Gorfinkiel

10:00 – 10:30

Carl Winstead, California Institute of Technology, USA
Recent progress with the Schwinger multichannel method

10:30 – 11:00

Rainer Johnsen, University of Pittsburgh, USA
Excited state formation in the dissociative recombination of HNC^+ ions with thermal electrons

11:00 – 12:30

Panel session on opportunities and challenges - Chair: Vincent McKoy

12:30

Closing Remarks

12:30 – 14:00
Farewell Lunch

List of Invited Papers

List of Contributed Papers

LIST OF INVITED PAPERS

BENCHMARK STUDIES OF ELECTRON (POSITRON) – MOLECULE (ATOM) SCATTERING

*Stephen J. Buckman**

Atomic and Molecular Physics Laboratories
Research School of Physical Sciences & Engineering
The Australian National University
Canberra, 0200, AUSTRALIA

This talk will attempt to review the current state of low energy electron and positron collision physics with an emphasis on where the field is with regard to “benchmark” studies. A well-known example of such a benchmark would be low energy elastic electron scattering from helium. Are there many others?

Benchmark measurements and calculations in a field such as ours are essential in providing a basis for assessing and improving experimental techniques, and for developing new theoretical tools and approximations. The capacity for accurate absolute measurements lies at the heart of these advancements, and in assessing the worth of such measurements in applied fields such as discharge technology, atmospheric processes and radiation biology. Benchmark measurements in ‘simple’ systems, which can be tested against the best available theoretical calculations, also provide some rationale for the extension of the calculations to more complex, reactive, or transient species, which are often difficult to study experimentally.

Experimentally, we have made significant advances in the last 10 years or so in the measurement of the simpler scattering processes, such as elastic scattering. For electrons, results from various groups around the world largely agree to within 20% on measured differential cross sections for a large range of atoms and molecules. Advances such as the Manchester magnetic angle changer have enabled the extension of DCS measurements to large angles to provide for a better comparison with theory and a better estimate of integral and momentum transfer cross sections. For inelastic collisions the situation is much more complex. The absolute scale is usually set by measuring the inelastic scattering intensity relative to that for the elastic channel. In doing so the energy dependence of the scattered electron analyser must be carefully determined, particularly for measurements close to threshold (the most interesting region!).

For positron scattering there are fewer ‘benchmarks’, although that is likely to change in the near future, as there have been major experimental developments in the field in recent years. Sophisticated techniques are being applied to the measurement of differential and integral cross sections, as well as measurements of positronium formation, ionization and annihilation.

In this talk I will attempt to cover some of the recent advances that have been made in experimental measurements and theoretical calculations for electron and positron interactions with atoms and molecules. Targets of interest will include He, N_2, NO, CO_2, CH_4, and if time permits, some recent measurements on electron scattering from laser-cooled and trapped, He (2^3S) atoms will also be discussed. Possible candidates for future ‘benchmark’ measurements will also be speculated upon.

*stephen.buckman@anu.edu.au

Use of the Feshbach-Fano R-matrix approach to the calculation of the discrete state and the coupling for solution of resonance nuclear dynamics in diatomics.

Přemysl Kolorenč[1], Vincent Brems[2] and Jiří Horáček[1]
[1]*Institute of Theoretical Physics, Charles University in Prague, Czech Republic*
[2]*Department of Chemical Physics, J. Heyrovský Institute, Prague, Czech Republic*

The Feshbach-Fano (FF) projection-operator formalism represents particularly useful tool for investigation of the resonant phenomena in quantum theory. Within this approach, a single square integrable wave function (the discrete state $|\varphi_d\rangle$) is associated with each resonance. Once the linear functional subspace $\mathcal{Q}$ spanned by the discrete states is defined, the FF formalism provides a detailed and intuitive understanding of the resonant processes. The major drawback of the the formalism is the need for *a priori* definition of the subspace $\mathcal{Q}$. Its choice is usually evident in the case of Feshbach resonances but can be difficult in case of shape resonances.

Nestmann [1] has proposed a systematic approach to determining $\mathcal{Q}$, the Feshbach-Fano R-matrix (FFR) method. The FFR method provides the discrete state, its position and the associated coupling terms to the background continuum. The method has been successfully applied to several molecules in the equilibrium geometry of the ground state (e.g. N_2, C_3H_6 and N_2O). More recently, detailed analysis of the FFR method was done on the ground of potential scattering [2] with the aim to determine the strengths and the limits of the method and to establish it as a general tool for investigation of the resonant phenomena. The FFR method can be applied to any system which can be studied via the R-matrix method. Once the standard R-matrix calculations are done the FFR procedure represents computationally very cheap way how to treat the results and obtain all necessary information about the resonances.

One of the most striking features of the FFR method is that it can be used directly to construct the so-called nonlocal resonance model (NRM) [3] of the nuclear dynamics of the low-energy electron-molecule collisions. Nonlocal resonance theory yields cross sections for vibrational excitation, dissociative electron attachment and associative electron detachment. It was used successfully to describe low-energy collisions of electrons with molecular hydrogen and hydrogen halides. The FFR method was used to provide model for the electron-F_2 scattering [4] and recently also for electron-Cl_2 scattering. Those systems are essential in plasma and laser physics and are also of great atmospheric and environmental interest. It is the lack of accurate data on inelastic electron scattering, both experimental and theoretical, that motivated our study.

References

[1] Bernd M. Nestmann. *J. Phys. B*, 31:3929–3929, 1998.

[2] Přemysl Kolorenč, Vincent Brems, and Jiří Horáček. *Phys. Rev. A.* accepted for publication.

[3] Martin Čížek, Jiří Horáček, and Wolfgang Domcke. *J. Phys. B*, 31:2571–2583, 1998.

[4] V. Brems, T. Beyer, B. M. Nestmann, H.-D. Meyer, and L. S. Cederbaum. *J. Chem. Phys.*, 117(23):10635–10647, 2002.

Low-Energy Electron Collisions of Molecular Ions in Ion Storage Rings

A. Wolf,[1] H. Kreckel,[1] L. Lammich,[1] H. Buhr,[1] H. B. Pedersen,[1] S. Novotny,[1] D. A. Orlov,[1]
A. S. Terekhov,[3] M. Lestinsky ,[1] F. Sprenger,[1] S. Altevogt,[1] V. Andrianarijaona,[1]
M. Motsch,[1] Y. Nevo,[2] D. Schwalm,[1] D. Zajfman[1,2]

[1] Max-Planck Institute for Nuclear Physics, Heidelberg, Germany
[2] Weizmann Institute of Science, Rehovot, Israel
[3] Institute of Semiconductor Physics, Novosibirsk, Russia

Collisions of molecular ions with low-energy electrons have large cross sections and reflect many types of energy exchange dynamics between electronic and ro-vibrational degrees of freedom in molecular systems. In particular the dissociative recombination between electrons and molecular ions is an important process in cold ionized media, whose rate coefficient depends on detailed aspects of molecular collision dynamics such as Rydberg resonances on a ro-vibrationally excited ion core.

Merged beams of cold electrons and molecular ions in storage rings are used successfully since several years to study such reactions in energy-resolved, event-by-event collision experiments. The lecture will present work at the storage ring facility TSR in Heidelberg, Germany, which recently achieved strong improvements in the energy resolution, in the control of initial molecular excitation, and in the analysis of the dissociation products. Systems under study are mostly light di- and triatomic molecular ions. In particular the hydrogen isotopomers (H_2^+, HD^+, D_2^+) [1,2], the triatomic hydrogen molecular ion H_3^+ and isotopomers [3,4], as well as the helium dimer He_2^+ [5]. The different landscapes of electronic potential curves for these systems lead to a large variation of the reaction rates, the underlying dynamics, and the dependence on initial ro-vibrational excitation.

Improvements of the energy resolution were achieved by a new electron target [6] using a cold (100-K) photocathode electron source [7], yielding a center-of-mass electron energy spread down to ~500 μeV. The internal excitation of the molecular ions can be monitored by fragment imaging techniques. Storage of the molecules over times up to ~90 s makes it possible to observe radiative cooling of the vibrational and rotational degrees of freedom of the molecular ions. In addition, the long storage times allowed us to observe vibrational and rotational cooling of the molecular ions by inelastic electron collisions.

Work partly funded by the German Israel Foundation for Scientific Research (GIF) under contract No. I-707-55.7/2001.

1. A. AlKhalili et al., Phys. Rev. A **68**, 042702 (2003)
2. S. Krohn et al., Phys. Rev. A **62**, 032713 (2000) ; V. Ngassam, et al., Phys. Rev. A **68**, 032704 (2003)
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7. D. A. Orlov et al., J. Phys.: Conf. Ser. **4**, 290 (2005)

Electron Transport in Dense Gases and more

A.F. Borghesani

Department of Physics, University of Padua
Padua, Italy

Electron transport in dielectric liquids has been investigated for several decades now and a large wealth of data is available. In simple high-mobility liquids the electric field dependence of the electron mobility closely resembles that in a dilute gas of hard-spheres and can be quite successfully described by means of the solution of the two-term expansion of the Boltzmann transport equation.

This approach, essentially due to Cohen and Lekner, retains the single scattering picture of kinetic theory, valid for dilute gases, because of the large electron mean free path in the liquid and introduces a suitable scattering cross section, which has to be considered as an adjustable parameter. Multiple-scattering corrections introduced by several authors have improved this approach and describe relatively well the density dependence of the electron mobility. A different route, directly based on multiple scattering, has been followed by Basak and Cohen, but it is not as satisfactory as the single-scattering picture to describe the density and electric field behavior of the electron mobility.

On the other hand, the equations of kinetic theory are correctly used in the realm of dilute gases in order to gather pieces of information on the electron-atom interaction potentials. However, for the same atomic species, there is no simple relationship between the cross section determined in the dilute gas and that in the liquid. Only at high electric fields, hence at high mean electron energy, the cross section in the liquid apparently approaches that of the single atom in the gas.

A way to bridge the gap between the description of the dilute gas and that of the liquid is to study the electron transport in a compressed gas as a function of density in order to see how multiple scattering effects develop and affect the dynamics and energetics of the electrons.

In this lecture the transport properties of electrons in the simplest gaseous systems, i.e. the noble gases, will be reviewed. It will be shown that from the experimental data a unified picture of the electron-atom scattering in the dense medium emerges, in which all multiple scattering effects cooperate with each other in a very predictable way in gases of very different polarizability so as to yield the apparently different experimental results. It will also be shown how the extrapolation of the dense gas results to even higher densities may suggest a way to interpret the experimental outcome in the simple dielectric liquids.

Other physical phenomena, some of which are not strictly related to electron transport, such as the self-trapping of electrons in bubbles, responsible of the low electron mobility in He and Ne, the resonant attachment of electrons to electronegative impurities like O_2, or even the density-dependent redshift of the infrared light emitted by noble gas excimers produced by electron impact excitation of noble gases will be presented and will find a coherent interpretation in terms of the unified picture of electron-atom scattering in a dense medium obtained from the analysis of the electron mobility.

Electron and Positron Induced Chemistry;
New Methods for studying chemical dynamics

N J Mason

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Electron and positron induced reactions in both gaseous and condensed phases initiate and drive many of the basic physical and chemical processes in science and technology with applications from industrial plasmas to radiation damage in living tissue. For example, in contrast to previous hypotheses radiation damage in the DNA of living systems has now been shown to arise primarily from collisions of very low energy (sub-ionization) secondary electrons through dissociative attachment to the components of DNA molecules or to the water around them. In the technological field electron induced reactions underpin most of the multibillion dollar modern semiconductor industry since it is those reactive fragments produced by electron impact of etchant gases that react directly with the silicon substrate[2].

Electron induced processes are also of extraordinary importance for determination of structure and chemical reactivity of species adsorbed on surfaces, while positrons are proving to be a useful new solid state probe for surfaces, interfaces and defect profiling. Indeed recently it has been demonstrated that, using STM based technology, discrete electron reactions may be performed at the individual molecular level thus introducing the prospect of designer synthesis on the nanoscale. New bond-selective molecular fragmentation induced by low energy positrons has also recently been demonstrated, positrons exhibiting a high chemical selectivity in the dissociative ionization of organic molecules. Thus it is now possible to develop a new *'antimatter chemistry'* that can lead to the development of novel chemical synthesis techniques.

The energy region below 3 eV is of particular interest since here the cross sections for both electron and positron-induced processes show a general reciprocal energy dependence. In addition, at energies where the positronium atom Ps (a bound state of an electron and positron) can no longer be formed, chemical reactions may be induced by low lying transient anion and cation states formed by the attachment of electrons and positrons, respectively. These quasi bound states are provided by the short range polarization interaction induced when an electron or positron approaches a target molecule. In the case of dissociative electron attachment (DEA) in many systems a 100 % selectivity with respect to the cleavage of a particular bond can be obtained! Dissociative positron attachment (DPA) is only just beginning to be studied but the first results indicate that hydrocarbons can effectively bind positrons while fluorocarbons do not, for electron attachment the situation is reversed. In particular breaking of single, double or triple bonds can be obtained in ring hydrocarbons by varying the positron energy between a few tenths and a few eV energies much lower than those needed with electrons, while studies of positron impact on halogenated hydrocarbons (eg CH_3F) have shown that ionized fragments emerge with much lower kinetic energy spread than in the case of electron induced ionization. This opens interesting prospects for a selective chemistry induced by electrons and positrons. It should also be noted that electron induced processes are often directly linked to photon induced processes since photons of sufficient energy excite or liberate electrons from targets which may then drive the local chemistry.

Modeling of rf and dc breakdown

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It is well known that studies of the non-equilibrium processes which occur in radio frequency (rf) discharges during breakdown are of interest, both for industrial applications and for a deeper understanding of fundamental plasma behavior. Capacitively coupled rf discharges are receiving an increased attention due to their wide applications in many technological processes such as plasma etching for semiconductor materials, thin film deposition and plasma cleaning. DC breakdown studies are of interest in a wide range of applications. One recent example are plasma displays. Finally studies of gas breakdown are of direct interest for development of gaseous dielectrics and circuit breakers. Most recently interest has been initiated in dc, rf and microwave breakdown at atmospheric pressures with an idea to develop micro discharges for applications for displays, nanotechnologies and light sources.

In order to optimize plasma technological processes it is often necessary to know gas breakdown conditions in a discharge device. On the other hand plasma models include numerous coefficients and some of the phenomenology that may be obtained most directly from the studies of breakdown. Therefore, it is of considerable interest to simulate and measure the breakdown curves in dc, rf or combined fields. However, as far as rf argon breakdown is concerned, agreement between the measured and predicted criteria is unsatisfactory.

The basic phenomenology of breakdown concurs with that of electron and ion swarms as space charges are negligible during the initiation of the discharge, thus a basic charged particle transport theory together with the kinetics of active species will suffice to model the breakdown. The breakdown is often epitomized in breakdown voltage (U_b) versus pressure (p) times gap (d) between the electrodes curves (Paschen curves) which basically reveal the importance of pd scaling which is valid in addition to E/N scaling.

Recently, Phelps and Petrovic [1] an analysis of the breakdown in argon. They have shown that it is possible to reconcile the data due to ion beam techniques and those from the application of Paschen law to the gas breakdown measurements which were otherwise different often by up to 2 orders of magnitude. At the same time the role of backdiffusion and nonequilibrium electron kinetics has been studied by Radmilovic and Petrovic [2,3]. Finally we should mention a large number of experiments performed at higher pressures that cover dc and high frequency breakdown data at very small gaps [4,5]. All of these studies were the basis from which we started our analysis presented here.

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STM investigation of single molecule surface processes

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Electrons tunneling inelastically from the tip of a scanning tunneling microscope through a molecule into a metal surface may induce chemical reactions. The method is based on high-resolution imaging at low-temperature (5K) that allows us to identify different groups within the molecule. Chemical reactions are induced by injecting selectively electrons into specific parts of the molecule. The success of the manipulation is visualized in the recorded tunneling current during the manipulation and in STM images taken afterwards. In this talk I will present reactions for a several molecules of different complexity, specifically water, substituted benzene molecules (chloronitrobenzene), and photochrome molecules (azobenzene). The molecular reactions include formation and destruction of external and internal bonds and isomerization. The energies needed for the reactions are remarkably low and involve excitations of molecular vibrations.

Electron swarms and cross section data

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Once a physically proper set of electron collision cross sections is determined, we can uniquely obtain electron swarm properties, which are even difficult to be observed experimentally, e.g. the electron energy distribution function $F(\varepsilon)$, using the Boltzmann equation. Cross section values are determined by a *beam method* or *swarm method*. The former gives basically detailed structure with high-energy resolution in the cross section, however, for a set of them in a gas it is not so easy. In particular in low electron energies the cross section resolution degrades. The latter method was introduced for evaluation of H_2 and N_2 cross sections by Phelps [1]. After that, a set of the cross sections in a wide range of electron energies ε for various gases have been studied using a swarm method. In general, electron swarm properties in a gas are determined by binary collisions between an electron and a gas atom (or molecule). The energy gain of an electron in a free flight path λ (= $(NQ)^{-1}$) is determined by E/N value (E: electric field strength in V/cm, and N: the particle number density in cm^{-3}, $10^{-17}Vcm^2$=1 Td).

In the present talk, a several gases with distinctive featured cross sections are taken and the electron swarm properties brought by the cross sections are described, such as,

1) A set of electron collision cross sections for He and Ne: An interesting point is that the momentum transfer cross section Q_m of Ne in low energies is smaller than that of He, though the atomic mass of Ne is larger than the He [2]. For many applications of both gases to be a buffer gas, this property should be considered.
2) Gases with strong ionization and attachment: In a swarm system with strong ionization and/or attachment, the electron number density in the swarm varies with time and is not conserved at all. In a such system, $F(\varepsilon)$ depends on position x in the direction of the field, i.e. $F(\varepsilon,x)$. Consequently the electron drift velocity W_V defined in $\boldsymbol{v}$-space differs from the average velocity of electrons $W_\mathbf{r}$ in real space [3].
3) Effect of Ramusauer-Townsend (R-T) minimum: The Q_m with R-T minimum affects the W and diffusion constant ND_L in low E/N, significantly. Featured structures in W and ND_L in Ar and its mixtures are seen for E/N around 0.005 and 5 Td [4]. In the mixtures the W depends strongly on the mixture ratio in low E/N.
4) Effect of Penning ionization in gas mixtures[4], effective value of excitation cross section for rare gases[5], and others.

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Current status of ion swarms

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It is now routine to compute transport properties of atomic ions in atomic gases *ab initio*, i.e. starting from computational chemistry calculations of the ion-neutral interaction potential, when the external fields are electrostatic. An illustration of this will be presented for O+ and O- ions moving in the rare gases. Systems with molecular ions and/or molecular gases are of more interest, but a brief review will show that *ab initio* calculations are still limited by the large amount of computation that would be required. Current research has turned to more complicated experimental situations, where there may be magnetic as well as electric fields and where either or both fields may vary with time and position. Recent progress in describing such experiments using momentum-transfer theory and moment theories obtained from the Boltzmann equation will be discussed, with particular attention given to comparison with data obtained in ion traps and field-asymmetric ion mobility spectrometers.

Transport coefficients of ions and electrons in pure gases and mixtures: Recent measurements and calculations

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The is a growing demand of swarm transport coefficients of electrons and ions in view of its importance for the simulation and modelling of electrical discharges. On the other hand, complex phenomena such as negative differential conductivity of electrons and Penning ionization, for example, are still in the process of being explained thoroghly. Ion motion is also a matter of intensive research since ion transport coefficients are now being widely used both in gas discharge modelling and in applied areas such as ion mobility mass spectrometry. In this respect, the refinement of models dealing with ion motion in the gas mixtures demand a knowledge of the ion mobility in the pure gases and in the gas mixtures. Moreover, recent calculations have shown the usefulness of the simultaneous combination of theory and experiment in order to test the cross sections sets in the calculations, and to extend, wherever possible, the range of calculations to regions of the density-reduced electric field where the experiment is still difficult to perform.

This talk will be dedicated to the discussion of recent measurements and calculations of the drift velocity (mobility) and diffusion coefficients of ions and electrons in several gases and gas mixtures, paying special attention to the processes such as negative differential conductivity, and also to the derivation of cross sections from measured swarm transport coefficients, an issue that may be controversial under some circumstances.

A GEOMETRICAL OPTICS MODEL FOR ELECTRON SCATTERING BY MOLECULES

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In calculating the electron elastic cross section of hydrocarbon isomers [1], we were surprised to verify that, for energies between 10eV and 40eV, the cross sections differed by a factor that could be calculated with a simple model burrowed from Geometrical Optics. The result was surprising because the range of energies implies electron wavelengths with the same order of the inter atomic distance. Therefore one would expect interference between the many atoms, which lies in the domain of the Wave Optics, while there is no such a thing in Geometrical Optics.

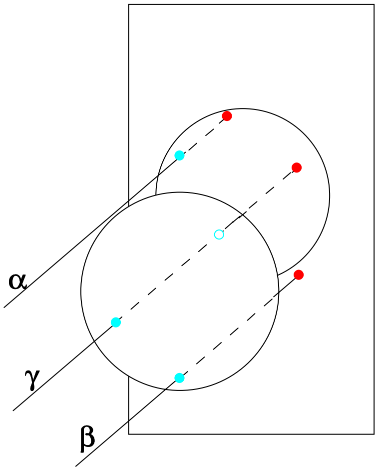

Fig. 1. Three light rays hitting 2 atoms. Ray α hits only the atom behind. Ray β hits only the atom in the front. Ray γ hits both atoms but its shadow in the screen is counted only once.

In Fig. 1 we explain the Geometrical Optics model. In this model the atoms are represented by spheres whose radii depend only on the atomic species and on the incident electron energy. The molecule is considered as a rigid assembly of these atomic spheres. We shine light with many orientations upon the molecule and then collect the molecular shadow in a screen behind the molecule (red dots in the figure). In the case of the hydrocarbon isomers [1] we verified that the area of the shadow, named "shadow cross section", is proportional to the electron-molecule cross section.

After the success of the model for the hydrocarbons the next natural step was to extend it to other atoms and molecules. In Fig. 2 we present some first results, which are still not optimized. In this figure we plot the ratio of the cross section obtained with the Schwinger multichannel method (SMC) and the shadow cross section for a collection of molecules.

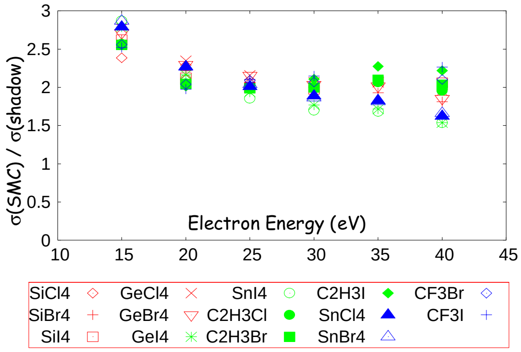

Fig. 2. SMC cross section $\sigma(SMC)$ divided by the shadow cross section. Observe that the ratio is approximately equal to 2 for many molecules and electron energies.

A question remains to be answered: how do the atomic sphere radii defining the shadows compare with those of standard tables (atomic and covalent radii) [2]? Or equivalently, how well the standard radii can be used to define the shadow spheres? The answer is that the comparison is poor, and the stardard radii are not a good choice to use as shadow sphere raddi. The shadow radii are not even monotonic with covalent or atomic radii. For instance, Sn and I have smaller shadow radii than Si and Cl respectively.

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ELECTRON SCATTERING BY MOLECULAR RADICALS (NO, CF)

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Low-energy scattering of electrons by radicals is of interest in a wide range of chemical and physical processes. Nitric oxide, for instance, is important in atmospheric processes and plays key functional roles in a variety of physiological systems. It is also used as a plasma gas. Knowledge of collision dynamics with CF is important in plasma etching processes. It is formed within plasmas under electron bombardment of C_2F_4, which has been proposed as a new feed gas due to its relatively benign impact on the atmosphere. Because of their high reactivity, radicals like CF are difficult to work with experimentally, making theoretical studies of collision processes crucial in the determination of cross sections, transition rates and other quantitative characteristics. Despite the need for *ab initio* results on electron scattering by NO and CF radicals, such calculations are scarce, particularly in the energy region below 2 eV, which is dominated by negative ion resonances. In the case of NO, recent experimental measurements of Allan [1] and of Jelisavcic *et al.* [2] allowed comparison and represented a test to theoretical models that could later be applied to radicals for which experimental data is unavailable, like CF. This prompted us to perform an *ab initio* study of elastic scattering and vibrational excitation of NO by electron impact in the low-energy (0-2 eV) region where the cross sections are dominated by resonance contributions [3]. We employed a nonlocal treatment of the nuclear dynamics, which was found to remedy the principal deficiencies of the local complex potential model. The complex-valued potential curves were obtained by combining large-scale configuration-interaction calculations for the resonance positions with fixed-nuclei, complex Kohn calculations for determining the resonance lifetimes. The resulting low-energy cross sections are dominated by shape resonance contributions associated with the $^3\Sigma^-$, $^1\Delta$ and, to a lesser extent, $^1\Sigma^+$ states of NO^- and display pronounced, overlapping boomerang structures that give irregularly shaped vibrational excitation cross sections.

We have also studied dissociative electron attachment to NO via the $^3\Sigma^-$ negative ion resonance which gives ground state $N(^4S) + O^-(^2P)$. Our results show that the dissociative attachment cross sections in this channel that originate from the ground vibrational state of NO are extremely small, as confirmed by several experimental studies. However, the dissociative attachment cross section is predicted by these calculations to increase by several orders of magnitude when the dissociation takes place from vibrational excited states of NO. We investigated the origin of this dramatic enhancement and predict that dissociative attachment cross sections producing ground state atomic products should be measurable starting from vibrational levels above approximately $\nu = 10$.

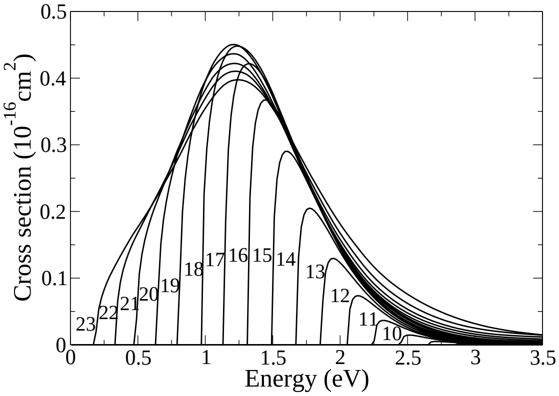

Fig. 1. NO Dissociative attachment cross sections from vibrationally excited states.

Preliminary results of low-energy electron scattering by radical CF, which is isoelectronic with NO, will also be discussed.

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Electron interaction with radicals; experimental observation of dissociative electron attachment to S_2O and S_2O_2

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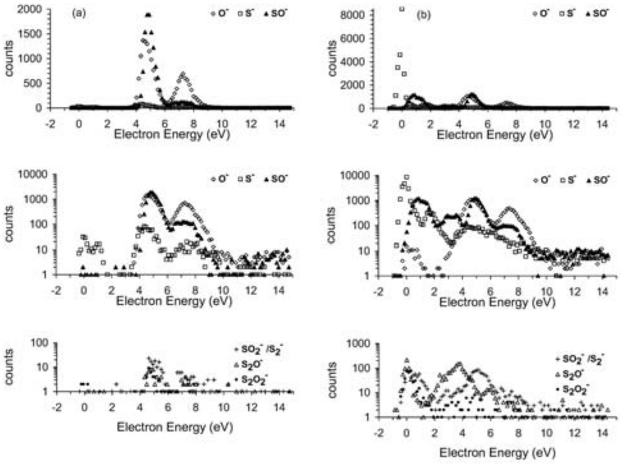

I. INTRODUCTION

Dissociative electron attachment (DEA) is a fundamental molecular fragmentation process and a major process in plasmas, electrical breakdown phenomena, combustion, the upper atmosphere and many other situations where there is a high density of free electrons. These are all environments where unstable free radicals have a crucial impact on the overall chemistry, but few studies of electron attachment to unstable molecules have been reported although many studies of stable molecules and clusters have been reported, *see e.g.* [1, 2]. It appears that DEA has only been observed experimentally to stable free radicals, such as NO [3], or partially stable ones, such as OClO [4, 5]. The experimental results for OClO are in agreement with theoretical calculations [6]. Theory has also been used to calculate the scattering of low energy electrons by free radicals such as ClO, CF, CF_2 and CF_3 [7–10] for which there are no experimental data. Electron attachment to excited states, such as SO_2 in the $\tilde{B}\ {}^1B_1$ state [11, 12], and some exotic species, such as S_2 [13] and Na_2 [14], has been observed experimentally. In this work a new spectrometer has been developed to study DEA to unstable molecular species such as free radicals; first results have been presented for S_2O and S_2O_2 [15].

II. RESULTS

The figure shows DEA spectra gathered for a mixture of He and SO_2 with the microwave discharge off, (a), and on, (b), with linear and logarithmic vertical scales. The results with the discharge off are consistent with previous measurements of dissociative electron attachment to sulphur dioxide, see *e.g.* [12, 16–18]. Several new resonances are observed with the discharge on, which have been assigned to the radicals S_2O and S_2O_2 [15].

Acknowledgments

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Electron and positron collisions with molecules

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Commendable studies of the fundamental interactions in electron- and positron-atom have been carried out based on discussions around the differences observed in the electrostatic, exchange (electron only) and polarization interactions [1]. However, even in positron-atom collisions, it has since been observed that the contribution of the virtual positronium formation mechanism, at energies below the positronium formation threshold, contributes significantly to the interaction – even leading to the production of either low-lying positron–atom virtual states or weakly bound states [2]. Formation of these states is expected to be even enhanced for molecules with dipole moments exceeding the critical value of 1.625 Debye [3].

In this report comparative studies of electron and positron total cross sections (TCSs) are carried out (as examples from the more than 70 molecular targets studied) for (I) CH_4, CH_3F, CH_2F_2, CHF_3 and CF_4 molecules for the *fluorination effect*, and (II) CH_3H, CH_3F, CH_3Cl, CH_3Br and CH_3I molecules for the *halogenation effect*. These TCSs have been measured using a retarding potential time of flight apparatus [4]. These effects are also jointly studied, for two molecular groups, in our electron impact differential cross sections (DCSs) are measured using a crossed-beam method [5]. In group (I), only the electron TCSs show the dipole moment characteristic enhanced long-range scattering at energies below 2 eV (also observed in DCSs at 1.5 eV at angles below 50°), as evidenced by the significantly rising TCSs for the polar molecules CH_3F, CH_2F_2 and CHF_3. Positron TCSs show a clear *fluorination effect* above 100 eV, where they are seen increasing in magnitude with increase in the number of F atoms substituted for the H atoms. This is not observed in electron TCSs, although it's clearly observed in electron DCSs as a conspicuous shoulder at 30 eV and angles 60° – 65°. In group (II), though the positron TCSs do not show, in the limit of the current lowest energy range of 0.2 eV, the low energy rise of TCSs expected for the polar CH_3F, CH_3Cl, CH_3Br and CH_3I molecules, the *halogenation effect* is observed over all the energy range 0.2 – 1000 eV. Though both electron TCSs and DCSs, on the other hand, show the typical dipole characteristic long-range scattering below about 1.5 eV, both the TCS and DCS magnitudes show a complicated ordering, i.e. deviating from the expected *halogenation effect*. These and other observations will be systematically discussed at the conference with reference to the dipole moments, molecular polarizabilities and molecular sizes.

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The use of isotope and site labeling for the identification of DEA peaks in biomolecules

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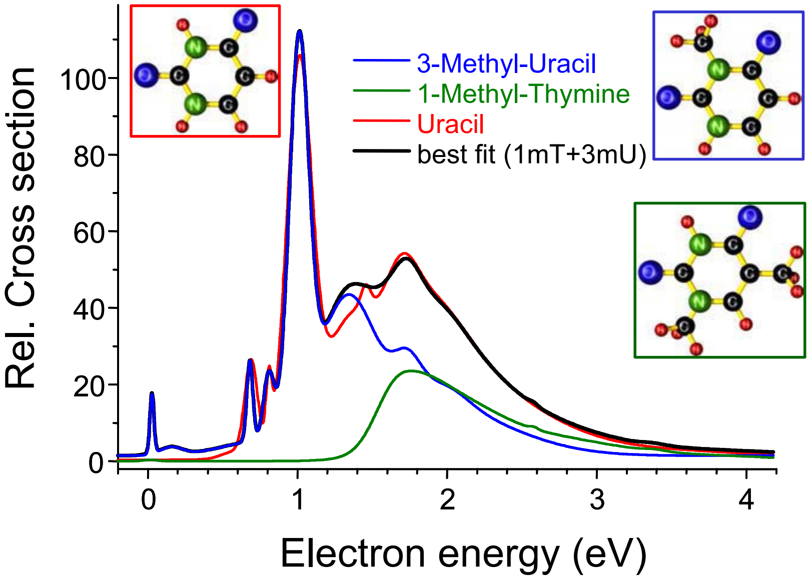
Free electron attachment to gas phase nucleobases (NB) leads exclusively to the formation of fragment anions. For most of the biomolecules studied so far, the most dominant reaction channel is

$$e^- + \mathrm{NB} \rightarrow (\mathrm{NB}^-)^\# \rightarrow (\mathrm{NB\text{-}H})^- + \mathrm{H}. \qquad (1)$$

For the pyrimidine bases uracil (U) and thymine (T) the attachment cross section in the electron energy range between 1 and 3 eV reveals several narrow resonances [1]. By using partially deuterated T with deuterium connected to all carbon atoms it is possible to show that all these resonances originate from the loss of hydrogen from the two nitrogen sites [2]. However, in DNA T forms a glycosidic bond between the 1N nitrogen and the 1C carbon atom of the deoxyribose and thus the 1N hydrogen atom is missing. Furthermore, the other N-hydrogen is part of a hydrogen bridge to adenine. Attachment cross sections for the H loss from thymidine and 1-methyl-thymine (1mT) show a smooth asymmetric resonance at about 2 eV that can be assigned to the loss of the N3 hydrogen atom. Alternatively, the use of 3-methyl-uracil (3mU) leads to hydrogen abstraction exclusively from the N1 position. The Figure below shows the relative partial cross sections for the dehydrogenated anions of U, 1mT and 3mU. The solid black line is a fit of a superposition of the $(1\mathrm{mT\text{-}H})^-$ and $(3\mathrm{mU\text{-}H})^-$ curves to the $(\mathrm{U\text{-}H})^-$ curve.



The complementary reaction channel of (1) is the formation of H^-. For the formation of H^- from U and T the attachment cross section shows four resonances in the energy range between 5 and 12 eV. Experiments with partly deuterated T and methylated pyrimidine bases show that the different peaks in the H^- ion yield can be associated to the loss from the different molecular sites [3]. The energy dependence for H^- abstraction from the carbon sites shows a remarkable resemblance to the energy dependence of strand breaks observed in plasmid DNA [4] suggesting that this reaction may be an important initial step towards strand breaks.

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Low Energy Electron Impact Excitation of Simple Diatomic Molecules – H_2 and N_2

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Recent progress regarding the electron impact excitation of the low-lying states of these important diatomics as well as comparisons with existing theoretical models, regarding differential scattering cross-sections, will be presented. In addition, new work on Rydberg-valence interactions[1] for the dipole-allowed states of N_2 will be discussed. These Rydberg-valence interactions result in complicated, but interesting interference effects in the differential scattering cross-sections and pose challenges for experiments and scattering models.

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Probing Electron Momentum Densities of Molecular Orbitals Using New Multichannel (e,2e) Spectrometers

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Electron momentum spectroscopy (EMS), based on the binary (e,2e) reaction under the high-energy Bethe ridge conditions, has been developed as a powerful means for investigating the electronic structures of atoms and molecules [1]. In particular, its unique ability to look at individual electronic orbitals in momentum space has been widely exploited in the last three decades with the aid of the plane-wave impulse approximation. Nevertheless, the potential of EMS has not been fully achieved for molecules as yet due mainly to the small cross sections involved and the fact that the experiments measure averages over all orientations of gaseous targets. Spherical averaging results in enormous loss of versatile information on collision dynamics and electronic structure; three-dimensional character of the (e,2e) scattering by molecules deteriorates into the one-dimensional momentum distribution or momentum profile.

Very recently, we have developed two types of multichannel (e,2e) spectrometers [2,3]. The first spectrometer [2] measures conventional (e,2e) cross sections, but it features remarkably high sensitivity by simultaneous detection in energy and momentum. The second spectrometer [3] has been developed for examining (e,2e) reactions in the molecular frame. In the axial-recoil limit of fragmentation of the residual molecular ion, measurements of vector correlations between the two outgoing electrons and the fragment ion are equivalent to (e,2e) experiments with fixed-in-space molecules.

In this contribution we report details and performances of the newly developed spectrometers. Our recent studies on several targets will also be presented. Applications to be discussed will involve the first observation of anisotropy of molecular frame (e,2e) cross section [3-5]. We will demonstrate a geometry effect of molecular orientation on the (e,2e) amplitude and how it depends on the nature of the final ion state.

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R-matrix calculations of electron-molecule collisions at low and intermediate energies

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The R-matrix method is now well-established as a reliable and flexible procedure for treating electron collision problems. In particular the UK molecular R-matrix codes have been applied to an increasing variety of electron molecule collision problems. Recent calculations on low-energy electron collisions with water have found outstandingly good agreement with published measurements of differential and momentum transfer cross sections. However the calculated elastic cross sections differ significantly from those inferred from experiment, suggesting that the published data still does not correctly measure the strong forward peak for this process. New calculations have been performed on the 13-atom organic ring molecule tetrahydrofuran with special attention paid to the low-lying resonances in this system: these are found to be numerous, narrow and Feshback in contrast to the standard interpretation of experiment in terms of a few, rather broad, (high energy) shape resonances. No evidence for such shape resonances has been found. A new
molecular R-matrix with pseudo-states (MRMPS) procedure has been developed which allows the correct ab initio treatment of electron collision processes, including ionisation, above the molecular ionisation threshold. Initial studies on benchmark systems suggest that this method works well.

Electrons attached by long-range forces: Quadrupole bound anions

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This talk addresses the notion of quadrupole bound states. First, the difference between dipole- or quadrupole-bound states, on the one hand, and conventional anions, on the other hand, is discussed. Possible criteria to distinguish the two and borderline cases are presented. Then, as a particular example electron binding to succinonitrile (NC-CH_2-CH_2-CN) is considered. For succinonitrile two anionic states have been observed, and these were interpreted as dipole- and quadrupole-bound states associated with two different conformers. Both states are analysed in terms of contributions to their binding energy and in terms of the excess electron's Dyson orbitals. Finally, candidates for molecules showing only quadrupole-bound states are discussed.

High resolution studies of dissociative electron attachment to molecules

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Experimental advances involving laser photoelectron sources have recently allowed detailed studies of low energy electron attachment to several small molecules at (sub)meV resolution [1]. For the first time, the limiting ($E \rightarrow 0$) threshold behaviour for s-wave (e.g. SF_6, CCl_4) and p-wave (e.g. Cl_2) electron attachment could be conclusively demonstrated [1]. At onsets for vibrational excitation, Wigner cusps due to channel interactions were clearly detected, and vibrational Feshbach resonances were observed for the first time in the dissociative electron attachment (DEA) channel [1]. Absolute DEA cross sections over the range E = 0.5 to 200 meV were established by normalizing the measured energy-dependent yields for anion formation to reliable rate coefficients, For comparison with the experimental results, semiempirical resonance R-matrix calculations have been carried out for several molecules; good agreement between the measured and calculated cross sections was achieved for the important cases Cl_2, SF_6, and CH_3I. The input for the theory includes the often known energetic and structural parameters of the neutral molecules and their anions while the parameters of the resonant anion curves are fixed with reference to the known thermal rate coefficients for the DEA process.

With the aim to provide benchmark DEA cross sections for some important molecules and to further test the theoretical calculations, we have extended the Laser Photoelectron Attachment (LPA) method towards higher energies by using a modified approach (EXLPA): it involves magnetically-guided combined acceleration/deceleration of zero-energy photoelectrons from a spatially separated photoionization region to the reaction volume, using as a molecular target either a static gas at 300 K or molecules in a seeded supersonic beam from a heatable nozzle (300 – 600 K). Typical resolutions of the EXLPA data are 20 –30 meV (FWHM). Joining the LPA with the EXLPA data in the energy range 50 – 200 meVyields highly-resolved absolute DEA cross sections from 1 meV up to several eV. At the conference results will be presented for the molecules SF_6 [3], CCl_4, $CHCl_3$, CCl_2F_2, CF_3I [4], and CF_3Br and compared with previous experimental and available theoretical work.

This work has been supported by the Deutsche Forschungsgemeinschaft and by the Forschungszentrum OTLAP. IIF acknowledges support from the US National Science Foundation.

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RECENT PROGRESS WITH THE SCHWINGER MULTICHANNEL METHOD

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When *ab initio* methods for studying electron–molecule collisions were developed, both experiment and theoretical studies were focused on small molecules such as N_2. Although small-molecule studies continue to be important, interest in recent years has increasingly shifted to electron interactions with larger polyatomics. Practical applications within the semiconductor industry, for example, demand electron collision data for molecules such as C_2F_6 or c-C_5F_8 [1]. An especially significant development in recent years has been the realization that slow electrons can directly damage DNA [2], which has spurred tremendous interest in low-energy collisions of electrons with DNA bases, sugars, and other biological molecules.

Owing to the low symmetry and the inherent many-electron nature of the problem, accurate calculations of low-energy electron–molecule collisions are computationally demanding. Moreover, as we will emphasize in this talk, the computational requirements scale rapidly with the molecular size, making studies of polyatomic targets especially challenging. To pursue such studies, we have adapted our computational procedure, known as the Schwinger multichannel method, to run efficiently on highly parallel computers, including workstation clusters, and we have made improvements to remove serial bottlenecks, decrease disk usage, and otherwise improve the overall scalability.

In this talk, we will present some of our recent results for elastic and inelastic collisions of low-energy electrons with biological molecules, in particular the DNA bases and the RNA base uracil. Special emphasis will be given to the characterization of low-energy resonances observed in gas-phase scattering [3] and dissociative attachment [4] studies. The assignment of these resonances is still a topic of discussion [5, 6], and by helping to clarify the assignments, theoretical studies may help to clarify the dissociation mechanisms.

Work by C. W. and V. M. was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, and by the U. S. National Science Foundation, Office of International Science and Engineering. S. d'A. S. acknowledges financial support by the Brazilian agencies FAPESP, CNPq, and CAPES.

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EXCITED STATE FORMATION IN THE DISSOCIATIVE RECOMBINATION OF HNC^+ IONS WITH THERMAL ELECTRONS.

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Dissociative recombination (DR) of molecular ions with thermal electrons often produces radiating molecular fragments. While it is straightforward to survey the resulting emission spectra, it is more difficult to obtain quantitative yields for particular electronic and vibrational states. We have deduced such yields from band intensities in recombining flowing-afterglow plasmas containing HNC^+. The first step in this work consisted of finding out which of the two isomeric ions, HCN^+ or HNC^+ is produced by the reaction Ar^++ HCN that is used to prepare the recombining ions. The reaction was studied in a separate drift-tube experiment. We found that the ionic products of this reaction (which could be either HCN^+ or HCN^+ or a mixture of both) charge-transfer only slowly with xenon. According to earlier reaction studies this indicates that HNC^+, somewhat surprisingly, is the by far dominant product of Ar^+ +HCN compared to HCN^+.

The spectroscopic measurements in the flow tube showed strong emissions of the CN (B-X) violet band around 400 nm which means that recombination of HNC^+ with electrons produces $CN(B^2\Sigma+)$ with a yield that we estimate to be on the order of 10 to 20%.. In addition we observe red-band emissions from the A-X transitions. One problem in this work is that the same emissions can be excited by metastable argon atoms that are known to be present in flow tube plasmas of the kind used in our experiment. Adding small amount of xenon to the flow tube was found to be effective in destroying argon metastables such that its contribution to the excitation of CN(B) could be subtracted. Quantitative recombination yields of CN(B) are then obtained by comparing the observed intensities to computer models of the plasma. At this time, only a limited set of data have been compared to computer models but we hope to be able to present credible yields at the meeting.

LIST OF CONTRIBUTED PAPERS

A NEW APPARATUS FOR THE INVESTIGATION OF ELECTRON IMPACT INDUCED IONIZATION AND FRAGMENTATION OF MOLECULES

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We present a new experimental approach for the investigation of low energy electron-molecule collisions. The goal is to determine the momenta of all charged particles emerging in molecular ionization and/or fragmentation processes. Therefore the collision kinematics of the reaction is completely determined and in many cases the detection of molecular fragments will allow to determine the molecular orientation in space during the collision and therefore enable electron scattering experiments on fixed-in-space molecules.

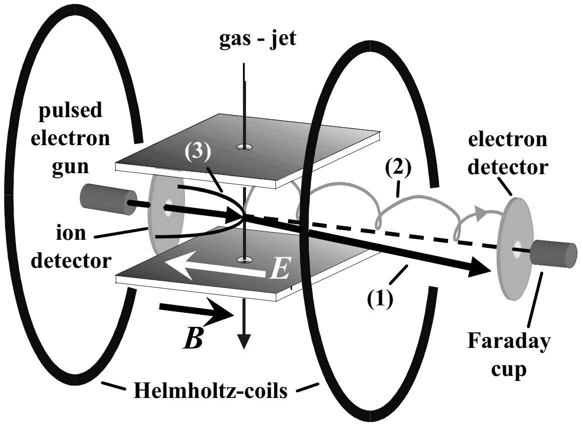

Figure 1: Schematic of the new reaction microscope. (1) Scattered projectile electron. (2) Ionized slow target electron. (3) Positive fragment ions.

The apparatus (Fig. 1) is a modified "reaction microscope" (COLTRIMS technique) in which a dense target gas jet is crossed with a pulsed electron beam. The charged fragments of a reaction are extracted by means of electric and magnetic fields and projected onto time and position resolving multi-hit-detectors with central bores to allow the passage of the primary projectile beam. In contrary to conventional COLTRIMS spectrometers the collision kinematics is not determined by means of the recoiling ion momentum but the scattered projectile electron itself is detected (in addition to all electrons emitted by the target). The coincident detection of one or several ions allows the additional characterization of the molecular fragmentation process. While so far projectile energies down to 20 eV where realized, in future energies in the few eV range with sub 100 meV energy resolution are envisaged using a GaAs photo emission electron source.

For illustration, in Fig. 2, the (e,2e) fully differential cross section for emission of a 10 eV electron is shown for the helium target and all possible emission angles. Presently first measurements on molecular hydrogen are performed.

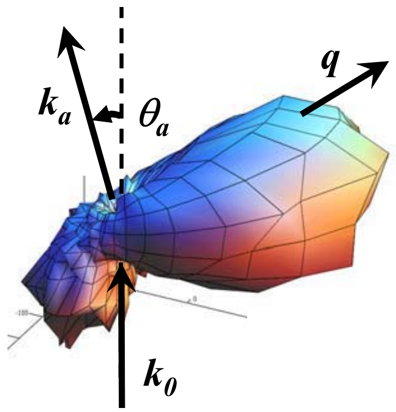

Figure 2: Fully differential cross section for emission of a 10 eV electron by impact of a 107 eV electron (momentum $\boldsymbol{k}_0$) on helium. The projectile scattering angle θ_a is 20° (momentum $\boldsymbol{k}_a$). $\boldsymbol{q}$: momentum transfer.

ON THE DESCRIPTION OF ELETRON – MOLECULE COLLISION IN THE SEMICLASSICAL PHASE – SPACE APPROACH

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1. Introduction

Phase-space representations of quantum mechanics play an important role in several branches of physics [1, 2]. Although there exist a large number of phase-space representations discussed in the literature, the Weyl – Wigner representation has come to play the role of a canonical phase-space representation, mainly because of its simplicity. In the present communication, we summarize how one could calculate the elastic differential cross section for the collision between an incident electron and a diatomic molecule. The method makes use of the quantum phase space Wigner function associated to a vibration degree of freedom for the target molecule.

2. Developments

Although the present method could be applied to any kind of reactions, for convenience we are considering a nonreactive collision represented by

$$A + BC\,(n) \rightarrow A + BC(m)$$

where n a m refer to any quantum vibration numbers to be specified.

It is assumed that the molecule vibrational motion can be described by a harmonic oscillator in an " n " state. The corresponding Wigner function is written as

$$W^{(n)} = (-1)^n \frac{1}{\pi\hbar} \exp\left(\frac{-2E_c}{\hbar\omega}\right) L_n\left(\frac{4E_c}{\hbar\omega}\right)$$

where E_c and ω are the classical energy and frequency of the harmonic oscillator and $L_n(x)$ is the Laguerre polynomial. In the present study we are considering the Yukawa type potential to describe the projectile – target interaction.

The quantum full time evolution of the Wigner function is governed by the Weyl-Wigner representation of the quantum von Neumann – Liouville equation. In particular, for harmonic potential interaction, we keep the lowest order term of the corresponding $\hbar$- power series for the Liouville operator,

$$\frac{\partial W(q,p,t)}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial q} + \frac{\partial V}{\partial q}\frac{\partial W}{\partial p}$$

where $dq/dt = p/m$ and $dp/dt = -\partial V/\partial q$ are the classical Hamilton's equations. In particular, the classical propagation of the Wigner distribution function leads to a exact description of the harmonic oscillator.[3] Each phase-space point of the initial Wigner distribution function (q,p) is propagated along a classical trajectories. Therefore, the resulting Wigner distribution function at time t can be used to determine the final oscillator quantum state. The classical trajectory picture leads to the description of the elastic differential cross section of the reaction.

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Low-Energy Electron Impact Dissociation of Molecules and Molecular Ions

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Electron collisions with molecules and molecular ions that lead to dissociationand excitation play a key role in a number of environments, since they produce the radicals and molecular fragments that initiate and drive the relevant chemistries. Examples of such systems can be found in biology as well as in chemistry and physics; they range from the technologically important plasmas used in plasma enhanced chemical vapor deposition, to planetary atmospheres and interstellar clouds, to DNA damage driven by secondary electron cascades produced by radiation. Since the mass of the electron is some three orders of magnitude less than that of the nuclei, it is a general prediction that in electron-molecule or electron-molecular ion collisions, there is little vibrational energy transfer or dissociation. However, there is an important exception to this rule, namely, systems where there is an intimate coupling between the electron interaction with the target and the nuclear dynamics of the target. The results of such an interaction can be quite dramatic. In these cases, the electron can temporarily attach to the molecule and change the forces felt between its atoms for a period of time comparable to a vibrational period. This can lead to resonant vibrational excitation and dissociative attachment, for neutral targets, or dissociative recombination in the case of ions.

We will outline the basic theory that underlies these processes, and our approach to study them. In the systems presented here, there exists one or more resonant states that lead to dissociation. The resonance parameters, the position and autoionization widths are taken from accurate electron scattering calculations using the Complex Kohn variational method. These parameters are then used as input to the dynamics calculations. The dyamics were studied using time-dependent wave packet methods, Multi-Channel Quantum Defect Theory (MQDT) and the solution of the time-independent equation using a Discrete Variable Representation (DVR) and exterior complex scaling. We will illustrate these methods with application to dissociative attachment in ClCN and BrCN, and dissociative recombination in the rare gas diatomic ions, He_2^+ and Ne_2^+ and in the HCN^+ and HNC^+ systems.

Electron collisions with CFX_3 and CF_2X_2 (X=Cl, Br, I) molecules: elastic and rotational excitations cross sections

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Dissociative electron attachment of molecules containing Carbon and halogen atoms have been widely studied over many years. These molecules are used in many practical fields as in chemical etching in plasma processing, which is an important step in the semiconductor fabrication. However, more information on the cross sections for electron collisions are needed. Experimental results on the cross sections are rare, and theoretical calculations are thus necessary. In the present work we report integral, differential and momentum transfer cross sections for elastic scattering of low-energy electrons by $CFCl_3$, $CFBr_3$, CFI_3, CF_2Cl_2, CF_2Br_2 and CF_2I_2 molecules. To calculate the cross sections we employed the Schwinger multichannel [1, 2] method with pseudopotentials [3] in the fixed-nuclei static-exchange approximation for incident energies up to 30 eV. We compared the differential and integral cross section of these molecules and found similarities between them. We also found a shape resonance in the integral cross sections of $CFCl_3$, $CFBr_3$ and CFI_3, and find two shape resonance in cross sections of CF_2Cl_2, CF_2Br_2 and CF_2I_2. We also compared our results with available experimental cross sections of $CFCl_3$ and CF_2Cl_2 and found good agreement. We also included the rotation effects to calculate cross sections for $J = 0, 1, 2, 3, 4, 5, 6$ excitation levels using the Adiabatic Nuclei Rotation approximation [4]. Since all molecules studied have permanent dipole moments, we included a first Born approximation [5] of the dipole potential correction to account for the long-range potential. $CFCl_3$, $CFBr_3$ and CFI_3 belong to C_{3v} symmetry group and are symmetric tops; CF_2Cl_2, CF_2Br_2 and CF_2I_2 belong to C_{2v} and are asymmetric tops. We compare the rotationally summed and rotationally unresolved cross sections for all molecules and we verify a very good convergence.

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ELECTRON ENERGY LOSS SPECTRA OF ALANINE

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In order to understand mechanisms of radiation damage in cells, we have been studying processes of elastic electron scattering, exitation and formation of resonances in molecules such as glycine (H_2N-CH_2-COOH) and alanine (CH_2-CH(NH_2)-COOH).

We have used an electron spectrometer ESMA [1] to record energy loss spectra. This spectrometer is equipped with the titanium oven heated by coaxial heater and hemispherical energy selectors both in monochromator and analyzer. The electron beam crosses the molecular beam perpendicularly.

Alanine exists under standard condition as a crystalline powder. The crucible of the oven was filled with 99% pure alanine. A sufficient vapour pressure for the formation of a molecular beam can be achieved at temperatures of about 450 K. The molecular beam was formed by effusing the molecules through a capillary into the interaction region. In the gas phase, alanine exists in the neutral tautomeric form only whereas in aqueous solution and in the solid phase the zwitterion is the predominant form of this amino acid [2].

An energy loss spectrum, focused on inelastic states, at 60 eV impact energy and scattering angle 6° is shown in figure 1. The pressure was in the range of 10^{-6} Torr during the experiment.

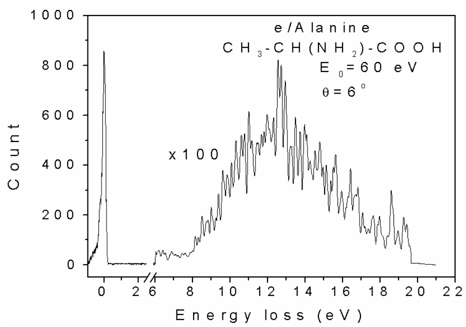

Figure *1. Electron energy loss spectrum of alanine .*

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ISOMER EFFECT BETWEEN PROPENE AND CYCLOPROPANE BY ELECTRON IMPACT

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We have carried out experimental and theoretical studies on electron scattering from the propene (C_3H_6) and cyclopropane (cyclo-C_3H_6). Total and differential cross sections (TCS and DCS) are reported for these molecules. Hydrocarbon molecules play an important role in several areas of applications, e.g. plasma diagnostics in the Tokamak fusion divertor [1]. To our knowledge, there are some few attempts that studied the isomer effect in these molecules by electron impact [2]. In this study, we examine the similarities and differences observed in the cross sections between these molecules due to the isomer effects and provide some rationale on the collision dynamics for electron impact.

A retarding-potential time-of-flight (RP-TOF) apparatus [3] was used for total cross section measurements, while the differential cross sections were measured using the crossed-beam setup, which was same as used in our previous studies [4].

Fig. 1 shows the TCSs for these molecules at energies 0.4 – 1000 eV. TCSs for C_3H_6 are larger than cyclo-C_3H_6 below 60 eV and show a lower energy peak at ~2.2 eV before the larger and broader one at ~9 eV, which is attributed to the shape resonance due to vibrational excitation of C_3H_6 molecules. Both TCSs become approximately equal above 60 eV.

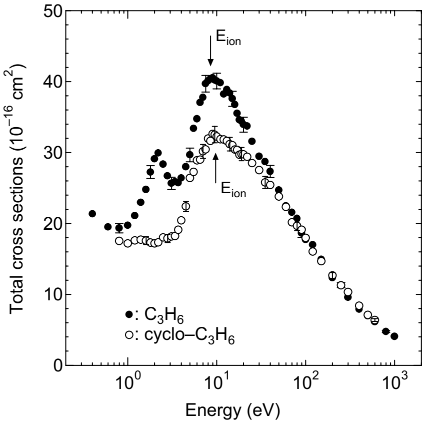

Fig. 1. TCSs for C_3H_6 and cyclo-C_3H_6 in energy range of 0.4 – 1000 eV. Arrows show the thresholds for ionization.

Fig. 2 shows the DCSs for elastic scattering from C_3H_6 and cyclo-C_3H_6 at 2 and 5 eV. These results show the most drastic difference between these two isomer molecules. As shown in Fig. 2, forward scattering for C_3H_6 is stronger than that for cyclo-C_3H_6. It was considered that this result was due to the presence of the dipole moment and larger polarizability in the C_3H_6 than the non-polar cyclo-C_3H_6.

At the conference, we will compare these experimental results with the cross sections calculated by the Continuum Multiple Scattering method [5] and discuss in detail the isomer effect in the cross sections for these molecules.

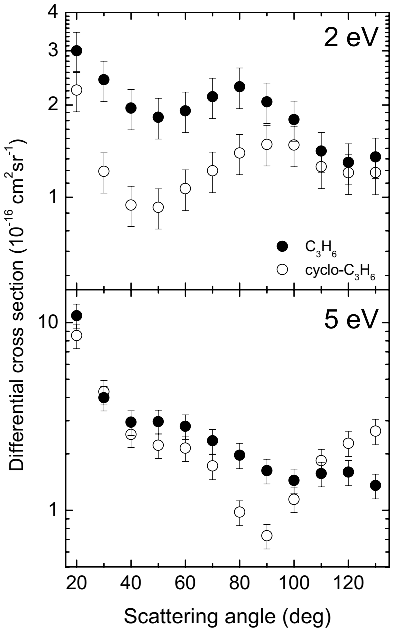

Fig. 2. DCSs for C_3H_6 and cyclo-C_3H_6 by electron impact at 2 and 5 eV.

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CH_3 Neutral Radical Formation from CH_4 by Electron Impact

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Absolute electron-molecule impact dissociation cross sections are of interest in many fields of physics and chemistry, and in industrial applications such as chemical vapour deposition and plasma etching of microelectronic devices. However, experimental data, especially on cross sections for neutral radical formation, is scarce mainly because of the difficulties involved in the measurements of neutral fragments [1].

In this work, electron impact dissociation of CH_4 molecules into the CH_3 radicals have been investigated over the energy range 15.0 – 37.0 eV. The experimental procedure involves a dual-electron-beam in a two-stage collision system in conjunction with a quadrupole mass spectrometer (QMS). This method also uses the threshold-ionization mass spectrometry method [2]. Significant differences, in magnitudes of up to four times at 100 eV, exist between the only available absolute measurements by Sugai *et al.* [2] and Moore *et al.* [3]. Our data shows very close agreement with the Moore *et al.* data, which show reasonable consistency with the available CH_4 total dissociation data by Winters [4].

At the conference we will discuss these results in detail and also hope to present results on the angular distribution measurement spectra of these radicals.

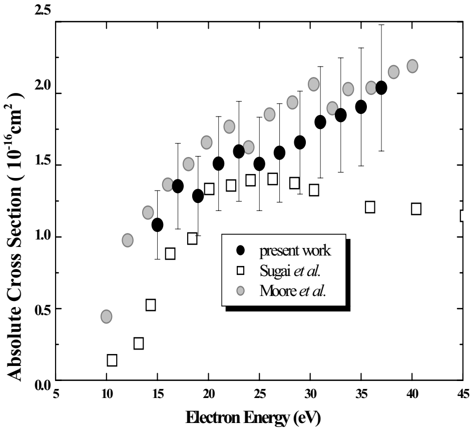

Fig. 1 Electron impact absolute cross sections for CH_3 neutral radical formation from CH_4 molecules.

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Comparative Study of Electron and Positron Scattering from ***c***-C_4F_8

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Perfluorocyclobutane (*c*-C_4F_8) molecules are a plasma processing gas employed in the plasma etching of semiconductors. Its CF_2 radicals have especially been used in the selective etching of SiO_2 [1]. These CF_2 radicals are also formed indirectly in a *c*-C_4F_8 plasma by dissociative electron impact with its C_2F_4 by-product [2]. On the other hand, as recently reviewed [3], predictions of positron bound states with neutral atoms, use of the positron emission tomography (PET) in the study of metabolic processes, and applications of positron scattering to the characterization of materials, have increased interest in positron scattering studies. In this study we carry out a comparative of electron and positron scattering total cross sections (TCSs) from *c*-C_4F_8 molecules.

The TCS measurements were carried out for 0.8-600 eV electron and 0.7-600 eV positron impact using a linear time-of-flight apparatus [4]. The results are shown in Fig. 1. Below 2.2 eV, electron and positron TCSs show the striking opposite trends. The rising trend in electron TCSs agrees well with the electron affinity (+0.63 eV) and increasing electron attachment cross sections below 1 eV, while the drop in positron TCSs could attributable to the near cancellation of the attractive and repulsive scattering in this region [5].

Detailed comparative studies of these and other features will be presented at the conference.

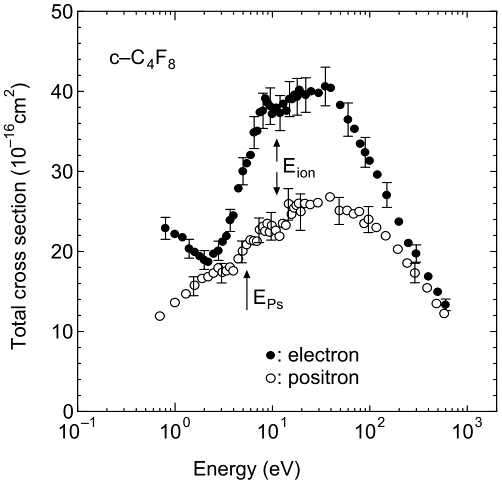

Fig. 1 *c*-C_4F_8 electron and positron TCSs. Arrows show the thresholds for ionization, E_{ion}, and positronium formation, E_{Ps}.

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ADDITIONAL DETAILS ON ELECTRON SCATTERING BY MOLECULAR RADICALS

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Low-energy scattering of electrons by radicals is of interest in a wide range of chemical and physical processes. Nitric oxide, for instance, is important in atmospheric processes and plays key functional roles in a variety of physiological systems. It is also used as a plasma gas. Knowledge of collision dynamics with CF is important in plasma etching processes. It is formed within plasmas under electron bombardment of C_2F_4, which has been proposed as a new feed gas due to its relatively benign impact on the atmosphere. Because of their high reactivity, radicals like CF are difficult to work with experimentally, making theoretical studies of collision processes crucial in the determination of cross sections, transition rates and other quantitative characteristics. Despite the need for *ab initio* results on electron scattering by NO and CF radicals, such calculations are scarce, particularly in the energy region below 2 eV, which is dominated by negative ion resonances. In the case of NO, recent experimental measurements of Allan [1] and of Jelisavcic *et al.* [2] allowed comparison and represented a test to theoretical models that could later be applied to radicals for which experimental data is unavailable, like CF. This prompted us to perform an *ab initio* study of elastic scattering and vibrational excitation of NO by electron impact in the low-energy (0-2 eV) region where the cross sections are dominated by resonance contributions [3]. We employed a nonlocal treatment of the nuclear dynamics, which was found to remedy the principal deficiencies of the local complex potential model. The complex-valued potential curves were obtained by combining large-scale configuration-interaction calculations for the resonance positions with fixed-nuclei, complex Kohn calculations for determining the resonance lifetimes. The resulting low-energy cross sections are dominated by shape resonance contributions associated with the $^3\Sigma^-$, $^1\Delta$ and, to a lesser extent, $^1\Sigma^+$ states of NO^- and display pronounced, overlapping boomerang structures that give irregularly shaped vibrational excitation cross sections.

We have also studied dissociative electron attachment to NO via the $^3\Sigma^-$ negative ion resonance which gives ground state $N(^4S) + O^-(^2P)$. Our results show that the dissociative attachment cross sections in this channel that originate from the ground vibrational state of NO are extremely small, as confirmed by several experimental studies. However, the dissociative attachment cross section is predicted by these calculations to increase by several orders of magnitude when the dissociation takes place from vibrational excited states of NO. We investigated the origin of this dramatic enhancement and predict that dissociative attachment cross sections producing ground state atomic products should be measurable starting from vibrational levels above approximately $\nu = 10$.

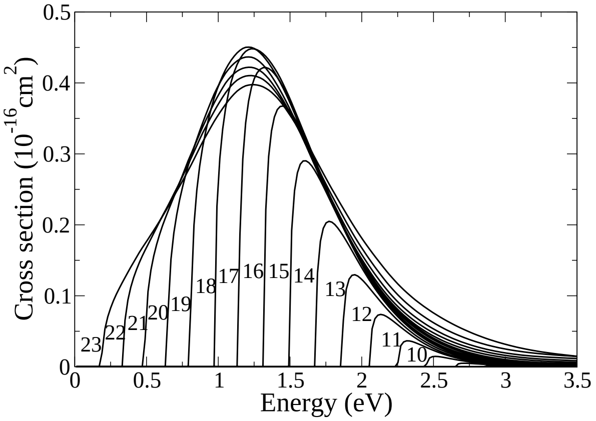

Fig. 1. NO Dissociative attachment cross sections from vibrationally excited states.

Preliminary results of low-energy electron scattering by radical CF, which is isoelectronic with NO, will also be discussed.

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Dissociative electron attachment to water

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Abstract

Dissociative electron attachment (DA) to H_2O is of direct importance for both biological and techological systems. The calculations on H_2O and H_2S presented comprise the first *ab initio* treatment of DA to a polyatomic molecule employing the full dimensionality of nuclear motion. Calculations of the DA cross section via the $^2B_1$ state of H_2O agree well with experiment, reproducing the high degree of vibrational excitation of the OH fragment. Several interesting features of the A' manifold of resonances for H_2O have been discovered, including a conical intersection between the $^2A_1$ and $^2B_2$ Feshbach resonances and a branch-point degeneracy between the $^2B_2$ shape and Feshbach resonances. This latter feature has no direct analogue in bound-state theory, although the theory of "hidden crossings" represents an interesting parallel. The two-seam structure of the $^2A_1$ / $^2B_2$ conical intersection is probed. Preliminary calculations on the Renner-Teller coupled $^2A_1$ and $^2B_1$ surfaces, and on electronically coupled diabatic $^2A_1$ and $^2B_2$ surfaces, will be presented.

In addition, the angular dependence of the H + OH channel for the $^2B_1$ state of H_2O and that of the analagous channel and state of H_2S have been calculated by incorporating the mixing of different partial waves into the entrance amplitude, and for H_2S, the variation of this mixing with geometry. The fact that the H_2S entrance amplitude is not factorable into a part dependent upon the internal coordinates and one dependent upon the relative orientation of the molecule and the incident electron beam is the most probable cause of the final-state-specific angular dependences observed in experiment.

RESONANCE SURFACES FOR H_2O^-

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Electron collisions with water are very important for the understanding of radiation damage in biological system, atmospheric processes, masers, etc.. These collisions can result in the rotational, vibrational and/or electronic excitation of the molecule but they can also induce fragmentation. Specifically, low-energy electrons can produce fragmentation via dissociative electron attachment (DEA) and electronic excitation into dissociative states.

Experimental work on water break-up has focused on dissociative attachment. More recently measurements of ground state OH production via electron impact have been performed [1] showing the different contributions of DEA and dissociative excitation. Few theoretical studies on the resonance curves for DEA of water are available [2]. Among them, one has been carried out taking into account a single dissociative coordinate [3], the assumption being that dissociation proceeds into the formation of H and OH. The discrepancy between the theoretical results and the experimental measurements of [1] suggest that full three-dimensional studies are needed.

The R-matrix method and the R-matrix polyatomic code [4] is used to treat the electronic part of the process. We have performed fixed-nuclei calculations for 840 geometries of H_2O. These were obtained by varying the internal nuclear coordinates of the molecule, using 8 different angles and 14 different OH internuclear distances. Following [3], we have incorporated nine target states in the close-coupling expansion and calculated cross sections for electronic excitation into the first 4 excited states as a function of geometry. In accordance with previous calculations and experiments [5] we found three Feshbach resonances below the ionisation threshold. In C_{2v} symmetry these resonances are labelled $^2B_1$, $^2A_1$ and $^2B_2$. The DEA process is likely to proceed via these resonances. Since the first four excited states of H_2O are dissociative, excitation into any of these will produce fragmentation.

We will present resonance positions and widths as a function of geometry and for the resonances. These results are the starting point for a full-dimensional study of the DEA and dissociative excitation processes.

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A THEORETICAL STUDY ON ELASTIC ELECTRON-CF_2 RADICAL COLLISIONS

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Electron-molecule collisions play an important role in a number of physical and chemical processes. In particular, interest on electron collisions with highly reactive radicals such as CH_x, CF_x, (x= 1,2,3), etc, has grown recently, in view of their important role in developing plasma devices. Specifically the CF_x radicals are some of such important fragments. These radicals can be produced from dissociation of CF_4 either by collisional and/or photodissociation processes. Since CF_4 is frequently used as a reactant gas plasma etching processes in the semiconductor industries, the knowledge of several cross sections for e -CF_x collisions is relevant. Unfortunately, experimental determination of such data is difficult. Therefore, theoretical calculations are presently an important manner to fill this lacuna. In this work we present a theoretical study on electron scattering by difluoro-methylene (CF_2) radical in the low energy range (1-30 eV). The present study made use of a optical potential, composed by static, exchange and correlation-polarization contributions, to represent the electron-radical interaction dynamics. The Iterative Schwinger variational method [1] is used to solve the scattering equations.

Fig. 1 shows our DCS's for elastic e $-CF_2$ collision calculated at incident energy of 3 eV. The recent theoretical DCS's for this radical [2], as well as calculated [3] and experimental ICS's [4] for electron scattering by O_3, which is an isoelectronic molecule of CF_2, are also shown for comparison. In general, there is a good agreement between the present calculated data and those of Rozum and Tennyson [2]. It is interesting to see that there is also a fairly good agreement between our results with the calculated DCS's for O_3, particularly at intermediate and large scattering angles. This fact may indicate the relavance of the intereaction between the scattering electron and the valence electrons of the targets. The discrepancy seen at small angles is probably due to the different dipole moments of CF_2 and O_3. Additional results will be presented during the Symposium. This work was partially supported by the Brazilian agencies CNPq and FAPESP.

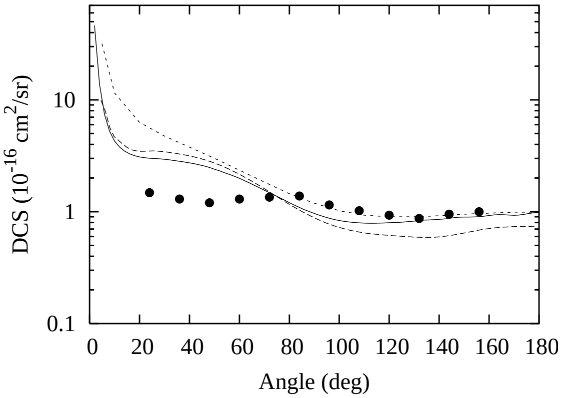

Fig. 1. DCS's for elastic electron scattering by CF_2 at 3 eV. Full curve, present results; dashed line, calculated results for e $-CF_2$ scattering of Rozum and Tennyson [2]; dotted line, the calculated results for e $-O_3$ scattering of Lee *et al.* [3]; full circles, experimental results for e $-O_3$ of Shyn and Sweeney *et al.* [4].

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ELECTRONIC EXCITATION OF COF_2 AND C_3F_6 MOLECULES BY ELECTRON IMPACT

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COF_2 has been advocated as a suitable cleaning gas in the Chemical Vapor Deposition (CVD) equipment, used in various processes in the semiconductor industry, and has thus attracted a lot of attention. Compared with other conventional cleaning gases, its global warming potential is as small as a few tens of thousandths. However, little is known about the physical and chemical properties of this molecule. On the other hand, C_3F_6 is invaluable as an etching gas in plasma processing, due to its small global warming potential and a short atmospheric lifetime. However, although there have been some works on photoelectron spectroscopy on these molecules [1-2], there is almost no data on electron scattering.

The experimental apparatus consists of a typical cross-beam method in conjunction with the relative flow technique [3]. The experimental resolution was about 40 meV (FWHM). Electron energy loss spectroscopy (EELS) spectra of COF_2 were measured at 30 eV and 100 eV at the fixed angles of 10º and 5º, respectively, while sweeping the energy losses over the range 5 – 18 eV. EELS spectra of C_3F_6 were measured at 20 eV and 100 eV at the fixed angles of 10º and 5º, respectively, while sweeping the energy loss over the range 2 – 14 eV. Part of the results from this study is shown in Fig. 1.

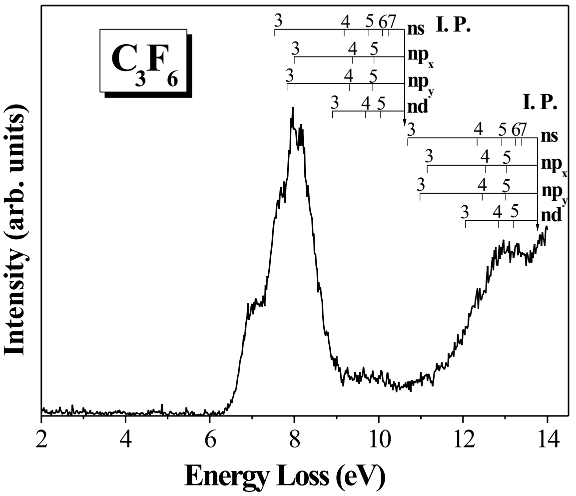

Fig. 1. EELS spectrum of C_3F_6 at the impact energy of 100 eV and angle of 5º.

In Fig. 1, the assignment of the observed broad features and the ionization potential (I. P.) for the 7.5 – 10.6 eV are from the VUV photoabsorption spectra of Ref. [2]. The second I. P. for the region 10.6 – 13.8 eV is from Ref. [4]. Three broad structures due to optically allowed transitions have been observed at about 7 eV and 7.5 eV and attributed to the $C = C\ \pi \rightarrow C - F\ \sigma^*$; $C = C\ \pi \rightarrow C = C\ \sigma^*$ (both dissociative); and at 8.2 eV, due to $C = C\ \pi \rightarrow C = C\ \pi^*$ excitations. The Rydberg states assignments shown at 7.5 – 10.6 eV are from Ref. [2], while we have assigned those at 10.6 – 13.8 eV using the standard Rydberg series equation and quantum defect values from Ref. [2]. Distinct differences have been observed in the EELS spectra above 11.5 eV between impact energies of 20 eV and 100 eV. Detailed discussions of these results and those for COF_2 will be presented at the conference.

This work was partially supported by the CUP program between Japan and South Korea. We also thank the Daikin Co. for kindly supplying us with the COF_2 gas sample.

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Inner-shell excitation of N 1(s) in N_2O molecules by electron impact.

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Abstract

Distorted-wave approximation (DWA) is applied to study excitation of core-level electron in N_2O molecules by electron impact. More specifically, we report calculated differential (DCS) and integral (ICS) cross sections for the $X\,^1\Sigma^+ \rightarrow^{1,3} \Pi(2s\sigma \rightarrow 3p\pi)$and $X\,^1\Sigma^+ \rightarrow^{1,3} \Pi(2s\sigma \rightarrow 3p\pi)$ transitions in the N_2O molecule and comparison is made with $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(1s\sigma_u \rightarrow 1p\pi_g)$and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(1s\sigma_g \rightarrow 1p\pi_u)$ transitions in the N_2 molecule in the 400 - 900 eV incident energy range. The ratios, named RI(3:1), calculated by dividing the distorted-wave integral cross sections(ICS), for transitions leading to the triplet and the singlet core-excited states as a function of incident energy are also reported. The present study shows the RI(3:1) behavior for the N 1s $\rightarrow$ π transition in each species here studied. The generalized oscillator strength(GOS) profiles for discrete N 1s excited states of N_2O and N_2 have also been calculated, and are compared with the available data reported in the literature. Quantitative agreement between the present theory and experiments is also satisfactory.

THESHOLD ELECTRON IMPACT STUDIES OF MOLECULES

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Threshold Electron impact studies, which distinguish and detect electrons scattered by atoms and molecules in the energy range from 0 to 10 meV, are very important, because the selection rules applied to it are much more relaxed compared with those applied to the photoionization process, or even to no-threshold electrons inelastically scattered. Various important process occur in threshold electron impact excitation of atoms and molecules, by instance, electron –electron correlation effects close to ionization potentials, resonance formation, and energy exchange due to post-collision integrations. In the present work we present the preliminary results from a threshold electron impact spectrometer built up in our laboratory. The spectrometer consists essentially of a monochromatized electron gun, an effusive gas source and an electron analyzer, which utilize the penetrating field technique [1] for the efficient collection of threshold (nearly – zero energy) electrons. It can be tuned to accept threshold electrons (< 20 meV) and work with a power resolution of 716, with a high signal/noise ratio. The electron gun operates continually in the energy range 1.5 to 20 eV, producing electron beam with 0.5 mm diameter and current intensity about 10 nA. This apparatus can also be tuned to operate as Electron Energy Loss Spectrometer, fixing its impact energy and scanning the collection energy of analyzer.

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Acknowledgments:

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ANOMALOUS MOBILITIES OF MOLECULAR IONS IN COOLED HELIUM GAS

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The dominant long-range ion-neutral interaction is the polarization potential which is in inverse proportion to the fourth power of the ion-neural distance. Because of this fact, the mobility of an ion in a gas generally approaches a finite constant value, which is called the polarization limit K_{pol}, as both an electronic field and temperature are lowered. However, more than ten years ago, we had found that the mobilities of CO^+ and O_2^+ in He at 4.3 K have much smaller values than K_{pol} in the low electric field region, and that of N_2^+ shows ordinary behavior. In order to understand this phenomenon, we had performed the mobility measurement for various molecular ions, i. e. NO^+, CH^+, CH_2^+, NO_2^+, CO_2^+, and CO_2^{2+}. Normalized mobility, which is defined as the ratio of reduced mobilities K_0 and K_{pol} is shown in Fig. 1 for five molecular ions. As the result of these experiments, it has been found that N_2^+ is only an exception.

To reveal the mechanism of this experimental finding, we had calculated the molecular ion mobility in He with the classical theories. It is necessary to obtain the interaction potential between the molecular ion and He atom for the calculation of the mobility. Therefore multi-reference SD-CI calculations using a *spdf* basis set were performed to obtain the potential energy surfaces for the N_2^+-He and O_2^+-He systems. Using the calculated potentials, we evaluated the momentum-transfer cross sections as a function of the collision energy with the classical trajectory method. Finally, by the calculation based on the two-temperature theory, we obtained the reduced mobility K_0 as a function of the effective temperature T_{eff} after the calculation of the collision integral $\bar{\Omega}^{(1,1)}$ which is the thermally averaged momentum-transfer cross section.

The experimental and calculated mobilities of O_2^+ in He gas are shown in Fig. 2. As can be seen in this figure, the reproduction by the theoretical calculation is satisfactory in this collision system. We analyzed each classical trajectory to find the reason why O_2^+ shows smaller mobilities than K_{pol} at the low T_{eff}. In the first half of the collision, the relative velocity is accelerated by the attractive potential between O_2^+ and He, and the rotational motion of O_2^+ is automatically excited due to the anisotropic interaction potential even if the collision energy is much lower than the lowest rotational excitation energy. In the very low collision energy, the kinetic energy of the relative motion becomes smaller than the depth of the potential well, and O_2^+ and He make a quasi-stable complex. This collision process resembles the quantal Feshbach resonance. In the latter half of the collision, the complex dissociates in the random direction and the rotational state returns to the initial one. This process does not change the relative energy, but the averaged velocity of O_2^+ in the initial direction is reduced by this type of collision. This mechanism has similarity with *the laser cooling.*

Because of such mechanism, the momentum-transfer cross section is enhanced to be much larger than the classical orbiting cross section, and the mobility becomes smaller than K_{pol}. This mechanism is also reproduced in the quantal calculation using wave packet propagation. By similar analysis, we found that the different behavior of N_2^+ is ascribed to small rotational rates due to the very isotropic potential energy surface.

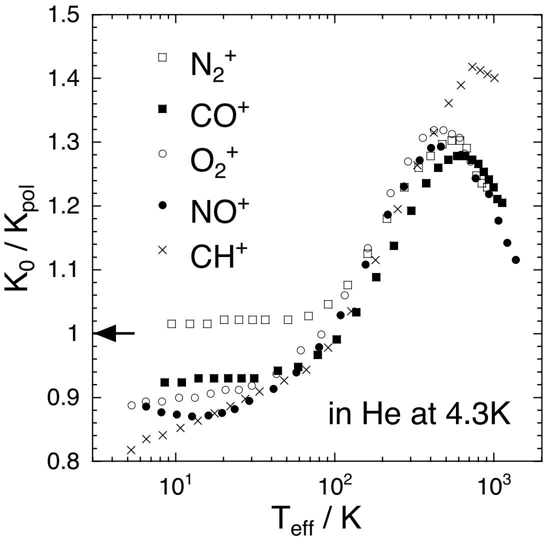

Fig. 1. Normalized mobilities of five molecular ions in He gas at 4.3 K.

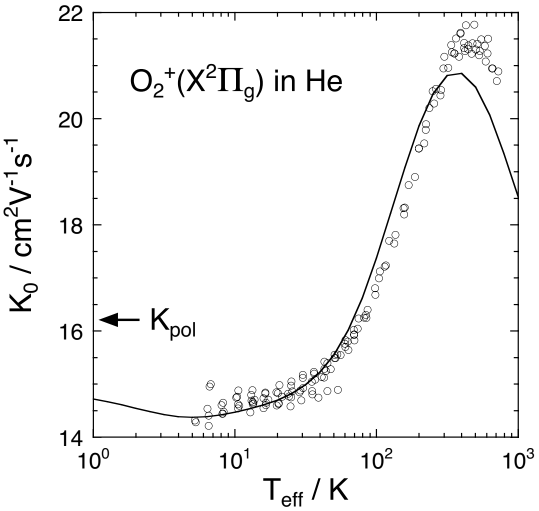

Fig. 2. Measured and calculated mobilities of O_2^+ in He gas at 4.3 K.

CROSS SECTIONS FOR ELASTIC ELECTRON-C_3H_8 COLLISIONS

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Electron- hydrocarbons scattering data are relevant to various applications such as combustion and interstellar clouds chemistry, and cometary and planetary's atmospheres[1] studies. They also play important role in fusion plasma modeling as some hydrocarbons are generated in fusion plasmas by the continuous sputtering of graphite lined *tokamak* walls. Hydrocarbons like C_3H_8 are used as source of carbon atoms during chemical vapour deposition reactions as well as in plasma processing in industries[2]. Although several groups have already measured total cross sections (TCS) in the intermediate energy range for e^--C_3H_8 much less is available on experimental elastic differential scattering cross sections (DCS)[3] and more information is needed.

In this work we report experimental DCS values for e^--C_3H_8 in the 100 to 500 eV energy range and for scattering angles of 7 to 130 degrees. The measurements were performed in a crossed-beam experiment and absolute values were obtained with the Relative Flow Technique (RFT). In Fig. 1, we show our experimental data at 100 eV in comparison to available values. Excellent agreement is seen between the two sets of experimental data. More results and discussion will be presented during the Symposium.

We thankfully acknowledge the financial support of FAPESP, CNPq, and FINEP-PADCT.

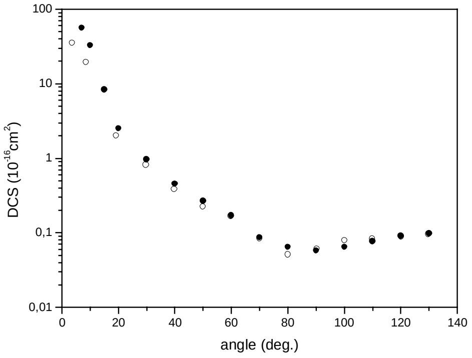

Figure 1 DCS for e^- - C_3H_8 scattering at 100 eV. Full circles, present experimental data; open circles, experimental results of Tanaka et al.[3].

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CROSS SECTIONS FOR ELECTRON-SIMPLE HYDROCARBONS COLLISIONS

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Electron-hydrocarbons scattering data are relevant for fusion plasma modeling. They also play important role to electron-initiated mechanisms present in the combustion of several commonly used materials, and to the chemistry of interstellar clouds and planetary and cometary's atmospheres[1]. Hydrocarbons are also important part of the building blocks that constitute living matter and are a source of carbon atoms for chemical vapour deposition reactions and plasma processing in industries[2]. Motivated by this relevance our group has recently engaged on developing systematic studies on electron-hydrocarbon interactions in the intermediate energy region where there is lack of cross sections values.

In this work we report experimental cross sections for e^--simple hydrocarbon scattering in the intermediate energy region. In Fig. 1, we show total cross sections (TCS) for the electron – C_2H_6 and C_4H_{10} collisions in the energy range of 200 to 1000 eV. (TCS) were measured in a linear transmission instrument[3]. More results and discussion will be presented during the Symposium.

We thankfully acknowledge the financial support of FAPESP, CNPq, and FINEP-PADCT.

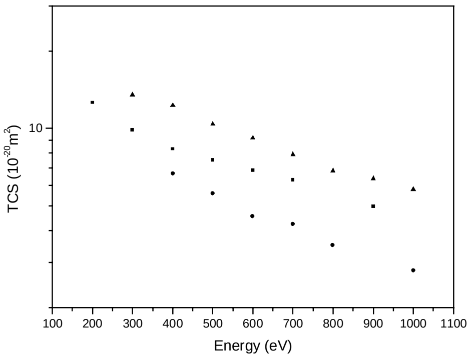

Figure 1 TCS for e^- - hydrocarbon scattering. Circles, C_2H_6 and triangles C_4H_{10}.

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AB INITIO R-MATRIX STUDY OF ELECTRON SCATTERING FROM TETRAHYDROFURAN

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In the last decade, low energy electron (LEE) scattering from biomolecules, and in particular from DNA constituents, has attracted considerable interest. It has been demonstrated [1] that not only primary high-energy radiation but also secondary LEEs can induce DNA damage. These electrons, produced by the ionizing radiation with energies below 20 eV, are the most abundant [2]. They can form resonant states when they scatter from DNA, which may lead to the fragmentation of the molecule via dissociative electron attachment (DEA). Indeed, DEA has been shown to be the main process of LEE induced DNA damage [3].

Tetrahydrofuran (THF), C_4H_8O, is of particular interest in the study of electron scattering on DNA, as it is the simplest model for the deoxyribose ring. Ptasińska et al. [4] recently showed that deoxyribose is extremely fragile compared to the nucleobases. Several experiments have been performed on this system (see [5] and references therein) both in gas and solid phase, but until now, no theoretical study was available.

In spite of the availability of several theoretical methods to treat low-energy electron-molecule collisions, processes involving DNA bases, sugars, etc. have hardly been treated. The size of these molecules (number of nuclei and electrons) presents an immense challenge to these methods that, until very recently, have been only applied to small molecules. Fortunately, this challenge is essentially computational.

We performed *ab-initio* calculations for electron collisions on THF within the fixed-nuclei approximation for incident electron energies up to 10 eV. For this purpose, we used the UK molecular R-matrix codes [6]. Of special interest were the lifetime and position of the resonant states that lead to DEA. THF is by far the biggest molecule ever treated with the R-matrix method. In addition, some of its low-lying electronic states have Rydberg character. This requires the use of diffuse basis sets and bigger R-matrix boxes (the standard box radius used in the calculations is 10 a_0).

Several target models using different basis sets and different state averaging procedures to generate natural orbitals were tested as the threshold for excitation is particularly sensitive to the diffuse character of the basis. Especial care was taken when testing the convergence of our results with the radius of the R-matrix box and the number of states included in the close-coupling expansion. No shape resonances were found for this system, but a few core-excited resonances were present in the energy region spanning the first 8 excited states.

Results for cross sections and resonance parameters will be discussed and analysed.

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DETERMINING IONIZATION CROSS SECTIONS WITH THE MOLECULAR R-MATRIX WITH PSEUDOSTATES METHOD

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The molecular R-matrix with pseudostates method (MRMPS) has been developed to calculate excitation and ionisation cross sections at energies straddling the first ionization threshold of the target. The method is fully general and has been implemented as part of the UK polyatomic R-matrix code [1]. This is the first *ab initio* method that provides information on molecular electron impact ionisation.

The MRMPS method, similar to the R-matrix with pseudostates method employed in electron-atom collisions [2], is based on the use of some states that represent a discretized continuum. These states, known as pseudostates, are eigensolutions of the molecular Hamiltonian within the basis set used but do not represent real eigenstates of the system. If chosen carefully, they will give a proper description of the continuum states of the target at short range. These pseudostates are included in the close-coupling expansion used to represent the basis states wavefunctions for the target plus electron in the inner region. Transition into the pseudostates that are above the ionization threshold can be interpreted as ionization. In practice, a projection technique may be required to extract the bound component from the pseudostates.

How to generate the pseudostates and ensure a good description of the ionized target is far from trivial. In our implementation, we use Gaussian Type Orbitals (GTOs) as basis functions for all (bound, continuum and pseudocontinuum) orbitals. This makes all integrals required analytical but leads to problems of linear dependence. A careful choice of exponents for the GTOs used to expand the pseudocontinuum orbitals can ensure that this linear dependence is avoided while at the same time providing a good distribution of pseudostates. We have chosen to use an even-tempered basis set for the pseudocontinuum orbitals, so their exponents follow: $\alpha_i = \alpha_0 \beta^{(i-1)}$. However, no systematic strategy for the choice of α_0 and β has yet been found.

Another problem that arises in these calculations is the presence of non-physical resonances associated with the pseudostates. This problem is particularly severe in the case of cationic targets (e.g. H_3^+) as there are an infinite number of Rydberg states of H_3 that converge to each of the H_3^+ thresholds. A convolution plus averaging technique has been implemented to deal with this problem. This technique requires performing calculations for several sets of pseudostates.

The MRMPS method was first applied to H_3^+ [3, 4] and then to H_2 [4]. Agreement with experimental data for ionisation of H_2 is very good. Experiments for H_3^+ are currently being performed. Use of pseudostates in the close-coupling expansion produced a converged polarizability for both systems. This results can have significant relevance in low energy collisions where polarization effects are very important.

We will describe in detail how the MRMPS method has been applied to the calculation of ionisation cross sections. In particular, a projection method recently implemented and based on collisional calculations of the bound states of the target plus electron system, will be presented at the conference.

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Metastable production from D_2O, H_2O and H_2O_2 following electron impact.*

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A channeltron has been used to detect metastable oxygen atoms $O(^5S)$ and hydrogen atoms H(2s) or D(2s), produced by electron impact dissociation of D_2O, H_2O and H_2O_2 over an incident energy range from threshold to 300eV. A crossed-beam apparatus with a pulsed electron beam is used to obtain time-of-flight (TOF), and hence energy, spectra of metastable H, D and O atoms. A sample of the TOF data obtained is shown in the Figure. Here a pulse of 300 eV electrons is incident on D_2O. The intense peak, A, at time zero is due to the VUV photons excited by the e-beam pulse. Peaks B and C, at short and long flight times respectively, are due to $D(2^2S)$ and $O(^5S)$ fragments respectively. Relative cross sections as a function of electron energy have been obtained for the different fragments. Some cross sections have been made absolute by comparison with data for production of H(2s) from H_2 [Ajello *et al* The Astrophysical Journal **371**, 422 1991]

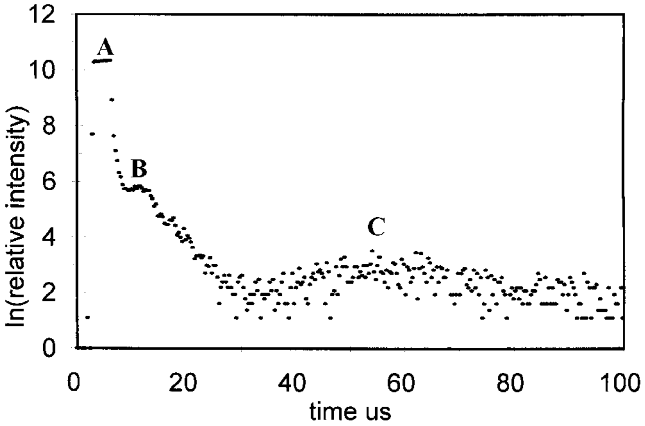

Figure 1 TOF data from D_2O at 300eV. See text for details.

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NUMERICALLY SOLVABLE MODEL OF LOW-ENERGY RESONANT ELECTRON-MOLECULE COLLISIONS WITHOUT BORN-OPPENHEIMER APPROXIMATION

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We suggest a simple model with one nuclear and one electronic degree of freedom that can be solved exactly (without the Born-Oppenheimer approximation) employing the exterior complex scaling method and the finite-element method with discrete variable representation [1]. Using this model it is possible to study basic electron-molecule collisions: the vibrational excitation of a molecule by electron impact

$$e \ + AB(\ _i) \rightarrow e \ + AB(\ _f), \qquad (1)$$

and the dissociative electron attachment to a molecule

$$e \ + AB(\ _i) \rightarrow A + B \ . \qquad (2)$$

The full Hamiltonian of our model is

$$H = -\frac{1}{2\mu}\frac{d^2}{dR^2} - \frac{1}{2}\frac{d^2}{dr^2} + V(R,r) \qquad (3)$$

where μ is the reduced mass of a molecule, R is the distance between atoms and r is the distance of the electron from the molecule. The potential $V(R,r)$ is written in the form

$$V(R,r) = V_0(R) - \lambda(R)e^{\ \alpha r^2} + \frac{J_e(J_e+1)}{2r^2} \qquad (4)$$

where $V_0(R)$ is a Morse potential for the vibrational motion of the neutral molecule, the second term describes the interaction between the molecule and the electron and the centrifugal term with $J_e \neq 0$ is added to provide a resonant behavior in our system.

The interaction of the electron with the molecule was chosen to possess one bound state for large R (dissociative attachment channel) that becomes a resonance state for a given $R = R_c$ (crossing point of the potential energy curves of AB and (AB)). Choosing $\lambda(R)$ appropriately we can get different types of resonance curves, with or without potential wells, to simulate various real systems.

The suggested model is used to compare various approaches to low-energy resonant electron-molecule collisions, for example the boomerang model [2] or the nonlocal resonance model [3].

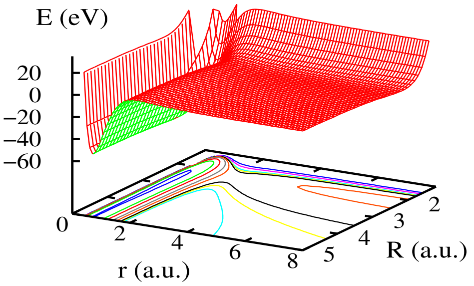

Fig. 1. Potential $V(R,r)$ of the NO-like model adjusted to data of [4].

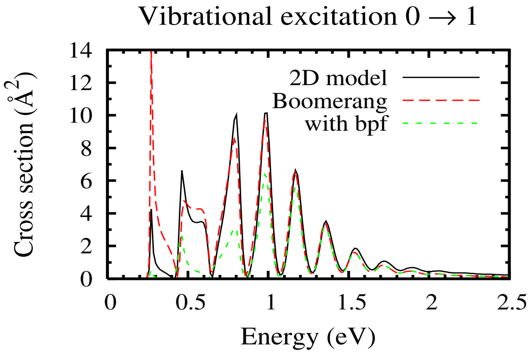

Fig. 2. Comparison of vibrational excitation cross sections for NO-like model obtained using the full 2D model (solid line) and the boomerang model without (long dashed line) and with (short dashed line) barrier penetration factor.

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Electron Cooling by Vibrational Excitation of Carbon Dioxide

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Abstract

We report new results for electron energy transfer rates [1] and electron cooling rates due to vibrational excitation of carbon dioxide (CO_2). The present model calculations are topical because at altitudes less than about 200 km, the neutral atmospheres of Mars and Venus are dominated by CO_2. Thus we expect electron cooling by CO_2 to be a significant energy transfer mechanism in their respective atmospheres, with vibrational excitation being the dominant process [2].

Our method was described earlier in Campbell *et al.* [1], although in this application our integral cross section (ICS) database has been meticulously constructed from the best available experimental and theoretical [e.g. 3-5] ICS for vibrational excitation in CO_2. Electron energy transfer rates from the present work are compared against those from the only previous corresponding study [2], with these results being presented at the meeting.

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A THEORETICAL STUDY ON ON e^{-}–CH$_3$ COLLISIONS IN THE LOW ENERGY RANGE

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The interest on electron collisions with highly reactive radicals such as CH$_x$, CF$_x$, (x= 1,2,3), etc, has grown recently, in view of their importance in the development of plasma devices. In particular, various cross sections of e$^-$–CH$_3$ collisions are expected to be important for the understanding and modelling of the chemistry in both planetary atmospheres and discharge plasmas.

Unfortunately, experimental determination of such cross sections for e$^-$-radical collisions are difficult. Only very recently, limited electron-impact ionisation cross sections of a few molecular radicals were reported in the literature. For e$^-$-CH$_3$ collisions, just two theoretical investigations were reported [1, 2]. In those works, total (TCS) and total absorption (TACS) cross sections in the (20-3000)-eV range were calculated.

In this work we present a theoretical study on elastic electron scattering by CH$_3$. Calculated cross sections for electron impact energies ranging from 0.1 to 30 eV are presented. In our calculation, the electron-molecule scattering dynamics is represented by an interaction potential (V^{SEP}) formed by the static, the exchange and the correlation-polarization contributions:

$$V^{SEP}(\vec{r}) = V_{st}(\vec{r}) + V_{ex}(\vec{r}) + V_{cp}(\vec{r}). \qquad (1)$$

The iterative Schwinger variational method [3] is used to solve the scattering equations.

Fig. 1 shows our calculated integral cross sections (ICS's) for elastic e^-–CH$_3$ collision, in the (0.1–30)-eV range. The calculated ICS's for e^-–CH elastic scattering [4] as well as calculated [5] and experimental ICS's [6–8] for e^-–CH$_4$ are also shown for comparison. The minimum seen at around 0.3 eV in our data was identified as a Ramsauer-Townsend minimum. Additional results and discussion will be presented at the Symposium.

This work was partially supported by Brazilian agencies: CNPq and FAPESP.

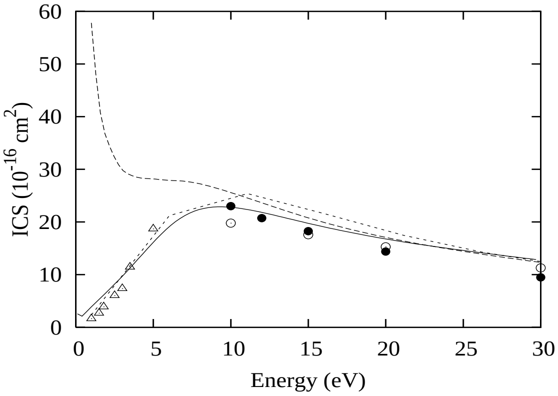

Fig. 1. ICS's for elastic e^-–CH$_3$ scattering in the (0.1-30)-eV energy range. Full curve, present calculated data; dashed line, calculated data for e^-–CH collisions [4]; short-dashed line, calculated ICS's for e^-–CH$_4$ [5]. Experimental results for e^-–CH$_4$ are: full circles, Boesten and Tanaka [6]; open circles, Shyn and Cravens [7]; open triangles, Sohn *et al* [8].

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THEORETICAL STUDY ON ELECTRON-NH$_2$ RADICAL COLLISIONS

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The interaction of electrons with highly reactive radicals has grown recently, in view of their importance in many plasma processes, including anisotropic etching, film deposition and surface modifications. Cross sections for electron scattering from a variety of such molecules are demanded in different fields of pure and applied sciences [1-3]. NH$_2$ is one of these radicals, also known as an important intermediate species in astrochemistry and various combustion processes.

In view of the above applications, the knowledge of cross sections for e −NH$_2$ collisions would certainly be of interest. Since the experimental determination of such cross sections is difficult, theoretical calculations are presently an important manner to fulfill the lack of data on this matter. However, except for the calculations of total cross sections by Joshipura *et al.* [7], no theoretical investigation on those collisions has been reported.

In this work we present calculated differential, integral and momentum-transfer cross sections for e −NH$_2$ elastic scattering at impact energies ranging from 1 to 30 eV. In our study, the electron-molecule scattering dynamics is represented by an interaction potential (V^{SEP}) composed of static, exchange and correlation-polarization contributions:

$$V^{SEP}(\vec{r}) = V_{st}(\vec{r}) + V_{ex}(\vec{r}) + V_{cp}(\vec{r}). \qquad (1)$$

The iterative Schwinger variational method [4] is used to solve the scattering equations.

Fig. 1 shows our calculated integral cross sections (ICS's) for elastic e −NH$_2$ collision, in the (1–30)-eV range. The calculated ICS's for e − NH radical scattering [5] as well as calculated ICS's for e −NH$_3$ collisions [6] are also shown.

Additional results and discussion will be presented during the Symposium.

This work was partially supported by the Brazilian agencies CNPq and FAPESP.

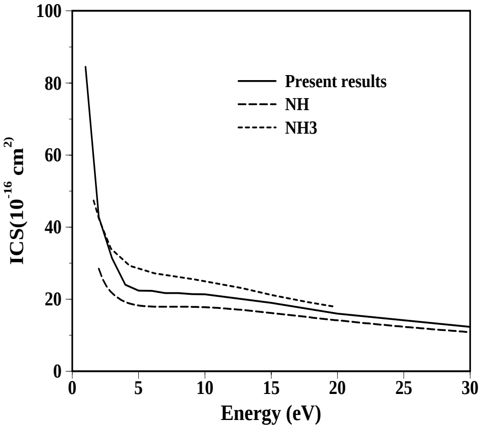

Fig. 1. ICS's for elastic e −NH$_2$ scattering in the (1-30)-eV energy range. Full curve, present calculated data; long-dashed line, calculated data for e −NH collisions [5]; dashed line, calculated ICS's for e −NH$_3$ collisions [6].

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A THEORETICAL STUDY ON ELECTRON-METHYLENE (CH_2) RADICAL COLLISIONS

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Electron-molecule collisions play an important role in a number of physical and chemical processes. In particular, interest on electron collisions with highly reactive radicals such as CH_x, CF_x, (x= 1,2,3), etc, has grown recently, in view of their important role in developing plasma devices. Specifically the methylene radical is one of such important fragments. This radical can be produced from dissociation of CH_4 either by collisional and/or photodissociation processes. Since CH_4 is frequently used as a constituent of feedgas in technological processing plasmas for deposition purposes (diamond films, diamond-like carbon films, amorphous carbon films), the knowledge of several cross sections for e -radical collisions is relevant. Unfortunately, experimental determination of such data is difficult. Therefore, theoretical calculations are presently an important manner to fill this lacuna. In this work we present a theoretical study on electron scattering by CH_2 in the low energy range (1-30 eV). The present study made use of a optical potential, composed by static, exchange and correlation-polarization contributions, to represent the electron-radical interaction dynamics. The Iterative Schwinger variational method [1] is used to solve the scattering equations.

Fig. 1 shows our calculated ICS's for elastic e −CH_2 collision, in the (1–30)-eV range. The calculated ICS's for e −CH scattering [2], as well as calculated [3] and experimental ICS's [4-6] for e −CH_4 are also shown for comparison. Qualitatively, a minimum located at incident energies around 1.2 eV is seen in our calculated ICS's for e −CH_2 collision. Eigenphase analysis has shown that it is not a Ramsauer-Townsend minimum. Additional results will be presented during the Symposium. This work was partially supported by the Brazilian agencies CNPq and FAPESP.

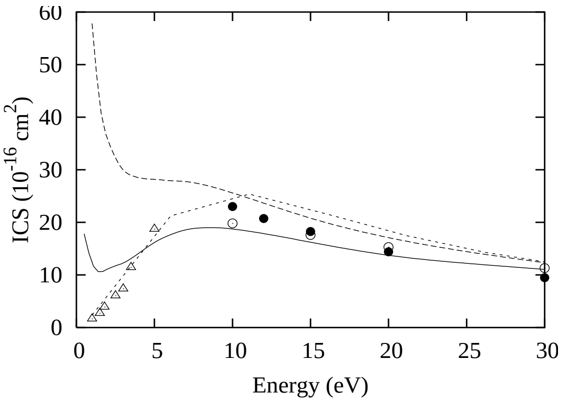

Fig. 1. ICS's for elastic electron scattering by CH_2 in the (1–30)-eV range. Full curve, present results; dashed line, calculated results for e −CH scattering of Lee *et al.* [2]; dotted line, the calculated results for e −CH_4 scattering of Machado *et al.* [3]. The shown experimental results for e −CH_4 are: full circles, Boesten and Tanaka *et al.* [4]; open circles, Shyn and Cravens [5]; open triangles, Sohn *et al.* [6].

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Core excitations processes of C1(s) in C_2 and C_2H_2 molecules by electron impact.

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Abstract

Distorted-wave approximation (DWA) is applied to study excitation of core-level electron in C_2 *molecules by electron impact. More specifically, we report calculated differential (DCS) and integral (ICS) cross sections for the* $X^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(1s\sigma_u \rightarrow 1p\pi_g)$ *and* $X^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(1s\sigma_g \rightarrow 1p\pi_g)$ *transitions in the* C_2 *molecule and comparison is made with* $X^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(1s\sigma_u \rightarrow 1p\pi_u)$ *and* $X^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(1s\sigma_g \rightarrow 1p\pi_u)$ *transitions in the* C_2H_2 *molecule in the 300 - 800 eV incident energy range. The ratios, named RI(3:1), calculated by dividing the distorted-wave integral cross sections(ICS), for transitions leading to the triplet and the singlet core-excited states as a function of incident energy are also reported. The present study shows the RI(3:1) behavior for the C 1s* → π *transition in each species here studied. The generalized oscillator strength(GOS) profiles for discrete C 1s excited states of* C_2 *and* C_2H_2 *have also been calculated, and are compared with the available data reported in the literature. Quantitative agreement between the present theory and experiments is also satisfactory.*

A comparative study for elastic electron collisions on the C_2N_2 and their isomers CNCN, CCNN and CNNC

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Abstract

In this work we present a theoretical study on elastic electron collisions with four isomers molecules (C_2N_2, CNNC, CCNN and CNCN) in the low and intermediate energy range. More specifically, calculated elastic differential, integral and momentum transfer cross sections as well as grand total (elastic+inelastic) and absorption cross sections are reported in the 1-300eV energy range. A complex optical potential is used to represent the electron-molecule interaction dynamics whereas the Schwinger variational iterative method combined with the distorted-wave approximation is used to solve the scattering equations. Comparison of the present calculated results with the available theoretical data for electron-C_2N_2 collisions has shown remarkable similarity for incident energies higher than 20 eV, In addition, probably due to importance of the interaction between the scattering electron and the target valence-orbital electrons in this range

ABSOLUTE TOTAL CROSS SECTION MEASUREMENTS FOR INTERMEDIATE ENERGY ELECTRON SCATTERING ON ETHANE AND PROPANE

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This work is part of the research program in our laboratory, which aims the study of properties of atmospheric pollutants. Nowadays the atmosphere is highly influenced by petroleum products and its derivatives. The burning of petroleum derivatives in domestic use, in industry and mainly in automotive transport, releases daily in atmosphere enormous quantities of carbon and other elements in gaseous form, some them extremely dangerous to human health. The hydrocarbons are one of the five most important atmospheric contaminants, representing more than 90% of pollution problem. We perform experimental and theoretical determinations of Absolute Total Cross Section (ATCS) for electron scattering by ethane and propane, in the energy range from 20 to 500 eV. Experimental data were acquired with an apparatus assembled in our laboratory, which uses the linear transmission technique [1]. The apparatus is composed by an electron gun, a gas cell, an analyzer system composed by desaccelerating electrostatic lenses and a Cylindrical Dispersive Analyzer 127º (CDA 127º) and a Faraday cup. The TCS, $\sigma(E)$, to the fixed impact energie E, was obtained by the measurement of the transmitted electron beam intensities, with (I_p) and without (I_o) sample the gas cell, applying the Lambert-Beer relation: $\ln(I_p/I_o) = -PL\sigma(E)/kT$, where k is the Boltzmann constant, L is the length of the interaction region, P the absolute pressure in the cell and T is the sample temperature. The energy resolution in all measurements was 0,7 eV (FWHM) and the overall systematic uncertainty at the TCS was evaluated to be less than 5%. The theoretical determinations of Total Cross Sections, also in the 20 to 500 eV energy range, was calculated using the Additivity Rule (AR) [1,2] and the Born-Bethe approximation [3-5]. These results were compared with our experimental data and also, with theoretical results from the literature. As it is expect, the theoretical calculations employing the Born–Bethe approximation overestimates the Total Cross Sections values in this energy range.

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MONTE CARLO SIMULATIONS OF LOW CURRENT TOWNSEND DISCHARGES IN NEON

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The studies of spatial profiles of excitation reveal non-hydrodynamic behavior close to the electrodes and at high *E/N*, effects of reflection and heavy particle excitation. Understanding the kinetics of excited neon is of practical importance for modeling collisional plasmas, gas discharge devices, in particular plasma displays. The data have been obtained from drift tube and were analyzed using Monte Carlo simulation, which involved an accurate representation of non-equilibrium effects and a complete set of initial cross sections. A complete excited state kinetics analysis is however required to obtain the electron, ion and fast neutral scattering cross sections for all the 2p levels.

In the present work, we show comparison between experimental data and results of Monte Carlo simulation (MCS) [1] for excitation coefficients in neon.

We have made measurements for charged and fast neutral particle transport neon [2]. The discharge vessel that we used in our experiment consists of parallel-plane electrode system (7.9 cm in diameter separated by 1.72 cm) inside a quartz tube. The cathode was made of stainless steel and the anode of vacuum-grade sintered graphite. Discharge between the electrodes is sustained by a dc voltage, typically we cover range from the total voltage of 200 V to 2000V. Pressures from 1 Torr down few tens of mTorr were covered respectively giving a wide range of E/N. The light emitted from the discharge was detected through the quartz window of the vacuum chamber by a monochromator, photomultiplier and a photon-counting chain. Spatial profile was obtained by using 1:1 optics with 1 mm wide collimators mounted on a movable platform.

We have performed the analysis of our data for neon by using a detailed Monte Carlo simulation scheme. Monte Carlo code is based on a null-collision technique because it is applicable to our steady state Townsend conditions [3]. The code contains electron kinetics part, ion kinetics part and fast neutral kinetics part and from the analysis for all these three elements we can obtain spatial profiles of emission, the excitation coefficients and as a result of the standard swarm analysis we can obtain the cross section data. In the present range of the analysis, only electron part was relevant. Swarm analysis is performed by comparing experimental and calculated transport (excitation) coefficients. Comparisons are repeated until a satisfactory agreement is achieved after modifications of the cross sections.

The spatial profiles of excitation coefficients of $2p_8$ neon emission have been used to obtain the cross section data. In particular, such data may be used to identify heavy particle excitation [4] that is recognized by the growth of emission towards the cathode. We were able to achieve a reasonable agreement with the experimental data but further modifications to the available cross section are required to take full advantage of the experimental data. The basic set of cross sections for electron scattering was taken from Hayashi [5] and Puech [6].

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CALCULATION OF PHOTOIONIZATION OF RELATIVISTIC ATOMS

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The calculations of photoionization cross section have faced two frequent problems. First, one frequently obtains different results for the so-named “length” and ”velocity” formulations. That difference results from the two Hamiltonians used in the definitions of the bound and of the scattered electron states [1]. Secondly, relativistic corrections may become very important. Indeed, even for low energy photoelectrons and the top bound states, the asymmetry parameter β resulting from the Dirac equation may differ much from the one resulting from the Schroedinger equation. The photoionization cross section is written as

$$d\sigma/d\Omega = \frac{\sigma}{4\pi}(1+\beta P_2(\cos\theta)) \tag{1}$$

where the parameter β is associated with the $L = 2$ component of the spatial distribution. In the case of the Dirac equation, expressions for the cross section and the asymmetry parameter β were given by Walker and Waber [2].

The calculation of photoionization of relativistic atoms, which have large numbers of electrons, suggests using *density functional* procedures instead of *ab initio*. One uses one of its approximations such as LDA, LSD or GGA. We chose LDA in our calculations. Further, as shown by Da Costa et al [3], the use of pseudopotentials requires special cares because they break the equality between the “length” and the “velocity” results. Thus pseudopotentials are preferably to be avoided and the present calculation was all-electron.

Using LDA, the proper way to calculate the ionization potential and a single one-electron Hamiltonian for the scattered electron and for the bound state, thus making the velocity and length results equal, is very old and was named in the seventies as the “transition state”. Its validity relies on a theorem formaly proven by Janak [4] as

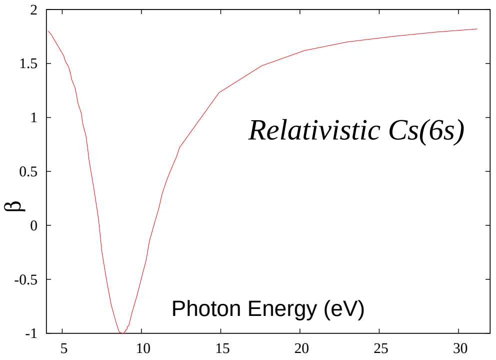
$$\frac{dE}{dn} = \epsilon \tag{2}$$

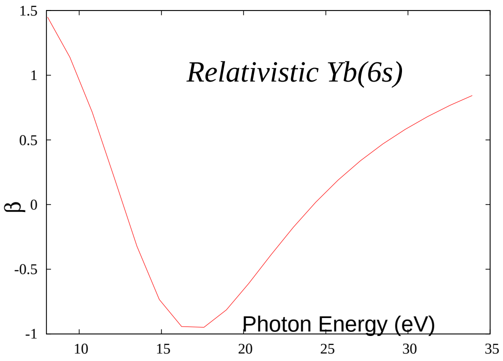
where E is the total energy and ϵ is the Kohn-Sham one-electron eigenvalue. The transition state procedure consists of using the one-electron self-consistent Hamiltonian of the electron system with half electron removed.

In the following we present some results for the asymmetry parameter of the photoionization of the 6s electron of Cs and Yb. The calculated ionization potentials agree very well with experiment, a feature that is only possible with the transition state. The asymmetry parameter β deviates much from the non-relativistic value of 2, even for the highest occupied orbital 6s. Of course, the length and velocity calculations are the same.

First Ionization Potentials (eV)

Atom	Calculated	Experiment[5]
Yb	6.71	6.25
Cs	4.00	3.89





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ELECTRON COLLISIONS WITH C_3H_6 ISOMERS

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Propene and cyclopropane are the two existing isomers of C_3H_6 molecule. Propene is an open chain molecule and belongs to the C_s group. Cyclopropane is a closed chain molecule and belongs to the D_{3h} group.

Experimental [1, 2, 3] and theoretical [4] studies investigated the *isomer effect* in the electron-collisions cross sections of the C_3H_6 isomers. They concluded that the cross sections for these isomers differ for energies below 40 eV. Another experimental [5] and theoretical [6, 7] studies investigated the electron-collisions with cyclopropane.

In this work we present results for electron-collisions with isomers of C_3H_6, propene and cyclopropane. Our calculations employed the Schwinger multichannel method with pseudopotentials at the static-exchange (SE) and static-exchange plus polarization (SEP) approximations.

Figure 1 shows a comparison of our elastic cross section for cyclopropane with those of Refs. [6, 7]. All calculations were performed at the SEP approximation. Our cross section agrees well with the results of Beyer *et al.*, except for the position of the shape resonance, and lies below the results of Curik and Gianturco.

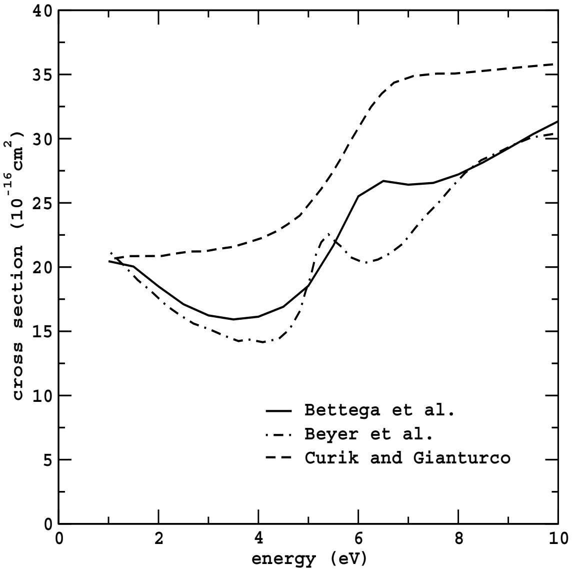

Fig. 1. Integral cross section for cyclopropane.

Figure 2 shows a comparison of our elastic cross section for propene at the SE and SEP approximations with total cross section of Ref. [3]. In particular our cross section shows a shape-resonance located at the same position of the resonance seen in the total cross section.

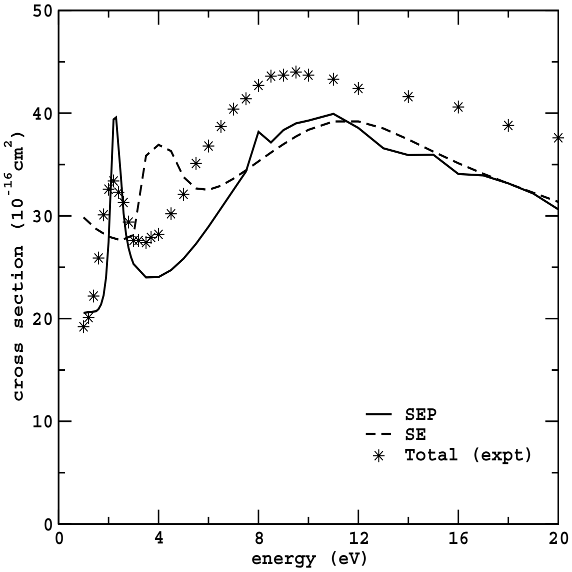

Fig. 2. Cross section for propene.

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LOW-ENERGY ELECTRON SCATTERING BY N_2O AND C_2H_4

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There have been several recent theoretical [1, 2, 3, 4, 5] and experimental [6, 7, 8] studies of elastic electron collisions with N_2O. One focus of interest has been the well-known Π shape resonance located near 2.2 eV, whose position has been correcty described by some calculations [1, 3, 5]. In particular, Winstead and McKoy presented a procedure to avoid target overcorrelation in resonant problems, which located the Π shape resonance at its experimental position. In general, the various calculated cross sections agree well with one another, and they also agree with experiment at energies above ~10 eV, but at lower energies agreement with experiment is poorer. As Kitajima *et al.* pointed out, the calculated differential cross sections differ most from the experiment at angles below ~ 60°, as shown in the figure. Similar behavior was noted in C_2H_4 and several other molecules that display low-energy resonances [9].

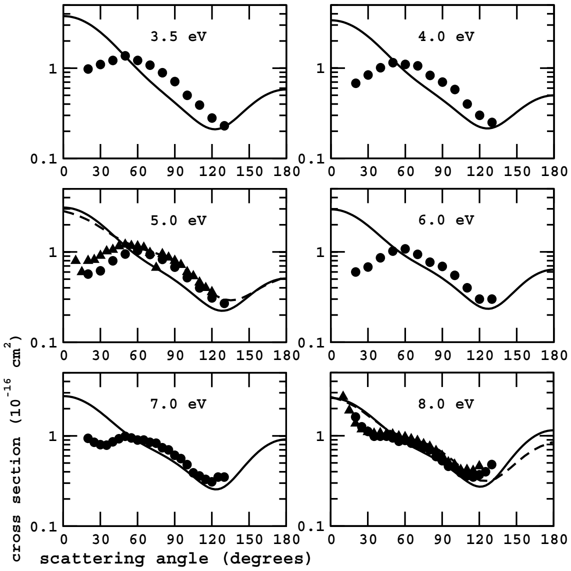

Fig. 1. Elastic differential cross sections for N_2O. Solid line, our recent calculation with a larger number of configurations; dashed line, results of Ref. [3]; squares, results of Ref. [7]; circles, results of Ref. [8].

Here we revisit the scattering of low-energy electrons by N_2O and C_2H_4 in order to understand the origin of the discrepancies seen between theory and experiment in the elastic differential cross section. Our calculations employ the Schwinger multichannel method at different levels of approximation: static–exchange, static–exchange plus polarization, and polarization with multichannel coupling. Our previous calculations at the static–exchange level indicated that the inclusion of nuclear motion (stretching and bending vibrations) does not significantly affect the behavior of the differential cross sections at angles below ~ 60°. This behavior is also unchanged by the inclusion of a few open channels in the calculation.

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SPINFLIP CROSS SECTIONS AND POLARIZATION FRACTION OF CCO RADICAL BY ELECTRON IMPACT

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Recently, we study theoretically the elastic cross sections of CCO radical by electron impact [1]. CCO is an open shell molecule with the ground state configuration $X^3\Sigma^-$ and the electron-radical interaction have two spin specific scattering channels, the doublet and quartet coupling between the scattering electron and the open shell electrons of the target. The results of integral cross section by symmetry shown that for incident electron with π symmetry we observed the existence of the shape resonance locate at around 3 and 4.5 eV corresponding to the quartet and doublet scattering channels. The shift of about 1.4 eV of the shape resonance in CCO is due to the different exchange potential operator used in the doublet- and quartet-coupling scattering calculations.

In this work, we calculate the spin-flip cross sections and the polarization fraction for electron collision with CCO molecules, in the energy range of 1eV up to 10 eV. The molecular wave functions are described at Hartree-Fock level and TZV basis set was used to represent the atomic orbitals. The scattering amplitudes for each channel was calculated using the Schwinger Iterative Method and the collision dynamic is represented for one interaction potential including the static, exchange, correlation and polarization effects. The results shown that the spin-flip cross sections and the polarization fraction are important around the resonance peak and bellow 10 eV. In figure 1, the results to the polarization fraction rotationally unresolved show that the spin-flip effect are more accentuated around of the resonance. We also calculated de spin-flip differential cross section and polarization fraction rotationally resolved for the transitions j=0→j'=0,1 and 2. Additional results will be presented during the symposium.

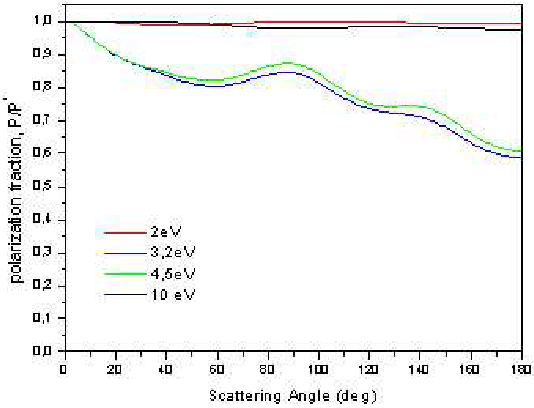

Figure 1: Polarization fraction for the electron scattering by CCO radical.

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THE STUDY OF THE INTERACTIONS OF LOW ENERGY ELECTRONS WITH OH

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Abstract:

The hydroxyl radical OH is an important component in a diverse array of physical environments. It is one of the most extensively studied diatomic hydrides as it is an important constituent of combustion gases, of both clean and polluted terrestrial atmospheres, of cometary gases and of diffuse, dense, and shocked regions of the interstellar gas. It is also an important species in biology being readily formed by the dissociation of water by radiation. Ionising radiation may form OH radicals in the body which can subsequently induced DNA damage which can lead to cell death or mutation. Within cells the major secondary species of any ionising irradiation are secondary electrons, therefore the interaction of electrons with OH is important in may areas of radiation chemistry. To date it has not been possible to prepare targets of OH radicals for electron bema experiments such it is necessary to develop theoretical models of such interactions.

We have used the UK R-matrix code for the low energy electron impact study on the OH molecule. The R-matrix method is now established as the most versatile and efficient method for the modelling of low energy scattering by electrons (and positrons) by atomic and molecular targets [1].The R-matrix method is used to treat electron collisions with the diatomic OH molecule as a function of inter-nuclear separation R. These calculations concentrate on obtaining low-energy (< 10 eV) elastic excitation cross sections of the seven lowest-lying electronically excited states of symmetries $^2\Pi$, $^2\Sigma^+$, $^2\Sigma^-$, $^2\Delta$, $^4\Sigma^+$, $^4\Sigma^-$ and $^4\Pi$. We used an equilibrium value for the O-H bond length $R_e = 1.8342\ a_o$. The basis set of slater type functions consisted of $24\,\Sigma$, $10\,\Pi$ and 2Δ orbitals and a complete active space configuration interaction model [2].The range of scattering energies is restricted to 12 eV. Resonance positions and widths are found using the RESON program. In order to study the dissociative behaviour of resonances we performed calculations in which the O-H bond was stretched for R = 1.3 a_o to 3.5 $a_{o.}$ We have calculated the total elastic cross sections for 6 geometries R = 1.3, 1.5, 1.6, 1.75, 1.8342 and 1.9 $a_{o.}$ Detailed results will be presented during the conference.

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A SET OF CROSS SECTIONS AND TRANSPORT COEFFICIENTS FOR ELECTRONS IN HBr

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In recent years HBr has become one of the key gases in plasma etching technologies [1]. Nevertheless there is a great shortage of data for plasma modeling, including both cross sections and swarm parameters. In the present work, we show compile a set of cross sections based on available theoretical and binary collision data and we proceed to calculate the corresponding transport coefficients.

The momentum transfer cross section was taken from Rescigno [2] and it was extrapolated to lower and higher energies. Rotational excitation was calculated on the basis of Takayanagi formulae. Vibrational excitation and dissociative attachment were taken from Čižek et al. [3]. Electronic excitation to three different states was taken from Rescigno [2] but we have supplemented it by effective total excitation cross section that was developed for HCl by Hayashi [4]. Finally ionization was calculated by Ali and Kim [5].

A Monte Carlo technique [6] was used to obtain transport coefficients for electrons in HBr. The momentum transfer cross section decays slowly with the energy and as it resembles a constant collision frequency cross section the transport coefficients are uneventful.

Data obtained by a two term theory were compared to exact Monte Carlo results. Due to a large vibrational cross section, there is a significant breakdown of the two term approximation (TTA) because of an extremely large vibrational excitation. The most characteristic feature in electron transport is the sudden increase of the D_T/μwhich has also significant nonconservative effects in the same range.

Due to lack of measured transport coefficients it was not possible to provide a unique and very accurate set of cross sections. However, based on the very accurate data for vibrational excitation, for momentum transfer cross section and for ionization cross section together with some reasonable extrapolations we are able to provide a set that will be good enough for modeling mixtures containing smaller amounts of HBr. For an improved set of cross sections it will be required to make measurements of swarm parameters, in particular ionization coefficients. In addition more studies of electronic excitation and dissociation are needed.

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Calculations of cross sections for vibrational EELS of cyclopropane

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Hydrocarbon species are known as sources of carbon atoms during chemical vapour decomposition reactions [1]. Among them cyclopropane, C_3H_6, is found to be present in cooler edges of fusion plasmas [2]. Therefore qualitative and quantitative understanding of different events during the electron-cyclopropane collisions is important for initiating a great variety of processes.

In this work we apply Discrete Momentum Representation (DMR) method for calculation of elastic and vibrationally inelastic cross sections for electrons scattered by the cyclopropane molecules. Static-exchange approximation is employed for the collision energy range of 2-20 eV.

We have analyzed all the 21 normal modes and the quantitative results have been compared with previous calculations of *Čurík and Gianturco* [3] where only 3 full-symmetric modes were computed. We also carried out a qualitative comparison with experimental data of Allan and Andric [4]. We have confirmed the presence of shape resonances of different symmetries in different vibrational modes and our cross sections compare well with those of *Čurík and Gianturco* for the excitations of modes where comparison is available, as can be seen on Fig.1.

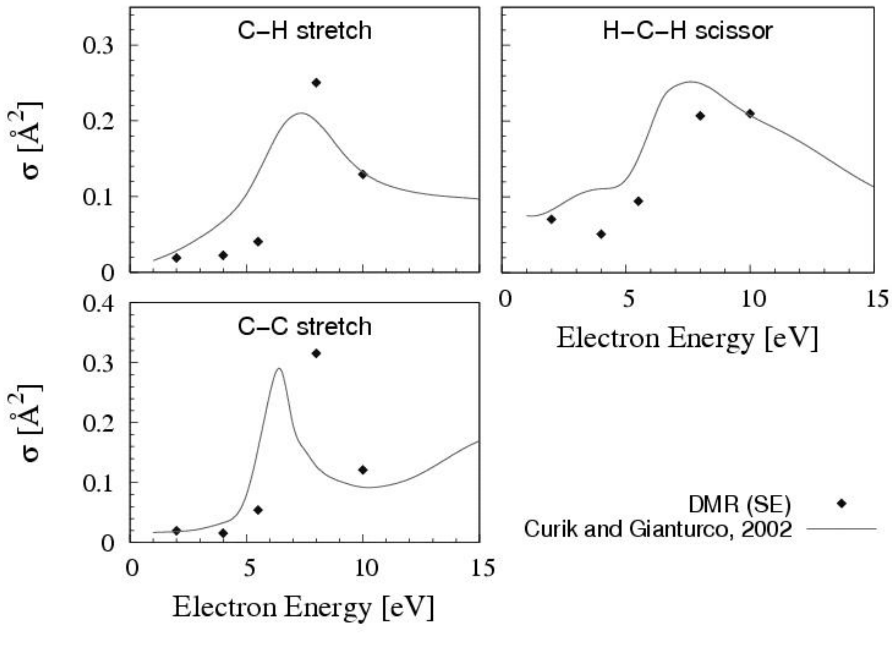

Fig. 1: Comparison of integral cross sections for the excitation of 3 vibrational modes. Diamonds represent DMR results and full curve are calculations of Curik and Gianturco [3].

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INELASTIC SCATTERING OF LOW-ENERGY (1.5 – 12 eV) ELECTRONS FROM CONDENSED ADENINE

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Research on low-energy electron scattering from DNA and its constituents aims to discover the mechanisms playing an important role [1] in several applications ranging from radiotherapy to nanotechnology. In continuation to our recent measurements on thymine [2], we performed a similar experiment on its complementary base, adenine.

Adenine is a purine base consisting of two rings with the amino group (NH_2) being attached to the six-member ring (C6). Within double-stranded DNA, it forms two hydrogen bonds with thymine. Previous studies of anion desorption from physiosorbed DNA bases [3] showed that electrons of energies below 15 eV produce bond cleavage via dissociative electron attachment. The aim of the present study is to investigate the formation of electron resonances (i.e. temporary negative ions) in adenine within the same energy range.

Measurements of the vibrational and electronic excitation were performed on a high-resolution electron energy-loss (EEL) spectrometer [2], housed in a cryogenically pumped ultra-high-vacuum chamber at a base pressure of ~ 5 x 10^{-11} Torr. EEL measurements were made on a very thin (from sub-monolayer up to a monolayer) film of adenine deposited on a six-layer spacer of argon condensed on a Pt substrate held at a temperature of 18 K. An incident electron beam of energy ranging from 1.5 to 12 eV was focused on the film at an angle $\theta_o = 15^o$ with respect to the normal to the surface. The number of electrons backscattered from the film was recorded at the fixed analyzer angle of 45^o. The vibrational EEL spectra show three distinctive spectral bands among 39 normal vibrational modes of the molecule: at EEL values ranging from 0.7 to 0.12 eV, from 0.15 to 0.22 eV and from 0.38 to 0.44 eV. A particularly interesting spectral feature is that the vibrations of the amino-group (mostly in the third band) reach their maximum intensity at incident electron energies between 3 and 5 eV. Since one of two adenine-thymine bonds involves hydrogen from adenine's amino group, possible resonance in this energy range could be of importance to DNA strand break. We have also measured the EEL spectra in the range from 4.5 to 7 eV where the electronic excitation of the molecule takes place. Both vibrational excitation of the molecule in its ground electronic state and the electronic excitation, and their possible consequences on DNA damage production will be discussed at the conference.

This research is financed by the Canadian Institutes of Health Research.

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Excitation of inner-shell states of C_2H_2 and C_2N_2 polyatomic molecules by electron impact.

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Abstract

Distorted-wave approximation (DWA) is applied to study excitation of core-level electron in C_2H_2 and C_2N_2 polyatomic molecules by electron impact. More specifically, we report calculated differential (DCS) and integral (ICS) cross sections for the $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(1s\sigma_u \rightarrow 1p\pi_g)$and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(1s\sigma_g \rightarrow 1p\pi_g)$ transitions in the C_2H_2 molecule and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(2s\sigma_u \rightarrow 2p\pi_u)$and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(2s\sigma_g \rightarrow 2p\pi_u)$ transitions in the C_2N_2 molecule in the 300 - 800 eV incident energy range. The ratios, named RI(3:1), calculated by dividing the distorted-wave integral cross sections(ICS), for transitions leading to the triplet and the singlet core-excited states as a function of incident energy are also reported. The present study shows the RI(3:1) behavior for the C 1s $\rightarrow \pi$ transition in each species here studied. The generalized oscillator strength(GOS) profiles for discrete C 1s excited states of C_2H_2 and C_2N_2 have also been calculated, and are compared with the available data reported in the literature. Quantitative agreement between the present theory and experiments is also satisfactory.

ELECTRON SCATTERING FROM FORMIC ACID

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Formic acid (HCOOH) is the simplest of the organic acids and it is thought that it could play a key role in the formation of simple biomolecules such as glycine and acetic acid in the interstellar medium. To date, the majority of studies of this molecule involving electron impact have been of the dissociative attachment cross sections [1,2]. To our knowledge there are no absolute differential scattering measurements in the literature, although there have been measurements of resonant contributions to vibrational excitation [3] and of the grand total scattering cross section [4]. There have also been recent calculations of electron scattering from both formic acid monomers and dimers [5], in which total and differential cross sections have been obtained.

We have studied elastic electron scattering from formic acid using a crossed-beam electron spectrometer. Formic acid [x], which has been further purified by a number of freeze-pump-thaw cycles, is admitted to the scattering system via a temperature-controlled needle valve and gas-handling system. The valve, gas lines, and beam-forming capillary tube through which the gas enters the collision region, are all set to a temperature of 70°C, at which value the beam is mostly comprised of the monomer. HCOOH dimers can also be studied by operating the apparatus at room temperature. The electron beam is obtained from a conventional electron monochromator and scattered electrons are energy analysed before being detected in a channel electron multiplier. The initial experiments have been performed with only moderate energy resolution (~100 meV). At energies above 10 eV this is not likely to lead to significant contributions from unresolved vibrational excitation, principally the $\nu_{7,9}$ modes with energy loss values of 0.077 and 0.079 eV respectively, as the cross sections for these modes appear to be very small at these energies.

Absolute cross sections are obtained using the relative flow technique. Flow rates for HCOOH, and the reference gas He, are measured at a number of temperatures, including both room temperature and 70°C. To establish the relative driving pressures of the two gases, such that the collisional mean-free-paths of the two gases in the beam-forming capillary are equivalent, we have used molecular bond lengths to estimate the hard sphere diameter of HCOOH.

Measurements at energies in the range 10-50 eV will be presented at the meeting and compared, where possible, with the recent theoretical calculations.

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MOBILITIES OF ATOMIC IONS IN COOLED HELIUM GAS

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Mobility of an ion in a gas is very sensitive to the shape of the interaction potential between the ion and the neutral gas. If a metastable ion is not de-excited by collisions with gases, we will be able to measure the mobility of the ion in the gas and to obtain the information about the interaction potential between the electronic excited ion and the gas molecule.

In our group, a low temperature drift tube mass spectrometer with a mass-selected-ion-injection system had been developed to measure mobilities of ions in helium gas cooled by liquid nitrogen and helium. In this work, we measured the motilities of C^+, N^+, O^+, Kr^+ and Xe^+ ions in He gas at 77 and 4.3 K by using the drift tube apparatus. Because all these ions are produced by electron impact in an ion source with electron energy of about 150 eV, the metastable states of C^+, N^+ and O^+ ions must be contained in the injected ions with fractions of several percents [1], and also the primary ions of Kr^+ and Xe^+ include two fine-structure states, namely the total angular momentum $J = 1/2$ and $J = 3/2$.

Fig. 1 shows the mobilities of the ground ($2s^22p\ ^2P^\circ$) and metastable ($2s2p^2\ ^4P$) states of C^+ in He, which are measured at 4.3 and 77 K, as a function of the effective temperature T_{eff}. As can be seen in this figure, the separation of the electronic states has been observed in the higher T_{eff} region above 500 K. The electronic state was identified from the intensity ratio in an arrival time spectrum.

We have performed the calculation of the interaction potentials for the ground-state and metastable ions with He by using the multi-reference CI method, and have calculated the mobilities with the two-temperature theory using the classical momentum-transfer cross sections. At the small internuclear distance, the potential of CHe^+ has splits into more than two molecular state. Therefore we have averaged cross sections taking into account the multiplicities of the molecular states. The solid and broken lines in Fig. 1 are the calculated values of mobilities for $C^+(^2P^\circ)$ and $C^+(^4P)$, respectively. The similar measurements and calculations have been performed for the mobilities of N^+ , O^+ and Kr^+ ions in He gas. However, the metastable state has been observed in the mobility measurements for only N^+ in these ions. The reason why the metastable state has not be observed separately from the ground state in many cases should be discussed.

In the mobility of Xe^+, the separation of the electronic states has not been observed. Fig. 2 shows the mobility of Xe^+ in He, which is measured at 4.3 and 77 K, as a function of T_{eff}. We can see a deep minimum around $T_{\mathrm{eff}} \sim 80$ K. Similar structure was observed for Kr^+. Such minimum has not been seen for the other ions, the mobility of which we have measured. According to the calculation by Viehland *et al.* using the model interaction potential, the large $-r^{-6}$ term in the potential $V(r)$ makes the minimum in the mobility. Therefore we consider the deep minimum in the mobility of Xe^+ in He indicates the large $-r^{-6}$ term in the Xe^+-He potential.

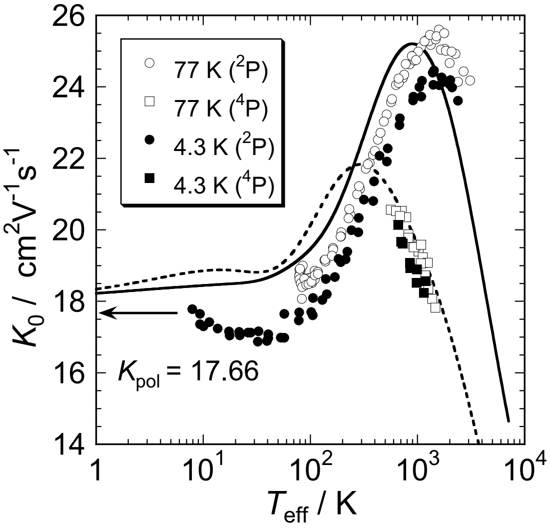

Fig. 1. Mobility of C^+ ion in He gas.

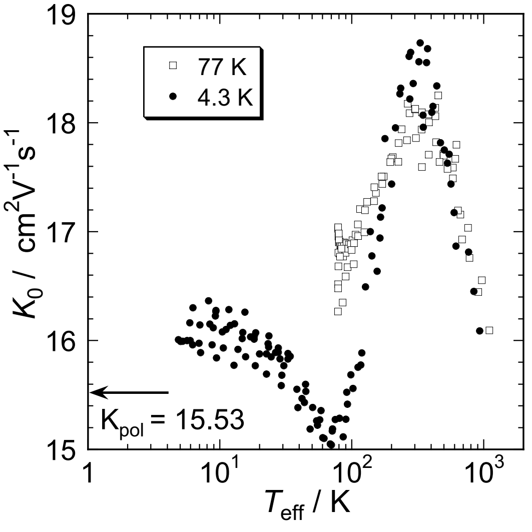

Fig. 2. Mobility of Xe^+ ion in He gas.

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Calculation of Isotropic, Partial Cross Sections and rate coefficients for Electron Ionization of CF_4

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Ionization processes play an important role in many applications such as discharges and plasmas, gas lasers, mass spectrometry, and chemical analysis. Even though cross sections for the single step multiple ionization of a molecule are significantly smaller than cross sections for single ionization, multiple ionization processes are important in fusion plasmas and other high-temperature environments.

In the present work we calculate the isotropic/ angular cross sections for the production of singly charged ions (CF_3^+, CF_2^+, CF^+, F^+, and C^+) produced through the dissociative channels and doubly charged ions (CF_3^{++} and CF_2^{++}) produced through dissociative- double ionization of the CF_4 molecule by electron impact using a semi-empirical formulation based on the Jain-Khare approach [1,2]. The calculations are made at fixed incident electron energy of 100 eV. As no previous data seem for these cross sections, we have derived the partial and total ionization cross sections from the corresponding angular cross sections in the energy range of ionization threshold to 500 eV. Where possible we compare the present results with the recent experimental data [3] and theoretical data including those of BEB- calculations [4] and DM- calculations [5]. A satisfactory agreement with the available theoretical and experimental data has been noticed.

From the perspective of applications, in particular applications to fusion plasmas, it s often more desirable to have ionization rate coefficients available rather than electron impact ionization cross sections. We have computed ionization rate coefficients for CF_4 as a function of incident electron energy using the calculated ionization cross sections.

Financial support from UGC and DST is acknowledged.

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Adventures in the wavepacket land: DEA of water

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A time-dependent description of the dissociative attachment of water is presented. The molecule is excited by an impinging electron to a resonance state . Water provides a serious challenge and test for theories of polyatomic resonant vibrational excitation, dissociative attachment and electron impact dissociation, and, not at last, is one of the key molecule to all known life in the Universe. It became clear that some of the most interesting phenomena arise from the interplay of the electronic scattering dynamics with the dynamics of nuclear motion, in particular vibration and dissociation of the molecule. Furthermore, recent developments on the time-dependent formulation of the low-lying theory and novel scattering experiments with low-energy electrons on water, encourage a deeper treatment of the molecular dynamics for the interpretation of the scattering cross section. Our approach breacks up into two parts: electron scattering and nuclear motion dynamics. The fixed-nuclei electron-molecule scattering calculations will be performed inside the framework of the R-matrix approach
[J. D. Gorfinkiel et al., J. Phys. B: At. Mol. Opt. Phys. 35 No 3, 543-555]. Wavepacket methods will be used to treat the nuclear motion. The formation and decay of resonances as modified by the coupling with the nuclear motion inform us that for systems with many degrees of freedom a time-dependent picture is needed. Computational methods and algorithms will also be presented to solve the nuclear problem in order to reduce the computational effort that scales exponentially with the number of vibrational degrees of freedom. The methods are sufficiently general and the subject enough multidisciplinary to be applied to the analysis and interpretation of different physical systems, such as other triatomic molecules and processes of interaction between matter and light.

LOW ENERGY ELECTRON SCATTERING FROM LARGE MOLECULES

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To describe the scattering of a low energy electron from a general polyatomic molecular target, we have implemented a three-dimensional finite element approach [1] in the framework of the R-matrix method. The potential is treated as a sum of three terms: electrostatic, exchange and polarization. The electrostatic term can be extracted directly from ab initio codes (GAUSSIAN 98 in the work described here), while the exchange term is approximated as a local density functional. A local polarization potential based on density functional theory [2] is then constructed in order to describe the long range attraction to the molecular target induced by the scattering electron without adjustable parameters. We have used this approach successfully in calculations of cross sections for small and medium sized molecules (like SF_6, XeF_6, C_{60}, Uracil and other DNA bases)[3].

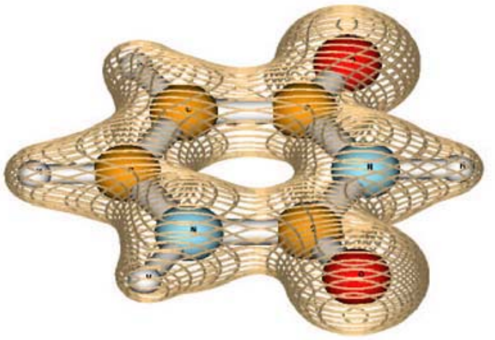

Fig. 1. Electron density and structure of the uracil ground state that we used as a target in our scattering calculations.

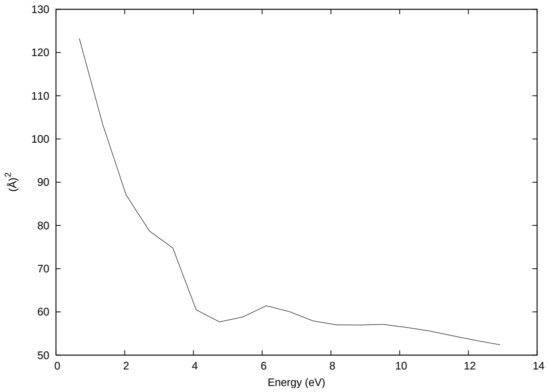

Fig. 2. Elastic cross section for electron scattering from Uracil, preliminary results.

This method will be very useful to treat the electron-induced dynamics of larger molecular systems, possibly of biological interest, difficult to tackle with more complex ab initio methods. This work has been supported by DOE-Office of Science and NERSC.

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RYDBERG-LIKE FESHBACH RESONANCES IN DISSOCIATIVE ELECTRON ATTACHMENT

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The dissociative electron attachment (DEA) spectra of saturated compounds (*i.e.*, without double and triple bonds) containig the O and N atoms have recently been shown to be generally dominated by Feshbach resonances with double occupation of Rydberg-like orbitals around a cationic core [1]. These resonances shift to lower energies with alkyl substitution, in contrast to the shape resonances, and are found at surprisingly low energies in amines. Feshbach resonances have been identified already earlier as being responsible for DEA in water [2], amonia [3], and other molecules [4, 5, 6].

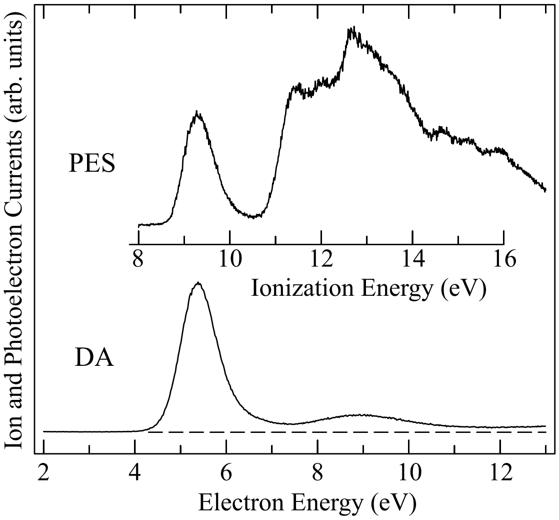

Fig. 1. Dissociative attachment spectrum (yield of the $(M-1)^-$ anion, bottom curve) and photoelectron spectrum (top) of *tert*-butyl amine.

This type of processes has gained interest recently in connection with the low-energy electron-driven chemistry encountered in radiation damage to living tissue and with plasma processing in material science. We therefore continue this work with the aim of gaining fundamental insight into the dynamics of dissociation of the Feshbach resonances. We study the dependence of the dissociation patterns on the energy of the resonance and the type of alkyl substitution of the amines. An example is shown in figure 1. The first photoelectron band, shifted to the left by 3.92 eV, corresponds to the first band in the yield of the $M-1$ fragment, a strong indication that the DA band is due to a Rydberg-like Feshbach resonance. The 3.92 eV are the binding energy of the two electrons in the Rydberg-like orbitals around a cationic core.

We plan to extend the studies to compounds containing several heteroatoms and thus having two grandparent cationic states split by the competing *through-bond* and *through-space* interactions [7, 8].

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ELASTIC AND VIBRATIONAL CROSS SECTION IN METHANE AND CYCLOPROPANE

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There is a general agreement about the elastic cross sections in methane in the literature, but substantial discrepansies exist about the vibrational cross sections. This work measures absolute differential elastic and vibrational cross sections from nearly threshold to 20 eV. The cross sections are measure over a large angular range using the magnetic angle changer.

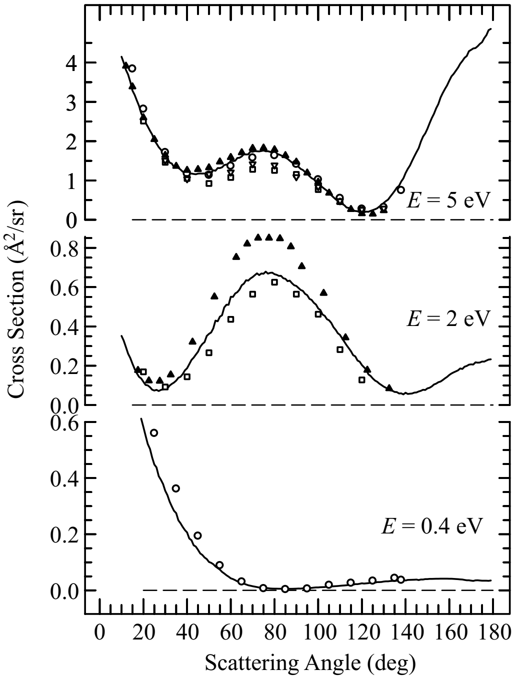

Fig. 1. Elastic cross sections in methane. Circles show the data of Sohn *et al.* [2], Squares of Rohr [3], black triangles of Bundschu *et al.* [1], white triangles of Tanaka *et al.* [4]

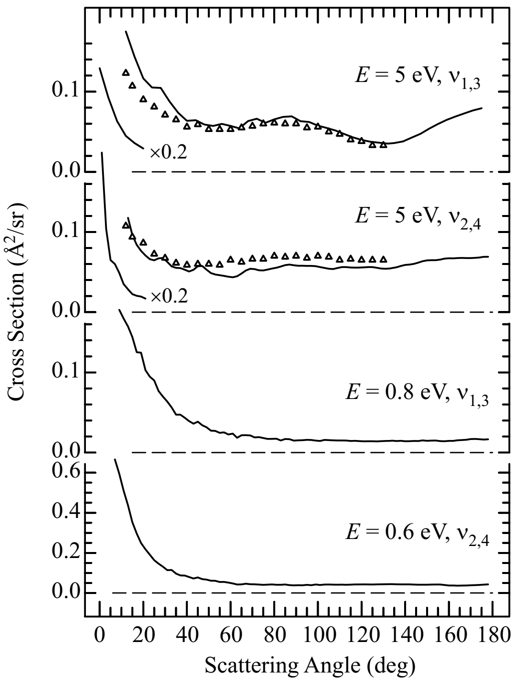

Fig. 2. Vibrational excitation cross sections in methane. Triangles show the data of Bundschu *et al.* [1].

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VELOCITY MAP IMAGING OF DISSOCIATIVE ELECTRON ATTACHMENT TO OXYGEN (O_2) AND NITRIC OXIDE (NO)

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Velocity map imaging (VMI) has been one of the recent techniques developed for the study of photo-ionization, photo-dissociation and photo-detachment by measuring the two momentum components in the given plane of interest [1]. We successfully modified this technique for low energy electron collision experiments [2]. This technique can provide simultaneous data on kinetic energy and angular distribution in the entire 2π angles, including the forward and backward directions with respect to the electron beam. This has helped us in solving two long standing problems regarding the DEA to two simplest molecules namely O_2 and NO.

Resonances in e^- - O_2 collisions has been a subject of much discussion in relation to vibrational and electronic excitation by electron impact [3], dissociative electron attachment [4] and electron collisions on condensed and adsorbed molecules [5]. The DEA to O_2 is known to show only one broad resonance in the O^- channel arround 6.5eV electron energy. This resonance is assigned to the $^2\Pi_u$ negative ion state based on the angular distribution studies using the conventional technique [6]. But the $^4\Sigma_u^-$ state of O_2^- is known to be the dominant resonance contributing to the vibrational excitation of the ground state of molecular oxygen under electron impact, as a broad peak centered at 9 eV in the vibrational excitation functions [3, 7]. Excitation to very high lying vibrational levels, close to dissociation threshold of the ground state has been observed at these electron energies [7]. Considering this, it is expected that the resonance would have long enough lifetime to manifest in the DEA channel. Based on the selection rules for DEA, the clear cut evidence for the presence of the $^4\Sigma_u^-$ state is likely manifest in the backward and forward directions in this case. Our measurements in the entire 2π angles using the VMI provide conclusive evidence for the first time on the contribution from this state to the DEA process.

DEA to NO is known to form O^- ions with the cross section curve showing a broad peak in the 8 to 11 eV region [8]. There are three possible channels through which O^- could be formed:

$$
\begin{aligned}
NO + e^- \rightarrow NO^{-*} &\rightarrow O^- + N\,(^4S) \qquad \text{(Channel 1)}\\
&\rightarrow O^- + N\,(^2D) \qquad \text{(Channel 2)}\\
&\rightarrow O^- + N\,(^2P) \qquad \text{(Channel 3)}
\end{aligned}
$$

The energy thresholds for these channels are 5.074 eV, 7.457 eV, and 8.650 eV respectively. There have been contradictory findings based on O^- kinetic energy measurements regarding the presence of these three channels in the DEA process. All the kinetic energy measurements carried out at 90 degrees to the electron beam direction showed that the first channel is absent and the process is dominated by the second channel, with one experiment pointing to the possibility of some contribution from the third channel [9, 10]. This is in contrast to the only measurements in the forward direction which showed the presence of all three channels, with the first channel being the most significant one [11, 12]. Our VMI data on DEA to NO show clearly distinct contributions from channels 2 and 3, in terms of both kinetic energy and angular distributions. The data also rule out the possibility of channel 1.

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FUNCTIONAL GROUP DEPENDENT SITE ELECTIVE FRAGMENTATION OF SIMPLE ORGANIC MOLECULES USING LOW ENERGY ELECTRONS

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Controlling the molecular dynamics has been considered to be one of the most effective ways to control the chemical reactions. There have been several ideas proposed in this direction that include the mode selective chemistry [1], and quantum interference of the various product channels leading to enhancement or suppression of a particular product channel [2]. With the advent of lasers these ideas were realized in actual experiments. The idea of mode selective chemistry has been demonstrated in a number of cases in reactive collisions involving molecules and in channel selective photo-dissociation of molecules [3]. Inelastic tunneling of electrons in a scanning tunneling microscope has also been used in a number of cases to break individual bonds and induce and control molecular motion on surfaces [4]. In our recent experiments we find that collision of free electrons to small organic molecules could be used to selectively fragment the molecules at specific sites using electron energy as a control parameter through the dissociative electron attachment process. We find that this selectivity is not due to specific energy thresholds as has been reported for some cases till now [5], but due to the core excited nature of the resonances.

In our studies of dissociative electron attachment (DEA) to some simple organic molecules like simple carboxylic acids, alcohols and an amine, some specific patterns in the resonant structure for the H^- channel are observed. These patterns are found to be specific to the functional groups associated with the molecules and in turn similar to the pattern shown by the precursor molecule of the functional group. For example, in the case of acetic acid (CH_3COOH), the prominent resonances are observed in the H^- channel at 6.7 eV, 7.7 eV and 9.1 eV. The study of DEA to partially deuterated acetic acid (CH_3COOD) revealed that the first two resonances are associated with the breaking of O-H bond. The corresponding energies are found to be close to the resonances observed for the same channel in DEA to the water molecule. The third resonance is found to be coming from the C-H bond breaking and energetically close to that observed for ethane. We also observed similar behavior in the alcohols. The H^- ion yield curve from the amine also provided results as expected from NH_3, thus conforming the functional group dependent selective fragmentation in the DEA process.

We explain our observations qualitatively in terms of core excited resonances. The core excitation by the incoming electron is similar to the case of photo-absorption in which a particular orbital electron is excited. The absorption spectra of molecules with same functional groups show remarkable similarity [6]. Once this electron is excited, the corresponding atomic core will have less screening of the nuclear charge. Subsequently the incoming electron is likely to be localized in the vicinity of this atom. This results in the localization of both the excess energy and the electronic charge. Since the DEA occurs in vibrational time scales, there will be relatively little energy redistribution. Due to the localization of energy, the fragmentation occurs at the site of core excitation and the excess charge is carried away by one of the fragments.

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ADF Calculation of Core-Electron Binding Energies

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Abstract

A total of 54 core-electron binding energies were studied with the ADF program and compared with the observed values. The results indicate that a polarized triple-zeta basis set of Slater-type orbitals is adequate for routine assessment of the performance of each method of computation. With such a basis set, seven density functionals were tested. In addition, the performance of twenty-one energy density functionals were computed from the density calculated with the statistical average of orbital potentials. Among all the choices tested, the best density functional for core-electron binding energies of C to F turns out to be the combination of Perdew-Wang 1986 functional for exchange and the Perdew-Wang 1991 functional for correlation, confirming earlier studies based on contracted Gaussian-type orbitals. For this best functional, five Slater-type orbital basis sets were examined, ranging from polarized double-zeta quality to the largest set available in the ADF package. For the best functional with the best basis set, the average absolute deviation of the calculated value from experiment is only 0.13 electron volts.

RATE COEFFICIENTS FOR VIBRATIONAL EXCITATION OF CF_4 IN CROSSED RF ELECTRIC AND MAGNETIC FIELDS

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Knowledge of electron transport coefficients as well as detailed understanding of the kinetic phenomena that may occur in rf plasma are two basic demands in plasma modeling nowdays [1]. Transport coefficients obtained under conditions of crossed RF electric and magnetic fields are the input data necessary for fluid models of plasma reactors such as ICP (inductively coupled plasmas). In particular, the behaviour of the transport coefficients is important for a fundamental understanding of processes leading to RF plasma maintenance. However, modeling of RF plasmas often relies on application of DC swarm data. Hence, there are some critical steps in plasma modeling. Apart from the application of time resolved fields in our calculations another critical step is proper inclusion of the effects of magnetic field as well as adequate treatment of the electron transport which is non-local in space and not fully relaxed in time.

The aim of this work is to investigate behavior of the rate coefficients for vibrational excitation under the influence of crossed RF fields in pure CF_4. CF_4 is one of the most frequently used gases in plasma applications in ultra large scale integrated (ULSI) circuit technologies. Therefore, a great effort has been made in order to complete sets of cross sections and related electron swarm data in order to employ them in plasma modeling [2,3]. The structure of cross section with the predominant inelastic electron scattering process at low energy range require non-trivial treatment of the electron transport. Rapidly rising cross section for vibrational excitation in the region of Ramsauer-Townsend minimum induce a strong anisotropy of the electron velocity distribution function (EVDF) and the most common techniques employed for calculating the electron transport parameters in plasma modeling may fail. Therefore the only recourse for CF_4 is the exact techniques such as the multi-term theory for solving the Boltzmann equation or Monte Carlo simulations.

Our calculations based on Monte Carlo simulation technique show that the effect of the magnetic field is strong and consequently produces complex behavior of the electron swarm transport coefficients and kinetic phenomena that should be accounted for in plasma models. In particular, we show the rate coefficients for vibrational excitation in order to analyze and understand electron kinetics at the region of Ramsauer-Townsend minimum.

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TEMPORAL RELAXATION OF ELECTRON SWARMS IN ELECTRIC AND MAGNETIC FIELDS CROSSED AT ARBITRARY ANGLES

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The theoretical investigations of electron swarms moving in an unbounded gas in electric and magnetic fields is a topic of great interest both as a problem in basic physics and for its potential for application to modern technology such as plasma processing. One of the major challenges in these investigations is an accurate representation of temporal and spatial relaxation of electrons. From a purely physical point of view, the knowledge of temporal relaxation is essential for a better understanding of electron-molecule interaction in short time intervals as well as a better understanding of transient transport phenomena in gases such as transient negative electron mobility [1]. The correct estimation of relaxation times for electron swarm transport parameters is important in experimental swarm physics, e.g., for design of the drift tubes. On the other hand, from an applied point of view, studies of temporal relaxation play a vitally important role in modeling of low-temperature, non-equilibrium plasmas. As an illistrative example, the relaxation times of the electron transport properties are necessary input data for fluid plasma models such as the relaxation continum model [2].

With these remarks as background, the groups at the Institute of Physics in Belgrade and James Cook University of Townsville have undertaken a program to understand the transient kinetic behavior of electron swarms under the combined action of electric and magnetic fields. The scope of this program covers a variety of hydrodynamic and non-hydrodynamic studies on the electron swarm relaxation by using a fully kinetic Monte Carlo simulation code [3] and multi-term theory for solving the Boltzmann equation [4]. In this work we study the temporal relaxation problem for the electron swarm in electric and magnetic fields crossed at arbitrary angles. Similar studies have been published previously for neon using the two-term approximation [5]. We extend these studies by (i) overcoming the inherent inaccuracies of the two-term approximation and (ii) addressing the temporal relaxation of spatial inhomogenities through a study of the diffusion tensor.

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ELECTRONIC EXCITATION OF N_2 MOLECULES BY ELECTRON-IMPACT: APPLICATION OF THE MINIMAL ORBITAL BASIS FOR SINGLE CONFIGURATION INTERACTIONS (MOB-SCI) STRATEGY

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Collisions between slow electrons and N_2 molecules play a key role for the understanding of a variety of natural phenomena that occurs in the Earth’s upper atmosphere as well as in other planetary atmospheres and in the interstellar media [1]. The knowledge of the cross sections related to collisional processes involving molecular nitrogen is also essential for the modeling of chemically active plasmas used in the fabrication of microelectronics devices [2]. In special, it has been pointed out in several publications that the electronic excitation processes strongly affects the reaction dynamics in such discharge environments [3]. In spite of the great interest in the compilation of reliable cross section data base for this collision process, the number of theoretical studies concerning the electronic excitation of nitrogen molecules by impact of low-energy electrons is still very scarce. Besides, the agreement among measured data and the results obtained by different methods is still far from satisfactory.

Motivated by this context we have decided to perform a study for the e^--N_2 electronic excitation by means of the Schwinger multichannel method [4]. Our scattering amplitudes are obtained within the minimal orbital basis for single configuration interactions (MOB-SCI) level of approximation [5]. Specific issues addressed by the present work may be summarized as follows:

(i) the representation of the target is improved by a CI-singles description of the excited states;

(ii) through the use of the MOB-SCI strategy we have investigated the coupling effects among ground state and first singlet and triplet states of the same symmetry representation, while keeping the pseudo-state associated space as minimum as possible;

(iii) the numerical stability of our scattering calculations is analyzed through the use of a check procedure similar to those developed by Chaudhuri and co-workers [6];

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VIBRATIONAL EXCITATION OF H_2 MEDIATED BY THE $^2\Sigma_g$ FESHBACH RESONANCE

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In low−energy electron scattering by polyatomic molecules, the coupling between electronic and vibrational degrees of freedom plays an important role when the incident particle is temporarily captured in the neighborhood of the molecule (resonance). This phenomenon is strongly responsible for the formation of reactive species (ions) in discharge environments (cold plasmas).

Hydrogen molecule has a number of nearby low-lying electronic states. In particular, there are experimental data on excitation to the lowest excited states, all of which have vertical excitation thresholds in the range 10-13eV. These studies yield a wealth of data including features which have been associated with several series of resonances [1]. While considerable effort has been devoted to the $^2\Sigma_u$ shape resonance in elastic $e^-{-}H_2$ collisions, reported theoretical data for core-excited and Feshbach resonances are sparse. Hydrogen may be viewed as a prototype system presenting the essential dynamical features and difficulties found in more complex molecules.

In this work, we study vibrational excitation and dissociation of H_2 mediated by the $^2\Sigma_g$ Feshbach resonance. Electron collisions are described with the Schwinger multichannel method (SMC) [2] in combination with a time-dependent formulation of the Local-Complex-Potential (or Boomerang) model [3] to account for the nuclear dynamics. We explore the $e^-{-}H_2$ $^2\Sigma_g$ resonance associated with the $a^3\Sigma_g^+$ parent state of H_2 and its influence on the elastic and $X^1\Sigma_g^+ \rightarrow b^3\Sigma_u^+$ excitation cross section. To the best of our knowlege, a systematic *ab initio* study of this resonance has never been carried out. In Fig. 1 we show the resonance position (upper panel) and width (lower panel) as a function of the interatomic distance (R). The upper panel also shows the potential energy curves for the electronic states of interest, obtained with restricted Hartree-Fock and improved-virtual-orbital SCF wave functions.

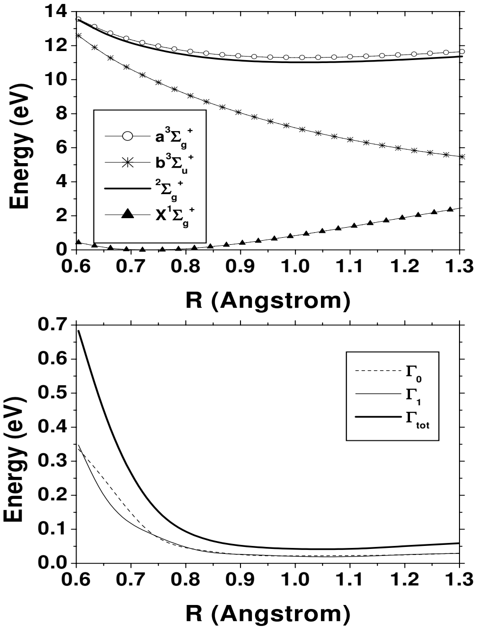

Fig. 1. Upper panel: Potential energy curves of H_2 and H_2^-. Solid line with triangle: ground sate ($X^1\Sigma_g^+$); solid line with asterisk: $b^3\Sigma_u^+$ state; solid line with empty circle: $a^3\Sigma_g^+$ state; thick solid line: $^2\Sigma_g^+$ resonance. Lower panel: resonance widths. Dashed line: partial width for decay to the ground state; thin solid line: partial width for decay to the $b^3\Sigma_u^+$ state; thick solid line: total width.

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VIBRATIONAL EXCITATION OF HYDROGEN MOLECULES BY ELECTRON AND POSITRON IMPACT

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We report results obtained with the Schwinger Multichannel (SMC) Method [1] for the vibrational excitation of H_2 by low-energy electron [2] and positron [3] impact.

We also report a comparative study of both integral and differential cross sections detailing the differences in the vibrational excitation cross sections related to important dynamic aspects such as projectile charge and exchange (antisymmetry), which is absent in positron scattering. Using a set of SMC scattering amplitudes calculated at specific quadrature points for the internuclear distance, we have obtained vibrationally resolved cross sections in the adiabatic aproximation[6]. The vibrational excitation cross section is given by

$$\frac{d\sigma_{\nu\to\nu'}}{d\Omega}(\theta)=\frac{1}{8\pi}\frac{k_{\nu'}}{k_{\nu}}*$$

$$\iint\left|\int\chi_{\nu'}(R)f^{\mathrm{Lab}}_{\vec{k}_{\Gamma,\nu},\vec{k}_{\Gamma',\nu'}}\chi_{\nu}(R)dR\right|^{2}d\Omega_{\vec{k}_{\Gamma}}d\phi_{\vec{k}_{\Gamma'}}$$

where ν and $\nu\,'$ are the vibrational quantum numbers of the molecule (initial and final vibrational states); Γ and Γ' are the eletronic channels; and R is the interatomic distance (irrotational molecule).

In the figures we show our theoretical results for excitation to the first excited vibrational state. The calculated integral and differential (5 eV) cross sections are shown in Figs. 1 and 2, respectively, and compared with existing experimental data. In Fig. 1, there is good agreement between theory and experiment for both positron and electron scattering. In Fig. 2, a sharp minimun at 90 degrees is noted in the e^+-H_2 croos section.

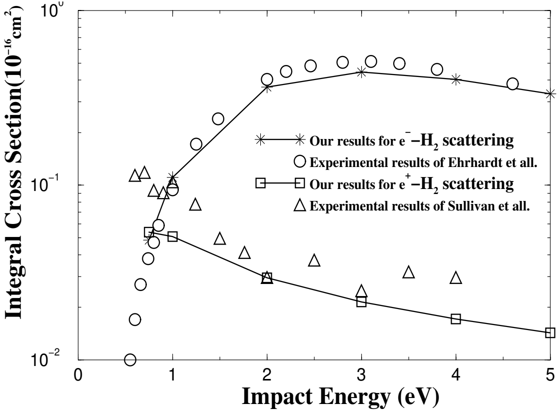

Fig. 1. Integral 0 → 1 vibrational excitation cross section of H_2 by e^- and e^+ impact. Present calculations: e^+, full line with squares; e^-, full line with stars. Experimental data: e^+, open circles[5]; e^-, triangles[4].

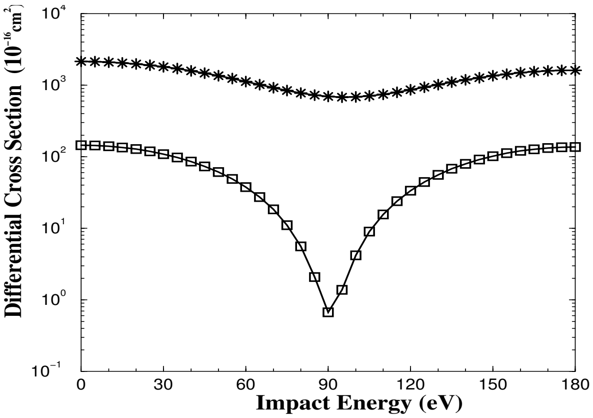

Fig. 2. Differential 0 → 1 vibrational excitation cross section of H_2 by e^- and e^+ impact at $E = 5.0eV$. e^+, full line with squares; e^-, full line with stars.

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Author Index