XIX International Symposium on Electron-Molecule Collisions and Swarms

Book of Abstracts

POSMOL 2015

17-20 July 2015, LISBOA, PORTUGAL

XVIII International Workshop on Low-Energy Positron and Positronium Physics &
XIX International Symposium on Electron-Molecule Collisions and Swarms
17 - 20 July 2015, Lisboa, Portugal

POSMOL 2015

XIX International Symposium on Electron-Molecule Collisions and Swarms

	Friday	Saturday		Sunday		Monday	
	17/07/2015	18/07/2015		19/07/2015		20/07/2015	
08:30 - 09:00		OPENING REMARKS					
09:00 - 09:45		PL01 - ALLAN		PL03 - BRAY		PL05 - TENNYSON	
09:45 - 10:15		TL01 - VARELA		TL09 - SUGAWARA		TLE 15 - ORLANDO	TLP 15 - KURODA
10:15 - 10:45		TL02 - DANIELSON		TL10 - CHIARI		TLE 16 - RACKWITZ	TLP 16 - STORRY
10:45 - 11:15		COFFEE BREAK		COFFEE BREAK		COFFEE BREAK	
11:15 - 11:45		TLE 03 - DENIFL	TLP 03 - GRIBAKIN	TLE 11 - URQUIJO	TLP 11 - LISZKAY	TLE 17 - SAJEEV	TLP 17 - ERIKSON
11:45 - 12:15		TLE 04 - PTASINSKA	TLP 04 - BETTEGA	TLE 12 - DONKO	TLP 12 - ASAI	TLE 18 - VÁSQUEZ	TLP 18 - NATISIN
12:15 - 14:00		LUNCH		LUNCH |COMMITTEES MEETING		LUNCH	
14:00 - 14:45		PL02 - BROMLEY		PL04 - PETROVIC			
14:45 - 15:15		TLE 05 - GAY	TLP 05 - MICHISHIO	TLE 13 - ALVES	TLP 13 - TATTERSALL		
15:15 - 15:45		TLE 06 - COSTA	TLP 06 - BRAWLEY	TLE 14 - BOYLE	TLP 14 - HOGAN		
15:45 - 16:15		COFFEE BREAK		COFFEE BREAK			
16:15 - 16:45		TLE 07 - SWIDEREK	TLP 07 - JONES	EXCURSION			
16:45 - 17:15	WELCOME RECEPTION AND REGISTRATION	TLE 08 - KUMAR	TLP 08 - MACHACEK			DEPARTURE	
17:15 - 19:00		POSTER SESSION | WG1CELINA MEETING					
19:00 - 00:00				CONFERENCE DINNER			

XIX International Symposium on Electron-Molecule Collisions and Swarms
Lisboa, Portugal
17-21 July, 2015

XIX International Symposium on Electron-Molecule Collisions and Swarms

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Editorial

Dear Colleagues,

Welcome to Lisboa and POSMOL 2015, the XVIII International Workshop on Low-Energy Positron and Positronium Physics & the XIX International Symposium on Electron-Molecule Collisions and Swarms. POSMOL 2015 permits to achieve a very privileged forum of sharing and developing our scientific expertise on current aspects of positron, positronium and antiproton interactions with electrons, atoms, molecules and solid surfaces, and related topics, as well as electron interactions with molecules in both gaseous and condensed phases. Particular topics include studies of electron interactions with biomolecules, electron induced surface chemistry and the study of plasma processes. Recent developments in the study of swarms are also fully addressed. We are very pleased to host in Lisboa for the first time POSMOL 2015 with 160 delegates from 25 countries.

POSMOL 2015 promises to be an exciting and stimulating conference with 5 plenaries, 4 joint topical lectures, 28 oral presentations and more than 100 posters providing a very privileged opportunity of scientific discussions on positron and positronium physics, electron-molecule collisions and swarms.

Just before the meeting, we have arranged to honour our loyal colleague and trusted friend Steve Buckman, Professor of Physics and School Director at the Australian National University, Canberra, Australia, on the occasion of his retirement in acknowledgement of his many achievements in Atomic and Molecular Physics.

POSMOL 2015 local logo has been envisaged from a Portuguese caravel, a sailing ship developed in the 15th century by the Portuguese to explore along the West African coast and into the Atlantic Ocean, together with two crows as symbol of Lisboa and guardians of the city. Both crows appear in red and blue colours which have been a while ago adapted as to represent the positrons and electrons & swarms communities.

We would like to express our gratitude to the local organizing committee, in particular to Susana Sério, Guilherme Meneses, Tiago Cunha, Emanuele Lange and Ana Luísa Cruz (local secretary) who worked so hard and made this meeting happen.

Last but not least, we wish you a successful meeting and a pleasant stay in Lisboa.

Paulo Limão-Vieira

Gustavo García

Filipe Ferreira da Silva

POSMOL 2015 Chairs

Lisboa, July 2015

General Information

ACCESS TO CAMPUS DE CAMPOLIDE

Lisbon airport is located in the city centre. It is easy to reach Campus de Campolide by metro from the airport, Red Line from Airport to S. Sebastião. Campus de Campolide can be reached within 10 minutes walking from S. Sebastião station.

REGISTRATION

The registration desk will be located at the atrium of the Rectorate building from 16:00 to 19:00 on Friday 17th July.

VENUE FOR SCIENTIFIC PRESENTATIONS

The POSMOL 2015 opening will be held on Saturday 18th July at 08:30 in room A. The plenary lectures, joint topical lectures and positron lectures will be held in room A, whereas EMS lectures will in room B. Poster session will be held on Saturday 18th July from 17:15 to 19:00 in the atrium of the building.

ORAL PRESENTATIONS

Room A and B are equipped with desktop computer. Speakers are recommended to bring their presentations in ppt, pptx or PDF format on a USB pen drive. Speakers should upload their presentations in advance. Speakers who want to use their Mac laptops should bring DVI-VGA or DisplayPort-VGA adapter.

POSTER PRESENTATIONS

Posters should fit A0 size suitable for the boards. Posters may be displayed from Friday 16th July and should remain until the end the conference.

BADGES

Please have your badge all the time.

WELCOME RECEPTION AND CONFERENCE DINNER

The welcome reception will be held on Friday 17th July at the atrium and front garden of the Rectorate building and the conference dinner on Sunday 20th July at "Estufa Real", Ajuda botanic garden.

POSTER PRIZE

The International Advisory Committees will award a poster prize to the best posters in EMS and Positrons. The winners will be announced during the conference dinner and awarded a € 50 prize each.

INTERNET ACCESS

There is free Wi-Fi internet access in the rooms and in the atrium of the Rectorate building. Details will be provided at the conference.

EPJD SPECIAL ISSUE

An EPJ D Special issue on "Advances in Positron and Electron Scattering" has been commissioned on topics related to the Workshop and Symposium.

Guest Editors: Paulo Limão-Vieira (Universidade Nova de Lisboa, Portugal), Gustavo García (CSIC Madrid, Spain), E Krishnakumar (Tata Institute of Fundamental Research, India), James Sullivan

(Australian National University, Australia), Hajime Tanuma (Tokyo Metropolitan University, Japan), Zoran Petrovic (Institute of Physics, Serbia & Montenegro).

1. This special issue of EPJ D provides an opportunity to have only original material, refereed and published quickly.

2. Accordingly, authors making a contribution should, on their own initiative, submit their paper to https://articlestatus.edpsciences.org/is/epjd . The style files of EPJ D must be used - they can be found at www.epj.org (in the pull-down of the LaTeX manuscript button in the left margin).

3. Articles submitted must be strictly journal length and quality and each will be refereed like any regular paper of its kind submitted to EPJ D.

4. All manuscripts should be submitted no later than December 31 2015.

MEALS

Lunch and coffee break are provided on 18th, 19th and 20th July.

SPONSORS

SCIENTIFIC PROGRAMME OF THE XIX INTERNATIONAL SYMPOSIUM ON ELECTRON-MOLECULE COLLISIONS AND SWARMS

Friday 17th July

16:45 – 19:00   REGISTRATION AND WELCOME RECEPTION (Campus Campolide)

Saturday 18th July

08:30 – 09:00   **Opening Remarks**

Plenary Lecture – Chair: E. Krishnakumar (Room A)

09:00 – 09:45   PL01: **M. Allan** (*University of Fribourg*)
"Nuclear dynamics in resonances, 2-dimensional EEL spectra, electrons and ionic liquids, electronic excitation and other stories"

Session A – Chair: M. Tachikawa (Room A)

09:45 – 10:15   TL01: **M. T. do N. Varella** (*University of São Paulo*)
"Electron-induced damage to biomolecules: from gas to condensed phase"

10:15 – 10:45   TL02: **J. R. Danielson** (*University of California*)
"Role of Vibrational Mode Coupling in Determining Positron Annihilation on Molecules"

10:45 – 11:15   COFFEE BREAK

Session B – Chair: O. Ingólffson (Room B)

11:15 – 11:45   TLE03: **S. Denifl** (*University of Innsbruck*)
"Low energy electron interaction with (hydrated) pyrimidine clusters"

11:45 – 12:15   TLE04: **S. Ptasinska** (*University of Notre Dame*)
"Evaluation of low energy electron-induced fragmentation of peptide model molecules"

12:15 – 14:00   LUNCH

Plenary Lecture – Chair: S. Buckman (Room A)

14:00 – 14:45   PL02: **M. W. J. Bromley** (*University of Queensland*)
"The remorseless AMO physics of Jim Mitroy"

Session C – Chair: R. Curik (Room B)

14:45 – 15:15   TLE05: **T. Gay** (*University of Nebraska*)
"Threshold Alignment Reversal and Circularly-Polarized Fluorescence in Rotationally-Resolved H2"

15:15 – 15:45   TLE06: **R. F. da Costa** (*Universidade Federal do ABC*)
"The role of multichannel coupling effects on the description of electron-molecule collisions"

15:45 – 16:15   COFFEE BREAK

16:15 – 16:45 **Session D** – Chair: N. J. Mason (Room B)
TLE07: **P. Swiderek** (*University of Bremen*)
"The electron-induced chemistry of FEBID: Beyond DEA and thermal fragmentation"

16:45 – 17:15 TLE08: **R. Kumar** (*University of Iceland*)
"Low energy electron induced fragmentation of potential FEBID precursors"

17:15 – 19:00 **Poster Session**
COST Action CM1301 CELINA WG1 Meeting (Room B)

Sunday 19th July

09:00 – 09:45 **Plenary Lecture** – Chair: Y. Nagashima (Room A)
PL03: **I. Bray** (*Curtin University*)
"Theory of low-energy positron scattering on atoms and molecules"

09:45 – 10:15 **Session E** – Chair: G. Laricchia (Room A)
TL09: **H. Sugawara** (*Hokkaido University)*
"Electron behavior under characteristic magnetic fields applied to inductively coupled plasmas for control of charged particle transport"

10:15 – 10:45 TL10: **L. Chiari** (*Tokyo University of Science*)
"Cross section measurements for positron and electron scattering from molecules of biological relevance"

10:45 – 11:15 **COFFEE BREAK**

11:15 – 11:45 **Session F** – Chair: M. Hoshino (Room B)
TLE11: **J. de Urquijo** (*Universidad Nacional Autónoma de Mexico*)
"Ion-molecule reactions and secondary ionization processes in gases of biological and atmospheric interest"

11:45 – 12:15 TLE12: **Z. Donko** (*Hungarian Academy of Sciences*)
"Coulomb collisions in electron swarms in heavy rare gases: effects on negative differential conductivity"

12:15 – 14:00 **LUNCH**

14:00 – 14:45 **Plenary Lecture** – Chair: H. Cho (Room A)
PL04: **Z. Lj. Petrovic** (*University of Belgrade*)
"Swarms as an exact representation of weakly ionized gases"

14:45 – 15:15 **Session G** – Chair: R. White (Room B)
TLE13: **L. L. Alves** (*Instituto Superior Técnico*)
"Electron scattering cross sections for the modelling of oxygen-containing plasmas"

15:15 – 15:45 TLE14: **G. J. Boyle** (*James Cook University*)
"Spatiotemporal evolution of electrons in gaseous and liquid argon"

15:45 – 16:15 **COFFEE BREAK**

16:15 – 19:00   **EXCURSION**

19:00   **CONFERENCE DINNER**

Monday 20th July

09:00 – 09:45

Plenary Lecture – Chair: I. Fabrikant (Room A)
PL05: **J. Tennyson** (*University College London*)
"Calculations of bound and continuum states of molecules using the R-matrix method"

09:45 – 10:15

Session H – Chair: P. van der Burgt (Room B)
TLE15: **T. M. Orlando** (*Georgia Institute of Technology*)
"Low energy (< 5 eV) electron interactions with DNA and RNA nucleotides"

10:15 – 10:45   TLE16: **J. Rackwitz** (*University of Potsdam*)
"Novel approaches to study low-energy electron-induced damage to DNA oligonucleotides"

10:45 – 11:15   **COFFEE BREAK**

11:15 – 11:45

Session I – Chair: H. Tanuma (Room B)
TLE17: **Y. Sajeev** (*Bhabha Atomic Research Centre)*
"Low-energy free-electron catalyzed chemical reactions"

11:45 – 12:15   TLE18: **F. J. Gordillo-Vázquez** (*Instituto de Astrofísica de Andalucía - CSIC*)
"Electron kinetics in upper atmospheric electrical discharges"

12:15 – 14:00   **LUNCH**

ABSTRACT INDEX

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Nuclear dynamics in resonances, 2-dimensional EEL spectra, electrons and ionic liquids, electronic excitation and other stories

Michael Allan and Khrystyna Regeta

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The talk will touch several subjects recently investigated in Fribourg:

2-D Electron Energy Loss spectra [1,2]. We show that 2D electron collision spectra contain rich information about the motion of a nuclear wave packet on a resonant potential surface - a key ingredient to understanding electron-induced chemistry. It is possible because the motion of the nuclear wave packet is characterized by a competition between propagation and detachment, the wave packet `rains down' along its path above the neutral potential surface and the final vibrational states carry (indirectly) information about where it rained down and thus allow us to `spy' on its trajectory. Changing the incident electron energy allows us to choose in which initial vibrational state (or boomerang state when the autodetachment is fast and the state is lifetime broadened) the resonance is prepared, i.e., into what direction (along what normal mode) is the nuclear wave packet initially sent. The spectra of the detached electrons carry information about the packet propagation, they tell us into what mode and into which quanta the wave packet dropped, and whether it changed modes by IVR.

Electrons and Ionic Liqids [3]. The instrument for low energy (0-30eV) electron impact spectroscopy, originally developed for gas phase molecules, is applied to room temperature ionic liquids (IL). Electron energy loss (EEL) spectra recorded near threshold, by collecting 0-2eV electrons, are largely continuous, assigned to excitation of a quasi-continuum of high overtones and combination vibrations of low-frequency modes. EEL spectra recorded by collecting 10eV electrons show predominantly discrete vibrational and electronic bands. The vibrational energy-loss spectra correspond well to IR spectra except for a broadening (~40 meV) caused by the liquid surroundings, and enhanced overtone activity indicating a contribution from resonant excitation mechanism. The spectra of four representative ILs were recorded in the energy range of electronic excitations and compared to density functional theory multireference configuration interaction (DFT/MRCI) calculations, with good agreement. The spectra up to about 8 eV are dominated by π-π^* transitions of the aromatic cations. The lowest bands were identified as triplet states. The spectral region 2-8 eV was empty in the case of a cation without π and π^* orbitals. The EEL spectrum of a saturated solution of methylene green dye in an IL band showed the methylene green EEL band at 2eV, indicating that ILs may be used as a host to study nonvolatile compounds by this technique in the future.

Electronic Excitation. Ethene, furan [4], benzene and pyrimidine will be compared and the common trends in the cross sections pointed out. The problem of connecting the electronic excitation cross section with neutral dissociation will be addresses by presenting an attempt to calculate the repulsive nature of the potential surfaces of the electronically excited states of $Pt(PF_3)_4$ [5].

References

[1]   K. Regeta and M. Allan, *Phys. Rev. Lett.*, **110**, (2013), 203201.
[2]   K. Regeta and M. Allan, *J. Chem. Phys.*, **142**, (2015), 184307.
[3]   K. Regeta and M. Allan, *Phys. Chem. Chem. Phys.*, (2015), DOI: 10.1039/C5CP01417D
[4]   K. Regeta and M. Allan, *Phys. Rev. A*, **91**, (2015), 012707.
[5]   M. Zlatar, J. Fedor and M. Allan, (2015), in preparation.

PL-02

The remorseless AMO physics of Jim Mitroy

Michael W.J. Bromley

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In this lecture I will survey and attempt to summarise the scientific contributions that Prof. Jim Mitroy produced before his unexpected passing away in August 2014 [1]. Whilst he was never a dedicated follower of fashion, the research topics that he tackled during his lifetime were generally aligned with the scientific times. Over three decades he relied on a combination of computational approaches underpinned by an excellent theoretical understanding of Atomic, Molecular and Optical Physics. Armed with a keen nose for which problems were interesting enough and that he could remorselessly solve with the current generation of computers, he managed to regularly reinvent himself whilst still using many of the techniques that he developed early in his career. I will discuss, in loosely chronological order, his key discoveries, some of his nearly 200 papers, ideas, and modus operandi:

e^- Decade (1977-1989): The early years involved developing atomic structure methods and accurate (at the time) computer codes with an emphasis on electron-atom collisions:

- 1977-1983: PhD thesis in "Studies in atomic structure and (e, 2e) reactions" supervised by Ken Amos at The University of Melbourne.
- 1983-1986: Postdoctoral Researcher with Ian McCarthy at Flinders University in Adelaide.
- 1986-1988: Research Associate with David Norcross at JILA in Boulder, Colorado.
- 1988-1989: Research Fellow in Theoretical Physics at ANU in Canberra.

e^+ Decade (1990-2002): Began with his appointment in 1989 as a lecturer at the University College of Northern Territory (shortly thereafter renamed the Northern Territory University), and initially this period saw an adaptation of the electron-atom scattering methods to positron-atom collisions:

- 1993-1996: Sabbatical in 1993 with Andris Stelbovics at Murdoch University in Perth, sparked off a series of papers on positron-hydrogen scattering including re-arrangement [2].
- 1997-2000: Employed Gregory Ryzhikh (Ryjikh) to work on positron scattering off alkali metals, ended up discovering positronic lithium, and consequently a number of other positronic atoms along with myself (his only PhD student: 1998-2002) [3].
- 2000-2002: Employed Igor Ivanov, they solved the positronium-atom scattering problem.

Final Decade (2003-2014): His university changed its name to Charles Darwin University. He moved into photon-atom and atom-atom interactions, whilst maintaining positron related research. He enjoyed visiting San Diego, USA and Wuhan, China a number of times during this period:

- 2002-2003: Employed Sergey Novikov and described spin-orbit quenching of positronium.
- 2003-2014: Employed Jun-Yi Zhang, Li-Yan Tang, Jun Jiang and Yongjun Cheng. Computed atom-atom and photon-atom interactions, published a major review article in 2010 [4].
- 2006-2013: Core member of the Australian National Centre of Excellence for Antimatter-Matter Studies, and contributed broadly to its success. Led major method review article [5].

References
[1] M.W.J.Bromley, S.J.Buckman, C.W.Clark , *Physics Today Obituary*, (2015). http://scitation.aip.org/content/aip/magazine/physicstoday/news/10.1063/pt.5.6137
[2] J.Mitroy, "Close Coupling theory of positron Hydrogen scattering", *Aust.J.Phys.,* **46,** (1993), 751.
[3] J.Mitroy, M. W. J. Bromley and G. G. Ryzhikh "Positron and Positronium binding to atoms", *J.Phys.B,* **35,** (2002), R81.
[4] J. Mitroy, M.S.Safronova, C.W.Clark, "Polarizabilities of atoms and ions", *J.Phys.B,* **43,** (2010), 202001.
[5] J.Mitroy, S.Bubin, K.Varga, Y.Suzuki, W.Horiuchi, L.Adamowicz, W.Cencek, et al. "Theory and application of explicitly correlated gaussians", *Rev.Mod.Phys.,* **85, (**2013), 693.

Theory of low-energy positron scattering on atoms and molecules

I. Bray, D. V. Fursa, A. S. Kadyrov, J. J. Bailey and M. C. Zammit

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In recent years there has been considerable progress in the theory of positron scattering on atoms and molecules. So much so that in the case of the atomic hydrogen target the collision system can be formulated without approximation and solved computationally. The major complexity, incorporation of the positronium (Ps) formation channels, can be done routinely with the usage of complete two-centre square-integrable expansions. The accuracy of such approaches can be tested internally, without reference to experiment.

In the case of targets more complicated than atomic hydrogen, such as helium or the hydrogen molecule, the complexities are immense. Yet from the perspective of theory the goal is to provide an accurate formalism that is valid at all energies, and is sufficiently general to apply to rearrangement collisions more broadly, such as in proton-atom/molecule scattering. In the talk we shall discuss the various unique aspects of the positron-atom/molecule collision systems and their computational complexity.

Swarms as an exact representation of weakly ionized gases

Zoran Lj. Petrović[1], Saša Dujko[1], Dragana Marić[1], Danko Bošnjaković[1], Srđan Marjanović[1], Jasmina Mirić[1], Olivera Šašić[1], Snježana Dupljanin[1], Ilija Simonović[1], Ronald D. White[2]

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Often swarms are regarded as idealized ensembles of charged particles that may be realized in specialized experiments to provide accurate transport coefficients, which after some analysis, yield "complete" sets of cross sections and accurate representations of non-equilibrium electron energy distribution function (EEDF) for a given *E/N*. Generally it is believed nowadays that swarms are just a tool for modeling non-equilibrium (low temperature) plasmas, as some kind of an interface through which atomic physics enters plasmas. In this review we shall show some new results that extend that picture into several directions:

- New results for the cross sections in systems where information from beam experiments and binary collision theories are insufficient such as $C_2H_2F_4$ that is commonly used as a cooling gas in modern refrigerators and air conditioners, but also it is used in particle detectors and has a potential for plasma processing applications.
- Ionized gases where swarms are exact representation of the system. Those include weakly ionized gases such as atmosphere, gas breakdown, afterglow (after the breakup of the ambipolar field), steady state Townsend regime of discharges, conduction of electricity through gases, interaction of secondary electrons produced by high energy particles with the gas or liquid background and many more. A special example will be modeling of Resistive Plate Chambers, the most frequently used gas phase detectors of elementary particles in high energy experiments.
- Swarm studies provide best insight into non-hydrodynamic (or as plasma specialists call it non-local) development of the ionized gas. It is not only that simulations are simple but also some of the accurate experiments operate in such conditions and thus allow testing of such theories. One such example are the Franck Hertz oscillations. Temporal and spatial relaxation of properties of ensembles to the final distribution belong to this group as well and are of interest for a number of positron applications and trapping in general.
- Fluid models when applied to swarms provide a good way to test the fluid models as used in more general plasmas. This has yielded the need to generalize fluid equations and extend them to a one step further while using a higher order transport coefficients.
- Finally we shall address the open issues for transport theorists and atomic and molecular collision population in the attempt to represent transport of electrons, positrons and other particles in liquids, especially in water that has a strong dipole moment. Hydrated electrons and positrons are the actually particles of interest for modeling these particles in the human tissue.

As an interface between atomic and molecular collision physics on a lower phenomenological (but deeper) level and plasmas on a higher (but less fundamental) level swarm physics has the responsibility of providing plasma physics with its intellectual basis and fundamental importance. It is how we combine the building blocks of atomic and molecular physics, transport theory and other relevant elementary processes that will define generality of the conclusions about non-equilibrium plasmas that are all different and require a special approach.

The models that we provide here are simple, yet realistic and real systems that may be described by swarm models and that may be regarded as low ionization limits of some more complex non-equilibrium plasmas.

Calculations of bound and continuum states of molecules using the R-matrix method

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The R-matrix method involves the division of space into an inner region, where the detailed physics of the process under consideration takes place, and an outer region where asymptotic methods can be applied. The method was originally developed by Wigner to look at resonances in nuclear reaction; it remains a particularly powerful procedure for characterising resonances. The R-matrix method is now widely used to study collision problems involving electrons and positrons, as well as photonisation [1]. In particular it is a popular method low-energy electron-molecule collision problems [2].

Besides the systematic push to study larger molecules, electron-molecule collision calculations are also becoming more reliable. Thus recent R-matrix studies of the bound [3] and continuum [4] states of N_2 have mapped out these states with an unprecedented level of detail and accuracy. Progress on the use of the R-matrix for electron-molecule collision calculations will be considered. This issue of how these studies might be adapted to incorporate uncertainties will be discussed.

Positron-molecule collision calculations are generally more challenging than their electron counterparts. The R-matrix with pseudostates method (RMPS) was originally developed to extend the energy range of low-energy electron collision studies. However the more rigorous treatment of polarisation effects obtained using RMPS procedures has been found to significantly improve the treatment of positron-molecule collisions.

References
[1] P. G. Burke. R-Matrix Theory of Atomic Collisions: Application to Atomic, Molecular and Optical Processes, (Springer, 2011).
[2] J. Tennyson, *Phys. Rep.*, 491, 29 (2010).
[3] D.A. Little and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.*, **46**, (2013), 145102.
[4] D.A. Little and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.*, **47**, (2014), 105204.
[5] R. Zhang, P.G. Galiatsatos and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.*, **44**, (2011), 195203.

TL-01

Electron-induced damage to biomolecules: from gas to condensed phase

Márcio T. do N. Varella, Lucas M. Cornetta, Fábris Kossoski, Sylvio Canuto, Kaline Coutinho

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The role played by secondary electrons in the radiation damage to biomolecules is well established both in the gas phase [1] and in aqueous solution [2]. In this process, electrons released along the track of high-energy photons attach to biomolecules and give rise to dissociative transient negative ions (TNIs) that induce DNA strand breaks.

In this talk, we will address the TNI spectra of 5-halouracils, a well-known class of radiosensitizing drugs (chemicals that can enhance the efficiency of the radiation treatment of cancer cells), as obtained from bound-state and elastic scattering calculations below the electronic excitation thresholds, i.e., accounting for stable anions and shape resonances. All 5-X-uracil molecules, with X=F, Cl, Br and I, present rich spectra comprising dipole bound states, valences bound states and shape resonances. While the energies of the π^* anion states are not strongly dependent on the halogen substituent, the σ^*_{CX} shape resonances are strongly stabilized from 5-F-uracil to 5-I-uracil, ultimately suppressing the electron-induced hydrogen elimination reactions in the heavier species.

We also address free-energy barriers for the dissociation of nucleotide anions in aqueous solution. While the gas-phase studies have proven essential to understand the basic mechanisms for dissociative electron attachment, at least some of these mechanisms would not be expected to be as important in aqueous environment, e.g., those triggered off by dipole bound states or those involving the elimination of hydrogen atoms (in gas phase) that take part in hydrogen bonding with solvent molecules. The nucleotides can be viewed as prototypes for the DNA strands, as they comprise the nucleobase, sugar and phosphate units. However, the study of these systems in solution would challenge the scattering methods, such that we restrict our calculations to stable anions, therefore employing bound-state electronic structure techniques. At the present stage, our main goal is developing a protocol to approach the dissociation in liquid phase, such that we explore a number of relevant technical aspects, namely the choice of basis sets, correlation-exchange functionals in density functional theory (DFT) computations, as well as the use of continuum (implicit) solvation models, wherein the solvent is treated as a polarizable dielectric, or explicit solvent (water) molecules.

We employ several well-established techniques in the present studies. The scattering calculations were carried out with the parallel implementation [3] of the Schwinger Multichannel Method implemented with pseudopotentials [4]. The implicit solvation studies employed the SMD approach [5], while explicit solvation was described with Monte Carlo techniques [6]. The bound state calculations were carried out with standard quantum chemistry techniques (DFT and coupled-cluster).

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Role of Vibrational Mode Coupling in Determining Positron Annihilation on Molecules.[*]

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Positron collisions with molecules at incident positron energies in the range of the molecular vibrations can result in attached states formed *via* vibrational Feshbach resonances (VFRs) [1]. While the resulting positron-molecule complexes are not a true bound states, but resonances, the attached positron has an increased probability of annihilation. The resulting annihilation rate is determined by a competition between annihilation and vibrational auto-detachment. This talk summarizes our current state of knowledge regarding these effects - processes that dominate positron annihilation on most molecules at low energies - and current outstanding questions are highlighted.

A theory of resonant annihilation on isolated VFRs (so-called "entrance channels") is successful in predicting the annihilation rates for selected small molecules such as methyl halides [1]. However, the picture is typically more complicated. A key consideration (e.g., in alkanes and molecules with additional halogen substitutions) involves vibrational coupling to other modes (a process known in the chemistry community as intramolecular vibrational energy redistribution or IVR) [2]. The auto-detachment rate depends critically whether the molecular vibrational energy resides (or does not reside) in a mode that couples the attached positron to a continuum state. The former is dubbed an "escape" channel and the latter a "dark state."

These mode-coupling effects can be greatly enhanced by the close proximity of multimode vibrations to the entrance channel (i.e., near-resonant combination and overtone modes). For example, if one of the components of a multimode vibration is an escape-channel vibration, the VFR is strongly suppressed; and if the entrance channel couples strongly to dark-state multimodes (e.g., alkane molecules), the resonant annihilation can be greatly enhanced.

A simple model will be discussed that highlights the role that vibrational mode coupling plays in determining the strengths of the annihilation resonances, and the multimode vibrational structure of specific molecules will be related to observed annihilation-rate spectra [3]. With these pictures in mind, the relationship between the mode coupling effects studied in typical IVR experiments and those responsible for resonant positron annihilation will be discussed. The talk concludes with a focus on issues yet outstanding that need be addressed in order to make quantitative predictions of annihilation rate spectra when mode-coupling effects are operative.

+ In collaboration with M. R. Natisin and C. M. Surko.

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Low energy electron interaction with (hydrated) pyrimidine clusters

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In recent years there has been a significant interest in processes induced by low energy electrons in biological systems, especially in relation to DNA damage [1-3]. Ionizing radiation releases a large number of secondary electrons in cells. This secondary species with initial kinetic energies of up to few tens of eV interacts further inelastically with building blocks of cells before they enter a (pre-) hydrated stage. It was shown that low energy electrons with energies < 15eV can induce single and double strand breaks in a film of plasmid DNA upon electron irradiation [1-3]. The underlying mechanism of DNA damage on the molecular level was identified as dissociative electron attachment (DEA). Subsequently a large number of gas phase studies was carried out with isolated building blocks of DNA (see for example [3,4]). In these mass spectrometric studies resonance energies as well as (charged) fragmentation products were determined.

However, studies with isolated molecules in the gas phase have the limitation that solvation effects are neglected. To bridge the gap between single molecules and the condensed phase we carried out low energy electron attachment with small biomolecular clusters. For our first study we chose pyrimidine which represents a model molecule for nucleobases. The studies have been carried out using a double focusing mass spectrometer. Neutral pyrimidine clusters were formed by supersonic expansion of pyrimidine vapour with argon as seeding gas.

The results showed that solvation causes a strong modification of the DEA process. While the isolated molecule dissociates into fragment anions by ring cleavage, pyrimidine molecules in clusters preferentially decay by loss a single hydrogen atom. Stable parent cluster anions can be observed close to zero eV as well as in the range of core-excited resonances above 5 eV. The monomer anion of pyrimidine can be only observed in the latter range. Hydration of pyrimidine altered this resonance yield substantially.

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Evaluation of low energy electron-induced fragmentation of peptide model molecules

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The dissociative electron attachment (DEA) to analogues of peptides/proteins, i.e., compounds containing a peptide bond or carboxyl and amino groups are crucial for development of understanding of DEA to larger cellular biocomplexes, thus are valuable in many fields, specifically radiation therapy research and biochemical modeling.

In this project, we have used our recently constructed experimental set-up to measure the anion yields resulting from DEA to N-methylformamide (NMF) [1] and dimethylformamide (DMF), simplest molecules containing a peptide linkage. DEA to both molecules produces several anionic fragments, which were confirmed by isotopic studies. Moreover, our results suggest that peptide bond (O=C-N-H) cleavage was one of dissociation channel, which resulted in CH_3NH^- and $(CH_3)_2NH^-$ for NMF and DMF, respectively, requiring higher energies (> 5 eV) to occur. The energetics of this channels was compared with the corresponding reactions for other peptide-like molecules. Similarly, like other biomolecules, but in contrast to DMF, DEA to NMF leads to dehydrogenation, which is also site-selective and occurs either at the aldehyde or amide sites. The thermodynamic thresholds for H loss from each possible location were estimated based on DFT (B3LYP functional) calculations of the bond dissociation energies for the homolytic scission to give H atoms and based on the calculated electron affinities of the neutral radical products. Both the thresholds for H loss from the aldehyde and amide sites agree well with the experimental anion thresholds, whereas the onset for dehydrogenation from the methyl site is slightly higher. This is consistent with the incident electron energy control observed for methylated thymine, uracil, and other nucleobases in which the dehydrogenation site could be precisely controlled and exhibits a preference for H loss due to N-H dissociation relative to C-H dissociation [2,3].

Further, the formation of cationic fragments due to electron impact ionization have been studied in the near-threshold ionization regions.

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Threshold Alignment Reversal and Circularly-Polarized Fluorescence in Rotationally-Resolved H_2

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Using targets of H_2 and D_2 in pure rovibrational quantum states, we have measured the polarization of Fulcher-band fluorescence resulting from spin-polarized electron-impact excitation of $d^3\Pi_u \to a^3\Sigma_g^+$ transitions, for incident electron energies from 14 to 29 eV [1]. Measurements of the linear polarization fraction P_1 near threshold yields negative values indicating a dynamic production of $M_N = 0$ states, which has not been observed to date in molecular systems. Agreement with the only available theory for electron impact excitation of diatomic molecules in pure quantum states [2] is poor.

The circular polarization fraction P_3 is measured to be nonzero, which constitutes the first observation of orientation of rotationally-resolved molecular states. For Q-branch transitions, we find P_3 values to be consistent with a newly-developed extension of the Blum-Jakubowicz theory [1,3], based on Hund's case (b), for the coupling of molecular multipole moments that includes incident electron spin polarization. The R-branch P_3 values do not agree with this theory equally well, indicating the effect of Σ-symmetry perturbation of the parent $d^3\Pi_u$ state.

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The role of multichannel coupling effects on the description of electron-molecule collisions

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The theoretical description of electron-molecule collisions is a problem that needs to be approximated in a realistic way so that one can be able to predict reliable results to be compared against existing experimental data. The way to deal with this problem in the most comprehensive way is by considering: (i) the potential due to the nuclei and the electronic molecular density (static potential), (ii) the potential due to the anti-symmetrization of the (N+1)-identical electrons wave function (exchange potential), (iii) the short and long range potentials due to the distortion of the electronic cloud due to the presence of the incident electron (polarization potential) and, finally, (iv) the flux competition among all possible electronic transitions, including ionization, with all being due to the electron impact (multichannel coupling effect). As denoted by several studies available in the literature, the many-body dynamics in electron-molecule collisions is strongly affected by the inclusion and by a proper balanced treatment of all those effects.

In this talk we will focus on the analysis of the influence of multichannel coupling effects upon calculated cross section results. According to our previous experience, the description as accurate as possible of the target states and the use of a strategy to construct the open-channel space (number and type of states that become energetically accessible during the collision process) represent crucial steps in the definition of the best (and computationally feasible) level of multichannel coupling to be used in the scattering calculations. Aiming to address these aspects in a unified way we have recently developed the so called minimal orbital basis for single configuration interaction (MOB-SCI) strategy [1]. Through the use of the MOB-SCI strategy we constructed an open channel space composed by a set of hole-particle orbitals which is capable of reproducing the spectrum of excitation energies obtained within a full single configuration interaction calculation for energies below a previously defined cut-off energy value. Comparison among theoretical results obtained with different channel-coupling schemes, clearly indicates that convergence of the elastic cross sections, in terms of the number of excited states included in the open-channel space, is relatively quickly achieved for energies below 30 eV. For electronic excitation processes, our calculations revealed that at energies near to the thresholds of the excited states are in good agreement with the experiment. However, for higher energies our results remain systematically above the experimental data, indicating that more open channels would probably be needed in order to lower the magnitude of the computed inelastic cross sections. This would be a problem, considering that molecular systems typically present a high density of energetically accessible states, and points out that convergence with respect to open channels is an important challenge to be addressed. All these findings are quite well exemplified by our most recent applications involving 33-channels for phenol [2], 45-channels for ethylene [3] and 63-channels for furfural.

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The electron-induced chemistry of FEBID: Beyond DEA and thermal fragmentation

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Focused Electron Beam Induced Deposition (FEBID) is a very promising direct deposition technique for nanofabrication capable of producing free-standing 3D structures of sub-10 nm size [1]. FEBID relies on electron-driven fragmentation at a surface of volatile precursor molecules. Ideally, their central metal or metalloid atoms define the nature of the deposited material while the ligands responsible for the volatility dissociate from the central atom and desorb completely from the surface. For example, the precursor $Fe(CO)_5$ yields pure Fe deposits under ultrahigh vacuum conditions [2]. However, in many cases ligand material is embedded in the deposit and deteriorates its properties. As an extreme case, trimethyl(methylcyclopentadienyl)-platinum(IV) ($MeCpPtMe_3$) yields a deposit with composition Pt:C = 1:8 [3] indicating that only one methyl group becomes a volatile fragment. Loss of one methyl group also dominates dissociative electron attachment (DEA) to $MeCpPtMe_3$ pointing to the important role of low-energy secondary electrons in FEBID [4]. Similarly, DEA predominantly induces loss of only one PF_3 ligand from $Pt(PF_3)_4$ [5]. Further electron exposure of surface-bound $Pt(PF_3)_3$ fragments leads to dissociation of remaining ligands so that phosphorous becomes embedded in the deposit [6]. Here, thermal reactions favour dissociation of further Pt-P bonds so that an elevated temperature can be used to obtain purer deposits [7].

When aiming at a full understanding of FEBID chemistry, however, reactions following the initial fragmentation processes must also be considered. Reactive fragments can form new bonds with remaining precursor molecules and thus lead to synthesis of less volatile material [8]. For example, methyl fragments are trapped by the precursor ligand acetylacetone, a reaction which most likely contributes to the incorporation of impurities in FEBID processes using acetylacetonate precursors [9]. As another example, deposits produced from $MeCpPtMe_3$ may be purified by electron-beam treatment in the presence of water vapour [10,11] with interesting implications concerning the use of cyclopentadienyl precursors that are so far deemed notoriously bad for FEBID.

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Low energy electron induced fragmentation of potential FEBID precursors

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Focused electron beam induced deposition (FEBID) is a 3D nanofabrication technique in which focused high-energy electron beam is used to create nanostructures on substrate surfaces. The physics behind FEBID are based on the electron beam induced dissociation of precursor molecule adsorbed onto the substrate. Therefore the composition and resolution of the fabricated structures strongly depends upon the behavior of the precursor molecules towards electron beam induced dissociation. Moreover, the deposit is largely formed through low energy secondary electrons (SEs) generated by the primary electron beam (PE), rather than the PE itself. Thus the energy distribution, the yield and the spatial extent of the SEs emitted from the substrate is an important factor in determining the performance of FEBID. However, not less important is nature of the interaction of this low energy SEs with the precursor molecules. In the typical SE energy range in FEBID dissociative electron attachment (DEA), dissociative ionization (DI), dipolar dissociation (DD) and neutral dissociation (ND) may all open active dissociation channels. These processes all show different energy dependency and result in different fragmentation products. To which extent the individual dissociation mechanisms contribute to the deposit formation will thus depend on the energy dependency of the efficiency of individual channels along with the energy distribution and yield of the SEs in the relevant energy range. This in turn will define the chemical composition and spatial extent, of the respective deposits.

In the current contribution we discuss the role of low energy electron induced dissociation in FEBID in relation to DEA, DI, DD and ND. In this context, we give a comparison of gas phase DEA and DI studies with surface studies on electron induced fragmentation of selected FEBID precursors, and we discuss these in context to the dissociation mechanisms governing FEBID with these precursors.

In the second part we discuss the role of DEA and DI in FEBID with the precursor molecules 1, 1-dichlorosilacyclohexane (DCSCH), 1, 3, 5-trisilacyclohexane (TSCH) and silacyclohexane (SCH). While DCSCH has fair cross sections for both DEA and DI [1], TSCH and SCH are as good as inert to DEA though it shows fair DI cross sections. The hypothesis in this work is that this different behavior towards DEA and DI should be reflected in performance of these molecules as precursors in FEBID. In this context we compare lateral broadening of pillars deposited with these precursors for a number of deposition times and the influence of the PE exposure of a growing pillar to the neighboring proximity pillars, i.e., the change in size of pillar due to the consequence of growing pillars very close to it so called proximity effect [2]. These results are discussed in context to the underlying mechanisms.

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Electron behavior under characteristic magnetic fields applied to inductively coupled plasmas for control of charged particle transport

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Electron motions in inductively coupled plasmas under characteristic magnetic fields ($\boldsymbol{B}$ fields), quadrupole magnetic field (QMF, fig. 1) and confronting divergent magnetic fields (CDMFs, fig. 2), are presented.

The QMF induced by three coaxial coils [1] consists of two pairs of antiparallel gradient magnetic fields (APGMFs) around a ring of $\boldsymbol{B} = 0$ called neutral loop (NL, corresponding to $x = z = 0$ in fig. 1). As well as gyration around magnetic field lines, electrons undergo directional drifts along the NL [2]. This directionality originates in the APGMFs [3] and is position-dependent; electrons under the weak $\boldsymbol{B}$ field near the NL meander to one direction, and those under the strong $\boldsymbol{B}$ field far from the NL gyrate and drift to the opposite direction [4,5] (the grad-$\boldsymbol{B}$ drift). This would result in a rectification of the loop plasma current along the NL in the coupling with the one-turn rf antenna. An experimental result [6] suggests an appearance of the rectification as an asymmetric rf emission. The rectification is an interesting effect to be confirmed by measurement.

The CDMFs formed by two coils [7] have a point of $\boldsymbol{B} = 0$ (X point). The plasma, driven by a planar spiral rf antenna, is divided into the upper and lower parts by the separatrix. The $\boldsymbol{B}$ field in the upper region guides the accelerated electrons sideways. This prevents the electrons from straight diffusion to the lower region. However, two ways of downward electron diffusion are considered. One is scattering near the separatrix. By the displacement of the gyrocenter, some of the scattered electrons transfer their guiding magnetic field lines from those of the upper region to those of the lower region. This is likely to occur for high-energy electrons with long gyroradii. The $\boldsymbol{E} \times \boldsymbol{B}$ drift synchronous to the rf $\boldsymbol{E}$ field also assists electrons to cross the separatrix. The other is passage through the weak $\boldsymbol{B}$ field around the X point. This process is easy even for low-energy electrons. The electron diffusion across the separatrix is controllable by the $\boldsymbol{B}$ field. Evaluation of the selectivity and efficiency would lead to active use of separatrix, e.g., as a magnetic shutter or filter.

Figure 1. Quadrupole magnetic field. Directionality appears in the azimuthal electron drift.
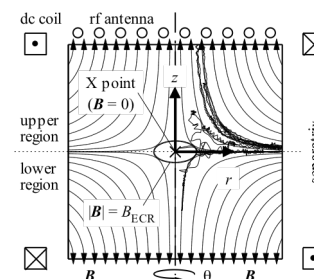
Figure 2. Confronting divergent magnetic fields. The separatrix suppresses downward electron diffusion. $B_{\mathrm{ECR}} = 2\pi(m/e)f_{\mathrm{rf}}$ is the rf-resonant magnetic field

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Cross section measurements for positron and electron scattering from molecules of biological relevance

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Ionising radiation is widely used in modern medical technologies, both for imaging and therapy. Positrons, in particular, lie at the heart of Positron Emission Tomography (PET), one of the most common tumour diagnostics. Positron thermalisation within the body, from the moment of release to positronium (Ps) formation or annihilation, involves an energy loss of six orders of magnitude and induces a cascade of ionisation events liberating several thousand low-energy electrons. Both the primary positrons and the secondary electrons may cause cell damage or mutations, e.g. by initiating DNA lesions. However, their energy deposition mechanisms remain mostly unknown. Hence investigations into low-energy charged-particle interactions with molecules of biological importance, such as the cellular components and their analogues, are needed to assess any potential charged-particle-induced damage.

We present cross sections measurements for positron and electron collisions with a variety of biologically relevant targets, including water [1], the sugars in the DNA backbone [2-4] and the nucleobases [5-7]. Total and integral cross sections, as well as angular distributions, are reported at incident energies from 1 eV to a few hundred eV. The positron experiments were carried out using two different spectrometers: the high-resolution buffer-gas trap and positron beam apparatus at the Australian National University and the very low-energy apparatus at the University of Trento. The electron-impact measurements were conducted using the cross-beam apparatus at Flinders University.

Accurate measured cross sections, in conjunction with energy loss and resonant dissociative electron attachment data, are fundamental in order to improve the current understanding of lepton interactions with living tissue. They also contribute to the development of more precise charged-particle track simulations and positron nano-dosimetry models, which will improve the current knowledge of the mechanisms of sub-cellular damage. This is essential for the future development of more efficient and safer positron-based medical technologies.

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Ion-molecule reactions and secondary ionization processes in gases of biological and atmospheric interest

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Selected cases of recent experimental work dealing with the measurement of ion mobilities and reaction coefficients are presented together with simultaneous calculations of collision cross sections. Additionally, recent work dealing with the generation of secondary avalanches from ion and photon feedback will be presented.

The talk starts by presenting the measurement of negative ionic avalanches in H_2O in the pulsed Townsend regime [1]. The analysis considered the formation of H^- followed by a fast ion-molecule reaction leading to OH^- and its reaction with H_2O to form the $OH^-(H_2O)_n$ species, with n=1-3. The use of an avalanche simulator adapted to the experimental conditions was necessary. Negative ion mobilities and reaction coefficients resulted from this experiment.

Measurements of the mobility of negative ions in N_2O and in the N_2O-N_2 mixtures were analized in terms of a reaction scheme considering the initial formation of O^-, followed by the formation of NO^-, on the one hand, and of $N_2O_2^-$ on the other hand [2]. NO^- is lost rapidly by electron detachment while $N_2O_2^-$ is stable at least during the characteristic drift times of this experiment. The momentum transfer integral cross section for $N_2O_2^-$ in N_2O and N_2 was derived from the above measurements. The unfolded cross sections were used as an initial guess and then further improved by ensuring good agreement between Monte Carlo calculations and the measured mobilities for the N_2O–N_2 mixtures.

This talk proceeds with a presentation of recent work on positive ions in N_2, focused on the formation of clusters the mass of which is assumed to be N_6^+, being formed by a chain of three-body reactions leading to the formation of N_4^+ and N_6^+ over the *E/N* range 100-400 Td. The shape of the measured waveforms suggests the presence of three positive ions drifting in the discharge gap. To gain more insight, the avalanches were simulated and compared successfully with those measured. The drift velocity (mobility) of N_4^+ and N_6^+ were derived, as well as the corresponding rate coefficients.

Finally, preliminary results of an investigation on photon feedback in the N_2 avalanche are presented. When the avalanche conditions are such that gas amplification is high, with *αd* products in the range 6-8 (*α* is the ionization coefficient and *d* is the drift distance), there results a copious formation of N_2 excited states, with that emitting at 337 nm being the most abundant. Some of these photons reach the cathode and start secondary avalanches. It is these secondary avalanches that would eventually lead the gas to breakdown, together with other processes such as secondary electrons produced by positive ion impact upon the cathode, a matter that will be looked at briefly. Measurements and simulations of these processes will be presented and discussed.

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Coulomb collisions in electron swarms in heavy rare gases: effects on negative differential conductivity

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An effect of the electron drift velocity decreasing with growing electric field is traditionally named as *negative differential conductivity*. During last few decades this phenomenon was comprehensively studied both experimentally and theoretically for a number of pure molecular gases (CH_4, C_2H_4, CF_4 and others), for mixtures of heavy rare gases with molecular gases ($Ar:N_2$, $Ar:CO$, and others), for Xe:He gas mixtures, and for pure heavy rare gases (see e.g. [1] and references therein). While the electron drift velocity in heavy rare gases is "normally" a monotonic increasing function of the reduced electric field, *E/n*, Coulomb (electron-electron) collisions have been found to change this behavior and to result in the appearance of the negative differential conductivity effect. It should be noted that so far there were no experimental observations of the effect in heavy rare gases and the theoretical predictions were based only on the conventional Boltzmann equation analysis.

Negative differential conductivity in Xe gas is investigated here for *E/n* values between 0.1 Td and 10 Td and electron to gas atom number density (n_e / n) ratios ranging between 10^{-8} and 10^{-4}. The gas pressure is set to values of 1, 10, and 100 atm, while the gas temperature is fixed at 300 K. In our calculations of the transport coefficients we apply a first-principles particle-based simulation technique [2] and a Boltzmann equation approach that adopts the usual approximations of (i) searching for the distribution function in the form of two terms ("two-term approximation"), (ii) neglecting the Coulomb part of the collision integral for the anisotropic part of the distribution function, (iii) treating Coulomb collisions as binary events, and (iv) truncating the range of the electron-electron interaction beyond a characteristic distance [3]. The particle-based simulation method is devoid of these approximations: the simultaneous many-body interactions between the electrons (situated in a cubic simulation box with periodic boundary conditions) with a true (un-truncated) Coulomb potential are described by a Molecular Dynamics algorithm, while the collisions between electrons and the background gas atoms are treated with a conventional Monte Carlo technique.

Test calculations (in Xe) performed without taking into account Coulomb collisions show a good agreement between the electron drift velocity values obtained from the Boltzmann equation, as well as with the Monte Carlo technique, and corresponding available experimental data. With taking into account Coulomb collisions the negative differential conductivity effect clearly shows up in the results obtained by both approaches. The quantitative differences observed between the results are believed to originate from the approximations used in the Boltzmann equation analysis.

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Electron scattering cross sections for the modelling of Oxygen-containing plasmas

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Oxygen-containing low-temperature plasmas, often produced in combination with other molecular gases and/or with noble gases, are the focus of a wide-range of interests spanning from fundamental studies to applications in various fields, such as material processing and functionalization, biomedical purposes and environmental/energy applications. The modelling of these plasmas requires reliable basic data, namely for the accurate description of the electron kinetics. This work proposes a set of electron–neutral scattering cross sections for (molecular and atomic) oxygen, which has been used in the modelling of oxygen-containing plasmas by the Group of Gas Discharges and Gaseous Electronics with IPFN/Técnico-Lisboa. These cross sections (compiled for kinetic energies up to 1 keV) are part of the IST-LISBON database with LXCat [1], being used as input data to the LoKI (LisbOn KInetics) numerical code [2] that couples the homogeneous two-term electron Boltzmann equation to the system of rate balance equations for the plasma (neutral and charged) species.

For ground-state molecular oxygen the set includes the following 14 cross sections [3,4]: elastic momentum-transfer; excitations to 4 vibrational levels; excitations to 7 electronic levels ($a^1\Delta g$; $b^1\Sigma g+$; $A^3\Sigma u+$, $C^3\Delta u$ and $c^1\Sigma u-$ bound states; $A^3\Sigma u+$, $C^3\Delta u$ and $c^1\Sigma u-$ yielding dissociation into $2O(^3P)$ and continuum Herzberg bands; $B^3\Sigma u-$ yielding dissociation into $O(^3P)+O(^1D)$; radiative levels with thresholds at 9.97 eV and 14.7 eV); dissociative attachment; and ionization. This complete set of cross sections yields calculated swarm parameters in agreement with measurements for *E/N* values between 10 and 1000 Td. Below 10 Td the set must be further completed to include rotational excitation / deexcitation mechanisms for the $J \leftrightarrow J + 2$ transitions (J=1,3,5…,29) [5], in order to reproduce measured swarm data within the 20% experimental dispersion. In this study we also show that the discrete collisional operator for rotations can be replaced by a convenient continuous approximation, including a Chapman–Cowling corrective term proportional to the gas temperature [6].

For ground-state atomic oxygen the set includes the following 8 cross sections [7]: elastic momentum-transfer; excitations to 6 levels ($O(^1D)$; $O(^1S)$; $O(^3P)$; the most important Rydberg states, lumped as $O(^4S^0)$, $O(^2D^0)$ and $O(^2P^0)$); and ionization. These cross sections, complemented by other electron-impact mechanisms (namely with ground- and excited-state O_2), are used in LoKI yielding predictions for the behavior of air plasmas in qualitative agreement with measurements [8].

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Spatiotemporal evolution of electrons in gaseous and liquid argon

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The study of electron transport in non-polar liquids is of fundamental interest for understanding the dynamics of electron processes in liquids and disordered, including dynamic and scattering processes. Applications to high-energy particle detectors and plasma medicine among others require knowledge of electron transport through liquid argon, liquid water and other biomolecules, typically under non-equilibrium conditions.

We have recently generalized the formalism of Lekner and Cohen, in which they describe ab initio modifications to the microscopic processes to account for dense fluid effects, overcoming several approximations which are no longer necessary in modern day transport and scattering theory [1]. A numerical solver for the full, spatiotemporally-dependent Boltzmann equation with a multi-term treatment of the velocity distribution has been developed. Operator splitting has been employed so that the energy-space and configuration-space components of the kinetic equation can be treated individually with specialized techniques. Specifically, the Boltzmann equation Green's function is solved numerically, which allows us to determine various experimental (time of flight, steady-state Townsend, pulsed Townsend etc.) configurations and applications from a single simulation. Cross-sections for the electron-argon system in the gas and liquid phases serve as inputs from which macroscopic transport properties can be calculated. We investigate the space-time evolution of electron swarms in gaseous and liquid argon, highlighting the non-hydrodynamic nature arising from source distributions etc., and their evolution to a hydrodynamic regime. Particular attention is paid to the impact of coherent scattering and modifications to the scattering potential arising from liquid effects.

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TLE-15

Low energy (< 5 eV) electron interactions with DNA and RNA nucleotides

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We have examined the low-energy electron (LEE) induced damage of DNA[1] and more recently several nucleotides using a novel graphene-platform and Raman micro-spectroscopy approach.[2] The single stranded DNA was shown to undergo significant damage due to the capture of electrons into primarily π* shape resonances initially localized on the bases. Adsorption on p-doped graphene can also lead to direct capture in phosphate σ*-type levels. Though simlar processes are expected for isolated nucleotides based on gas-phase studies of the constituent sugars and bases, we observe only limited damage of all RNA constituent nucleotides studied following < 5 eV electron bombardment. However, significant LEE-induced damage of DNA nucleotides such as deoxyadenosine monophosphate (dAMP) occurs after bombardment of only 2 eV electrons. The much higher stability of the RNA nucleotide adenosine monophosphate (AMP) is correlated with a change in the electronic structure associated with the simple addition of an –OH group to the $2'$-C site on the sugar. This dramatically changes the attachment energies and lifetimes of the transient negative ion resonances. The DNA nucleotides have lifetimes long enough to allow base damage and glycosidic bond cleavage at energies < 2 eV. This is not the case for the RNA nucleotides. The general radiation stability of important RNA sub-units relative to those in DNA is consistent with an RNA or RNA-like polymer based origin of life hypothesis.

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Novel approaches to study low-energy electron-induced damage to DNA oligonucleotides

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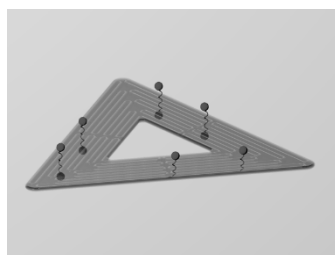
Figure 1. 3D model of a triangular DNA origami structure carrying six well-defined oligonucleotides and Streptavidine at the 5' end.

Secondary low-energy electrons (LEEs) belong to the most important intermediates in DNA radiation damage. Strand breaks in the DNA backbone can be initiated by resonant electron attachment at different electron energies.[1] Recent experiments suggest that single strand breaks (SSBs) strongly depend on the nucleotide sequence due to efficient coupling of the electronic states of the nucleobases by stacking interactions.[2] A novel approach using DNA origami templates carrying different oligo-nucleotide target sequences provides access to efficient and systematic determination of electron induced DNA strand break cross sections (Figure 1).[3]

We assembled a new instrument to irradiate specific oligonucleotide sequences on DNA origami templates with electrons of defined but variable energy from 2 to 50 eV (Figure 2). First experiments are performed at 10eV, where a maximum of DNA single and double strand breaks was previously observed.[4]

The damaged oligonucleotides are analysed with atomic force microscopy (AFM) and the well-defined shape of the DNA origami templates allows for a precise localization and thus quantification of DNA strand breaks at a single-molecule level. The influence of the DNA sequence, e.g the telomere sequence, shall be explored. Furthermore, potential radiosensitizers such as 2-Fluoroadenine are used to study their influence on DNA strand break cross sections.

Figure 2. 3D model of the instrument for oligonucleotide irradiation, equipped with vacuum pump, electron source, sample stage and manipulators.

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TLE-17

Low-energy free-electron catalyzed chemical reactions

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Low-energy free-electron can be used as a reactant to initiate chemical processes such as bond formation (known as associative electron attachment) or bond dissociation (known as dissociative electron attachment) reactions. In sharp contrast to using free-electrons as reactants in this way, recently we have shown that they can also be used as catalysts for chemical reactions [1]. The free-electron catalyzed chemical reaction is initiated when the molecule captures a low-energy free electron of a particular energy, i.e. resonant capture of electron, to form an electron- molecule compound state. The compound state thus formed can further undergo chemical reactions yielding neutral molecular products and a free-electron. Our work on the electron-molecule compound states that can act as molecular precursors for the energy- and site- selected electron-catalyzed chemical reactions [1] will be presented here. I shall also present the formulation, implementation and the advantages of the variants of *stabilization methods* and *analytical continuation methods* that we have developed for the electron correlated calculation of energy position and a decay rate of electron-molecule compound states [2,3].

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Electron kinetics in upper atmospheric electrical discharges

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We will present an overview of the kinetic studies carried out in our group towards the understanding of the so called Transient Luminous Events (TLEs), which are a diversity of weakly ionized low temperature plasmas occurring in the upper atmosphere of the Earth between thundercloud tops (15 km) and the lower ionosphere (95 km). Optical flashes from upper atmospheric air plasmas were first recorded 25 years ago (in the summer of 1989) [1] as hypothesized in 1925 by C.T.R Wilson [2]. Their occurrence is linked to the electrical (lightning) activity in the Earth troposphere (0 - 15 km). Our research tries to answer questions such as, what are the chemical and electrical impacts of TLEs in the Earth atmosphere?. What are the physical (kinetic and electrodynamic) mechanisms underlying the ignition of TLEs?. What are the key spectroscopic features (and fundamental underlying kinetic processes) of TLE optical emissions in the UV-visible-NIR range?.

In order to study the chemical and electrical influence of TLEs in the Earth upper atmosphere, we have followed a kinetic approach (including the study of non-equilibrium vibrational kinetics) to investigate the upper atmospheric air plasmas originated by the presence of different types of TLEs such as sprites, halos and beads. The kinetic studies of TLEs aim at understanding the basics of the nonequilibrium plasma chemistry triggered by sprites (streamers and afterglow), halos and beads in the Earth upper atmosphere. In this regard, our kinetic models have allowed us to explore and identify chemical species affected by TLEs (like nitrogen oxides, metastables and ions) [3] together with key kinetic processes (like electron detachment) that influence the ignition and dynamics [4] of sprites and halos as well as the upper atmosphere electrical conductivity [5] affected by TLEs.

Special attention is paid to the vibrational kinetics of N_2 triplets ($A^3\Sigma_u^+$, $B^3\Pi_g$, $C^3\Pi_u$, $W^3\Delta_u$ and $B'^3\Sigma_u^+$) and singlet ($a^1\Pi_g$) states. Several hundreds of reactions and 130 chemical species are considered with more than 200 reactions involving vibrational states. The main processes considered are electron-impact reactions, vibrational - vibrational (V-V) and vibrational - translational (V-T) excitations, energy pooling, electronic quenching (with vibrationally dependent rates) of the A, B, W, and B' electronic states of N_2, intersystem collisional transfer, radiative de-excitation and vibrational re-distribution (within the N_2 ($A^3\Sigma_u^+$) state).

Our electron kinetic studies of upper atmospheric electrical discharges have allowed us to calculate and compare with available observations and measurements the following magnitudes:

- Nonequilibrium VDFs of singlet $N_2(a^1\Pi g)$ and triplet $N_2(B^3\Pi_g)$, $N_2(C^3\Pi_u)$ electronic states involved in UV-visible-NIR optical emissions from TLEs.
- Calculate synthetic spectra, from modeled VDFs, of the first and second positive systems of N_2 together with that of the Lyman Birge Hopfield (LBH) band and compare with available TLE spectra.
- Identify key electron-driven kinetic mechanisms underlying the production of NO_x, key ions (like O^-) influencing TLE ignition dynamics as well as atomic and molecular metastable species of atmospheric interest influenced by the presence of TLEs.

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A comprehensive cross section study of e-Cyanoacetylene

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The cyanoacetylene or propiolonitrile (HCCCN) has been detected for the first time in the intra stellar medium (ISM) by microwave spectrocopy [1] due to its strong permanent dipole moment. HCCCN has been widely detected in the carbon and nitrogen rich atmosphere of Titan [2], comets [3,4], interstellar gas clouds [5, 6] and circumstellar envelopes [7]. The vibrationally excited spectra of this molecule has been used to derive physical properties of protoplanetary nebula [8]. There has also been tentative detection of HCCCN in external galaxies and constellations such as Orion [9]. Ionizing radiations such as cosmic rays and solar wind create an electron rich environment. Hence, electron cross section data for molecule like HCCCN are, therefore, important for modelling these environments. Moreover, HCCCN has a major role to play in the exobiological world, since it is an intermediate in the prebiotic synthesis of cytosine [10]. There are previous reports of dissociative electron attachment (DEA) studies [11-13] and an ionization study [13] on this molecule. However, there is a void in total, excitation and momentum transfer cross section dataset for this molecule. The scarcity in data and important implications of HCCCN in diverse fields of applied sciences has motivated us to carry out an extensive study to find e-HCCCN cross section for a wide energy range. The present paper reports the elastic, total and ionisation cross section of HCCCN molecule. Excitation, differential and momentum transfer cross sections are also reported for the molecule in the low energy region. The low energy calculations are accomplished using R-matrix method [14], while the intermediate to high energies studies are done through SCOP & CSP-ic formalisms [14].

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Rescaling procedures for Monte Carlo simulations of electron transport in strong electronegative gases

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Electron attachment often imposes practical difficulties in Monte Carlo (MC) simulations of electron transport in strong electronegative gases at low electric field strengths. If the attachment rate is too high, the entire electron swarm can be consumed before steady state is achieved. In such extreme cases the transport data cannot be calculated. An obvious solution would be to use a very large number of initial electrons. However, in order to obtain the results with reasonable statistical accuracy, this would usually require computing resources which are beyond practical limits.

In order to address this issue in an optimal fashion, two distinctive procedures for electron compensation were proposed. The first one, which we refer to as *discrete rescaling*, is based on duplication of electrons randomly chosen from the remaining swarm at certain discrete time instants [1]. The other one we refer to as *continuous rescaling* introduces a fictitious ionization process with constant collision frequency chosen to be roughly equal to the attachment rate [2]. Both of these procedures were devised with the aim not to alter the electron distribution function and its evolution. However, it can be shown theoretically that only continuous rescaling meets this requirement [2].

In this work, we investigate the effects of MC rescaling procedures on the electron transport in CF_3I and SF_6 gases. Additionally, we propose a new implementation of continuous rescaling procedure which does not require the fictitious ionization rate to be defined *a priori*. Transport data is calculated using our electron impact cross sections for CF_3I [3] and a cross section set for SF_6 developed by Itoh et al. (1993). The results show that in case of CF_3I the transport parameters obtained using these two rescaling procedures can differ as much as 30% for the flux drift velocity or the attachment rate. Figure 1 shows the calculated flux drift velocity for CF_3I over a range of reduced electric field strengths. The results calculated using two term approximation for solving Boltzmann equation (BE TTA), are also shown for comparison.
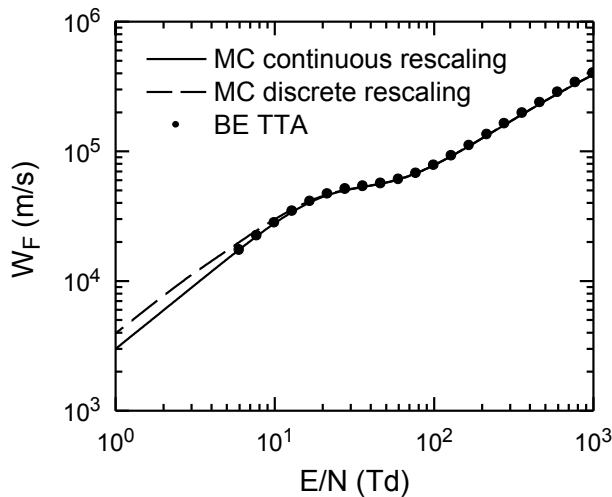
Figure 1. Flux drift velocity for CF_3I calculated over a range of reduced electric field strengths using two different MC rescaling procedures. Values obtained using two term approximation for solving Boltzmann equation are also shown (BE TTA).

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Negative ion formation in potassium- adenine and -9-methyl-adenine collisions

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The most abundant secondary species produced by the primary ionizing radiation within the biological environment are low-energy electrons ($\sim 4\times10^4$ by a 1MeV particle) with energies typically below 30 eV [1]. Their interactions with DNA/RNA subunits lead to the formation of short lived anions yielding molecular dissociation and hence single and double strand breaks [2, 3]. However, due to the lack of free electrons in the physiological environment, electron-transfer processes may be prevalent and appear to be a key process in the decomposition of such units [4]. Collision induced dissociation in pyrimidines results in site- and bond-selective excision of N_1-H against N_3-H by just tuning the proper collision energy [4].

Dissociative electron attachment (DEA) experiments to purine molecules and their derivatives (9-methyl-adenine) have been performed by Denifl *et al*. [4], where resonances below 1.4eV yield H abstraction from the N_9 position in pristine adenine. However, methylation at the N_9 site supresses such resonance, where site selectivity yielding the dehydrogenated parent anion was shown to be a relevant process.

We have been exploring negative ion formation in collisions of neutral potassium atoms with adenine and 9-methyl-adenine by time-of-flight (TOF) mass spectrometry. Such anionic yields have been obtained as a function of the collision energy and significant differences are noted from DEA experiments. Preliminary ab initio calculations have been performed in order to help interpreting the experimental data. Such details will be presented at the meeting.

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Shape resonances of polyatomic molecules – their impact on vibrationally inelastic electron-molecule collisions

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We would like to report on our recent results on vibrationally inelastic collisions of electrons with diacetylene molecules [1]. The results combine the experimental work [1,2] with ab initio calculations [1]. The theoretical modeling was carried out by employing our Discrete Momentum Representation (DMR) method. The electron-molecule interaction is, within the DMR method, described by a SEP approximation. The correlation-polarization component of the interaction is modeled by a local DFT potential.

Our aim was to identify the origin and symmetries of shape resonances that were observed in the experimental inelastic cross sections [2] in the energy range from 1 to 10 eV. The presence of these resonances is demonstrated in Fig. 1. While the strong $^2\Pi_u$ resonance seen in C≡C and C–H stretch modes at 1 eV (left panel of Fig. 1) was well documented before, the origin and symmetry components of the other four resonances has been unknown. Deeper insight into the nature of these resonances is important especially for their possible role they may play in the DEA channel (loss of H atoms) that peaks resonantly around 5.2 eV [2].
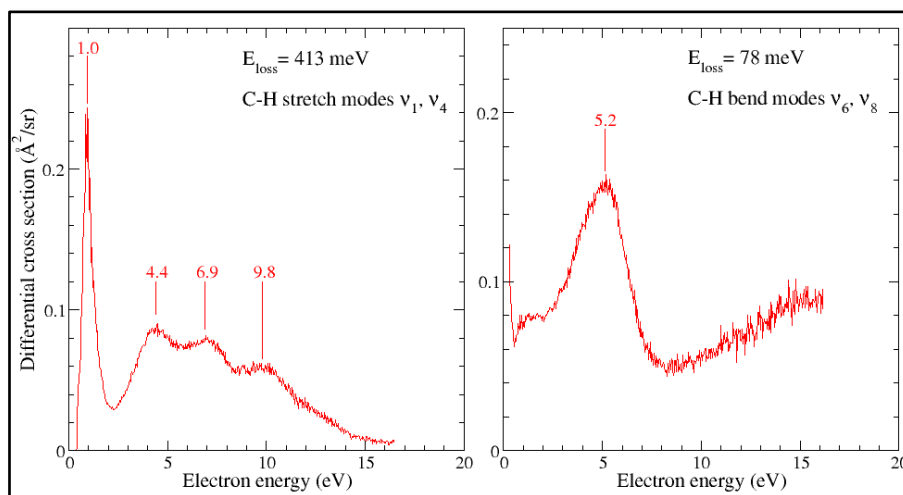
Fig 1. Absolute inelastic differential cross section [1] measured at energy loss of 143 meV (left panel) and 78 meV (right panel).

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Fulcher α radiation after electron impact excitation of hydrogen molecule

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Fluorescence radiation of Fulcher α system $d^3\Pi_u \rightarrow a^3\Sigma_g^+$ was measured for a few vibronic bands after electron impact. For study of elementary collision processes between electrons and molecules we use the electron induced fluorescence apparatus, which implements a cross – beam geometry. Near-monochromatic electron beam formed by a trochoidal electron monochromator collides the molecular beam effusively flowing from a capillary into the reaction chamber. High vacuum is required for the experiment to maintain purity of the sample and single-collision conditions. Such reactions can lead to generation of excited neutral, ionized and fragmented species which subsequently emit a photon. For studied species we measure fluorescence spectra in UV/VIS region and emission functions in the electron energy range of 0-100 eV.

Measurements of a few bandheads of Fulcher α system were done and preliminary results are presented. The emission functions were calibrated to obtain absolute emission cross section values. Only a few studies of energetics of Fulcher systems are available, and usually only Fulcher α (0,0) band is discussed [1] [2] [3]. Our results correspond well with some of them. Thanks to implementing of the electron monochromator, we also provide results with higher energy resolution as before.
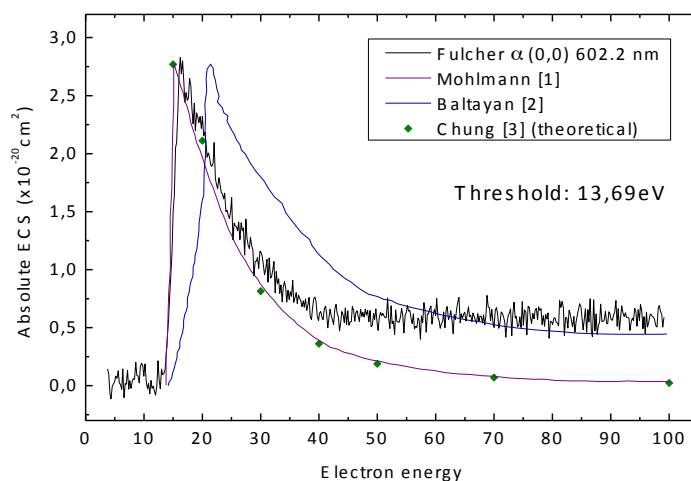
Figure 1. Emission function of the Fulcher α radiation, vibronic band $d^3\Pi_u \rightarrow a^3\Sigma_g^+$ (0,0). The present data are compared to previous measurements and calculations.

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Mechanisms of Chiral Sensitivity in Electron-Molecule Interactions

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We present the results of our search for asymmetric interactions between longitudinally spin-polarized electrons and different chiral halocamphor molecules. The asymmetry is defined as

$$A = \left(\frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow}\right)_L - \left(\frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow}\right)_R,$$

where $I_\uparrow$ ($I_\downarrow$) is the current measured for spin-up (spin-down) electrons and the "L" and "R" subscripts correspond to the left- and right-handed chirality of the molecules [1]. Two electron-molecule interaction channels were studied: electron transmission (related to the total scattering cross section) and dissociative electron attachment (DEA). Three halocamphor molecules were investigated: 3-bromocamphor ($C_{10}H_{15}BrO$), 3-iodocamphor ($C_{10}H_{15}IO$), and 10-iodocamphor.

While the transmission asymmetry data do not show a strong molecular dependence, the DEA asymmetries collected for bromocamphor and iodocamphor are qualitatively different, suggesting that the atomic number of the heaviest atom in the molecule plays a crucial role in the asymmetric interactions. The DEA asymmetry data for 3- and 10-iodocamphor have the same qualitative behavior, but the 10-iodocamphor asymmetry is about twice as large at the lowest energies investigated, so the location of the heavy atom in the camphor molecule also affects the asymmetries.

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Electron transport in planetary atmospheric discharges

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The occurrence of plasma discharges in the planetary atmospheres due to the electrical activity in the underlying thunderstorms is a subject of intense research in the last two decades [1]. In particular, sprites are large luminous discharges, which appear in the mesosphere at 40 to 90 km altitude above large thunderstorms [2]. They represent one of the most spectacular forms of the so-called transient luminous events (TLEs) in the atmosphere of our planet. Sprites are always associated with positive cloud-to-ground lightning discharges which lower positive charge from clouds to the ground. After removal of positive charges from the cloud by a lightning stroke, the remaining negative charges in the thundercloud produces a large quasi-electric field above the thundercloud up to the conducting ionosphere. This field appears at all altitudes above the thundercloud, and endures for a time equal to approximately the local relaxation time at each altitude. The local relaxation time depends on the local conductivity and can be calculated from the profile of electron density and electron mobility. This temporarily existing electric field heats the electrons and controls transition from avalanches into streamers.

In addition to sprites, other forms of TLEs are possible. These include the blue jets, the gigantic jets and elves. Though physical mechanisms behind of these TLEs are different comparing to sprites, the knowledge of electron transport properties for their modeling is of an essential importance.

In this work we discuss the elementary physical processes of electrons in the mixtures of gases used to model planetary atmospheric discharges. First, we investigate the possibility of sprites in the atmosphere of other planets using the quai-electrostaic model to calculate the electric field above the cloud after an intensive positive cloud-to-ground lightning. Electron transport coefficients are calculated for all planetary atmospheres and the influences of specific physical processes on electron kinetics are identified. For example: (i) for Earth's atmosphere the effects of 3-body attachment on electron transport is studied; (ii) for Venusian atmosphere the effects of the gas temperature is examined and used to simulate propagation of positive streamers in the mixtures of N_2 and CO_2; and (iii) the influence of planetary magnetic fields on electron transport in the atmospheres of gas giants is illustrated by solving Boltzmann's equation. Additional issues including thermalization of high-energy electrons and runaway phenomena are also discussed and illustrated by numerical examples in various gas mixtures.

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Electron attachment properties c-C_4F_8O: from single-collision conditions to swarm

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In this contribution we address the question how the environment – namely the pressure and the closely related collisional frequency – influences electron attachment properties of c-C_4F_8O. This gas has been chosen due to its high technological potential: it is considered for use as a radiating medium in Cherenkov detectors, as a cleaning agent for CVD chambers or as an SF_6 replacement in high voltage insulation. We determine its attachment cross sections using two complementary setups: (i) an electron-beam experiment equipped with a time-of-flight mass analyzer and (ii) pulsed swarm experiment that uses low concentrations of c-C_4F_8O in various buffer gases. The attachment cross sections in the two experiments are more than one order of magnitude different [1].

The explanation of this extreme difference is based on the properties of the transient negative ion $(C_4F_8O^-)^*$. A certain fraction of these anions survives long enough to be detected even at single-collision conditions of the beam experiment (microseconds). This long lifetime leads to efficient collisional stabilization of anions in the swarm experiment where the collisional frequency is approximately five orders of magnitude larger. Such collisional stabilization (three-body attachment) causes effective attachment rate which is much higher than the one corresponding to the beam cross sections. We argue that a convenient cross section scaling that would describe attachment properties at various pressures is basically impossible due to dependence of the stabilization rate on the buffer gas.

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Electron induced chemistry in $Fe(CO)_5$ deposited on argon nanoparticles

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A lot of effort has been put recently into understanding electron-induced chemistry of molecules that serve as precursors for focused electron beam deposition (FEBID). The ultimate goal is to use the knowledge of the elementary processes in isolated molecules (e.g., fragmentation pathways, cross sections ...) for optimizing the deposition performance. The biggest drawback of gas phase studies is that they completely ignore the effect of environment that certainly plays a strong role in determining the outcome of electron-induced reactions.

In the present study we bridge the gap between the gas phase and surface approach by depositing $Fe(CO)_5$ molecules on the surface of argon nanoparticles. This is achieved by supersonic expansion of argon gas under controlled conditions (leading to production of argon clusters with the mean size of 330 atoms), skimming the cluster beam and passing it through a pickup cell filled with $Fe(CO)_5$ vapor. The mixed clusters are then ionized by an electron impact and the product ions are analyzed in a high-resolution reflectron time-of-flight mass spectrometer.

The most important results can be summarized as follows:

- The most abundant aggregates of guest molecules are those with a mixed composition $Fe_n(CO)_m^+$. We detect such composites with sizes up to $n = 5$. The relative abundances reveal that the argon support partially stabilizes the precursor molecule and suppresses the fragmentation.
- The pure iron aggregates Fe_n^+ are observed as well, however, only up to the size of $n = 3$ and with very small abundance.
- By varying the electron energy and determining the appearance energies of various fragment ions we clearly see the effect of the nanosubstrate and of secondary electron-induced processes. When compared to the gas phase measurement the appearance energies are shifted to higher values and coincide with the ionization potential of argon. The ionization thus proceeds via ionization of cluster constituents and subsequent charge transfer to the aggregates of $Fe(CO)_5$.

Elastic scattering and electronic excitation of ethylene by electron impact: an investigation on the role of multichannel coupling effects

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It is a challenge to provide reliable cross sections for electron scattering by molecules. In spite of this fact, there is a growing interest in describing these processes especially due to a need to establish a cross section database to be used in the modeling of chemical plasmas of industrial importance [1] and in investigations involving biological molecules that dissociate through the formation of temporary negative-ion states (resonances) [2].

In this work we report elastic and electronically inelastic cross sections for low-energy electron collisions with ethylene. The calculations were performed with the Schwinger multichannel method with pseudopotentials (SMCPP) [3,4] according to the so-called N_{open}-channel-coupling scheme at the static-exchange-plus-polarization approximation [5]. More precisely, up to 45-states of ethylene obtained within a single configuration interaction representation of the target states were included in the open-channel space. This scheme enabled a detailed analysis of the influence of multichannel coupling effects on the cross section results. In particular, we investigate how the number of excited states included in the open-channel space impacts the convergence of the elastic and the ($X^1A_g \rightarrow \tilde{a}^3B_{1u}$) excitation cross sections as long as the electron impact energy increases. For elastic scattering we found that the agreement with experimental data is quite good over the whole energy interval covered by the present study. Comparison among theoretical results obtained with different channel coupling schemes indicates that the convergence of elastic cross sections in terms of the number of excited states included in the open-channel space is relatively quickly achieved. For the excitation of the $\tilde{a}^3B_{1u}$ state our calculations revealed that at 5.7 and 7 eV our results are in good agreement with the experiment. However, for energies above 7 eV our results lie systematically above the experimental data, indicating that perhaps even more open channels would be needed so as to cause the appropriate reduction in the magnitude of the computed inelastic differential cross sections. We also introduce a simple but rather effective method of representing multichannel coupling effects through the use of ficticious thresholds and show that it also provides cross sections in good agreement with experiments.

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Electron collisions with phenol: a joint experimental and theoretical investigation

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It has long been recognized that lignocellulosic biomass is a potential sustainable source of mixed sugars for fermentation to biofuels. During the last decades many technologies have been developed that allow this conversion process to occur and, nowadays, the clear objective is to make the use of such technologies cost-effective. Recently, it has been found that free-electrons and radical species formed within atmospheric plasmas have the ability to overcome the natural resistance of plant cell walls thus allowing for an enhancement of microbial and enzymatic deconstruction [1]. In this context, low-energy electrons which are produced within the plasma environment have the potential to induce breakage of chemical bonds through dissociative electron attachment, electron-impact excitation and other fragmentation processes.

In this work we report a joint experimental and theoretical effort in order to determine reliable elastic and electronically inelastic cross sections for low-energy electron collisions with phenol [2], a key structural subunit of lignin.

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Electron collisions with hydrocarbons and chlorofluorcarbons: isomer and halogenation effects

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In this meeting we report integral and differential cross sections for elastic scattering of low-energy electrons by C_4H_8 isomers, namely 1-butene and 2-methylpropene, and by CF_3Cl, CF_2Cl_2 and $CFCl_3$ molecules. The scattering cross sections were obtained using the Schwinger multichannel method [1,2] with pseudopotentials [3], in the static-exchange and in the static-exchange plus polarization approximations. Our goal is to study different features in the cross sections due to the different geometrical structures of C_4H_8 isomers and also due to the substitution of F atoms by Cl atoms in the sequence CF_3Cl, CF_2Cl_2 and $CFCl_3$.

Our calculations indicate that 1-butene molecule has a shape resonance at around 2.1 eV, in agreement with the experimental data of 2.3 eV as reported by Mozejko *et al.* [4]. The 2-methylpropene molecule has also a shape resonance located at around 2.8 eV and also in good agreement with the experimental results of Mozejko *et al.*[4] of 2.4 eV. The differential cross sections from 6 eV to 12 eV showed different wave patterns in their behaviour, 1-butene has a clear f-wave pattern and 2-methylpropene has a d-wave behaviour. Our results for C_4H_8 have been recently published in ref. [5].

For the set of chlorofluorcarbons we have found up to four shape resonances for each molecule, for energies below 10 eV. We analyze the effects of atoms substitution in the position of the resonances and in the magnitude of the elastic cross section. The resonances are located at: 0.45 eV, 1.9 eV, 4.1 eV and 9.6 eV for CF_3Cl; 1.1 eV, 2.8 eV, 4 eV and 6.5 eV for CF_2Cl_2; 2.1 eV, 6.6 eV and 9.8 eV for $CFCl_3$. There is a good agreement between our results and the available experimental data of Jones [6] Mann and Linder [7] and Hoshino *et al* [8]. We also compared the calculated differential cross sections with the experimental results of Hoshino *et al.* and found a very good agreement between them.

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A comparative study of pyrimidine and water as molecular backgrounds for describing radiation damage

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Radiotherapy for cancer tumour treatment is reliant on the interactions of secondary species (electrons, positrons, radicals, molecular fragments) with important biomolecules within cells to cause (ideally) apoptosis of cancer cells[1]. In order to control the effects of radiotherapy, both to minimise damage to healthy tissue and increase site specific damage to tumours, a detailed understanding of the physicochemical processes occurring between the biological system and the primary and secondary particles is necessary[3].

Charged particle track simulations for the interaction of secondary electrons with biomolecules are usually performed using water as the medium. This is an oversimplification of the living cell, which is composed of approx. 70% water, 24% macromolecules (proteins, nucleic acids, polysaccharides) and 4% inorganic ions, sugars, amino acids, nucleotides, fatty acids and other small molecules[2]. This work compares the track simulations of a 10keV primary ionizing particle in the water medium with the same in pyrimidine ($C_4H_4N_2$), the commonly used prototypical structure for RNA/DNA bases. As expected, the results for the two mediums differ, including in the secondary electron penetration depth, indicating that a shift towards mixed media modeling is appropriate to truly determine the physicochemical effects and biological implications of radiation treatment.

The simulations used the Low-Energy particle Track Simulations code LEPTS[4], a Monte Carlo code for event by event simulation to describe the underlying mechanisms of electron and positron interactions with the relevant target molecules. This includes not only the energy deposition and the stopping power, but also the number and types of interactions taking place along the particle track. Also presented is a database for the scattering cross sections and stopping power of electrons with Pyrimidine, with recommended values chosen from experiment and calculation to cover the incident electron energy range from 1 - 10000 eV. The data for water has been previously compiled.

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Dissociative Electron Attachment to Carbon and Nitrogen Rich Molecules

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Carbon- and Nitrogen-rich molecules have been observed in a number of environments outside of Earth, such as comets, nebulae and in the atmosphere of Saturn's moon titan. A very recent paper by the team at Atacama Large Millimeter/submillimeter Array (ALMA) identified and mapped out the distribution of HCN and HCCCN in Titan's atmosphere. In particular, HCCCN "is abundant at a [broad] range of altitudes", from 70-600km above Titan's surface. This information, along with the revelation that a large number of negative ions exist in Titan's atmosphere (Cordiner, M. A., et al. 2014 *ApJL* 795.2 L30), highlights the importance of having cross sections for electron scattering processes for a complete understanding these alien environments.

Graupner et al (2006 New J. Phys. 8 117) has previously presented dissociative electron attachment spectra for this molecule, which identified the electron energy resonance bands where negative ions are found and the relative abundances of these ions. These measurements were made using ERIC, the electron radical interaction chamber, which has been described previously (Field, T. A., *et al.* 2005 J. Phys. B 255). In light of recent demands for better data pertaining to gaseous and plasma processes, a reanalysis of Graupner *et al's* data was done. Using some straight forward inference methods, absolute cross sections for dissociative electron attachment to HCCCN were obtained. As part of the re-analysis, it was necessary to determine absolute cross sections for electron-impact ionization of HCCCN with the binary-encounter Bethe method. Full details are available in reference [1].

Similar work has been carried out for the azines, the isomers of $C_4H_4N_2$. Pyridimine, the most well-known of the azines, is a component of the nucleobases Thymine, Cytosine and Uracil. R-Matrix scattering calculations for the azines are available for comparison and thus benchmarking of the code. CN- was found to be the dominant dissociation channel for these molecules, occurring at approximately 5.1 eV and 8.2 eV electron impact energies for all the azines. Hydrogen anion formation was also observed. Further details, including cross sections and theory comparisons, will be available in "Absolute cross sections for dissociative electron attachment to the azines" (in preparation).

Using the R-matrix codes via Quentemol-N, potential energy curves were calculated for the CS and CO molecules. For CS, 17 bond-lengths from 1.1 to 2.7 Angstroms were analysed (Varambhia 2010), while for CO 20 bond-lengths from 0.8 to 2.4 Angstroms were analysed. These curves were correlated with various distinct appearance potentials for the dissociative electron attachment at various energies (5.43 eV, 6.40 eV and 6.70eV for CS, 9.63 eV, 9.8 eV and 10.88 eV for CO).

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E-15

Study of dissociative electron attachment to thioacetic acid

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Chemical control by controlling molecular dynamics has been pursued by many researchers over the past century. Most of those efforts have been concentrated on the usage of photons to direct the chemical reaction to a specific out-come. Recent discovery of functional group dependent site specific fragmentation of organic molecules using dissociative electron attachment has opened up a new possibility in chemical control [1]. Although electron based chemical control has been investigated earlier, such selectivity in bond breakage based on the functional group present in the molecule has been seldom found..This functional group dependent dissociative electron attachment (DEA) has been established recently for molecules with hydroxyl, amine and alkyl groups [2]. Here we probe the functional group dependent DEA for the thiol (SH) group by studying the DEA dynamics for thioacetic acid (CH3COSH).

So far there has been no report of DEA studies of thioacetic acid. Our measurements on DEA to thioacetic acid show formation of H^-, S^-, SH^- and $CH3COS^-$ fragments. The H^- is found to peak at 5.5eV, and 9.5eV with the later peak being very broad and much intense. The SH^- and $CH3COS^-$ were found to peak around 1.5eV electron energy. The S^- channel is found to peak around 9eV. We studied the DEA dynamics by measuring the absolute cross sections as well as kinetic energy and angular distributions of various anion fragment channels as a function of electron energy. The absolute cross sections were measured using relative flow technique [3] where the O^- from O_2 was used as the standard molecule to put the measured signal from thioacetic acid on the absolute scale [4].

The angular distribution and kinetic energy of the fragment ions was measured using velocity slice imaging technique [5]. Resonance positions for the S^- and SH^- channel show close resemblance with those found for H_2S. There is also a resemblance in the resonance positions for the H^- channel from H_2S and thioacetic acid. However, the relative intensities of various resonance peaks are way different from that observed in H_2S. The angular distribution of the H^-, S^- and SH^- ions are compared with those from H_2S [6]. We also note that in comparison with the acetic acid (CH_3COOH), the fragmentation patterns observed in thioacetic acid are way different. Many ions like O^-, OH^-, CH_2^- etc. are not found to be formed in the case of thioacetic acid. This also highlights the dominance of the S^- atom in the DEA process.

In this poster we will report the details of the measurements and present the comparison of the DEA dynamics with that from H_2S and acetic acid exploring the functional group dependence DEA in the thiol groups.

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Dissociative electron attachment to molecular chlorine

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Velocity slice imaging (VSI) is a well-established technique to investigate the molecular dynamics involved in dissociative electron attachment (DEA) to simple molecules [1]. This technique enables one to measure the kinetic energy and angular distribution of the fragment ions produced in the DEA process. The kinetic energy distribution of the fragment ions points to the kinematics of the process leading to DEA. On the other hand the angular distribution of the fragment negative ions with respect to the incoming electron beam indicates the symmetry of the negative ion resonant states involved in the DEA process. This information in combination with the kinetic energy distribution unravels the dynamics of the DEA process. Due to their high electron affinity, the halogen molecules form a class of interesting diatomic molecules. These molecules are known to show more than one resonances in the DEA channel with very little threshold for the formation of halide anion. This leads to the substantial kinetic energy release in the fragmentation process in DEA. Particularly for chlorine, the DEA studies are important from the plasma processing point of view. Chlorine is known to affect the properties of electrical plasmas considerably and hence the efficiency of technologies utilizing the plasma, such as those generated in either pure chlorine or mixtures of chlorine with other gases. Chlorine being a highly oxidizing agent much attention has been paid to the investigation of its properties.

Dissociative electron attachment to chlorine has been extensively studied in the past with reports of measurements of absolute cross-section [2] and angular distribution in the limited angular range [3]. However the kinetic energy distribution and the angular distribution for the entire 0-360° angular range have not been reported so far. Here we report the study of DEA using velocity slice imaging at various resonances observed in the DEA to chlorine molecules [1]. The VSI spectrometer was modified with longer flight tube and larger (75mm diameter) phosphor screen based position sensitive detector. In our measurements we measured the ion yield curve up to 90eV electron energy and we found that the chloride anion yield show three resonances at 0eV, 2.5eV and 5.6eV which is consistent with earlier measurements. The velocity slice images obtained at various electron energies across the resonances are shown in Fig. 1. In this poster we will describe the dynamics involved in DEA to chlorine molecule based on the kinetic energies and angular distributions obtained using these velocity slice images.
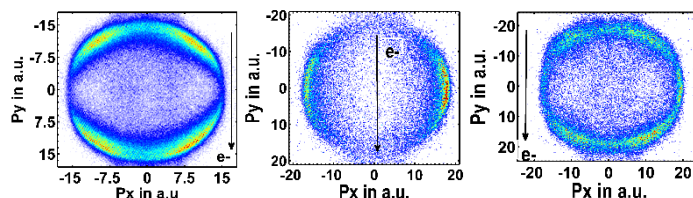

Figure 1. Image of Cl$^-$ from Cl$_2$ at 2.5eV, 4eV and 6eV electron energy.

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Dissociative electron attachment to chlorine dioxide probed by velocity slice imaging

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Chlorine dioxide (OClO) is an important molecule in atmospheric chemistry as a major source of atomic chlorine in the stratosphere as it de-composes photo-chemically forming O_2 as the other product. Dissociative electron attachment (DEA) to OClO can also lead to atomic chlorine formation. DEA to OClO has been studied in the past with reports of absolute cross-section measurements [1]. However, the dynamics that leads to DEA has not been reported so far. Here we report the study of DEA dynamics for OClO using velocity slice imaging technique.

We observed Cl^-, O^-, O_2^-, and OCl^- ions from the DEA measurements on OClO formed at various electron energies. The OCl^- being the most dominant channel was found to peak around 0.7 eV, whereas Cl^- and O_2^- signals peaked around 0.7 eV, 4 eV, 8 eV. Out of these the peak at 0.7 eV was found to be the dominant peak. The O^- ion yield was found to peak at 1.2 eV, 4 eV, 8 eV.

We carried out the momentum imaging of various fragment ions across different resonances using velocity slice imaging [2]. The VSI spectrometer was modified with longer flight tube and larger (75 mm diameter) phosphor screen based position sensitive detector [3]. For each of the ion fragments, we obtained the kinetic energy and angular distribution data. The velocity slice images obtained for Cl^- channel at 8 eV is shown in Fig. 1 as an example. For Cl^- channel, with very low energy threshold (-3.37 eV) [1], it was expected to carry good amount of kinetic energy from the 8 eV resonance. However, the low kinetic energy observed in Cl^- channel indicates an interesting many body fragmentation dynamics behind the DEA process. The angular distribution also shows a forward-backward asymmetry.

In this poster we will describe the dynamics involved in DEA to OClO based on the kinetic energies and angular distributions measured using velocity slice images for all the fragments observed at various resonances..
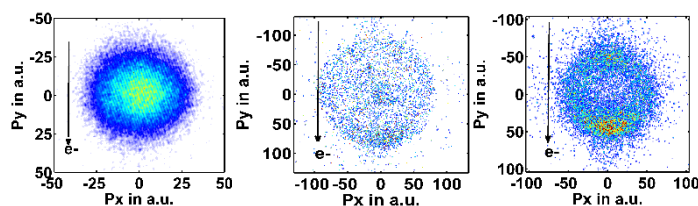
Figure 1. Momentum image of OCl^-, O^- and Cl^- from OClO at 0.7eV, 4eV and 8eV electron energy respectively.

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Dissociative electron attachment dynamics of ozone using velocity slice imaging

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Dissociative electron attachment (DEA) to ozone has been studied in the past including measurement of absolute cross-sections [1]. However, the dynamics that leads to DEA has not been reported so far. Here we report the study of DEA dynamics for ozone using velocity slice imaging technique.

Here we report the study of DEA dynamics of O_3 using velocity slice imaging [2]. The VSI spectrometer was modified with longer flight tube and larger (75 mm diameter) phosphor screen based position sensitive detector [3]. We observed O^-, and O_2^- ions from the DEA measurements on Ozone formed at various electron energies. The O^- being the most dominant channel was found to peak around 1.4 eV along with 3 eV and 7.5 eV whereas O_2^- signals peaked around 1.2 eV, 3.2 eV, 7.5 eV.

We carried out the momentum imaging of various fragment ions across different resonances using velocity slice imaging. Around 3 eV peak the angular distribution shows a forward-backward asymmetry in the O^- channel and that asymmetry is reversed in the O_2^- channel as shown in Fig. 1. Around 1.5 eV there is considerable kinetic energy release (~1.4 eV) in the O^- channel.

In this poster we shall describe the dynamics involved in DEA to ozone using velocity slice images for both the fragments observed at various resonances.
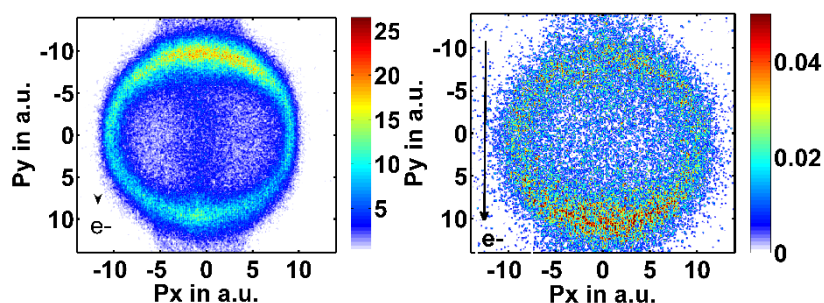
Figure 1. Image of O^- and O_2^- from O_3 at 2.5eV and 3.7eV electron energy.

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Doubly excited states of molecular nitrogen by scattered electron-ion coincidence measurements

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Doubly excited states of molecules lie above the first ionization threshold. They converge to ionic excited states of the molecular, which decay through auto-ionization or neutral dissociation processes. There are some studies about molecular nitrogen (N_2) by electron impact. A dipole (e, e+ion) experiment by Wight et al. [1], and a Co-EELS experiment by Odagiri et al. [2] are representative of their experimental works. In particular, the Co-EELS experiment which observes both fluorescence from excited neutral atoms and electron energy-loss values is useful to obtain information on forbidden states and their decay processes. In the present work, we observed both scattered electron and ion in coincidence, and determined the generalized oscillator strengths for the creation of N_2^+ and N^+. The experimental apparatus used for this scattered electron-ion coincidence (SEICO) experiments has been described in previous publication [3] in detail. Briefly, the SEICO spectrometer consisted of a pulsed electron-gun, an electron energy analyzer, and a time-of-flight mass analyzer. After the incident pulsed electrons collided with molecules,

Fig. 1: Scattered electron-ion coincidence spectra for (a) N_2^+ and (b) N^+, under 200 eV incident energy and a scattering angle 6 degrees.

scattered electrons were analyzed with the electron energy analyzer, while formed ions were analyzed with time-of-flight mass analyzer. We measured intensities of ions as a function of electron energy-loss values, as a scattered electron-ion coincidence spectrum. Figure 1 (a) and (b) show the scattered electron-ion coincidence spectra for N_2^+ and N^+, respectively. The experiment was performed under 200 eV incident energy and a scattering angle 6 degrees. Some structures are shown in Fig. 1(a). The peak around 23 eV indicates the vibrational structure of the doubly excited $(C^2\Sigma_u^+)4s\sigma$ Rydberg states assigned by Codling [4]. These doubly-excited states produce N_2^+ ions caused by auto-ionization, but never produce N^+ ions. In fact, theses structure is seen in the similar spectra obtained by the dipole and photon-impact experiments. Overall, our results agree well with the previous experiments.

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E-20

Combined experimental and theoretical study on the dynamics of rearrangement reactions triggered by low energy electrons in p- and o-tetrafluorohydroquinone

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Similar to pentafluorophenol [1,2]; both *ortho*-tetrafluorohydroquinone (*o*-TFHQ) and *para*-tetrafluorohydroquinone (*p*-TFHQ) capture electrons through two distinct low-energy resonances. In dissociative electron attachment (DEA) these result in maxima in the ion yield close to 0 and 1.5 eV. As is the case for many fluorinated organic molecules [1-6], DEA to *o*-TFHQ and *p*-TFHQ leads to complex rearrangement reactions involving multiple bond ruptures and new bond formations; reactions that are energetically enabled by the formation of highly stable neutrals such as HF and CO.

The dominating DEA channels for *o*-TFHQ and *p*-TFHQ are the spontaneous loss of one or two HF molecules, leading to the formation of $[M - HF]^-$ and $[M - 2\,HF]^-$, respectively. The former channel is observed in both molecules at close to 0 and at 1.5 eV, although with distinctly different branching ratios. The formation of $[M - 2HF]^-$ is also observed through both resonances from p-TFHQ, but from o-TFHQ this channel only proceeds through the higher lying resonance. In addition to the loss of HF and 2HF, a considerable contribution to the ion yield from *o*-TFHQ is observed through the loss of both HF and CO (formation of $[M - HF - CO]^-$) close to 1.5 eV, while this channel barely exists for *p*-TFHQ.

While simple DEA reactions, involving single bond ruptures can easily be explained by their thermodynamics, this is often not the case for complex DEA reactions, where multiple bonds are broken and new bonds are formed. The key to this lies in the reaction path and the associated reaction barriers along the potential energy surface (PES).

In the current contribution we present experimental data and quantum chemical calculations on DEA to o-TFHQ and p-TFHQ. Calculations of the PESs were carried out using ORCA and Chemshell at the B3LYP/ma-def2-TZVP level, and multiple reaction pathways, leading to HF and CO formation were considered. In good agreement with our experimental findings, the calculations show that the reaction barrier for the loss of two HF units from *o*-TFHQ is about 1 eV higher than for *p*-TFHQ, a finding that readily explains the experimental observations. Also in good agreement with our experimental results, the calculations reveal a low-energy reaction pathway to $[M - HF - CO]^-$ that is enabled by a proton-shuttling mechanism. Such a mechanism is only possible for *o*-TFHQ as there is an insurmountable barrier on the corresponding reaction path for *p*-TFHQ through the low energy resonances.

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Dissociative electron attachment to H₂ and D₂: Reliable magnitude of the isotope effect at 4 eV resonance

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Absolute measurement of dissociative electron attachment (DEA) cross sections for H_2 and D_2 at 4 eV and 14 eV resonances is presented in this contribution. The isotope effect at the former resonance is stronger than previously reported.

The $^2\Sigma u$ 4 eV hydrogen molecule resonance is the most elementary resonance in electron-molecule collisions. The resonance is very broad and the production of H^- from DEA to H_2 has a very low cross section. Another consequence of the large width is a very large isotope effect: The cross section for D^- from D_2 has been reported to be 200 times lower than for H^- from H_2 [1].

The experiment has been performed using a quantitative DEA spectrometer with trochoidal electron monochromator in combination with ion time-of-flight (TOF) analyzer [2]. An effective separation of signal from background has been achieved with the aid of delay-line time-and-position sensitive detector (RoentDek). This separation is essential when measuring such a low cross sections as presented in this study. The measurements of absolute cross sections have been performed in a mixture of studied molecule (H_2 or D_2) together with CO_2 and HCOOH used as calibration gasses with known cross sections and positions of resonances [3].

The DEA cross sections for H_2 and D_2 at 14 eV have been recently reported in a velocity-map imaging study [4] and are in a good agreement with the present experiment. For the 4 eV resonance in D_2 we report a cross section approximately two times lower than reported in [1].
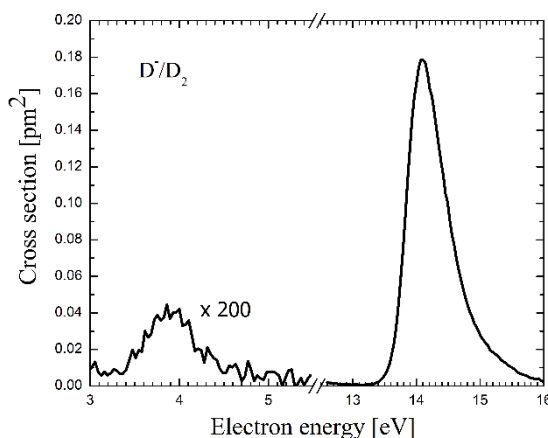
Figure 1: Absolute cross section for production of D^- in DEA to D_2 molecule.

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Electron induced ionization of astrophysically relevant cyanide molecules

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Electron impact ionization has numerous applications in various fields ranging from analytical mass spectrometry or mass filter, plasma studies, fusion modeling, radiation physics and gas discharges to more abstract applications such as astrophysical applications and modeling of planetary atmospheres [1]. The present work presents the electron impact ionization cross section of four preliminary cyanide molecules namely methyl cyanide (CH_3CN), ethyl cyanide (CH_3CH_2CN), propyl cyanide (C_3H_7CN) and iso-propyl cyanide (i-C_3H_7CN). The calculation to obtain cross section is performed using spherical complex optical potential (SCOP) formalism and complex scattering potential-ionization contribution (CSP-ic) method [2]. These molecules are of much interest due to their presence in the interstellar medium. Recently, it was found that the strongest methyl cyanide emission arise in hot cores in the regions of massive star formation [3]. Ethyl cyanide has a very dense rotational-vibrational spectrum as observed in laboratory characterization and astrophysical detection [4]. Belloche *et al* has reported the presence of propyl cyanide and its isomer in the giant gas cloud in the star-forming region of Sagittarius B2 [5,6]. Hence, cross seciton for such molecules are very important to study these environemnts. However, the dearth of cross section data has crippled the modeling community. Due to these reasons the present study finds significance.

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Electron driven reactions in aminotiols: the case of cysteamine and N-acetylcysteamine

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The investigation of collisions between electrons and neutral molecules is of importance for the understanding and the development of many naturally and technologically occurring processes [1]. Owing to many applications dissociative processes received a great deal of interest in recent years, among them dissociative electron attachment (DEA) processes.

Recent years have witnessed a considerable increase of interest in the studies of DEA processes in sulphur containing molecules. This has been mainly stimulated by the importance of these compounds in many biochemical processes as they can be implicated, *e.g.*, in aging [2] or oxidative stress [3]. Besides, they can undergo reductive processes. Recent dissociative electron attachment experiments on thiolated nucleobases, *e.g.*, 2-thiothymine [4] and 2-thiouracil [5], have demonstrated that the presence of the sulphur atom within the molecular structure strongly influences the fragmentation of the molecule, which is visible via the formation of the sulphur containing anionic fragments.

In this contribution we will present the results from low energy electron driven reactions in cysteamine ($NH_2CH_2CH_2SH$) and N-acetylcysteamine ($CH_3C(O)NHCH_2CH_2SH$). Cysteamine is the simplest stable aminothiol and a degradation product of the cysteine. N-acetylcysteamine is the N-acetylderivative of the cysteamine, which besides the thiol group contains the peptide group within the structure.

The results from cysteamine and N-acetylcysteamine have been obtained utilizing the electron-molecular crossed beam apparatus. Dissociative electron attachment to these compounds results in the formation of various negative ions, which are generated preferentially at the very low energy range < 3 eV. The predominant fragment generated from both compounds is the $(M - H)^-$ ion, which is most likely generated from the loss of the H atom from the thiol group. Surprisingly we observe the fragments at higher masses then the respective intact molecules. This observation indicates that in the presence of a trace amount of the air the molecules polymerize to form dimers via most likely formation of the S–S bond. This phenomenon will be discussed in more detail during the conference.

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Electron energy loss distributions from pyrimidine

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Pyrimidine is a prototype molecule for numerous biological molecules, such as cytosine, thymine, uracil thiamine, and alloxan. For this reason, it is one of the most interesting molecular targets to perform electron interaction studies. Pyrimidine is stable to moderate heating with a melting point close to room temperature, which makes it easily accessible for scattering experiments in the gaseous phase [1].

Here, we present novel experimental results on electron energy loss distributions from gaseous pyrimidine at 20eV obtained in a magnetically confined electron scattering system (see Fig. 1). This system is based on a strong axial magnetic confinement of the beam (0.1T) inside a collision chamber [2]. The results obtained show that energy resolution of the beam in the given configuration is around of 1.5 eV. In order to improve the energy resolution, some modifications in the system will be implemented. Namely, a nitrogen trap will be introduced in the system to reduce the electron energy spread. The electrons produced by a filament will pass through the chamber filled with nitrogen and will be cooled down to about 50 meV via vibrational excitations of the molecular nitrogen. These electrons will be extracted and accelerated to the energy of the interest while keeping their relative energy spread. The observed energy loss distribution will be compared with that simulated in our Low Energy Particle Track Simulation code [3] in order to check the reliability of the input parameters used in this model. In a future work, the improved system will be used to determine total electron scattering cross sections for different molecules in the energy range (1-1000 eV).
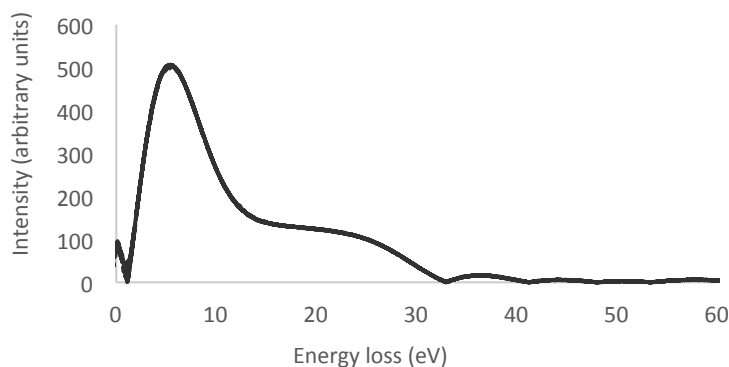

Figure 1.Electron energy loss distribution measured for pyrimidine at incident energy of 20 eV.

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E-25

Low Energy Electron Induced Reactions in Condensed Methanol

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Site selective reactions in molecules can be induced by low energy electrons (LEE) through dissociative electron attachment (DEA) [1]. Indications of selectivity in surface reactions could be seen in the electron induced desorption of negative ions from condensed molecular films [2]. Methanol (CH_3OH) is one of the simplest compounds with two different functional groups (CH_3 and OH). DEA to gas phase methanol showed the site-specific fragmentation of C-H and O-H bonds using incident electron energy as a control parameter [1]. A recent study of electron stimulated desorption (ESD) from condensed methanol has identified the formation of H^- and O^- by DEA using electrons of energy above 5 eV [3].

We have carried out ESD experiments from condensed methanol films of varying thickness using our newly built condensed phase experimental setup. We form cold molecular films by depositing them on a gold substrate cooled by a closed cycle helium cryostat. The ions desorbed from the surface following irradiation by a magnetically collimated and pulsed electron gun are analyzed using a time of flight mass spectrometer (ToFMS) mounted normal to the substrate. The composition of and any chemical changes taking place in the molecular film is probed in situ by using Fourier transform infra-red (FTIR) spectrometry throughout the experiment.

The measurements on the desorbed anions show the resonant formation of O^- at 3 - 4 eV and H^- at 5 - 6 eV. FTIR measurements show signature of ethylene glycol ($OHCH_2CH_2OH$) in the same energy range (5 - 6 eV). Production of glycol in methanol ice indicates formation and recombination of (CH_2OH) radicals in the irradiated film. It is possible that (CH_2OH) and H^- are generated in the same channel in the 5 - 6 eV energy range. These observations suggest a new reaction path way involving bond breaking and bond formation at specific electron energies in condensed methanol.

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E-26

Electron ionization and attachment to Dicyclohexyl Phthalate molecule

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Dicyclohexyl phthalate (DCP) molecule belongs to the group of phthalates used in production of PVC as a plasticizer. Many of the phthalates represent a potential risk for human health and their concentrations in everyday products are strictly limited [1]. The analysis of concentration and identification of the phthalates type is mostly done by gas chromatography-mass spectrometry technique. The electron ionization (EI) and dissociative electron attachment (DEA) to DCP molecule was measured at the Comenius University in Bratislava with a crossed electron-molecular beams technique (CEMBA) [2].

The mass spectrum of DCP ($C_6H_4(COO(C_6H_{11}))_2$) has a characteristic feature typical to other phthalates with a strong peaks m/z 149 ($C_6H_4(CO)COOH^+$) and 167 ($COOH(C_6H_4)C(OH)_2^+$), and a weaker ionic product at m/z 249 ($(DCP-C_6H_{10})^+$). Several peaks under m/z 83 represent the fragmentation of cyclohexane. The DEA to DCP is more useful for distinguishing the DCP from other phthalates as the DCP^- ion with m/z 330 is the dominant product. Almost 0 eV kinetic energy of the attaching electron is enough to initiate the attachment and other dissociative channels to products with m/z 148 ($C_6H_4(CO)COO^-$) and 45. The m/z 148 product is the only with two resonances at low energy single particle region and higher energy core-excited region ~7.5 eV. Other core excited products are the $C_6H_4(COO)^-$ with m/z 121, phenyl anion with m/z 77 and $C_6H_{11}O^-$ with m/z 99.

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Electron ionization of Diiron nonacarbonyl

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Diiron nonacarbonyl ($Fe_2(CO)_9$) is a potential precursor for FEBID (focused electron beam induced deposition) technology. Study of interaction of precursors with low energy electrons is important for description of the processes originated from secondary electrons emitted from the surface. Formation of positive ions via electron ionization and dissociative ionization of $Fe_2(CO)_9$ is presented in this work and compared with previous experimental and theoretical study of similar iron precursor, iron pentacarbonyl ($Fe(CO)_5$) [1]. The experiment was performed using a crossed electron and molecular beam technique [2]. Diiron nonacarbonyl in solid state was sublimated via small capillary into the reaction region where it collided with a mono-energetic electron beam created by trochoidal electron monochromator (with FWHM ~200 meV). Ionic products were accelerated with a weak electric field into a quadrupole mass analyzer and finally detected by channeltone electron multiplier. For estimation of appearance energies (AE) we used modified Wanier formula [3]

$$\sigma(E) = b + a(E - AE)^d$$

were E is represented by electron energy and a,b are variable fitting parameters.

In the mass spectrum of $Fe_2(CO)_9$ a weak formation of parent ion $Fe_2(CO)_9^+$ can be visible. Also, dissociation of CO ligands resulting into a creation of $Fe_2(CO)_8^+$, $Fe_2(CO)_7^+$, $Fe_2(CO)_6^+$, $Fe_2(CO)_5^+$ and $Fe_2(CO)_4^+$ ions is typical for this precursor. The relative intensity of these products is increasing with the number of lost CO group. The creation of other positive ions containing two iron atoms was not detected. All ions with masses below m/z 200 are similar to the products of electron ionization of $Fe(CO)_5$ [1]. However, higher ion yields of some of the products were observed in comparison to the dominant intensity of m/z 84, $FeCO^+$. The most intensive increase (around six times) was detected for creation of $Fe(CO)_5^+$ ion, followed by $Fe(CO)_4^+$, $Fe(CO)_3^+$ as well as CO^+ ions.

Below m/z 200 no multiply charged products for $Fe_2(CO)_n^{2+}$ were detected, contrary to $Fe(CO)_3^{2+}$, $Fe(CO)_2^{2+}$, $Fe(CO)^{2+}$ and Fe^{2+} visible both in the mass spectrum of $Fe(CO)_5$ [1] and $Fe_2(CO)_9$. The products like $FeC(CO)_n^+$ and/or $FeO(CO)_n^+$ [1] were detected in the spectrum of $Fe_2(CO)_9$ also but again without corresponding cationic fragments with two Fe atoms included.

Appearance energies was estimated for creation of $Fe(CO)_n^+$ (n = 0 - 5) ions, as well as for CO^+ ion. The values of AE´s are close to corresponding AE´s estimated for $Fe(CO)_5^+$ ion [1] with variation cca 0.3 eV witch can be compared to standard error of electron energy resolution. The most visible offset is observed for production of $Fe(CO)_2^+$ ion around 0.5 eV.

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Elastic differential cross sections for acetone by 7-50 eV energy electron impact

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Acetone (C_3H_6O) is the simplest carbonyl and aliphatic compound largely used as an industrial solvent for the plastic and fiber industries, and is closely related to human health as a biomarker in the breath of untreated patients with diabetes [1]. Acetone, can also be used in radiobiology, as a radiosensitizer since the presence of ketones may modify the structures of DNA bases, which are sensitive to low-energy interactions along ionisation tracks [2].

Electron interactions with organic compounds, such as acetone, are a powerful tool to determine elastic and inelastic differential cross sections, which can be used as input data in radiotherapy dose planning [3]. As such, in this joint theoretical and experimental study, we present comprehensive elastic differential cross sections for electron scattering from acetone in the 7 to 50 eV energy electron in the angular range 15 to 90°. The experimental measurements have been obtained in an high-resolution electron-energy-loss spectroscopy (HREELS) setup [7], while the theoretical calculations have been performed by the Independent Atom Model-Screening Corrected Additivity Rule (IAM-SCAR) [4] and Schwinger Multichannel Methods [5,6]. The level of agreement between these calculations and our measurements is found to be quite remarkable

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Secondary electron yield in low-pressure H$_2$O vapour discharge

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Two main mechanisms govern the electrical breakdown event in gases: ionization in the gas phase and secondary electron emission from electrode surface. In the case of low-pressure breakdown, the ionization coefficient (α) and the secondary electron emission yield (γ) are related by the Townsend's condition for creation of self-sustaining discharge. In principle, Townsend's theory is deduced under the assumption that only ions can induce secondary electron emission. However, this theory requires extension, as discussed by Phelps and Petrović [1], by taking into account all possible mechanisms producing secondary electrons: emission induced by ions, metastables, fast neutrals and photons. This addition is necessary particularly when modeling complex systems, such as discharges in vapours of liquids. One of the solutions is determination of the effective secondary yields from low current Townsend discharge, where flux of electrons at the anode is proportional to fluxes of species reaching the anode [1].

In our experiment the effective secondary electron yield for water vapour discharge is determined for copper cathode in plane parallel geometry of electrodes. For calculation of the secondary yield we utilize formula for self-sustaining condition using experimentally attained ionization coefficient obtained from axial emission profiles and Paschen curve [2,3]. This approach has an advantage as it takes into account non-hydrodynamic effects close to the cathode, as well as possible effects of gas impurities, thus giving actual electron multiplication from the slope of emission profile recorded in the experiment. However, in water vapor discharges in spatial emission profiles at high reduced electric fields (*E/N*) principal part of emission comes from excitation in heavy-particle processes in front of the cathode. This emission screens emission from electron-induced excitations taking place before the anode. Hence, determination of ionization coefficient from discharge profiles is limited to the range of conditions where dominant emission is induced by electrons. Moreover, for *E/N* values where heavy-particle emission start to emerge, determination of the length of non-hydrodynamic region at the cathode (d_0) can be imprecise due to the shape of the profile. At higher *E/N* this is not critical, as overall multiplication is small so d_0 does not influence determination of secondary yield considerably.

Taking into consideration all limitations, we calculated effective secondary electron yield in *E/N* the range between 680 Td and 6500 Td with the equilibration length (d_0) where that was possible to attain and without the d_0 length. Comparison with the results by Hasegawa *et al* [4] obtained with a cathode made of stainless steel showed that the agreement was very good having in mind different cathode materials.

By recording breakdown voltages (i.e. Paschen curve) and spatial profiles of low-current discharge and subsequently obtaining ionization coefficient and secondary electron yields consistently from the experimental results we provided a complete set of breakdown data for low-pressure water vapour discharge. The next step should be to couple the breakdown data to the Volt-Ampere characteristics to determine the energy (effective *E/N*) dependence of the secondary yield [1].

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Recent developments in R-matrix applications to molecular processes

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Advances in experimental atomic and molecular physics (e.g. the advent of femto and attosecond laser pulses) and the increased need in technological areas for quantitative data involving the electronic continuum of molecules (e.g. electron-molecule scattering cross sections required to model industrial plasmas and the interaction of radiation with biological material) is driving the development of new methodology and software to treat correlated multielectron dynamics in molecules.

The UKRmol suite [1] is based on 30+ years of software development. Initially a set of codes that enabled the study of low energy electron scattering from molecules (and partly based on prior electron-atom scattering software) the suite has developed and is now used to study positron molecule scattering, scattering from molecular clusters and to generate data necessary to perform calculations for photon induced processes (photoionization, high harmonic generation, etc) as well as other processes involving nuclear dynamics like associative detachment. In recent years, the suite has been significantly improved, both in terms of its efficiency (for example, the parallelization of various programs in the suite has allowed us to perform sophisticated calculations for electron scattering from uracil [2] as well as the bound and continuum electronic states of N_2 [3]) and the addition of new functionality (e.g. a program, CDENPROP [4], that determines transition moments between bound and (discretized) continuum states as well as Dyson orbitals has been developed). Many of these applications entail the calculation of scattering and other data (in particular, resonance energies and widths) for a large number of molecular geometries. A set of scripts has been developed that significantly simplify this task. The suite of codes and scripts are freely available for download [5].

We will present recent developments as well as some examples of the physics being investigated with the UKRMol suite.

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Benchmark cross sections for electronic excitation to $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ levels and elastic scattering for H_2O molecule by low energy electron impacts

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Electron impact excitation of water molecules is of particular relevance to radiation-driven chemistry in biological systems because several of the lowest-lying states are strongly dissociative, producing H atoms and OH radicals [1]. Itikawa and Mason noted in their review [2] that the angular differential cross sections (DCSs) and angular integral cross sections (ICSs) data for excitation of water by low-energy electron impact were poorly characterized. Therefore, in contrast to the elastic scattering, vibrational and rotational excitation, they were unable to recommend a cross sectional dataset for electronic excitation. Recently, the DCSs for electronic excitation to the $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ lowest-lying states, which correspond to the $1b_1$ to $4a_1$ transitions, have been reported by two different research groups [1, 3]. However, these results have shown serious discrepancies in the angular distributions of the electronic excitation cross sections of these lowest-lying states below 20 eV impact energy. In the present work, in order to fully address this discrepancy, we have performed comprehensive quantitative measurements of the electronic excitation cross sections at impact energy of 15, 20, and 30 eV. In addition, we also obtained comprehensive DCSs for elastic scattering from water molecules in the energy range of $2.0 - 100$ eV, which has been used for normalization.

The present measurements have been carried out using an original crossed-beam electron spectrometer described in detail many times before, see e.g. ref. [4] and performed in the scattering angle range of $10 - 130^o$. The energy resolution was typically 55 - 60 meV (FWHM). The absolute scale has been obtained by the standard relative flow technique. The H_2O sample was obtained from the vapour of ultra-pure water supplied by Wako Pure Chemical Industries, Ltd. The liquid sample was purified to remove dissolved gases by a repeated freeze-pump-thaw procedure.

In the present measurements, for the DCSs for electronic excitation to the $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ states, our present measurements and those of Ralphs *et al* [1] are generally consistent, but for the $\tilde{A}^1B_1$ state, we observed quantitative differences at the impact energy of 15 eV. In order to explain this difference, we compared the present elastic DCSs with those of other groups. The agreement between the present elastic DCSs and those of Nishimura and Danjo [5] is found to be good in all range of impact energies. Further details of the results will be presented at the conference.

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Electron-induced processes in helium droplets – experiment and theory

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In experiments utilizing electron ionization of pure and doped helium droplets we observed the excited metastable anions He*- and He_2*- [1]. Although they are formed at similar electron energies [2], they show rather different behaviour. The atomic helium anion is heliophilic and of high mobility, whereas the molecular helium anion is heliophobic and surface-bound [3]. This leads to very different reactivities with foreign molecules embedded in helium droplets. In Figure 1 we graphically summarize the properties of atomic and molecular helium anions in helium droplets.

Here we present evidence for single-charge transfer from He*- to SF_6- [1] embedded in helium droplets, as well as the formation of dianions via double-charge transfer from He*- to clusters of fullerenes [4,5]. For the latter, we also discuss the internal stability of fullerene clusters against Coulomb explosion, which enables the observation of these dianions. Furthermore we explain the formation of He^+ via He*- at electron energies below the ionization energy of the free helium atom [6].

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Electron interactions with aminomethane sulphonic acid and taurine as probed by experimental and theoretical methods

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Seminal studies of Sanche and co-workers revealed the capability of secondary electrons, with energies ≤ 20 eV, to induce single and double strand breaks to DNA [1]. Given the resonant-like behavior of the quantum yield profiles for induction of Double Strand Breaks (DSBs), Single Strand Breaks (SSBs) and loss of the supercoiled DNA form, several theoretical and experimental studies concerning dissociative electron attachment (DEA) to biological relevant molecules in the gas-phase have been performed. In the last few years, special attention has also been given to electron transfer processes in potassium-(bio)molecule collisions [2]. This dissociation mechanism represents an alternative approach to mimic electron driven dissociation reactions within the physiological medium.

The scientific community has become more aware of the importance of studies on electron driven reactions in sulphur containing biomolecules, in order to further investigate the role of sulphur in redox reactions. Recent studies on DEA to sulphur containing analogues of thymine and uracil show that the main fragmentation is assigned to sulphur containing anions [3,4].

Here we give the first set of comprehensive experimental and theoretical analysis on the electron interactions with aminomethane sulphonic acid and taurine, two sulphur containing compounds. Taurine is an amino acid comprising several physiological functions. Aminomethane sulfonic acid represents the taurine molecule with one less CH_2 group in the carbon chain.

The experimental results have been obtained through DEA and electron transfer, from the Siedlce and Lisbon laboratories with negative ions detected by quadrupole and time-of-flight mass spectrometry. From the ionic yields we note a rich fragmentation pattern where the parent anion was not observed. The anionic yields show evidence of resonance-like features with main contributions centered at ~4.7 eV. These resonances are consistent with theoretical predictions obtained through Schwinger multichannel implemented with pseudopotentials, where the data from the Brazilian group indicates a π* a shape resonance around 4.75 eV and suggests a σ* shape resonance around the same energy. Results of electron transfer to taurine reveal that this mechanism may promote further dissociation of the molecule when compared to free electron attachment.

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Benchmark cross sections of lowest-lying 4s[3/2]₁ and 4s'[1/2]₁ levels for argon by electrons in the 15 – 300 eV impact energy range

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We have been studying electron impact excitation of rare gases in order to extract absolute differential and integral cross sections (DCSs and ICSs), and more dedicated to obtain a comprehensive set of measurements on the lowest-lying levels ($ns[3/2]_1$ and $ns'[1/2]_1$) of optically allowed transitions. Recently, we reported the benchmark cross sections for electron excitation of n = 3 for Ne in the energy range from 20 to 300 eV [1]. In this study, we focused on the electronic excitations of Ar in n = 4 and the ICSs obtained from the corresponding DCSs for low-lying levels have been compared with the BE*f*-scaled ICSs [2].

The present measurements were performed at Sophia University using a crossed-beam apparatus of a conventional high resolution electron spectrometers in impact electron energies of 15 to 300 eV and at scattering angle range of 1° to 130° with their energy resolution of 45 meV (FWHM). The absolute scale of the DCSs was obtained by the relative flow technique using the well-known elastic DCS of He [3]. Errors in the DCS and ICS are estimated about 20 % and 30 % in this work, respectively.

Figure 1 shows present results of DCSs for both (a) $4s[3/2]_1$ and (b) $4s'[1/2]_1$ levels at an impact energy of 30 eV. In Fig. 1, the results from previous measurements and computations are also shown [4]. The ICSs for the excitations to $4s[3/2]_1$ and $4s'[1/2]_1$ levels were obtained by extrapolating the DCSs with the Vriens fitting formula [1].

We compared present ICS with the previous experimental and theoretical ones in the energy range 15 to 300 eV. It is found that the BE*f*-scaled ICS for the both transitions in Ar reproduce well the present experimental results, except for low energy region below 30 eV. In addition, we also compared our ICS with the large-scaled B-spline R-matrix computation for Ar reported recently [5]. Further details will be discussed at the conference.
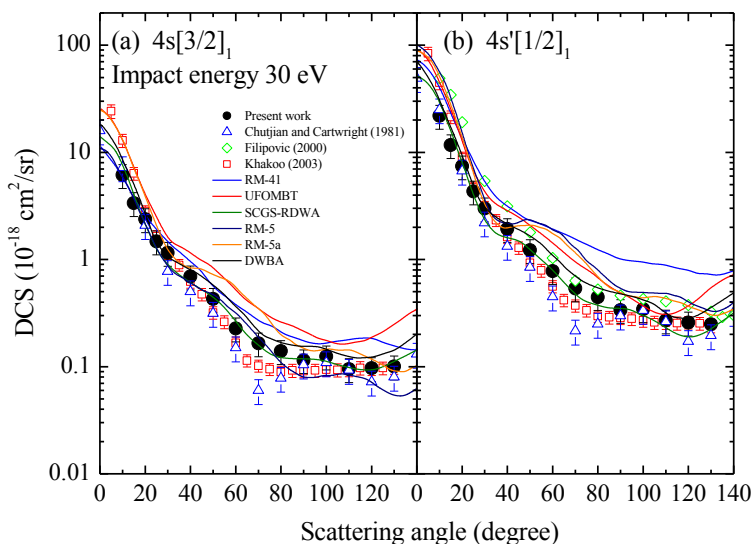

Figure. 1 Present DCSs for electron impact excitation in Ar at an electron incident electron energy of 30 eV.

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Reaction equilibrium in electric field of an ion drift tube: stepwise formation of $H_3O^+(H_2O)_n$ cluster ions

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For decades, the stepwise formation of ionic cluster has been investigated under relevance to various scientific fields. For instance, stepwise formation of ionic cluster is a significant subject as an early stage of the ion-induced nucleation since it governs the subsequent growth stage of nucleation. However, in many of experimental researches, the core ions have been produced in reactant gases by discharge, a pulsed electron beam, radiation sources, and so on. In general, various ionic species are generated together with desired core ions in such a setup and the initial ionic reactions are complicated. In order to eliminate reactions involving undesired ions, we developed an ion drift-tube with selected-ion injection [1-5], where only specific parent or seed ions are injected into the drift-tube reactor.

The ions drift with their own average velocities determined by the electric field and the number density of the molecules in the drift tube. They simultaneously react with molecules and the sizes of the ionic clusters become up and down in the drift tube. Thus, the electric-field dependence of ionic cluster formation is presumably governed by the quantities determining the drift motion of ionic clusters, e.g., collision cross sections. Most of preceding investigations for ionic-cluster formation using drift tubes were performed using conditions where influence of electric-field strength could be ignored [4, 5,] or using extrapolation of observed quantities at non-zero field to zero electric field [3].

In the present study, we filled the drift-tube reactor only with water vapor and measured produced $H_3O^+(H_2O)_n$ yields using CO^+ injection in the temperature range from 242 K to 329 K. We obtained the reaction equilibrium constants, $K_p(T, E)$, for non-zero electric fields, E, and the gas temperature, T, in stepwise attachment/detachment of a water molecule, where $K_p(T, E)$ were determined by normalizing yield-ratios of $H_3O^+(H_2O)_n$ to $H_3O^+(H_2O)_{n-1}$ (n=4-8) with the water vapor pressure. $K_p(T, E)$ was found to be reproduced well using a functional form of $A\exp(-BE^2)$, where the parameters A correspond to the ordinary reaction equilibrium constants at zero electric field, $K_p(T, 0)$. The enthalpy and entropy changes for the stepwise association were estimated from the parameters $A = K_p(T, 0)$. We also investigated the pressure dependences of the parameters B and obtained empirical effective temperatures representing the reaction equilibrium constants, $K_p(T, E)$, for the present conditions. In this symposium, we're going to report the estimation of the enthalpy/entropy changes and the analysis of the electric field dependence of $K_p(T, E)$.

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Measuring electron-impact excitation cross sections of XF$_4$ (X = C, Si and Ge) molecules

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CF$_4$ is one of the most commonly used etchant gases in dry-etching processes, where the fluorine atoms created in CF$_4$/O$_2$ mixing plasma discharge on silicon surfaces, yield SiF$_4$ formation. GeF$_4$ has been also used for the manufacturing of semiconductors in plasma discharges. Therefore, the electron spectroscopic studies of XF$_4$ (X = C, Si and Ge) play important roles on our understanding of the fundamental underlying chemical processes in the plasma environment [1]. Recently, our group has carried out a series of comprehensive experimental electron energy loss spectroscopy studies with CF$_3$Y (Y = F, Cl, Br and I) molecular targets [2], as well as angular-resolved EELS measurements in CF$_4$ at 3 keV [3].

In this work, we report on the generalized oscillator strengths (GOSs) and integral cross sections (ICSs) for low-lying electronic excitations of XF$_4$ molecules. GOS analysis [4] is employed to derive the oscillator strength, f_0 value, which is compared with the optically oscillator strength (OOS) from photoabsorption measurements. ICSs for electronic excitation are also obtained from the GOS analysis. The present ICS are compared with the binary-encounter and f-scaled (BEf) Born cross section [5]. The electron spectrometer used in this work has been described before [6]. In brief, the spectrometer is of crossed-beam type with a hemispherical monochromator and analyser differentially pumped and the electron lens system controlled by computer-driven voltages. The apparatus was operated at electron impact energies from 50 to 300 eV and a scattering angle range from -6° to 50°, with typical energy resolution of 50 meV (FWHM) and angular resolution of ±1.5^o. The electron energy scale was calibrated against the 19.37 eV, ^{2}S resonance of He whereas the angular scale was determined from the symmetry in the intensity profile of the He 2^{1}P excitation measured at the 0° nominal scattering angle. The absolute scale of the excitation cross sections has been obtained by the relative flow technique [6] with He cross sections as the reference species.

From present measurements, it is found that the BEf-scaled ICS for CF$_4$ intense optically allowed transition from 4t$_2$ to 3s level in the energy loss around 14 eV, seems to generate more reliable values than unscaled Born ICS over the intermediate impact energies between 50 to 300 eV.

These results on SiF$_4$ as well as on CF$_4$ molecules will be discussed in more detail at the conference.

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Dissociative excitation of iron pentacarbonyl by impact of slow electrons

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The investigation of dissociative excitation reaction of $Fe(CO)_5$ induced by electron impact was performed using electron induced fluorescence. The emission spectrum was measured in the range from 200nm to 470nm, and photon efficiency curves were recorded for particular spectral lines such as in the Figure 1. The spectrum was dominated by Fe I and Fe II lines with the presence of CO I (b-a), CO I (d-a) and CO II (A-X), CO II (B-X) and CO II (B-A) band lines. The density of the lines in spectrum was very high and despite the optical resolution of approximately 0.3nm many of them were mixed. The Fe I emissions are related to dissociative excitation of $Fe(CO)_5$, leading to removal of all CO ligands from the molecule and subsequent Fe excitation to different excited states. The photon efficiency curves we measured for selected lines. More than one threshold was usually detected, resulting from the line mixing. Mechanisms and energetics of the dissociative processes leading to the emission of CO and Fe bands will be discussed.
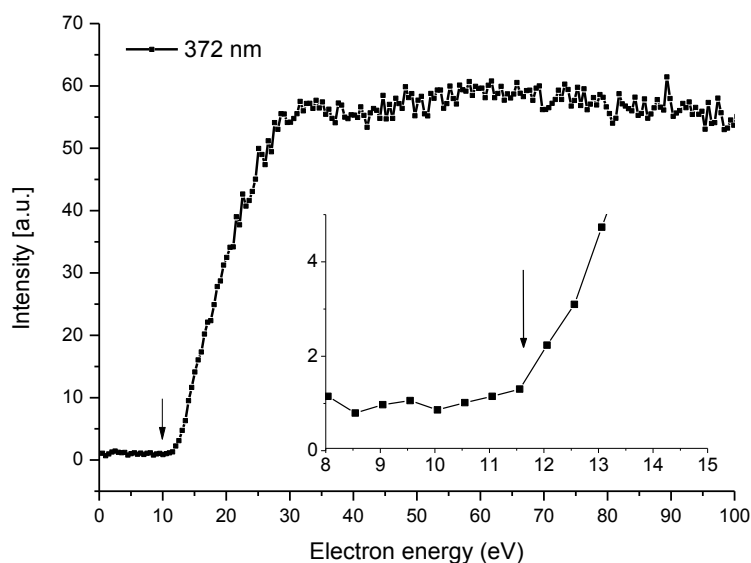
Figure 1. Photon efficiency curve recorded at 372 nm and ascribed to the Fe I transition $w^5F°$ (4) $\rightarrow$ a^5P (3) originating from $Fe(CO)_5$.

Comparing electron impact ionization and multi-photon ionization of nucleobases: new insights into electronic excited state dynamics and reactivity

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Radiation induced processes in biomolecules have been investigated intensively recently, notably in order to better understand the fundamental processes that can initiate DNA lesions [1]. While studies of isolated molecules generally provide the clearest data interpretations, equivalent measurements on hydrogen-bonded complexes enable closer analogies to be drawn with biological environments where different unimolecular or intermolecular reactive pathways can be significant. By comparing fragment ion production by electron impact ionization (EII) and UV multi-photon ionization (MPI) of isolated and clustered nucleobases, we have obtained the first experimental evidence supporting neutral CO loss due to ring opening at the crossing seam of the S_2 and S_1 electronic excited states of uracil [2]. Equivalent experiments on deuterated uracil confirm the identification of neutral CO loss as opposed to CNH_2 loss, while no evidence for a comparable ring opening pathway is observed in thymine and 5-fluorouracil. Clustering with water suppresses this channel, indicating a new mechanism by which the hydrogen-bonded environment stabilizes the molecule with respect to radiation damage.

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A protocol to study low energy electron collision with molecules in a aqueous media

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The interest in the collision processes of low energy electrons (LEE) with molecules, in particular biomolecules, is growing every day [1]. In order to understand the processes by which the electron is able to modify the structure of molecules of biological relevance, it is necessary understand the influence of the biological media in these processes [2].

In the present work we present a protocol to study low energy electron collision with furan (C_4H_4O) molecules in an aqueous media. This protocol involves two steps. In the first step we carried a Monte Carlo (MC) Simulation [3] to generate statistical relevant structures of the $C_4H_4O…H_2O$ complexes. After the MC simulation we apply a cluster analysis [4] to select the cluster with the major statistical relevance. The second step consists to carry out LEE-complexes scattering calculation. We apply the Schwinger multichannel method [5] with pseudopotentials of Bachelet, Hamann and Schlüter [6].

We show that after the MC simulations is possible to divide all $C_4H_4O…H_2O$ complexes in clusters. Each cluster stores information about the proton donor / acceptor character of the water molecules in the hydrogen bond with the furan molecules.

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A protocol to study low energy electron collision with molecules in a aqueous media

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We show that after the MC simulations it is possible to divide all $C_4H_4O{\ldots}H_2O$ complexes in clusters. Each cluster carries the information about the proton donor / acceptor character of the water molecules in the hydrogen bonds with the furan molecules.

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Electron transfer in potassium-tryptophan collisions: an experimental and theoretical fragmentation study

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It is known that ionizing radiation bring adverse effects to living cells. In the femtosecond regime, multiple ionizations may occur in the human body leading ultimately to the formation of radical and/or ionic species. In fact, for every MeV of radiation energy deposited in matter, about 5×10^4 secondary electrons (<100 eV) are generated [1, 2]. In the 10^{-15}-10^{-12}s time window, these entities may propagate through nanometer distances in the biological medium, leading to several inelastic events [3]. Low energy electrons, with energy below 20 eV can be resonantly captured in unoccupied molecular orbitals (virtual orbitals) [4, 5]. This process results in an unstable excited transient negative ion, which can further decay via auto detachment, dissociation or, in a comparatively long time scale, via photon emission.

In the present communication electron transfer studies upon potassium collisions with tryptophan, are presented as well as theoretical DFT analysis. Experimental results have been obtained by means a crossed molecular beam apparatus coupled with Time-of-Flight mass spectrometer. It is clear that for energy collision below 75 eV in the lab frame, the main fragment corresponds to the scission of C_β indole bond, with hydrogen transfer. This has been also described by means to DFT calculations, CAM-B3LYP and BHandHLYP codes.

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Two-dimensional spectra of electron collisions with acrylonitrile and methacrylonitrile reveal nuclear dynamics

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We have measured the elastic and vibrationally inelastic differential cross sections of acrylonitrile (in absolute units) and methacrylonitrile (relative units) at a scattering angle of 135°. In the energy dependence spectra of vibrational excitation of acrylonitrile the bands at 2.9 and 4.4 eV were observed which must be due to shape resonances, at low energy sharp structures were found, they are due to either boomerang structure of a shape resonance or vibrational Feshbach resonances.

Acrylonitrile is a suitable target to study the coexistence of the dipole-bound and the valence states of the anion because electron transmission spectroscopy revealed sharp structures – narrow resonances – in electron scattering at low energy [1] and it was shown that acrylonitrile due to its large dipole moment (3.86 D) supports dipole-bound states [2].

We measured methacrylonitrile hoping that it can help us to define the nature of the first resonance in acrylonitrile and assign it to either shape resonance or vibrational Feshbach resonance because it is known that a methyl substituent destabilizes the π^* orbitals by hyperconjugation, i. e., admixture of occupied pseudo-π orbitals of the methyl group, shifting the resonance up by 0.1–0.2 eV. The first resonance in methacrylonitrile appeared shifted up by about 0.1 eV compared to acrylonitrile, proving that it has to be a simple shape resonance.

The detailed view of the autodetachment dynamics is gained from a two-dimensional electron impact spectrum, in which cross section is plotted as a function of the incident electron energy, which determines the initial state of the negative ion, and of the energy loss, which carries information about the final state of the neutral molecule. The 2D spectrum provides a detailed insight into the autodetachment dynamics of the anion. The 2D spectrum of acrylonitrile reveals diagonal patterns, which are not evident in the more conventional presentation of cross section as a function of incident energy or of energy loss. The dominant process is $\Delta n = 0$ – no change of vibrational quanta during the detachment. Many of the remaining peaks are arranged along two other diagonals [3].

We have measured energy-loss spectra of methacrylonitrile and 2D energy-loss spectrum in the range of incident energies up to 1 eV where the incoming electron is temporarily captured in the lowest π^* orbital (region of the first resonance) and compared it to the 2D spectrum of acrylonitrile. The inelastic peaks are about two times weaker relative to the elastic peak than in acrylonitrile. The lower intensity and the fact that the resonances are much broader indicate that the methyl group substantially shortened the resonance lifetime. The interesting feature found in acrylonitrile – the diagonal patterns – are also observed in methacrylonitrile, although they become much broader.

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Absolute cross sections for electronic excitation of pyrimidine

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Pyrimidine is an important molecule since DNA and RNA bases are pyrimidine derivatives.

Electron scattering from pyrimidine has been studied in the past both experimentally [1-3] and theoretically [4-6], however there are still open questions.

We measured absolute differential cross sections (DCS) for elastic scattering and for electronic excitation of five electronically excited states of pyrimidine (shown on Figure 1) at 0°, 45°, 90°, 135° and 180°, then integrated them over angle and received integral cross sections. One example of energy dependence spectrum – excitation of the state at $\Delta E = 4.26$ eV (see Figure 2) shows three clear bands which must be due to $^2(\pi, \pi^{*2})$ core-excited shape resonances.
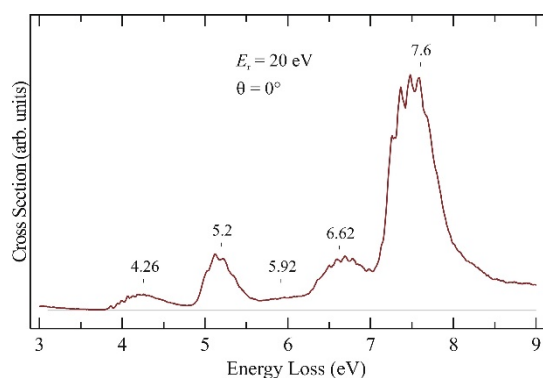
Figure 1. EEL spectrum of pyrimidine.
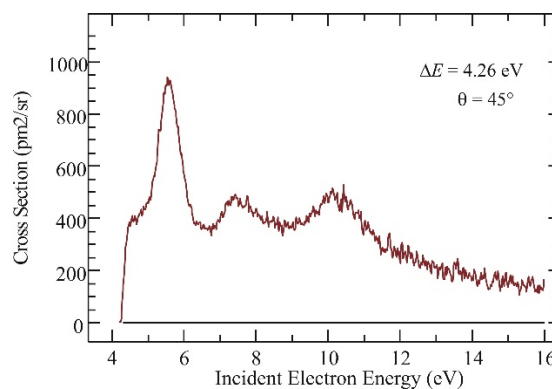
Figure 2. DCS for exciting the state at ΔE=4.26 eV.

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Electrons and ionic liquids – a novel approach to study electron scattering from nonvolatile compounds

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Ionic liquids (ILs) have numerous applications many of which involve their interactions with electrons.

We have applied the technique of low-energy electron impact spectroscopy, normally used for gas phase studies [1, 2], to ionic liquids. For this a droplet of ionic liquid was suspended on a loop of molybdenum wire (see Figure 1) and electrons scattered from ionic liquid were collected at an angle of 135° with respect to the incident beam.
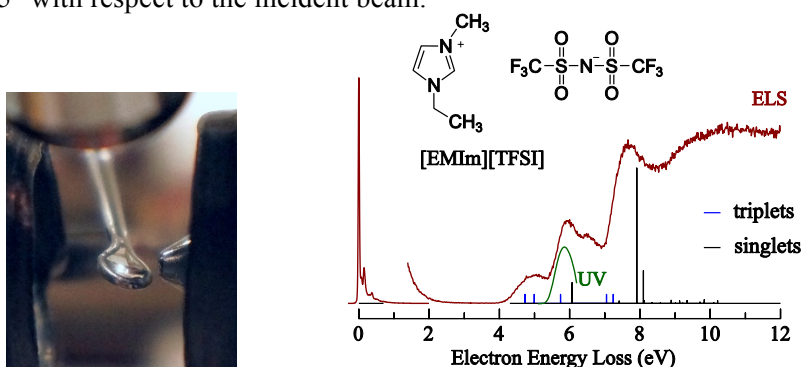
Figure 1. The IL droplet.   **Figure 2.** EEL, UV, DFT/MRCI spectra of one of the ILs.

Excited states of four representative ionic liquids were characterized by electron energy-loss spectra (EELS) and DFT/MRCI calculations, with good agreement. The capacity of EELS to induce spin-forbidden transitions revealed triplet states. Bands in the 3-8 eV range were assigned to (π, π^{*}) transitions of the cations; anion states are at energies above 7 eV (Figure 2). The spectrum of the piperidinium cation is 'empty' in the energy-loss range 2-8 eV, reflecting the absence of a (π, π^{*}) system.

Energy-loss spectrum of a saturated solution of methylene green (MG) in [EMIm][BF$_4$] showed a MG band at $\Delta E = 2$eV, demonstrating that ionic liquids may serve as hosts for nonvolatile compounds. Surprisingly, the band of MG was missing in the energy-loss spectrum when it was dissolved in a different IL, [BMPipe][TFSI]. This may indicate that it is displaced from the surface in this case and cannot be reached by electrons as they have a limited penetration depth.

This study demonstrates power of EELS to investigate surface structure.

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Effects of hydrogen bonding on pyridine resonances

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The collision of low-energy electrons (E<20 eV, secondary products of the radiation interacting with biological material), with isolated DNA bases has been studied for more than a decade [1]. A number of experimental works have been reported, focused on dissociative electron attachment (DEA). This process leads to the break-up of DNA via the formation of a temporary negative ion or resonance. From the theoretical point of view DEA is a highly complex process to describe, requiring use of sophisticated methods as well as large amount computational resources, even to treat the electronic part of the problem. Theoretical work has therefore concentrated on studying the formation of the temporary negative ions (except for a handful of small targets), and looked at model molecules as well as the bases themselves. DNA, however, is surrounded by water molecules. Understanding how solvation affects resonance formation (and the subsequent break-up) is therefore crucial.

We have performed calculations of electron collisions with pyridine (C_5NH_5) and the pyridine-water dimer using the R-matrix method [2]. Calculations for isolated pyridine at the SEP [3] and CC level revealed the presence of several shape and core excited resonances. Cross sections as well as a detailed analysis of the resonances will be presented at the conference.
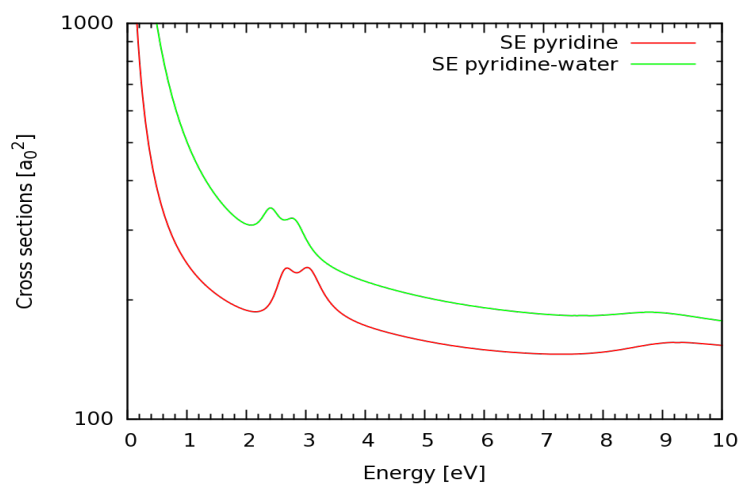
Similar calculations have been performed for pyridine-water. Results are consistent with earlier work on formic acid-water dimer [4] that shows a downshift of the shape resonance when the molecule acts as proton acceptor. The elastic cross section determined at SE level for both targets is shown in Figure 1. Two of the shape resonances are clearly visible in both cross sections.

Figure 1. Low energy integral elastic cross section for electron scattering from pyridine and pyridine-water.

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Higher order transport coefficients for electrons and positrons in gases

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Higher order transport coefficients usually have not been included in the interpretations of traditional swarm experiments where it is assumed that electrons have a Gaussian profile in space. However, recent application of a Monte Carlo simulation technique has revealed that the spatial distribution of electrons is not well described by a perfect Gaussian [1,2]. It has also been demonstrated that third order transport coefficients are generally required for conversion of hydrodynamic transport coefficients to those measured under steady-state Townsend (SST) conditions [3]. Finally, it has been shown in [4,5] that third order transport coefficients are much more sensitive with respect to the energy dependence of cross sections for elementary processes than transport coefficients of lower order, including drift velocity and diffusion coefficients.

The behavior of third order transport coefficients for electrons under the influence of electric field only was analyzed by several authors. Solutions of the Boltzmann equation and Monte Carlo simulation by Penetrante and Bardsley [4] and momentum transfer theory developed by Vrhovac et al [5] were used to study the behavior of skewness tensor for electrons in atomic gases. A molecular dynamic simulation and a three-temperature treatment of Boltzmann's equation were used by Koutselos to evaluate the third order transport coefficients for ions in rare gases [6,7].

In this work we extend these previous studies by addressing the structure of skewness tensor when both electric and magnetic fields are present and by considering the effects of inelastic and non-conservative processes (e.g. ionization and electron attachment for electrons and Positronium formation for positrons) for electrons and positrons in model and real gases. A group projector technique is employed to determine the structure and symmetries along individual elements of the skewness tensor. Calculations are performed by a multi term theory for solving the Boltzmann equation [8] and Monte Carlo simulation technique [1,2]. Various aspects in the behavior of skewness tensor elements are investigated, including the existence of correlation with low-order transport coefficients, sensitivity to post-ionization energy partitioning and errors of two-term approximation for solving Boltzmann's equation. Special attention is paid to the comparison between skewness tensor elements for electrons and positrons in H_2, N_2 and CF_4.

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Low energy electron attachment to molecules of biological interest

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Understanding the interactions of various types of radiation with the constituent cellular molecules (DNA in particular) underlay new DNA damage models formulation. Such models should be able to predict not only the patterns of ionizations but also the spectra of damage complexity that different types of radiation can induce in DNA. Hence knowledge of the relationship between the amount of energy deposited within a given region of the DNA helix and the type and severity of the damage that is produced is required [1]. In irradiation studies extracted plasmid DNA is being used that requires stabilisation, e.g. is suspended in EDTA solution. Therefore, the accurate determination of the influence of DNA stabilizers on the experimental outcomes is of great importance [2]. We have investigated by means of 70~eV electron impact and low energy (0-20~eV) electron attachment two most popular compounds used in DNA irradiation studies; EDTA often used as stabilizer [3] and TRIS used as OH radical scavenger [4], since it has already been noticed that EDTA may impact irradiation outcome [5]. Our results indicate that upon LEE attachment as well as at 70~eV electron irradiations, vast quantities of charged OH and O are being produced from both compounds. We also derived most probable dissociation channels throughout thermochemical calculations.

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PePa: Photoelectron-Photoabsorption Database

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This website was created to gather all the spectra collected by various members of our group over the past years. The simplicity of the data access and browsing was particularly stressed in order to provide a quick and easy-to-use tool for database users. Both photoelectron and photoabsorption spectra that were measured, can be found there. The data gathered in the database is accompanied by the reference to the peer-reviewed journals. In order to see the data, one needs to simply point the name of compound of interest. For individuals interested in obtaining data files for scientific use, a data request form is also provided.

A brief description of experimental setups that were used during the measurements was provided on the website. These can be found under the "Experimental setup" tab.

Figure 2. A screenshot of Photoelectron-Photoabsorption Database.

Cross Sections for Electron Collisions with Acetylene

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Acetylene (C_2H_2) is a hydrocarbon and the simplest alkyne. It is linear, symmetric and isoelectronic with N_2 and CO. It has triggered many theoretical and experimental studies. Electron collisions with C_2H_2 are important in the plasma processing, and acetylene has been detected in natural environments where free electrons may occur, including the interstellar medium and the atmospheres of Jupiter and other planets [1]. Electron collision cross sections with acetylene for various processes have been reported and reviewed in the literature [2].

In this report, cross section data have been compiled from the literature for electron collisions with acetylene molecules. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, ionization, excitations of rotational, vibrational and electronic states, and dissociative attachment. The data extracted from swarm experiments are also considered. For each of these processes, the recommended values and associated uncertainties for the cross sections are derived if possible. The literature has been surveyed through early 2015.

As group we are actively collaborating on the evaluation and recommendation of electron collision cross sections with key molecules, especially those of interest for plasma studies. A comprehensive review of electron-methane data was our first project [3]; this was followed by the present study on acetylene. Further reviews will follow in due course.

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E-50

Collisions of slow electrons with proline molecule

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Since 2000's a lot of work has been devoted to explain the interaction of slow electrons with molecules of biological relevance, mainly due the fact that low-energy electrons can cause single and double strand breaks to the DNA [1]. The damage caused by the low-energy electron is associated with its temporary attachment (resonance) within the molecule [2,3], such that many theoretical and experimental groups aim to properly obtain and classify the resonant processes in those biomolecules. One example of biomolecules are the amino acids, such as proline. Furthermore proline belongs to the group of amino acids encoded by the DNA.

In this work we present calculated integral, momentum transfer and differential cross section for low-energy electrons collisions with proline molecule. We employed the Schwinger multichannel method [4] implemented with pseudopotentials [5] in the static-exchange and static-exchange plus polarization approximations, for energies up to 20 eV. We identify the shape resonances as pronounced structure present in the integral cross sections and compare their energy positions with available data in the literature [6,7].

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Scattering of low-energy electrons by benzene

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Low-energy electron collisions play an important role in many areas, such as in high temperature plasma and in biological systems. Benzene is an interesting target molecule for many reasons, such as the symmetry and the fact it can be seen as a prototype for bigger systems.

In this work we present calculated integral and differential cross sections for low-energy electron scattering by benzene. It was employed the Schwinger multichannel method [1] implemented with pseudopotentials [2] in the static-exchange and static-exchange plus polarization approximations, for energies up to 20 eV. We compare the calculated cross sections with experimental differential and integral cross sections [3], experimental total cross sections [4,5,6] and with theoretical [7,8] data available in the literature. Benzene belongs to the D6h symmetry group and experimental data indicates two low-lying resonances at 1.15 eV and at 4.85 eV [9], where the first resonance belongs to the degenerated E_{2u} symmetry of the D_{6h} symmetry group. However our calculations were carried on the D_{2h} symmetry group such that the first resonance splits in two components, belonging to the A_u and B_{1u} symmetries of the D_{2h} symmetry group, located at the same energy.

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Transport parameters of Ar$^+$ in CF$_4$

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Charge transfer reactions of ions with molecules are essential elementary processes in modelling kinetics in industrial, terrestrial and astrophysical plasmas. In studied case charge transfer reactions are known to represent the most significant part of a cross section set [1]. Thus, in this work we assessed complete cross section set for Ar$^+$ in CF$_4$ by using existing experimental data [2] for charge transfer collisions producing radical ions of CF$_4$ and simplest extrapolations. We also calculated transport parameters by using Monte Carlo simulation technique. In Figure 1 we present drift velocities as a function of E/N where also temperature was used as a parameter.
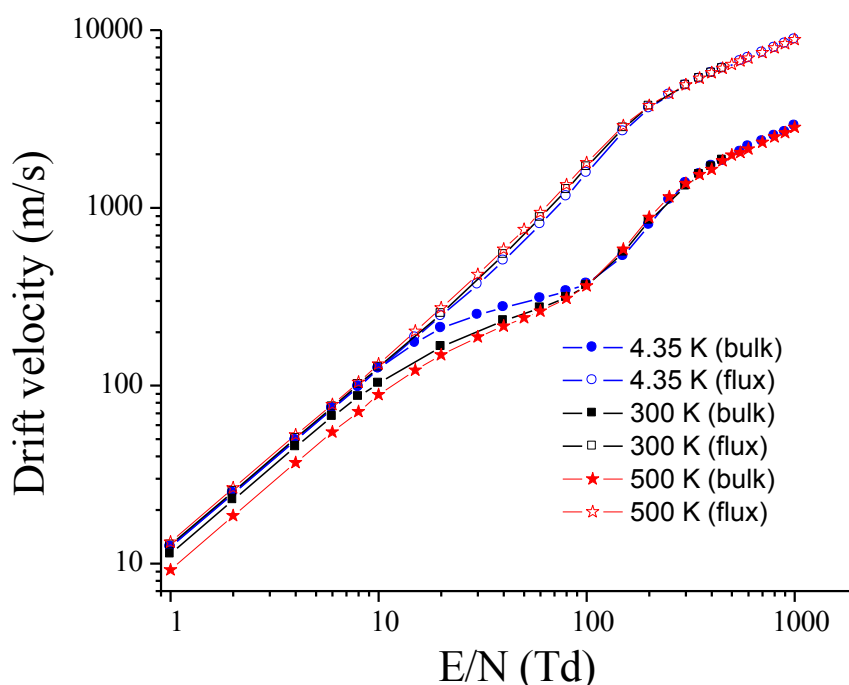
Fig. 1 Drift velocity for Ar$^+$ ions in CF$_4$ as a function of E/N.

In addition to presenting the data we show here effects of non-conservative collisions on ion transport. Due to non-conservative cross sections that are larger than the elastic scattering cross section differences between flux and bulk transport coefficients are quite large - comparable to the strongest cases observed for electrons, even positrons.

Data for swarm parameters for ions are needed for hybrid and fluid codes and the current focus on iquids or liquids in the mixtures with rare gases dictates the need to produce data compatible with these models.

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E-53

The interaction of $Co(CO)_3NO$ precursor with porphyrin-covered $TiO_2(110)$: Preparation of carbon-free cobalt nanoparticles by FEBIP

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The preparation of clean and morphologically controlled nanosized particles is a challenging task. One promising route to attack this goal is Focused Electron Beam Induced Processing (FEBIP) in which a highly focused electron beam is used to deposit the dissociation products of suitable precursor molecules [1]. Co nanoparticles are very important in many field of chemistry and physics. Deposition of Co allows the precise writing of thin ferromagnetic structures [2]. In this regard $Co(CO)_3NO$ is a suitable source of Co deposits with FEBIP.

We demonstrate in analogy to recent FEBIP experiments with $Fe(CO)_5$ on Ag(111), pre-covered with thin layers of organic molecules, namely 2H-Tetraphenylporphyrin (2HTPP), in UHV [3], that it is possible to fabricate carbon-free Co deposits on rutile $TiO_2(110)$ also pre-covered 2HTPP. Since $Co(CO)_3NO$ decomposes unselectively on the pristine $TiO_2(110)$ surface it is important to ensure that 2HTPP forms a closed layer which exhibits the autocatalytic decomposition of the precursor already at room temperature. The Co deposition is either realized via Electron Beam Induced Deposition (EBID), or Electron Beam Induced Surface Activation (EBISA). In EBISA, the 2HTPP layer is irradiated in the absence of the precursor, leading to active sites where catalytic decomposition occurs once the precursor is dosed onto the surface. All deposits show a district contrast in SEM between the central part and the periphery. AES reveals that the central part consist only of Co and minor parts of N and O. Furthermore, we pointed out that additional dosage of $Fe(CO)_5$ on this structures leads to its autocatalytic growth of pure bcc Fe. The AFM investigations provided information on the topography of the corresponding layered structures formed via catalytic processes.

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Ion mobility of the ground and metastable states of molecular ions

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Mobility of molecular ions, NH^+, NH_2^+, and NH_3^+, in cooled He gas has been measured by using a low temperature drift tube. In the arrival time spectra of NH^+ and NH_3^+, we have observed two peaks that might correspond to the ground and metastable excited states of molecular ions.

Ion mobility is very sensitive to the interaction potential between an ion and a buffer gas molecule. Therefore, it is able to distinguish the electronic states of the ions by means of ion mobility measurements because the interaction potential strongly depends on the electron state of the ion [1, 2]. We have already observed the separation of ground and metastable states of C^+, N^+, and O_2^+ ions that are produced in an electron-impact ion source with mobility measurements in He gas using a low temperature ion-injected drift tube mass spectrometer cooled by liquid nitrogen and liquid helium [3].

In this work, we have measured the mobility of NH^+, NH_2^+, and NH_3^+, which are produced by electron impact from NH_3 gas, in He gas at 77 and 4.3 K. At higher effective temperature, $T_{eff} > 20$ K ($E/N > 10$ Td at gas temperature of 4.3 K), each arrival time spectrum of NH_3^+ has only a single peak as usual. On the other hand, at lower effective temperature, $T_{eff} < 15$ K ($E/N < 7$ Td at 4.3 K), two peaks have observed in arrival time spectra. This result suggests that two peaks observed in the low electric fields correspond to the ground and metastable states of the NH_3^+ ions.

According to theoretical calculations [4], the NH_3^+ ion in the ground state is planar (D_{3h}). On the other hand, that in the metastable electronic state has a pyramid structure (C_{3v}). It is reported that the molecular axis of ions in the drift tube is not random by collisions with buffer gases but orients to the electric field direction [5, 6, 7]. We suppose that a planar molecular ion flights like a Frisbee in the drift tube as the result of the collisional alignment. Such alignment gives the smaller collisional cross section between ions and gases and the shorter arrival time. Therefore, the fast peak in the low electric filed will correspond to the ground state. On the other hand, the pyramid style ions have no alignment effect and larger cross sections than that of the planar molecular ions. Then the slower peak will be due to the metastable state.

In measurements of NH^+, we have observed two peaks in arrival spectra. We consider that two peaks correspond to the ground ($X\ ^2\Pi$) and metastable ($a\ ^4\Sigma^-$) states of NH^+ [8, 9].

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Swarm analysis of electron transport in biomolecules: Water and THF

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The determination of a comprehensive set of electron-biomolecule cross-sections is fundamental to understanding electron induced processes arising in plasma medicine and radiation damage modelling. Formulation of complete sets is generally based on a critical assessment of available experimental `beam' studies and theoretical calculations, and interpolations/extropolations. Issues of completeness and accuracy of cross-section sets arise and it is here that swarm experiments play a key role. Here, excess electrons under the action of an applied electric field are passed through a gas of biomolecules and measured currents are interpreted in terms of transport coefficients such as drift velocities, diffusion coefficients, and ionization/attachment rates. Through comparison of measured transport coefficients with those calculated from transport theory/ simulation, one can assess the ability of the cross-section set to accurately treat particle, momentum, and energy balance.

In this presentation we report on recent swarm measurements in the biomolecules of water and tetrahydrafuran (THF) using the pulsed-Townsend technique of the de Urquijo group. We present and assess the consistency of cross-section sets for water and THF through a comparison of calculated transport coefficients using a multi-term Boltzmann equation solution with the available experimental swarm measurements provides a discriminating test on consistency and accuracy of the cross-section. Cross-section degeneracy (i.e., different sets of cross-sections can produce the same field dependence of the transport coefficients) is an issue. Additional handles to assess the degeneracy, accuracy and completeness of the cross-section set can be through measurements in admixtures with well known cross-sections which can considerably modify the distribution function. To this end, results for water/He, water/Ar and THF/N_2 mixtures will be presented.

Electron induced ionization and fragmentation of the nucleobases

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Using computer-controlled data acquisition we have measured mass spectra of positive ions for electron impact on the five nucleobases, with electron energies up to 100 eV in 0.5 eV steps. An effusive beam of the nucleobase under study is generated using a resistively heated oven and is collimated using a skimmer. The molecular beam is crossed with a pulsed electron beam and positive ions are extracted into a reflectron time-of-flight mass spectrometer.

Ion yield curves for the fragment ions have been determined by fitting groups of peaks in the mass spectra with sequences of normalized Gaussians. Partial ionization cross sections have been obtained by normalizing the sum of the yield curves to the average of calculated total ionization cross sections. Appearance energies have been determined for most fragment ions. Results for thymine, cytosine and adenine have been published [1 - 3]. New results will be presented and will be compared with other fragmentation studies involving electron and photon impact, e.g. [4 - 6].

For a number of fragment ions of each of the nucleobases, the ion yields rise very rapidly just above threshold $\propto (E - E_0)^p$ with powers $p \geq 2$. We attribute this to several onsets very close to each other due to the presence of parallel fragmentation pathways with similar appearance energies. Second onset energies have been determined for a number of fragment ions, with energy differences between the first and second onsets of 2 eV and higher. These high energy differences may indicate that there are distinctly different fragmentation processes producing these fragments.

The appearance energies exclude some fragmentations proposed in the literature. For example, for thymine 83 u and 55 u have the same appearance energy, so loss of HNCO loss followed by CO loss does not occur near threshold. For cytosine 95 u has a 3.7 ± 1.0 eV higher appearance energy than 68 u, so NH_2 loss followed by HCN loss does not occur.

Several of the nucleobases exhibit successively higher appearance energies for successively smaller fragments in a group (e.g. 53-52-51 u, 40-39-38-37 u for thymine), which is consistent with successive loss of single H atoms.

In each of the nucleobases we encounter a few groups of two fragments with 1 u difference in mass, with ion yield curves with very similar shapes above around 30 - 40 eV (e.g. 118-119 u, 107-108 u, and 91-92 u for adenine). We attribute these constant yield ratios to H atom rearrangement (tautomerization) immediately preceding the fragmentation, but the presence of tautomers in the molecular beam may also contribute to this. Two groups of cytosine fragments (67-69 u and 41-44 u) also have ion yield curves with very similar shapes above 40 eV. This may be due to charge localization on an ion in the one or in the other group, or to a successive fragmentation of the 67-69 u ions to fragments of size 41-44 u, but the explanation of the similar shapes is not clear.

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Momentum imaging of dissociative electron attachment in biologically relevant molecules

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Since Pan et. al. [1] showed that dissociative electron attachment (DEA) is an important process which can lead to the creation of strand breaks in DNA, much effort has been put into investigations of this process. Most experimental work however only identifies fragmentation channels while studies of the dissociation angles or kinetic energy transfer to the fragments are scarce. Our experimental setup is designed to perform those tasks. Based on the design of Adaniya et. al. [2], a pulsed electron beam from a photo-emission source with an energy spread of 200 meV (FWHM) is crossed with a supersonic gas jet. The created anion is pushed into the spectrometer by a pulsed extraction voltage applied after 1 μs. The potentials of spectrometer and extraction electrode as well as the extraction delay can be set to compress the time of flight of different momenta. This operation mode allows to significantly improve the mass resolution while still recording the momentum projection in the detector plane. Due to the axial symmetry of the problem, the complete information about the momentum distribution can be reconstructed.

An analysis of the distribution of dissociation angles in DEA to ammonia leading to production of NH_2^- ions shows a broad peak around 110° up to 5.7 eV electron impact energy, in agreement with measurements by Ram et. al. [3] who investigated H^- production at the same resonance. At higher energies, we observe a shift of the peak towards higher angles and a second peak in the forward direction that has not been described before.

The kinetic energy release of the reaction has its maximum at 0.95 eV and a FWHM of 0.5 eV. This distribution is constant over the investigated energy range from 4.3 eV to 7.3 eV, showing that excess energy has to be stored in internal degrees of freedom, i.e. a vibrationally excited state of the fragment.

The improved mass resolution of the setup has been demonstrated using the dissociation of furan by attachment of electrons with energies around 6 eV. Here, production of $C_4H_3O^-$ (67 amu), C_4H^- (49amu), C_2HO^- (41 amu) and $C_3H_3^-$ (39 amu) can be observed [4]. Although the fragment with a mass of 39 amu is created with a significant amount of momentum, corresponding to a kinetic energy release up to 0.5 eV, it can be separated in time of flight from the fragment at 41 amu.
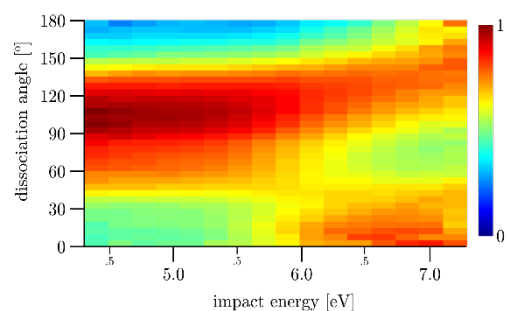
Figure 3: Distributions of fragment dissociation angles for the production of NH_2^- ions by electrons of different energy. Results have been normalized for each energy to compensate the varying total cross section.

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Electron and positron scattering from vibrationally excited H_2^+ and H_2

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The newly developed *ab initio* adiabatic-nuclei convergent close-coupling (CCC) method has been formulated in both the spherical [1, 2] and spheroidal coordinate systems for electron and single centre positron scattering. Our recent studies of positron scattering from vibrationally excited H_2 and electron scattering from vibrationally excited H_2^+ [1] indicate a large dependence on the initial vibrational state of the molecule. Results are presented over a broad energy range for elastic, vibrational excitation, electronic excitation, grand total and total ionisation cross sections and are converged in both the multichannel and partial-wave expansions.
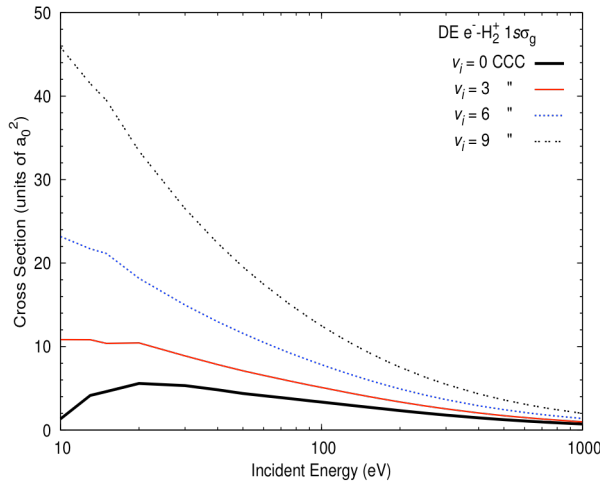
Figure 1. Dissociative excitation (DE) cross sections for electron scattering from H_2^+ in the vibrational state v_i.

Figure 2. The grand total cross section (GTCS) for positron scattering from the $v_i = 0$ and $v_i = 1$ vibrational states of H_2. Adiabatic-nuclei convergent close-coupling (CCC) results are compared with the mean internuclear distance $R_m = 1.448$ a_0 fixed-nuclei CCC calculations.

In Fig. 1 we present dissociative excitation (DE) cross sections for electron scattering from H_2^+ in the initial vibrational state v_i. The DE cross sections have a major dependence on v_i. For example at 20 eV the $v_i = 9$ DE cross section is around five times larger than the $v_i = 0$ state.

In Fig. 2 the grand total cross section (GTCS) is presented for positron scattering from H_2 in the initial vibrational state $v_i = 0$ and $v_i = 1$. The vibrational ground state mean internuclear distance $R_m = 1.448$ a_0 fixed-nuclei results are in excellent agreement with the adiabatic-nuclei $v_i = 0$ results. In the low-energy region the $v_i = 1$ results are approximately 20-25% larger than the $v_i = 0$ cross section.

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Electron ionization of Iron pentacarbonyl clusters

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The Iron pentacarbonyl FEBID precursor was studied in the past [1] using the crossed electron/molecular beams technique [2] built at the Comenius University in Bratislava (CEMBA). Interactions of low energy electrons with $Fe(CO)_5$ molecule were performed [1] to describe the processes of secondary electrons with the precursor in the volume close to surface during the deposition with FEBID. Except those processes running between low energy electron and isolated molecule of $Fe(CO)_5$ we have recently carried out new measurements on the electron ionization of iron pentacarbonyl clusters in argon gas. Experimental technique built at the Freie Universitaet in Berlin [3] (CLUSTER) was successfully moved and installed in Bratislava and used for the purpose of CELINA COST Action measurements. Similarly to the CEMBA experiment the CLUSTER experiment uses trochoidal electron monochromator and quadrupole mass analyzer to initiate the ionization reactions and detect the ionic products.

Except the molecular ion of $Fe(CO)_5$ the strong feature of sequential carbonyl losses was described with the CEMBA experiment [1], the more carbonyls were dissociated the higher ion yield of $Fe(CO)_n^+$ was obtained up to the final decomposition to Fe^+. The same processes were observed in the mass spectrum of $Fe(CO)_5$ clusters. Except the expected ions we have detected the adoption of one carbonyl to the molecular ion and its clusters, the ions with m/z which is exactly 28 amu above the m/z of molecular ion and its dimer, trimer… Contrary to the spectrum of isolated $Fe(CO)_5$ under electron impact, in the clusters there are no dissociations of C=O bond in the ligand(s).

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