



EIPAM06
Second Annual Meeting of
ESF Programme on Electron
Induced Processing at the
Molecular Level



Valletta, Malta
16 – 20 September 2006



Co-funded by
EU-ESF COST Action
P9 on Radiation
Damage



Programme

Saturday 16th September 2006

14.00 to 18.00 Registration

18.00 Committee Meeting

19.30 Committee Dinner.

Sunday 17th September 2006

Title

09.00	Opening of EIPAM06	
09.15 to 10.00	Low Energy Electron and Positron Interactions with Atoms and Molecules: Benchmark Measurements and Measurements with Bio-Molecules	Prof Steve Buckman
10.00 to 10.30	Formation and stability of anions upon free electron attachment to biomolecules in the gas phase and embedded in superfluid helium droplets	Prof Paul P Scheier
10.30 to 11.00	<i>Coffee</i>	
11.00 to 11.30	Electron scattering from hydrogenated micro- and nano-diamond: resonant, DOS and size effects	Prof Roger Azria
11.30 to 12.00	Modification of materials and surfaces by low-energy electrons	Prof Petra Swiderek Miss Eliza Burean
12.00 to 12.30	Low Energy Electron Transmission through Acetic Acid, Fluorobenzene, and Water	Dr Peter Cicman
12.30 to 14.00	<i>Lunch Break</i>	
14.00 to 14.45	Low-energy electron induced damage of hydrated DNA: The role of resonance scattering and diffraction	Prof Thomas Orlando
14.45 to 15.15	IR photon enhanced dissociative electron attachment to SF ₆ : dependence on photon, vibrational, and electron energy	Prof Hartmut Hotop
15.15 to 15.45	<i>Tea</i>	
15.45 to 16.00	The valence anions of pyrimidines in the DNA π -stack: how stable or unstable might they be?	Prof Janusz Rak

16.00 to 16.15	Feshbach-Fano R-matrix method: resonances in electron-H ₂ scattering	Dr Premysl Kolerenc
16.15 to 16.30	Dissociative electron attachment to water	Dr Juraj Fedor
16.30 to 16.45	Ultrafast Electron Transfer and Solvation Dynamics at the NH ₃ /Cu(111) Interface	Miss Julia Stähler
16.45 to 17.00	Intermolecular reactions in thin molecular films induced by low-energy electrons	Dr Imre Ipolyi
17.00 to 17.10	Quantemol-n Presentation	Camille Herreman
17.15	<i>Welcome Reception</i>	
18.30 to 20:00	Poster Session 1.	

Monday 18th September 2006

	<u>Title</u>	
09.00 to 09.45	Femtochemistry with feedback-optimized Laserpulses	Prof Gustave Gerber
09.45 to 10.15	Threshold Two-Photon Electron Spectroscopy From A Cu(100) Surface	Dr Jesus Tornero
10.15 to 10.45	<i>Coffee</i>	
10.45 to 11.15	Atom-Scale Electronic Processes	Prof Gerald Dujardin
11.15 to 11.45	Organic and Biological Ad-species on Solid Surfaces: Dynamics and Self-Assembly	Prof Roberto Otero
11.45 to 12.15	Scanning tunnelling spectroscopy on single molecules and molecular nanostructures	Dr Katarina Franke
12.15 to 13.15	<i>Lunch</i>	
13.15	<i>Coaches Leave for Harbour Cruise</i>	
14.00	Afternoon Grand Harbour Cruise	

Tuesday 19th September 2006

Title

09.00 to 09.45	Similarities and Differences between Electron and Positron scatterings from molecules	Prof Mineo Kimura
09.45 to 10.15	The big Chill : electron scattering from molecular gases at low and ultralow energies	Prof Franco Gianturco
10.15 to 10.45	<i>Coffee</i>	
10.45 to 11.15	Quantum theory of electron transfer at interfaces	Prof Peter Saalfrank
11.15 to 11.45	Simulating high-resolution scanning tunnelling microscopy: providing a detailed understanding of electronic processes	Prof Werner Hofer
11.45 to 12.15	Vibronic effects in electron transport through atomic and molecular systems	Prof Nicolas Lorente
12.15 to 12.45	Detachment of ionized clusters and graphene islands by ultrafast charging of graphite surface	Dr Andrey Kaplan
12.45 to 14.00	<i>Lunch Break</i>	
14.00 to 14.30	Transient negative ions of valine; formation and decay	Prof Oddur Ingolfsson
14.30 to 15.00	High resolution studies of low energy electron attachment to SF ₅ Cl: product anions and absolute cross sections	Dr Chris Mayhew
15.00 to 15.30	Electron Attachment to CS and HCCCN	Dr Tom Field
15.30 to 16.00	<i>Tea</i>	
16.00 to 16.30	Dissociative electron attachment to the bromo-chloro substituted hydrocarbons.	Dr Stefan Matejcik
16.30 to 17.00	Differential ionization of molecules by positrons impact	Dr Akos Kover
17.00 to 17.30	Photoionisation at atmospheric pressure of biomolecules: implication of the photoelectrons	Dr Alexandre Guiliani
17.30 to 17.45	Why positrons, unlike electrons, do not show Ramsauer-Townsend effect?	Dr Gregorz Karwasz
20:00	Poster Session 2	

Wednesday 20th September 2006

	<u>Title</u>	
09.00 to 09.45	Significance of Electron-Molecule Interactions in the Development of Materials for New Technologies	Prof Loucas Christophorou
09.45 to 10.15	Electron driven reactions in free and bound molecules	Prof Eugen Illenberger
10.15 to 10.45	<i>Coffee</i>	
10.45 to 11.15	Two topics in the calculations of electron molecule collisions	Prof Petr Carsky Prof Jiri Horacek
11.15 to 11.45	Elastic electron scattering by amino acids: glycine and alanine	Prof Bratislav Marinkovic
11.45 to 12.15	Stopping power of electrons in water from 10 to 10000 eV	Prof Gustavo Garcia
12.15 to 14.00	<i>Lunch Break</i>	
14.00 to 14.30	Low-energy elastic electron scattering and vibrational excitation in tetrahydrofuran	Prof Mariusz Zubek
14.30 to 15.00	Lowest energy excited states of small organic molecules induced by low energy electron impact	Prof Marie Hubin Franksin
15.00 to 15.15	Positron scattering off polyatomic molecules with the <i>ab initio</i> the R-matrix method	Dr Jan Franz
15.15 to 15.30	Correlation effects in electron scattering of F ₂ – R-matrix approach	Mr Michel Tarana
15.30 to 16.00	<i>Tea</i>	
17:00	<i>Coaches Leave for Mdina</i>	
19:00	<i>Conference Dinner Mdina</i>	

Thursday 21st September 2006

Departure

Elastic electron scattering by amino acids: glycine and alanine

B. P. Marinković¹, F. Blanco², V. Pejčev¹, D.M. Filipović¹, G. García³, D.Šević¹, D.Pavlović¹ and N. J. Mason⁴

¹Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia

²Departamento de Física Atómica Molecular y Nuclear, Facultad de Ciencias Físicas, Universidad Complutense, Avda. Complutense s/n, 28040 Madrid, Spain

³Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 121, 28006 Madrid, Spain

⁴Department of Physics and Astronomy, Open University, Milton Keynes MK7 6AA, U.K.

Current studies of electron interactions with amino acids have been motivated by the need of deeper understanding of the fundamental processes at the molecular level connected to the biologically relevant molecular systems. Also, there are recent results that indicate that both UV and electron radiation of ice mixtures of organic molecules can lead to the formation of the simplest amino acids such are glycine and alanine [1].

We have recorded the first elastic electron differential cross sections for glycine and alanine at the incident energies of 20, 40, 60 and 80 eV over the angular range of 20° to 150°. We have supported these measurements with calculations using a corrected form of the independent – atom method known as a SCAR (Screen Corrected Additive Rule). The level of agreement between experiment and calculations is excellent except at low scattering angles where the theoretical method has substational limitations.

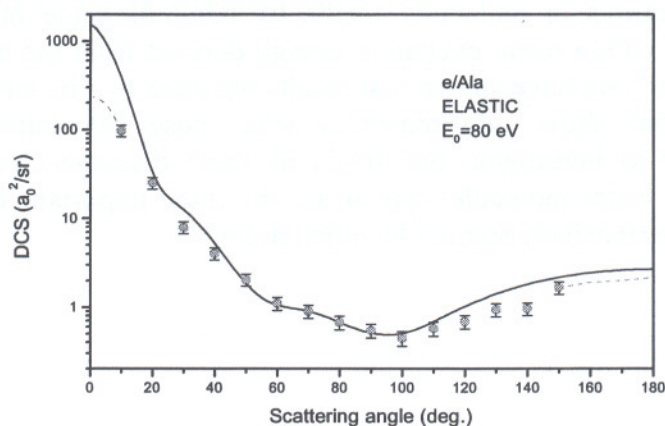


Figure 1. Differential cross sections for elastic electron scattering by alanine at 80 eV impact energy

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[1] G. M. Muños-Caro, U. J. Meierhenrich, W. A. Schutte, B. Barbier, A. Arcones Segovia, H. Rosenbauer, W. H.-P. Thiemann, A. Brack and J. M. Greenberg, *Nature* **416** (6879) 403 (2002).

Poster Abstracts

Vibrational excitation of tetrahydrofuran by low energy electron impact

M. Zubek^{1*}, A.R. Milosavljević², M. Dampc¹, I. Linert¹ and B.P. Marinković²

¹Department of Physics of Electronic Phenomena, Gdańsk University of Technology,
80-952 Gdańsk, Poland

²Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia
*mazub@mif.pg.gda.pl

Vibrational excitation of tetrahydrofuran (THF), C₄H₈O has been studied at the incident electron energies of 7 and 10 eV which correspond to the position of a previously observed broad resonance [1]. The measurements have been carried out in a wide scattering angle range, 20°-180° using a recently constructed double hemispherical electron spectrometer [2] equipped with the magnetic angle changer [3] to detect backscattering of electrons.

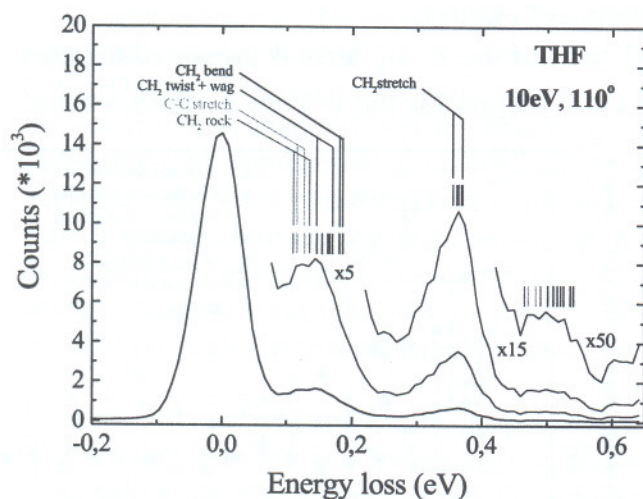


Fig. 1 Energy loss spectrum obtained in THF at an incident electron energy of 10 eV and a scattering angle of 110°.

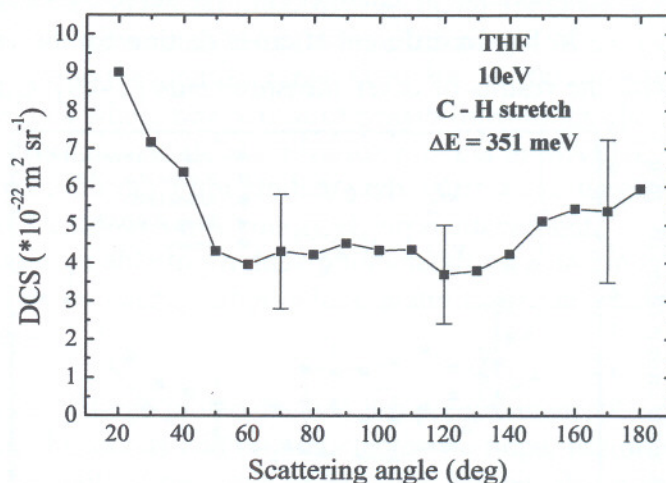


Fig. 2 Differential cross section for excitation of a group of C-H stretch vibrational modes at 351 meV energy loss

In the energy loss spectra (Fig. 1) two prominent peaks have been observed at energy losses of 141 and 351 meV respectively. The peaks are 20 to 30 meV wider than the elastic scattering peak indicating excitation of groups of vibrational modes of similar types having close frequencies. Excitation energies of the fundamental vibrational modes [1] that are most likely responsible for the energy loss peaks are indicated in Fig. 1. Combination modes around 500 meV involving the C-H stretch modes and the 141 meV bands are also visible in the energy loss spectra. These results are similar to that obtained previously for cyclic alkanes (cyclopentane) [4].

Fig. 2 presents the differential cross section obtained for the excitation of vibrational modes at 351 meV energy loss which correspond to a group of α - and β -CH₂ stretch modes. This cross section has been normalized against the absolute elastic cross section measured using relative flow technique.

- [1] Lepage M. *et al* 1998 J. Chem. Phys. **109** 5980.
- [2] Linert I. and Zubek M. 2006 J. Phys. B, submitted.
- [3] Linert I. *et al* 2004 J. Elect. Spect. Rel. Phenom. **134** 1.
- [4] Allan M. and Andric L. 1996 J. Chem. Phys. **105** 3559.

Resonances in the integral cross sections for scattering of 1.5 – 12 eV electrons from condensed adenine

Radmila Panajotovic, Marc Michaud, and Léon Sanche

Groupe en sciences des radiations, Faculté de médecine, Université de Sherbrooke, 3001, 12^e Av. Nord, Sherbrooke (Québec), Canada, J1H 5N4
e-mail : radmila.panajotovic@USherbrooke.ca

One of the major research areas in biological physics is focused on the nanoscopic aspect of radiobiological damage, i.e. the effects of radiation which produces charged particles in live tissue such as secondary electrons. The results from measurements on short DNA strands impinged on by 1-30 eV electrons indicate that the damage they induce is due to the chemical nature of the nucleic bases and/or their sequence [1].

In the cell, besides from being constituents of the DNA, nucleic acid bases are important elements of its complex metabolic network. Adenine is a part of the essential energy supply molecule, ATP, whose intercellular concentration reaches the highest abundance of all nucleotides in the cell. In DNA and RNA, adenine is supposed to play a role in the electron transport, which couples to the vibrational motion of the molecular wires formed by hydrogen-bonded and stacked nucleic bases. Furthermore, stable negative ion formation on the DNA bases and base pairs can also affect the electron transport along the helix.

As in previous studies on thymine and pyrimidine [2], our aim was to investigate a possibility of resonance formation (temporary negative ions) in adenine for electrons of incident energies below 12 eV. Measurements of the vibrational and electronic excitation were performed on a high resolution electron energy-loss (EEL) spectrometer [2], housed in a cryogenically pumped ultrahigh- vacuum chamber at a base pressure of $\sim 5 \times 10^{-11}$ Torr. EEL measurements were made on a sub-monolayer up to a monolayer film of adenine deposited on a six-layer spacer of argon condensed on a Pt substrate held at a temperature of 18 K. An incident electron beam of energy ranging from 1.5 to 12 eV was focused on the film at an angle of 15 deg with respect to the normal to the surface. The number of electrons backscattered from the film was recorded at the fixed analyzer angle of 45 deg.

The integral cross sections (over the half-space angle) for excitation of the normal vibrational modes of the ground electronic state and electronically excited states are calculated from reflectivity EEL spectra following the procedure applied earlier on thymine and pyrimidine [2]. Most of cross sections for vibrational excitation are of the order of 10^{-17} cm², the largest being the out-of-plane wagging of the amino-group and the six-member ring deformations. A wide resonance feature appears at incident electron energies of 3-5 eV, while at 7-8 eV a weak shoulder is present in the cross sections for combined ring deformations and bending of hydrogen atoms.

[1] L. Sanche, *Mass Spectr. Rev.* 21 (2002) 349-369

[2] P. L. Levesque, M. Michaud, and L. Sanche, *Nucl. Instr. Meth. Phys. Res. B* 208 (2003) 225-230 ; P. L. Levesque, M. Michaud, W. Cho, and L. Sanche, *J. Chem. Phys.* 122 (2005) 224704

Vibrational excitation of condensed thymidine by low-energy electrons

Radmila Panajotovic, Marc Michaud and Léon Sanche

Groupe en sciences des radiations, Faculté de médecine, Université de Sherbrooke, 3001, 12^e Av.
Nord, Sherbrooke (Québec), Canada, J1H 5N4
e-mail : radmila.panajotovic@USherbrooke.ca

Investigation of the vibrational excitation of nucleosides leading to dissociation through formation of temporary negative ions aims at understanding the correlation of nucleic base-sugar moiety conformational coupling and its consequences on the bond cleavage in DNA. The conformation of the 2'-deoxyribose moiety with respect to the base is expected to influence which species are formed upon exposure of nucleosides to ionizing radiation [1]. Extensive results from measurements on short DNA strands impinged on by 1-30 eV electrons indicate that the damage they induce is due to the chemical nature of the nucleic bases and/or their sequence [2].

Thymidine is one of the most important nucleosides of DNA and an important component of antiviral compounds [3]. In the condensed phase, thymidine's 2'-deoxyribose ring is in the pentose sugar ring form, which is a true conformation of this nucleoside in DNA. As in previous studies on thymine and pyrimidine [4], our aim was to investigate a possibility of resonance formation (temporary negative ions) in adenine for electrons of incident energies below 12 eV. Measurements of the vibrational excitation of thymidine were performed on a high resolution electron energy-loss (EEL) spectrometer [4], housed in a cryogenically pumped ultrahigh- vacuum chamber at a base pressure of $\sim 5 \times 10^{-11}$ Torr. EEL measurements were made on a monolayer film of thymidine deposited on a six-layer spacer of argon condensed on a Pt substrate held at a temperature of 18 K. An incident electron beam of energy ranging from 1 to 5 eV was focused on the film at an angle of 15 deg with respect to the normal to the surface. The number of electrons backscattered from the film was recorded at the fixed analyzer angle of 45 deg.

Electron energy-loss spectra of thymidine for electrons of energy between 1 and 5 eV will be presented at the conference. Possible resonance enhancement of vibrational motion of thymidine and the energy shift with respect to the resonance features found in the previous study on thymine, as well as how they compare with the results from dissociative ionization of thymidine [5] will also be discussed.

[1] C. H. Görbitz, W. H. Nelson, and E. Sagstuen, *Acta Cryst. E* 61 (2005) o1207-o1209

[2] L. Sanche, *Mass Spectr. Rev.* 21 (2002) 349-369

[3] J. C. Martin, *Nucleotide Analogues as Antiviral Agents; ACS Symp. Ser.*, Vol. 401 (1989) American Chemical Society, Washington, DC

[4] P. L. Levesque, M. Michaud, and L. Sanche, *Nucl. Instr. Meth. Phys. Res. B* 208 (2003) 225-230 ; P. L. Levesque, M. Michaud, W. Cho, and L. Sanche, *J. Chem. Phys.* 122 (2005) 224704

[5] S. Ptasińska, P. Candori, S. Denifl, S. Yoon, V. Grill, P. Scheier, T. D. Märk, *Chem. Phys. Lett.* 409 (2005) 270-276