RADIATION DAMAGE IN BIOMOLECULAR SYSTEMS

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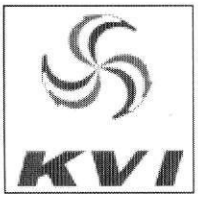

RADAM'06 Local Committee

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Marjorie Imhoff

RADAM'06 Programme

Tuesday, 6 June 2006

17:00 - Registration

Wednesday , 7 June 2006

8:45 Welcome Thomas Schlathölter/Groningen

"Electrons and biomolecular interactions"

Chair: Nigel Mason, Milton Keynes, United Kingdom

9:00 - 9:30 Colin Latimer, Belfast, United Kingdom
Irradiation of water and DNA with soft x-rays

9:30 - 10:00 Janusz Rak, Gdansk, Poland
Electronically Stable Valence Anions of Pyrimidine Bases: Possible Pivotal Species Responsible for the Formation of Single-Strand Breaks in DNA Induced by Excess Electrons

10:00 - 10:30 Anne Lafosse, Orsay, France
Chemical modifications following low-energy electron irradiation of condensed molecular films: the case of carboxylic acids

10:30-11:00 Coffee Break

"Ions and biomolecular interactions"

Chair: Reinhard Morgenstern, Groningen, Netherlands

11:00 – 11:35 Marjorie Imhoff, Groningen, Netherlands
Low Energy (1-500eV) Ion-Biomolecule Interactions in the Condensed Phase

11:35– 12:10 Bernadette Farizon, Lyon, France
Proton impact on biomolecules in the Bragg peak velocity range

12:10 – 12:45 Nico Stolterfoht, Gainesville, Florida
Electron capture and fragmentation in collisions of multi-charged ions with water molecules

12:45 Lunch at the "Nieuwe Academie"

"Radiation in physiological environments"

Chair: Kevin McGuigan, Dublin, Ireland

14:00 - 14:45 Michèle Martin, Evry, France
Plenary lecture:
"Radiation and gene regulation in human skin cells"

14:30 – 15:05 Brenda H. Laster, Ben Gurion University Israel
The Therapeutic Effect of Photon Activation Therapy by a Platinum Porphyrin and ^{103}Pd Brachytherapy Seed Irradiation for Photon Activation Therapy

15:05 – 15:40 Fiona M. Lyng, Dublin, Ireland
Radiation induced bystander effects: Signalling pathways induced in cells exposed to medium from irradiated cells

15:45 – 16:15 Coffee Break

"Theoretical developments for radiation damage"

Chair: Marie-Christine Bacchus, Lyon, France

16:15 – 16:50: Andrzej Sobolewski, Warsaw, Poland
Theoretical Studies of the Mechanisms of Photostability of Selected Building Blocks of Life

16:50 – 17:25 Chantal Daniel, Strasbourg, France
A DFT and TD-DFT theoretical study of Ru(II) polypyridyl complexes used as intercalators in DNA

17:25 – 18:00 Andrey V. Solov'yov, Frankfurt, Germany
Structure and Dynamics of Polypeptide chains

Time for Dinner

20:00 – … Poster session

Thursday , 8 June 2006

"Track structure in cells"

Chair: Michal Waligórski, Krakow, Poland

8:45 – 9:20 Pavel Kundrat, Prague, Czech Republic
Cell killing effects of proton and light ion tracks: Probabilistic modelling

9:20-9:55 José Manuel Pérez, Madrid, Spain
Simulation of low energy electron tracks in media of radiological interest

9:55-10:30 Werner Friedland, Neuherberg, Germany
Biophysical Simulation of Radiation Damage in Cells: Influence of Chromosomal Structure

10:30-11:00 Coffee Break

Chair: Sandrine Lacombe, Orsay, France

11:00-11:10 Kevin McGuigan, Dublin, Ireland
Presentation: RADAM'07 in Dublin/Ireland.

11:10-11:45 Rob Coppes, Groningen, Netherlands
Physiological Radiation effects; from membrane damage to DNA signaling

11:45 12:20 Leticia Gonzalez, Berlin, Germany
Quantum-mechanical modelling of mutations in DNA base pairs

12:20 12:35 Elena Zaharieva, Sofia, Bulgaria
Bystander effect in gamma irradiated peripheral blood

12:45 Lunch at the "Nieuwe Academie"

"Electrons and biomolecular interactions"

Chair: Ronnie Hoekstra, Groningen, Netherlands

14:00 - 14:35 Elspeth Garman, Oxford, United Kingdom
Radiation Damage in Cryo-cooled Protein Crystals

14:35 – 15:10 Yann Gauduel, Palaiseau, France
Radiation Induced Ultrafast Electron Attachment on Disulfide Biomolecule: the Prethermal Regime

15:10 – 15:30 Sandrine Lacombe, Orsay, France
Ice Radiolysis: Application to Radiobiology

15:30 – 16:00 Coffee Break

"Ions and biomolecular interactions"

Chair: Melvyn Folkard, Northwood, United Kingdom

16:00 – 16:30 Claude Le Sech, Orsay, France
Monochromatic X-rays and fast atomic ions irradiation of DNA loaded with platinum containing molecules

16:30 – 17:00 Steen Brøndsted Nielsen, Aarhus, Denmark
Electron capture dissociation of multiply charged peptides

17:00 – 17:30 Bruno Manil, Caen, France
Pure and Mixed Charged Clusters of Nucleobases

17:30 – 18:00 Arnaud Le Padellec, Toulouse, France
Electron spectroscopy in H^+ to dry DNA, RNA collisions in the 25 – 100 keV energy range

18:30 Guided tour through Groningen

20:00 Conference Dinner at the "De Apedans"

Friday, 9 June 2006

"Radiation in physiological environments"

Chair: Rita Plukiene, Vilnius, Lithuania

8:45 -9:20 Kevin G. McGuigan, Dublin, Ireland
Solar UVA Inactivation of Waterborne Pathogens for Use in the Aftermath of War, Famine or Disasters: Identifying the Limits.

9:20-9:55 Krzysztof Bobrowski, Warszawa, Poland
Stabilization Of Sulfide Radical Cations Through Complexation With The Peptide Bond.

9:55-10:30 Dimitra Markovitsi, Saclay, France
Collective Behaviour Of Excited States And Energy Transfer In DNA Double Helices

10:30-11:00 Coffee Break

"Theoretical developments for radiation damage "

Chair: Jack Sabin, Gainesville, Florida

10:45 – 11:35 Luis Serrano Andrés, València, Spain
Tutorial lecture:
Quantum Chemistry and Biological Systems: Theoretical Studies on Photobiology

11:35 – 12:10 Remigio C. Trujillo, Gainesville, Florida
Fragmentation of molecules by collisions of swift heavy ions: A theoretical and experimental study

12:10 – 12:45 Denis Duflot, Lille, France
Ab initio study of core excited molecules

12:45 Lunch at the "Nieuwe Academie"

"Track structure in cells"

Chair: Werner Friedland, Neuherberg, Germany

14:00 - 14:35 Michal Waligórski, Krakow, Poland
What can track structure modelling tell us about about radiation damage in cells?

14:35 – 15:10 Maria Grazia Pia, Genova, Italy
Geant4 capabilities for microdosimetry simulation

15:10 – 15:45 Aliaksandr Bantsar, Ottwock, Poland
Nanodosimetry of low energy electrons

15:45 – 16:00 Lukasz Czopyk, Krakow, Poland
The new analytical model for calculation of microdosimetric distributions for heavy ions

16:00 – 16:30 Coffee Break

16:30 – 18:30 Posters and Refreshments

19:00 - … Management Committee Meeting/Dinner

Saturday, 10 June 2006

departure

Posters

1. Fresia Alvarado, Sadia Bari, Ronnie Hoekstra, Thomas Schlathölter
   Ion-Induced molecular fragmentation of isolated deoxyribose molecules
2. Inge Hald Andersen, Jens Ulrik Andersen, Anne I.S. Holm, Preben Hvelplund, Steen Brøndsted Nielsen, Jean-Christophe Poully, Esben S. Worm
   Statistical vs. non-statistical dissociation of dinucleotide cations after photoexcitation in a storage ring
3. Baccarelli, M. Campetella, F.A. Gianturco, A. Grandi, R.R. Lucchese and N. Sanna
   Resonant electron capture by Glycine Zwitterion : bond-breaking routes and the possible effects on the pH of the medium
4. M.C. Bacchus-Montabonel, M. Łabuda, Y.S. Tergiman, J.E. Sienkiewicz
   Ion-biomolecule interaction : charge transfer processes induced by collision of C^{q+} ions with uracil
5. W. Y. Baek and B. Grosswendt
   Energy Loss Spectra of Electrons in TriEthylamine in the energy range 20 ev-1.0 kev
6. S. Bari, F. Alvarado, R. Hoekstra, T. Schlathölter, V. Bernigaud, B. Manil, J. Rangama, B. Huber
   Fragmentation of adenine and its clusters by atomic particles
7. V. Bernigaud, B. Manil, O. Kamalou, J. Lenoir, J. Rangama and B. A. Huber, F. Alvarado, S. Bari, A. Lecointre and T. Schlathölter
   Formation of charged clusters of nucleobases
8. Lluís Blancafort
   Excited states of stacked nucleobase dimers studied with CASSCF and CAS-PT2
9. L.Chen, R.Brédy, J.Bernard, S.Martin, M.C.Buchet-Poulizac,
   Ion induced fragmentation of biomolecules
10. D. Duflot, S. Zeggari, J.-P. Flament
    ***Ab initio* study of core excited cyclopropane**
11. Melvyn Folkard, Kirk D Atkinson, Kevin M Prise, Giselle Flaccavento, Alan G Michette, Borivoj Vojnovic
    A Variable-Energy Soft X-Ray Microbeam for use as a sub-cellular probe
12. F. Francerics, A Le Padellec and P Moretto-Capelle
    Delayed fragmentation of doubly charged adenine observed in 100 keV proton collisions
13. Muñoz, J. M.Pérez, J. C. Oller, F. Blanco, M. Vinodkumar, P Limão-Vieira and G. García
    Inelastic scattering and stopping power of electrons in H2 and H2O
14. Monika Gołębiowska and Janusz Rak
    Influence of DNA Sequence on the Electron Affinity of Cytosine
15. J. D. Gorfinkiel
    R-matrix studies of electron collisions with the water dimmer
16. Grandi, I. Baccarelli, M. Campetella, F.A. Gianturco, R.R. Lucchese and N. Sanna
    Electron-molecule scattering calculations for systems of biological interest

17. Anne I.S. Holm, Tapas Chakraborty, Søren Vrønning Hoffmann, Steen Brøndsted Nielsen, Jesper Wengel, and Esben S. Worm
Synchrotron radiation circular dichroism on DNA segments: Unraveling new information in the vacuum UV region

18. C.A. Hunniford, D.J. Timson and R.W. McCullough
Conformational changes to plasmid DNA induced by low energy carbon ions

19. Z. Juhász, R. Ricsóka, N. Stolterfoht, B. Sullik
Fragmentation of H_2O and CH_4 molecules following 800 keV He^+ impact

20. Magdalena Maciejewska and Jerzy L. Gebicki
An attempt to perform the hydroperoxide assay with ferric-xylenol orange c complex in reverse micellar system

21. Christel M. Marian
The Guanine Tautomer Puzzle: Assignment of the UV Spectra

22. R. Milosavljevic, D. Ševic and B. P. Marinkovic
Electron energy loss by tetrahydrofurfuryl alcohol

23. D. Markovitsi, S. Marguet, Laboratoire Francis Perrin
Time-Resolved Study of Thymine Dimer Formation

24. K.G. McGuigan, S.C. Kehoe, W. Heaselgrave, N. Patel, S. Kilvington, B.P. Meyer, S. Ramalingham, and E.A. Meyer
Solar UV inactivates Polio virus and cysts of the protozoan pathogen *Giardia muris* in drinking water – a laboratory study using simulated sunlight.

25. J. R. Sabin, S.S.P. Sauer, J. Oddershede
Directional Dependence of the Mean Excitation Energy and Spectral Moments of the Dipole Oscillator Strength of Glycine and its Zwitterion

26. M. Śmiałek, P. Cahillane, K. M. Prise, M. Folkard, N. Mason
Low energy radiation damage to DNA

27. V. Štísová, S. Goffinont, M. Spotheim-Maurizot, M. Davídková
Radiation damage to specific complex of estrogen response element DNA with estrogen receptor protein

28. B. Sulik, K. T_kési, T. Ricsóka, Z. Berényi Gy. Víkor, Sz. Nagy, and D. Berényi
Fast electrons from accelerating multiple electron scattering by ion impact: Contribution to radiation damages

29. Marian Wolszczak
Electron Transfer in DNA Solution

30. E. S. Worm, J.U. Andersen, T. Chakraborty, A.I.S. Holm, P. Hvelplund, S. Brøndsted Nielsen, J.-C. Poully, S. Ptasinska, A.V. Streletskii, E. Williams
Electron capture induced dissociation of peptide cations

31. F. Zappa, S. Denifl, S. Ptasińska, I. Mähr, M. Beikircher, P. Scheier, T. D. Märk
Hidden resonances in Dissociative Electron Attachment to Thymine?

Electron energy loss by tetrahydrofurfuryl alcohol

A. R. Milosavljević, D. Šević and B. P. Marinković

Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia

We report preliminary results on experimental investigation of inelastic electron interaction with gaseous tetrahydrofurfuryl alcohol (THFA). The THFA can be considered as an analogue to DNA sugar deoxyribose. Therefore, the investigation of low (medium) electron interaction with THFA is of interest in radiation damage research [1-4]. According to our knowledge, the electron-THFA energy loss spectra have not been reported.

The present experiment has been performed using a cross-beam arrangement, with an electron gun (without a monochromator), a double cylindrical mirror energy analyzer (fitted with cylindrical electrostatic zoom lenses), and a single channel electron multiplier as a detector. The molecular beam has been obtained using a stainless still needle connected to a glass container heated to a temperature of about 70 ^{o}C. The electron gun can be rotated around the gas needle (angular resolution about $\pm 2^{o}$). The anhydrous THFA was purchased from "Merck KGaA" with a declared purity of >98% and was used after several cycles of freeze-thaw under vacuum. The energy resolution was about 0.5 eV. An energy resolution was about 0.5 eV. The spectra have been obtained for different incident electron energies (E_0) from 20 eV to 100 eV and at different scattering angles from 10^{o} to 30^{o}. An example for E_0 = 40 eV is presented in Figure 1.

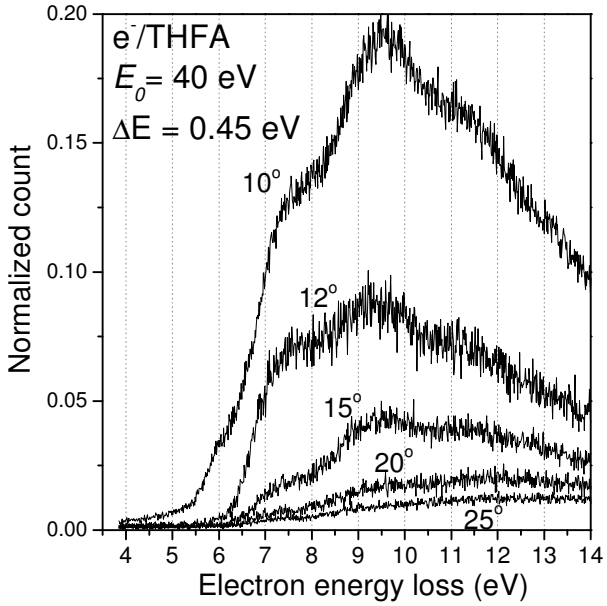

Figure 1. Electron energy loss spectra for THFA.

Generally, the spectra show broad peaks, the positions of which are similar to those obtained for tetrahydrofuran molecule and can be fitted to Rydberg series. Furthermore, the obtained electron energy loss spectra are in a very good agreement with the most recent, still unpublished, VUV absorption data [5].

References:

[1] D. Antic, L. Parenteau, M. Lepage, L. Sanche, *J. Phys. Chem. B* 103, 6611 (1999)
[2] D. Antic, L. Parenteau, L. Sanche, *J. Phys. Chem. B* 104, 4711 (2000)
[3] P. Možejko, L. Sanche, *Radiat. Phys. Chem.* 73, 77 (2005)
[4] A. R. Milosavljević, F. Blanco, D. Šević, G. Garcia and B. P. Marinković, *Eur. Phys. J. D* (*in press*)
[5] M.-J. Hubin-Franskin (*private communication*)