RADAM Conference 2007

Radiation Damage in Biomolecules Conference

19th – 22nd June 2007

The Royal College of Surgeons in Ireland

The Final Conference within COST Action P9
supported by the European Science Foundation

RADAM
COST P9

RADAM07 Programme June 19th-22nd, 2007

Registration begins at 8.30am each morning in Front Hall.
Conference Venue is the Albert Theatre unless otherwise indicated.
(CH) = College Hall, (BR) = Board Room, Video-Conference Room

Tuesday 19th June ***Early Researcher Tutorial Day***	Wednesday June 20th **RADAM'07 Day 1**	Thursday June 21st **RADAM'07 Day 2**	Friday June 22nd **RADAM'07 Day 3**
09:00 WG3 Tutorial	**09.00 WG3-A** Radiation in physiological environments	**09.00 WG5-A** Track structure in cells	**08.30 WG4-B** Theoretical developments for radiation damage
10:00 WG5 Tutorial	***10.30*** *Tea/Coffee (CH)*	***10.30*** *Tea/Coffee*	***10.00*** *Tea/Coffee*
11:00 *Tea/Coffee*	**11.00 WG1-A** Electron and biomolecular interactions	**11.00 WG1-B** Electron and biomolecular interactions	**10.30 WG5-B** Track structure in cells
11:30 WG2 Tutorial	***12.30*** *Lunch (CH)*	***12.30*** *Lunch*	**12.00 Conference Tour** *(Packed Lunch Provided)* 1. Walking Tour of Dublin City Centre 2. Bus Tour to Brú na Bóinne Neolithic Site and Interpretive Centre
12:30 *Lunch*	**13.30 WG2-A** Ions and biomolecular interactions	**13.30 WG2-B** Ions and biomolecular interactions	
14:00 WG1 Tutorial	**15.00** *Tea/Coffee (CH)*	**15.00** *Tea/Coffee*	
15:00 *Tea/Coffee*	**15.30 WG4-A** Theoretical developments for radiation damage	**15.30 WG3-B** Radiation in physiological environments	
15:30 WG4 Tutorial	**17.00** *Break*	**17.00** *Break*	
16:30 Summary	**20.00** Poster Session + Reception- *(CH + BR)*	**18.00 Management Committee Meeting (VR)** **20.00 Management Committee Dinner (BR)**	**19.30** Conference Dinner *(CH + BR)*

RADAM 07 Tutorial Day Programme

Tuesday June 19th

Early Researcher Tutorial Workshop

Venue: Albert Theatre

Coordinator: Jimena Gorfinkiel, Open University, UK.
Isabella Baccarelli, CASPUR, IT.

08.30 – 09.00	***REGISTRATION.***
09.00 – 09.10	**Introduction (J. Gorfinkiel)**
09.10 – 10.00	**<u>Tutorial 1</u>: Working Group 3 - Radiation in physiological environments.** Adrian Meade, Dublin Institute of Technology: *Radiation Damage in Biological Systemsd*
10.00 – 11.00	**<u>Tutorial 2</u>: Working Group 5 - Track structure in cells.** Andreas Hauptner, Munich: *Damage structure along ion tracks in cell nuclei*
11.00 – 11.30	*Tea/Coffee*
11.30 – 12.30	**<u>Tutorial 3</u>: Working Group 2 - Ions and biomolecular interactions.**
11.30-12.00	Experiments 1: Sam Eden, Lyon: *Ion sources and collisions with isolated Biomolecules*
12.00-12.30	Experiments 2: Adam Hunniford, Belfast: *Ion irradiation of large biomolecules and clusters*
12.30 – 14.00	*Lunch*
14.00 – 15.30	**<u>Tutorial 4</u>: Working Group 1 - Electron and biomolecular interactions.**
14.00-14.30	Theory: Isabella Baccarelli, Rome: *Electron-driven molecular processes induced in biological stystems by ionizing sources*
14.30-15.00	Experiments: Stephan. Denifl, Innsbruck: *Inelastic electron interactions with biomolecules: from gas phase to complex systems*
15.00 – 15.30	*Tea/Coffee*
15.30 – 16.30	**<u>Tutorial 5</u>: Working Group 4 - Theoretical developments for radiation damage.**
15.30-16.10	Ines Corral Perez, Berlin: *Quantum chemical and dynamical tools for solving photochemical problems.*
16.30 -	***SUMMARY***

Wednesday June 20th

08.30 – 09.00 ***REGISTRATION.***
Venue: Front Hall

09.00 – 10.30 WG3-A: Radiation in physiological environments
Venue: Albert Theatre
Chair: Nigel Mason, Open University, UK

09.00 – 09.40 Ron Chesser, Texas Tech University, USA.
Mechanisms of Adaptive Radiation Responses in Mammals at Chernobyl

09.40 – 10.05 Neil O'Hare, St James Hospital, Dublin, IRELAND
Risks & potential damage from Ultraviolet (UV) Radiation used for Phototherapy

10.05 – 10.30 Melvyn Folkard, Grey Cancer Institute, UK
The use of X-ray and particle microbeam techniques for investigating DNA damage in cells

10.30 – 11.00 ***Tea/Coffee***

11.00 – 12.30 WG1-A: Electron and biomolecular interactions.
Venue: Albert Theatre
Chair: Ron Chesser, Texas Tech University, USA

11.00 – 11.30 Kevin Prince, Elletra, ITALY
Synchrotron radiation studies of biomolecules

11.30 – 12.00 Dr.Peter Papp, Comenius University, BRATISLAVA
Theoretical calculations of parameters characterising electron impact with biomolecules.

12.00 – 12.30 Yann-A. Gauduel, Groupe de Femtochimie Bioradicalaire, Laboratoire d'Optique Appliquée, CNRS, FRANCE
Prethermal radiation events in aqueous environments: the teneous borderline between direct and indirect molecular damages

12.30 – 13.30 ***Lunch***

13.30 – 15.00 WG2-A: Ions and biomolecular interactions.
Venue: Albert Theatre
Chair: Paulo Limao-Vieira, New University of Lisbon, Portugal

13.30 – 14.10 Michaels Huels, University of Sherbrooke, CANADA
Hyperthermal Ions Damage to DNA Components

14.10 – 14.35 Maria Elisabetta Palumbo, Catania Astrophysical Observatory, ITALY
Ion processing of astrophysical ices

14.35 – 15.00 Fresia Alvarado, University of Groningen, NETHERLANDS
Energetics of ion induced fragmentation of DNA building blocks

15.00 – 15.30 ***Tea/Coffee***

15.30 – 17.00 WG4-A: Theoretical developments for radiation damage.
Venue: Albert Theatre
Chair: Herwig Paretzke, GSF-Institut für Strahlenschutz NEUHERBERG Germany

15.30 – 16.00 Adalgisa Sinicropi, University of Siena, ITALY
Recent applications of the QM/MM method in photochemistry and photobiology

16.00 – 16.25 Lluis Blancafort, Institut de Química
Computational, Girona, SPAIN Photochemistry and photophysics of DNA nucleobases

16.25 – 16.45 Jimena Gorfinkiel, The Open University, Milton Keynes, GB
Theoretical studies of electron-molecule collisions

16.45 – 17.05 Ágnes Vibók, Department of Theoretical Physics, Debrecen, HUNGARY
Renner-Teller/Jahn Teller intersections along the collinear axes of polyatomic molecules

17.00 – 20.00 ***Break***

20.00 – 22.00 **POSTER SESSION AND WELCOME RECEPTION**
Venue: College Hall and Board Room.

Thursday June 21st

Venue: Albert Theatre

08.30 – 09.00 ***REGISTRATION.***
Venue: Front Hall

09.00 – 10.30 WG5 - A - Track structure in cells.
Venue: Albert Theatre
Chair: Fiona Lyng, FOCAS, DIT, Dublin, Ireland

9.00 – 9.30 Vaclav Stepan, Nuclear Physics Institute, Prague, CZECH REPUBLIC
Effect of oxygen on DNA damage caused by ionizing radiation - theoretical modeling approach

09.30 – 10.00 Martin Falk, Academy of Sciences of Czech Republic, Brno, CZECH REPUBLIC
Local changes of higher-order chromatin structure during DSB-repair

10.00 – 10.30 Stanislaw. Pszona , Soltan Institute for Nuclear Studies, Otwock/_wierk, Poland
A nanodosimetric experiment with Auger electrons of I-125

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10.30 – 11.00 ***Tea/Coffee***

11.00 – 12.20 WG1-B: Electron and biomolecular interactions.
Venue: Albert Theatre
Chair: Kevin McGuigan, RCSI, Dublin, Ireland

11.00 – 11.30 Gosia Smialek: The Open University, Milton Keynes, UK
VUV irradiation of DNA

11.30 – 12.00 Stephan Denifl, Univeristy of Innsbruck, AUSTRIA
Electron attachment to gas phase biomolecules in superfluid helium

12.00 – 12.30 Aleksandar Milosavljevic, Institute of Physics, Belgrade, SERBIA
Electron interaction with DNA and deoxyribose analogues

12.30 – 13.30 ***Lunch***

13.30 – 15.00 WG2-B: Radiation in physiological environments
Venue: Albert Theatre
Chair: Dimitra Markovitsi Laboratoire Francis Perrin, CEA, France

13.30 – 13.40 Bela Sulik, ATOMKI, Debrecen, HUNGARY
RADAM '08 Conference, Debrecen, HUNGARY

13.40 – 14.10 Bela Sulik, *ATOMKI*, Debrecen, HUNGARY
Orientation sensitivity of capture fragmentation channels: a study with small molecules of different degree of symmetry

14.10 – 14.35 Adam Hunniford, Queen's University Belfast, UK
Low Energy Ion Induced Radiation damage to DNA and its components

14.35 – 15.00 Kristian Støchkel, Univ of Aarhus, DENMARK
Electron capture induced dissociation of peptide cations

15.00 – 15.30 ***Tea/Coffee***

15.30 – 17.00 WG3-B: Radiation in physiological environments.
Venue: Albert Theatre
Chair: David Field, University of Aarhus, Denmark

15.30 – 16.00 Claudia Lage, Universidade Federal do Rio de Janeiro, BRAZIL
Targeting DNA in therapies: using damages to design strategies on cell sensiti\ation

16.00 – 16.30 Herwig Paretzke, GSF Neuherberg, GERMANY
Polonium 210: The German Experience

16.30 – 17.00 Brenda Laster, Ben Gurion University of the Negev, ISRAEL
It may not take a shillelagh to end a controversy among radiation scientists

17.00 – 20.00 ***Break***

18.00 – 20.00 **MANAGEMENT COMMITTEE MEETING**
Venue: Video Conference Room

20.00 – 22.00 **MANAGEMENT COMMITTEE DINNER**
Venue: Board Room

Friday June 22nd

Venue: Albert Theatre

08.30 – 09.00 *REGISTRATION.*
Venue: Front Hall

8.30 – 10.00 WG4-B: Theoretical developments for radiation damage.
Venue: Albert Theatre
Chair: Thomas Schlatholter, University of Groningen, NETHERLANDS

08.30 – 09.00 Jack Sabin, *University* of Florida, Gainesville, USA
Theoretical study of the fragmentation of small biomolecules by swift ions

09.00 – 09.30 Dimitra *Markovitsi*, Laboratoire Francis Perrin, CEA, FRANCE
UV interactions with DNA helices

09.30 – 10.00 Martial *Boggio*-Pasqua, Imperial College, London, UK
Photostability of DNA : ultra-fast deactivation of an excited Guanine-Cytosine base pair

Tea/Coffee

10.30 – 12.00 WG5 - B - Track structure in cells.
Venue: Albert Theatre
Chair: Marie-Christine Bacchus, Université Claude Bernard Lyon 1, France

10.30 – 11.00 Sergey Andreev, Institute of Biochemical Physics, Moscow, RUSSIA
Interphase chromosomes: structure and radiation damage.

11.00 – 11.30 Andrea Ottolenghi, University of Pavia, ITALY
Models and simulations of radiation induced chromosome damage

11.30 – 12.00 Werner Friedland. GSF Neuherberg, GERMANY
Biophysical modelling of DSB repair processes

12.00 – ***CONFERENCE TOUR***

1. Walking Tour of Dublin City Centre
(Packed Lunch Provided)
2. Bus Tour to Brú na Bóinne Neolithic Site and Interpretive Centre
(Packed Lunch Provided)

19.30 – 22.00 **CONFERENCE DINNER**
Venue: College Hall and Board Room.

ORAL PRESENTATION ABSTRACTS

Electron interaction with deoxyribose analogue molecules in gaseous phase

Aleksandar R. Milosavljevi_, Dragutin _evi_
and Bratislav P. Marinkovi_

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We present recent results on elastic and inelastic low(medium)-electron interaction with tetrahydrofuran (THF) – C_4H_8O, tetrahydrofurfuryl alcohol (THFA) – $C_5H_{10}O_2$ and 3-hydroxytetrahydrofuran (3HTHF) – $C_4H_8O_2$ molecules in gaseous phase. These cyclic compounds have been used in recent years to model the deoxyribose ring in DNA with respect to low-energy electron interaction [1-3]. It has been suggested [4] that although with energies below the ionization threshold, the secondary electrons which are produced on the track of the primary high-energy particle can induce damage of DNA (single and double strand breaks) through dissociative electron attachment to building blocks of DNA, which proceed via negative-ion resonances. Therefore, a great deal of work has been performed to investigate interaction of low-energy electrons with the basic DNA components, namely the purine and pyrimidine bases, the phosphate group and the deoxyribose sugar including its simpler analogues of the furanose structured molecules (THF, THFA and 3HTHF). Considering the analogue molecules, the most of the results for gaseous phase have been reported for the simplest representative – THF (see [5] and references therein), while experimental data for THFA and particularly 3HTHF are scarce [6,7].

In this work, a comparative study of absolute differential cross sections (DCSs) for elastic electron scattering from THF, THFA and 3HTHF and electron energy loss (EEL) spectra, in a wide incident electron energy range, has been presented. The measurements were performed using a standard cross-beam experimental setup, with an electron gun which can be rotated around the molecular effusive beam produced from a stainless still needle and a double cylindrical energy analyzer (see [8] for details). The elastic DCSs were obtained both as a function of scattering angle and incident electron energy and normalized to the absolute scale according to relative flow measurements and reliable calculations. The experimental elastic DCSs are compared with the most recent theoretical results and capability of different theoretical methods is discussed. Both for elastic and inelastic scattering a special attention has been paid to investigate potential differences in electron scattering processes upon substitution of one of the H-atom in THF by the OH group (in 3HTHF) or CH_2OH group (in THFA).

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] L. Sanche, *Eur. Phys. J. D* **35**, 367 (2005).
[4] B. Boudaiffa, P. Cloutier, D. Hunting, M. A. Huels, and L. Sanche, *Science* **287**, 1658 (2000).
[5] M. Dampc, A. R. Milosavljevi_, I. Linert, B. P. Marinkovi_, and M. Zubek, *Phys. Rev. A* (2007) (*accepted*).
[6] Pawe_ Mo_ejko, Alicja Domaracka, Elizbieta Ptasi_ska-Denga, Czes_aw Szmytkowski, *Chem. Phys. Lett.* **429**, 378 (2007).
[7] A. R. Milosavljevi_, F. Blanco, D. _evi_, G. García, and B. P. Marinkovi_, *Eur. Phys. J. D* **40**, 107 (2006).
[8] A. R. Milosavljevi_, S. Mad_unkov, D. _evi_, I. _ade_, and B. P. Marinkovi_, *J. Phys. B: At. Mol. Opt. Phys.* **39**, 609 (2006).

Electron interaction with deoxyribose analogue molecules in gaseous phase

Aleksandar R. Milosavljević, Dragutin Šević and Bratislav P. Marinković

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References:

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[4] B. Boudaiffa, P. Cloutier, D. Hunting, M. A. Huels, and L. Sanche, *Science* **287**, 1658 (2000).
[5] M. Dampc, A. R. Milosavljević, I. Linert, B. P. Marinković, and M. Zubek, *Phys. Rev. A* (2007) (*accepted*).
[6] Paweł Możejko, Alicja Domaracka, Elizbieta Ptasińska-Denga, Czesław Szmytkowski, *Chem. Phys. Lett.* **429**, 378 (2007).
[7] A. R. Milosavljević, F. Blanco, D. Šević, G. García, and B. P. Marinković, *Eur. Phys. J. D* **40**, 107 (2006).
[8] A. R. Milosavljević, S. Madžunkov, D. Šević, I. Čadež, and B. P. Marinković, *J. Phys. B: At. Mol. Opt. Phys.* **39**, 609 (2006).

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