RADAM 2010

7th International Conference on Radiation Damage in Biomolecular Systems

30th June – 4th July 2010

Madrid, Spain

UNED

MINISTERIO DE CIENCIA E INNOVACIÓN

CSIC

ECCL

VAMDC Virtual Atomic and Molecular Data Centre

http://www.uned.es/074150/radam10

RADAM 2010 Scientific Programme

Wednesday 30 June

18:00-20:00 Registration and welcome reception

Thursday 1 July

	Session	Speaker	Title
09:15-09:30	1. Biomedical applications of radiation Chair: H. Hotop	Introduction	
09:30-10:00		K. Prise	Spatial and temporal aspects of radiation response in cell and tissue models
10:00-10:30		M.E. Sánchez	Advances in radiation therapy and related techniques
10:30-11:00		K. Belkic	Optimized Molecular Imaging through Magnetic Resonance for Improved Target Definition in Radiation Oncology
11:00-11:30	Coffee Break		
11:30-12:00	2. Ion interactions Chair: J. Sabin	A. Solov'yov	Multiscale approach to radiation damage induced by ion beams: current status and perspectives
12:00-12:30		R. Rivarola	Interaction of ion beams with water and other small molecules of biological interest
12:30-13:00		S. Bari	Peptide dissociation by keV ions and VUV photons
13:00-13:30	Lunch		
13:30-14:00			
14:00-14:30			
14:30-15:00	3. Theoretical methods Chair: L. González	F. Gianturco	Modelling the quantum dynamics of electron-induced reactions in biosystems
15:00-15:30		J. Tennyson	Resonances in electron collisions with small biomolecules using the R-matrix method
15:30-16:00	Coffee Break		
16:00-16:20	4. Energy deposition and induced damage Chair: P. van der Burgt	John R. Sabin	Swift Ion Energy Deposition in the DNA and RNA Nucleobases: Mean Excitation Energies
16:20-16:40		R. Garcia Molina	Simulation of the spatial distribution of energy deposition by proton beams in liquid water
16:40-17:00		M. Falk	Induction and repair of DNA double-strand breaks in the context of higher-order chromatin structure
17:00-19:00	Poster Session		
19:00-			

Friday 2 July

	Session	Speaker	Title
09:30-10:00	5. Electron interactions (I) Chair: M. Brunger	L. Sanche	Low energy electron damage to DNA under vacuum, atmospheric and cellular conditions
10:00-10:30		K. Nixon	Low Energy (e,2e) Studies of Methane
10:30-11:00		H. Tanaka	Electronic Excitation and Ionization Cross Sections by Electron Impact
11:00-11:30	Coffee Break		
11:30-12:00	6. Electron interact. (II) Chair: H. Cho	J. Kopyra	Electron driven reactions in amino acids: from canonical to zwitterion structure
12:00-12:30		P. Limão-Vieira	Dipole and valence anion states of thymine: negative ion formation in atom-molecule collisions
12:30-13:00		T. Field	Dynamics of electron stimulated molecular decomposition
13:00-14:30	Lunch		
14:30-15:00	7. Positrons Chair: H. Telle	G. Laricchia	Interactions of positrons and positronium with molecules
15:00-15:30		J. Sullivan	Positron interaction data for radiation damage models
15:30-16:00	Coffee Break		
16:00-16:20	8. Low energy electron interaction models Chair: S. Eden	J. Gorfinkiel	Low energy electron collisions with HCOOH and its dimer
16:20-16:40		M. Brunger	Modelling electron tracks in ethylene
16:40-17:00		M. Fuss	Modelling electron and photon interactions for applications of brachytherapy: the role of low energy secondary electrons
17:00-19:00	Poster Session		
19:00-			

Saturday 3 July

	Session	Speaker	Title
09:30-10:00	9. Radiation dosimetry Chair: M. Falk	A. Rosenfeld	Solid State Micro and Nano dosimetry and its applications
10:00-10:30		C. Muñoz-Ferrada	Research and Development of an Automatic Optically Stimulated Light (OSL) Reader for Patient Verification
10:30-11:00		H. Rabus	Nanodosimetry - bridging the gap to radiobiology
11:00-11:30	Coffee Break		
11:30-12:00	10.Data for radiation	N. Mason	Data needs for modelling radiation damage
12:00-12:30		B. Marinkovic	Current research on electron interactions

	modelling (VAMDC)		relevant to modelling of radiation damage processes
12:30-13:00	Chair: L. Méndez	R. White	On the application of swarm techniques to the study of electrons and positrons in gaseous and soft-condensed bio-systems
13:00-14:30	Lunch		
14:30-14:50	11. DNA models (VAMDC)	M. Huels	Does Nature Care (what, where, or how we ionize): hyperthermal ion versus VUV and soft X-ray damage to DNA components studied by ion and electron spectroscopies
14:50-15:10	Chair: J. Gorfinkiel	C. Champion	Theoretical predictions for ionization and capture cross sections of DNA nucleobases impacted by light ions
15:10-15:30		H. Abdoul-Carime	Probing Radiation Damage to Biological Systems at the Molecular Level by the "Event-by-Event" Analysis Technique
15:30-16:00	Coffee Break		
16:00-16:20	12. Damage and repair mechanisms Chair: I. Baccarelli	L. Errea	Charge exchange in ion-molecule collisions
16:20-16:40		P. Bolognesi	Inner shell excitation and fragmentation of halopyrimidines
16:40-17:00		L. Feketeova	Kangaroos and clues to the repair of cyclobutane pyrimidine dimers
17:00-19:00	ECCL WG-1 Meeting		
21:00	Conference Dinner		

Sunday 4 July

	Session	Speaker	Title
09:30-10:00	13.UVB damage, clusters and condensed phase Chair: J. Horacek	S. Denifl	Biomolecules and Clusters in He droplets: synthesis and characterization
10:00-10:30		O. Ingólfsson	Low-level UVB induced strand breaks in pUC19 plasmid DNA
10:30-11:00		A. Lafosse	Low-energy electron induced damages - A chemical & physical approach dealing with model systems
11:00-11:30	Coffee Break		
11:30-13:00	- Round table: VAMDC and RADAM perspectives (moderator: A. Solov'yov) - Concluding remarks (G. García)		
13:00-14:30	Lunch		
15:0	Departure		

Current research on electron interactions relevant to modelling of radiation damage processes

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The important activity within RADAM research is modelling of radiation damage processes by photon, electron and ion interactions [1,2]. Electron interactions with deoxyribose analogue molecules in gaseous phase have been previously reviewed by our group at the same series of conferences [3]. Basic interactions of low energy electrons include elastic scattering and excitation cross sections from molecules relevant for biological systems, such as H_2O, amino acids, nucleotide bases, etc. On the other hand, there is a revival of interest for basic interactions of electrons by metal atoms and their clusters since they are proved as the chemotherapeutic agents (like cisplatin, gold nanoparticles, etc.) [4]. There are relatively few groups in the world who are dealing with experimental investigations of electron scattering by metal atoms as well as theoretical groups who calculate respective cross sections. Measurements with metal vapour atoms had been recently critically evaluated [5,6].

Elastic scattering cross sections have been obtained for several metal atoms and molecules in experiments of crossed beam arrangement with monochromatic electron beam and effusive atomic particle beam. The relative cross sections have been obtained after applying the effective scattering volume correction factor (V_{eff}) to angular distributions of scattered electrons. In the case of metal atoms, the absolute scale has been established through normalization process to the experimentally known optical oscillator strength for the resonant transition and respective intensity ratio of elastic-to-inelastic scattering. For molecules, a relative flow technique is used to normalize cross sections to the known referent gas. The excitation cross sections were obtained through energy loss spectra which on the other side had been compared with high resolution photoabsorption cross sections.

Comprehensive set of collisional data, both experimental and theoretical, have been accumulated during the time. There are certain efforts to organize data base in the way such that it can be used by different communities, radiation chemists been one of them [7,8].

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[1] M. Fuss, A. Muñoz, J. C. Oller, F. Blanco, C. Huerga, M. Télez and G. García, *Proc. VI Int. Conf. on Radiation Damage in Boimolecular Systems* – RADAM 2009, Ed. A. V. Solov’yov, (FIAS, Frankfurt, 2009) Invited lecture W-I-2, p. 26.
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[8] B. P. Marinković, G. García, D. Šević, and N. J. Mason, “Electron Collision Cross Section Data Base”, *Proc. Third Annual Meeting of ESF Programme on Electron Induced Processing at the Molecular Level* (EIPAM 07) Hveragerði, Iceland, 25-29 May 2007. Eds. N J Mason and O Ingólfsson, Invited Talk No.6.

User-friendly software for resolving some of the parameters in electron spectrometry experiments: scattering volume correction factor and metal vapour pressure curves

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In electron spectrometry experiments, in order to obtain differential cross sections from angular distributions, the effective scattering volume correction factor (V_{eff}) has to be determined exactly. Following the early considerations of Brinkmann and Trajmar [1] for crossed beam experiments, we have made a software to determine the V_{eff} for different atomic species (with specific gas kinetic cross section, σ) and for various vapour pressures in back reservoir, p. For each scattering angle, we interpolate the calculated V_{eff} curves [1] from limiting values of σ and p. The limiting curves has been determined for the present experimental conditions i.e. tube aspect ratio, geometry of monochromator and analyser, diameters of defining diaphragms, distance of scattering volume from the tube, which supplies effusive atomic beam, etc. [2-4]. The screen shot of the program window is shown in Fig.1.

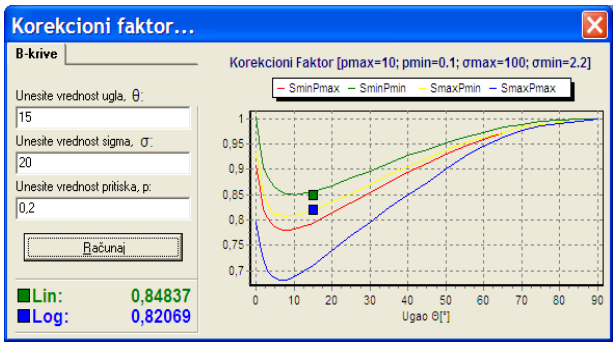

Figure 1. Screen shot of the program window showing determination of V_{eff} at 15 deg. scattering angle and for species with σ=20 Å^2 and p= 0.2 Torr.

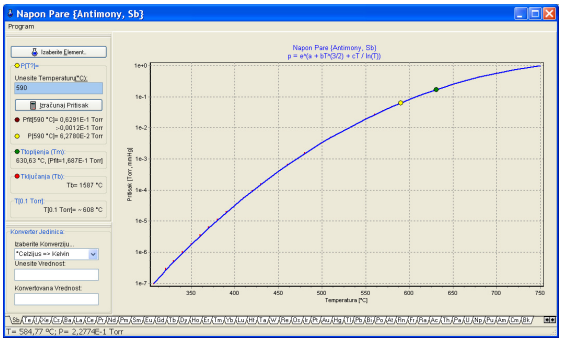

Figure 2. Screen shot of the program window showing determination of vapour pressure for Sb (antimony) atoms at temperature of 590 °C.

For experiments with metal atom vapours, the back pressure in reservoir, p, is determined by the temperature of the crucible. That temperature is measured by thermo pair placed at the bottom of the crucible, while the nozzle temperature is maintained at approximately 50 K higher temperature in order to avoid clogging. Relationship between temperature and vapour pressure is nonlinear [5] and it is fitted by the appropriate analytic curve (Fig.2).

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