LEEMI IV – NEGATIVE IONS; experiment and theory

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Smolenice Castle, 6th – 9th October 2005

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Conference timetable

Thursday, October 6

14:00 – 18:00	Registration
18:00	Dinner
20:30	Opening Lecture by E. Illenberger, Chairman W. Schmidt

Friday, October 7

7:30 – 9:00	Breakfast
9:00 – 9:45	T. D. Märk, *Low energy electron interactions with complex molecules*
9:45 – 10:30	J. Simons, *Mechanisms of electron-capture and electron-transfer dissociation*
10:30 – 11:00	Coffee Break
11:00 – 11:20	J. M. Weber, *Photodetachment from Doubly Charged Negative Ions*
11:20 – 11:40	J. Langer, *Electron-driven Reactions in van der Waals Clusters*
11:40 – 12:00	A. F. Borghesani, *O_2^- formation and transport in dense noble gases*
12:00 – 12:20	M. Braun, *High resolution studies of electron attachment to the molecules CCl_4, $CHCl_3$, and CF_2Cl_2 over the electron energy range 0.001 – 2 eV*
12:30 – 14:00	Lunch
14:00 – 14:20	P. Swiderek
14:20 – 14:40	S. Ptasinska, *Explosives detection by low energy electrons*
14:40 – 15:00	S. V. K. Kumar
15:00 – 15:20	O. Ingolfsson, *Metastable decay of negatively charged oliginucleotides*
10:30 – 11:00	Coffee Break
15:50 – 16:10	A. Domaracka, *Low energy electron interactions with condensed films of CH_3COOD/NH_3 mixtures*
16:10 – 16:30	P. Mozejko, *Low energy electron-initiated ion-molecule reactions of the DNA deoxyribose analogues*
16:30 – 16:50	T. Solomon, *Application of Microarray Technology to Study the Interaction of Slow Electrons with DNA*
16:50 – 17:20	Oral poster presentation
18:00 – 20:00	Dinner
20:00	Poster session

Saturday, October 8

7:30 – 9:00	Breakfast
9:00 – 9:45	J. Horáček, *Low-energy electron-molecule scattering. Theory and computation: where do we stand?*
9:45 – 10:30	S. Price, *Using coincidences to study the dynamics of ionic reactions*
10:30 – 11:00	Coffee Break
11:00 – 11:20	V. Staemmler
11:20 – 11:40	M. Probst, *Negative Ions in Condensed Phases*
11:40 – 12:00	J. Kalcher, *Ground and Excited State Electron Affinities of Selected Cyanocarbens and Cyanosilylenes XCCN and XSiCN*
12:00 – 12:20	R. Čurík
12:30 – 14:00	Lunch
14:00 – 14:20	I. Fabrikant, *Condensed-Matter and Cluster Effects in Low-Energy Electron-Molecule Scattering*
14:20 – 14:40	P. Skurski, *Mechanism for Damage to DNA by Low-Energy Electrons*
14:40 – 14:55	B. Nestmann, *Strong electron correlation in resonant electron-molecule collision*
14:55 – 15:10	J.Fedor, *Temperature effects on dissociative electron attachment to HBr*
15:10 – 15:25	I.Bald, *Electron Induced Reactions in Cyclic Sugar Molecules*
15:25 – 15:55	Coffee Break
16:30	Castle wine degustation and banquet

Sunday, October 9

7:30 – 9:00	Breakfast
9:00	Departure

Inelastic electron interaction (attachment/ionization) with furan and tetrahydrofuran

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We report experimental results on electron induced formation of cations and anions of furan (C_4H_4O) and tetrahydrofuran (C_4H_8O) molecules, which can be considered as simplest analogues to DNA sugar deoxyribose. Recently a detailed experimental investigation of inelastic electron interaction (attachment/ionization) with deoxyribose was published [1]. The authors pointed out that damage to DNA and RNA strands, induced by secondary electrons produced upon ionizing radiation, may start preferentially at the sugar-phosphate backbone. The present experiments are performed at the Institut für Ionenphysik Innsbruck, using a crossed electron/molecule beam apparatus [1]. A monochromatized electron beam is produced by an electrostatic hemispherical energy filter and crossed perpendicularly with a molecular beam of furan (F) or tetrahydrofuran (THF). The ions formed, are extracted into a quadrupole mass spectrometer and detected by a single channel electron multiplier. Anhydrous F and THF are used after several freeze-thaw cycles under vacuum.

Electron attachment to F and THF is investigated in the electron energy range of about 0 – 15 eV. In case of dissociative electron attachment (i.e. $e + XY \leftrightarrow [XY]^{-*} \rightarrow X^- + Y$) to furan the following anions (X^-) are observed within the detection limit of the instrument: $(F\text{-}H)^-$, C_2HO^- and $C_3H_3^-$. All these anions exhibit a strong resonance at about 6 eV, as well as a broad structure between 8 and 12 eV. Detailed measurements of $(F\text{-}H)^-$ yield reveal two processes in the energy range 8-12 eV and a further weak resonance at about 3.7 eV. For THF and electron energies above 2 eV no anion formation is observed. However, preliminary measurements show low cross section resonances for $(THF)^-$ and $(THF\text{-}2H)^-$ at about 1.2 eV.

Positive ion formation upon electron impact ionization is studied for both F and THF. The mass spectra obtained at the electron energy of 70 eV agree very well with data taken from the NIST database [2]. Appearance energies (AE) are determined for the most abundant fragments (F: F^+, $C_3H_3^+$; THF: THF^+, $C_4H_7O^+$, $C_3H_6^+$, $C_3H_5^+$) by fitting a Wannier type threshold function (see e.g. [1]) to the measured ion efficiency curve. Our AE values are in good agreement with published values [2]. For the fragment ions CH_3O^+ and CH_3^+ from THF AE are measured for the first time. These cations have also been detected upon electron impact ionization of deoxyribose [1].

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References:
[1] S. Ptasińska, S. Denifl. P. Scheier, and T. D. Märk, J. Chem Phys **120**, 8505 (2004)
[2] NIST Chemistry WebBook, http://webbook.nist.gov

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Conference organizers

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