

Dr Aleksandar Milosavljevic
Institute of Physics Belgrade
Pregrevica 118
11080, Zemun, Belgrade (RS)
vraz@phy.bg.ac.yu

REFERENCE: Short Term Scientific Mission, COST P9
Beneficiary: Dr Aleksandar Milosavljevic, Institute of Physics Belgrade
Host: Prof Stefan Matejcik, Depart. Plasmaphysics, Comenius University
Period: from 06/08/2007 to 02/09/2007 Place: Bratislava (SK)
Reference code: COST-STSM-P9-02813

SCIENTIFIC REPORT

PURPOSE OF VISIT

The purpose of visit was the exchange of experiences and joint work related to the investigation of dissociation and fragmentation of biomolecules in the gas phase upon low (medium)-energy electron impact. The emphasis was put on two molecules: tetrahydrofurfuryl alcohol (THFA), $C_5H_{10}O_2$ and 3-hydroxytetrahydrofuran (3HTHF), $C_4H_8O_2$, which have been used recently to model DNA sugar deoxyribose. The objective was the experimental study of molecules that are substantial parts of DNA, which should lead to better understanding of effects linked to chemical and structural changes of cellular DNA connected with radiation damage.

DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT

The measurements have been performed at the Comenius University Bratislava, using a crossed electron/molecule beam apparatus. A monochromatized electron beam was produced by a trochoidal electron monochromator (TEM) and crossed perpendicularly to the molecular beam, which was formed by effusion of the target gas from a single stainless steel tube. The incident electron energy resolution was about 150 meV. The ions formed were extracted into a quadrupole mass spectrometer and detected by a single channel multiplier operating in the counting mode. Anhydrous both THFA and 3HTHF were purchased from Aldrich with a declared purity of >99.8% and have been used after several degassing cycles under vacuum. The yield of an ion, with a mass/charge ratio defined by the quadrupole filter, was recorded as a function of electron energy. The energy scale was calibrated according to well known values of ionization energies of krypton and argon.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

Positive ion formation upon electron impact ionization of both THFA and 3HTHF has been studied. Recorded mass spectra are presented in the figure below. For both molecules, the spectra show several intensive groups of positive fragments corresponding to combination of either C, O and H atoms or C and H atoms. However, the spectra do not appear to be very similar considering the most abundant fragments. For THFA, the most intensive peak is at $m/q=71$, most probably due to a simple detachment of the CH_3O group from the furanose ring, while in the 3HTHF spectrum, the most abundant fragment is at $m/q=57$, with also very intensive signal at 58. Also, while the parent cation is rather intensive in the 3HTHF spectrum (88 au), it is very weak in the THFA spectrum (102 au). Appearance energies (AEs) were obtained for about 15 most abundant fragments in both spectra by fitting Wannier type

threshold function to the measured ion efficiency. According to our knowledge, these are the first gas phase ion energetic data for the THFA and 3HTHF molecules. Preliminary results for appearance energies of parent ions – 9.23 eV for THFA and 9.57 eV for 3HTHF – appear to be in a very good agreement with the existent photon electron spectra, recently published by Ibanescu et al (PCCP, 2007).

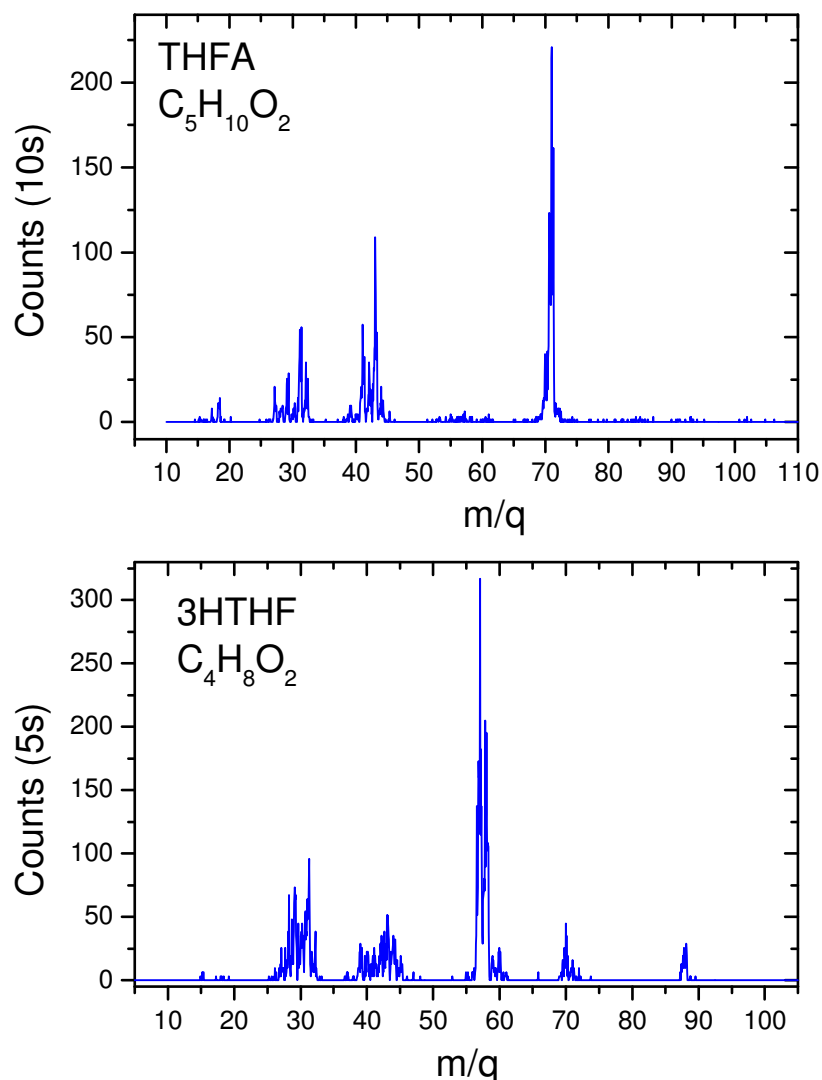


Figure 1. Mass spectra of cations formed by electron impact ionization of tetrahydrofurfuryl alcohol (THFA) and 3-hydroxytetrahydrofuran (3HTHF) at the electron energy of 70 eV.

FUTURE COLLABORATION WITH HOST INSTITUTIONS

The future collaboration with host institution will involve further investigation of binary collisions of electrons with molecules of biological interest. The experimental set-up in Bratislava has facilities for measuring of a yield of mass selected both positive and negative ions as a function of incident electron energy, as well as energy distributions of a specific ionic fragment upon electron induced dissociation. The experimental set-up in Belgrade allows differential cross section measurements for a specific electron scattering process, as well as measurements of energy and angular distributions of positive ions upon electron induced dissociation of a molecule.

***PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT
FROM THE STSM***

We expect at least one publication in a leading international journal in a near future and several contributions to international conferences.

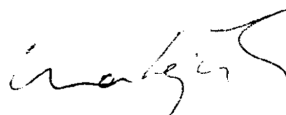


Aleksandar Milosavljević
Institute of Physics, Belgrade

Belgrade, September 6th 2007

***CONFIRMATION BY THE HOST INSTITUTE OF THE SUCCESSFUL
EXECUTION OF THE MISSION***

Herewith I confirm that Aleksandar Milosavljevic, PhD, successfully worked in the Depart. Plasmaphysics, Comenius University from August 6th until September 2nd 2007. The obtained results are interesting and this first contact between the participating institutions suggests further collaboration in the future. It was a pleasure to have Aleksandar Milosavljevic working in my group.



Stefan Matejčík

Bratislava, September 10th 2007