Scientific report

REFERENCE: Short Term Scientific Mission, COST CM0601
Beneficiary: Mr Dusan Kubala, Comenius University
Host: Mariusz Zubek, Gdansk University of Technology
Period: from 14/01/2008 to 29/01/2008 Place: Gdansk (PL)
Reference code: COST-STSM-CM0601-03385

Purpose of the visit

The purpose of the visit was to initiate studies of electron impact dissociation of fragments of biological molecules especially analogues of deoxyribose ring and nuclei bases. These processes are related to the investigation of radiation damage. The study was planned to be carry out using trochoidal electron monochromátor coupled with the optical spectrometer. The part of the aim was to learn a technique of measuring the fluorescence emission spectra induced by the electron impact which is introduced in our laboratory at the Comenius University in Bratislava in the group of Professor Stefan Matejcik.

Report

Present electron impact studies of dissociative excitation of Tetrahydrofurfurylalkohol (THFA) refer to the previous study of Tetrahydrofurane (THF) carried out in the group of Professor Mariusz Zubek. [1,2]. Here the THF itself could be considered as a simplest model of the deoxyribose building block of DNA. The backbone of DNA may be seen as a series of THF molecules held together by phosphate bonds to which the basis are attached [3].

The fluorescence spectrum of THFA obtained at electron energy of *70 eV*, using *0.5 mm* slit at the entrance and the output of the optical spectrometer shows significant emission bands in the range *260-340 nm* (Figure 1). These bands correspond to Δv=0 (around *310 nm*) and Δv=1 (*283.5nm*) transitions of OH ($A^2\Sigma^+ \rightarrow X^2\Pi$).

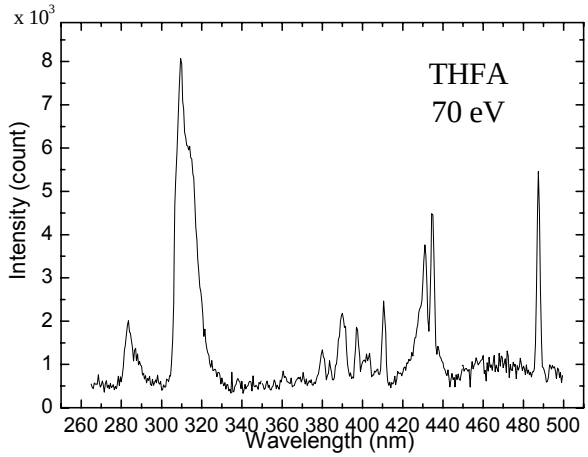

Fig.1: Fluorescence spectrum of THFA at electron energy *E=70eV* using *0.5 mm* slit.

During my scientific mission we focused just on the OH bands. We measured near-threshold emission cross-section of mentioned Δv=0 OH ($A^2\Sigma^+ \rightarrow X^2\Pi$) transition (Figure 2) at the wavelength of *310 nm* (close to maximum of the band). Repeating the measurement several times and using N_2 calibration [4] the value of *9.10 ± 0.1 eV* was estimated as the threshold energy.

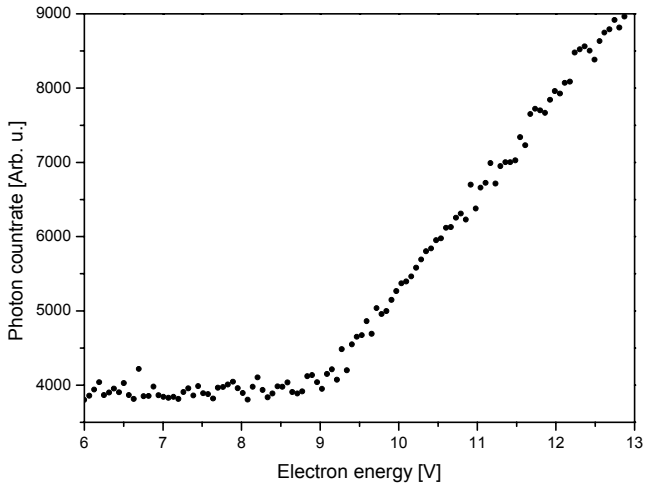

Fig. 2: Near-threshold emission cross section for the Δv=0 OH ($A^2\Sigma^+ \rightarrow X^2\Pi$) transition.

Afterwards we measured the same emission cross-section in the interval *5 – 95 eV* (Figure 3).

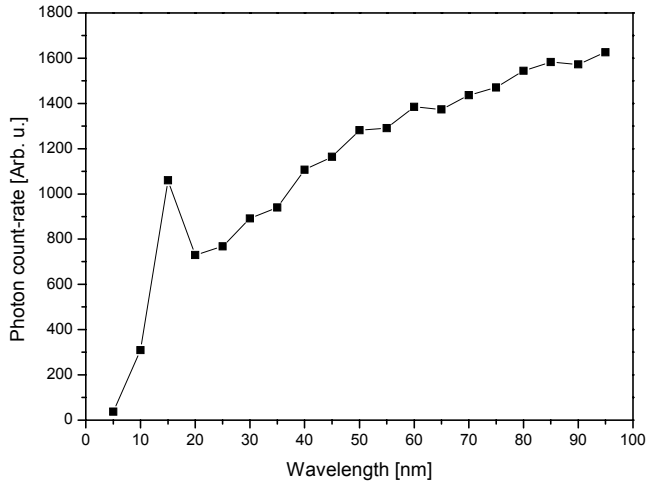

Fig. 3: Emission cross-section of Δv=0 OH ($A^2\Sigma^+ \rightarrow X^2\Pi$) transition.

The cross-section showed a peak structure close to energy of *15 eV*. Analyzing that structure and comparing the emission spectrum of THFA with the spectrum of N_2 we found out around *19%* contribution of Δv=0 $N_2(C^3\Pi_u \rightarrow B_3\Pi_g)$ band to the cross-section measured at *310 nm*. In order to decrease the influence of N_2 to negligible level we set the optical spectrometer transition to the wavelength of *307 nm*, where the Δv=0 OH

($A^2\Sigma^+ \rightarrow X^2\Pi$) transition produces still very intense signal. Repeating the wide range measurement we have obtained final emission cross-section of Δv=0 OH ($A^2\Sigma^+ \rightarrow X^2\Pi$) shown in the Figure 4. Here we may see the persisted peak structure at around 15 eV, which indicates new unexpected process induced by impinging electrons.

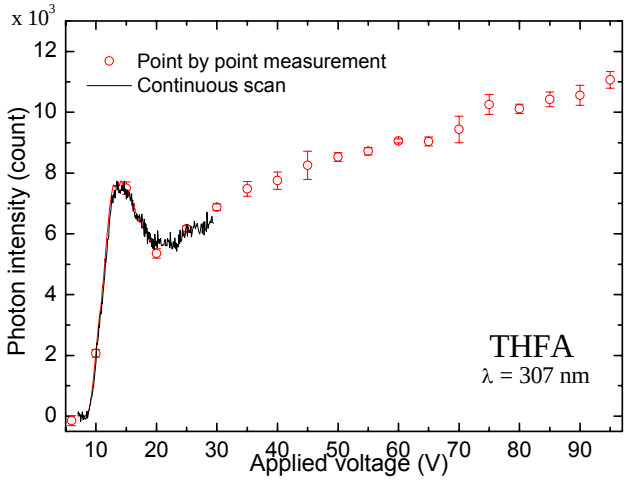

Fig. 4: Emission cross-section of Δv=0 OH ($A^2\Sigma^+ \rightarrow X^2\Pi$) transition at λ=307nm.

Besides the above described measurements we have measured an emission spectrum at 15 eV and analyzed the rotational structure of mentioned OH band as shown in the Figure 5.

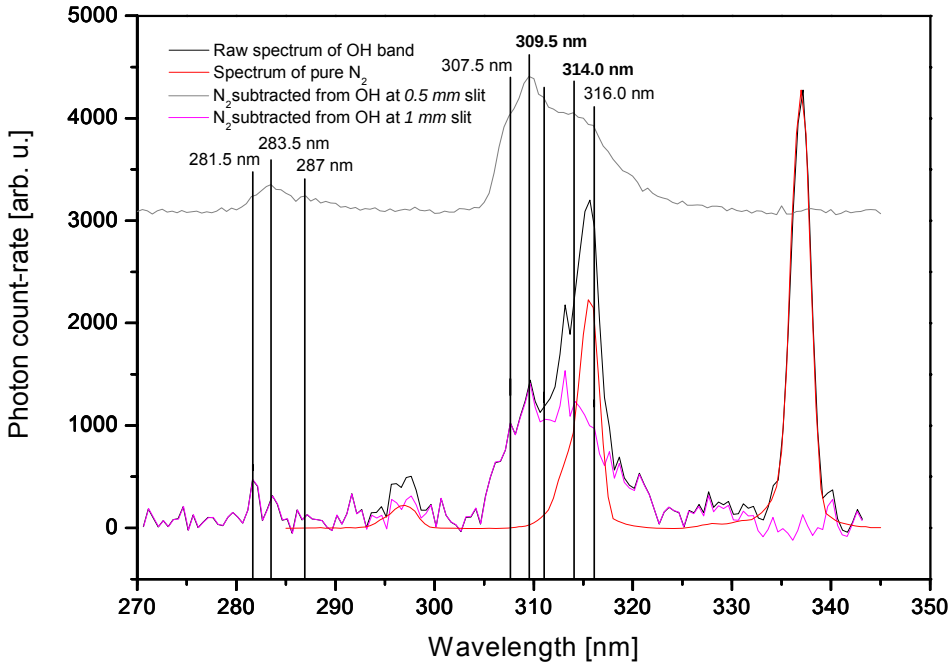

Fig. 5: Analysis of rotational structure of Δv=0 OH ($A^2\Sigma^+ \rightarrow X^2\Pi$) band

Finally I may conclude that my stay at the Technical University of Gdansk in the laboratory of professor Zubek was fruitful. I got new practical knowledge of the technique of dissociative excitation measurements which will be utilized in our laboratory in the short time. The results obtained during my mission will help us more deeply to understand the behaviour of the molecules of biological interest after irradiation by slow electrons and will be published in one of physical or chemical journals. My scientific stay in Gdansk was also good base for further collaboration between our group at Comenius University in Bratislava and the research group of Professor Zubek.

Acknowledgement

I would like to express my thanks to the COST office for support of my scientific mission in Gdansk. Thanks to Professor Zubek for the possibility to spend time in his laboratory and for many fruitful discussions and advices. Thanks to mgr. Marcin Dampc for his invaluable help during the measurements and data processing and to all other members of the research group in Gdansk for their hospitality.

References

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[2] M. Dampc, I. Linert, A. R. Miloslavljevic, M. Zubek; *Chem. Phys. Lett.*, **443** (2007) 17-21.
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