Scientific Report on the EIPAM Exchange Visit

Aleksandar R. Milosavljević, Institute of Physics Belgrade, Pregrevica 118, 11080 Zemun, Serbia and Montenegro (email: vraz@phy.bg.ac.yu)

Host: Professor Mariusz Zubek, Department of Physics of Electronic Phenomena, Faculty of Applied Physics and Mathematics, Gdansk University of Technology, G. Narutowicza 11/12, 80-952 Gdańsk, Poland (email: mazub@mif.pg.gda.pl)

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Title of the project: Investigation of elastic and inelastic low-energy electron interaction with DNA deoxyribose analogue molecules

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Purpose of the visit

The purpose of the visit was the investigation of low energy electron interaction with gaseous molecules that can be considered as simple analogues to DNA deoxyribose. It has been pointed out [1] that investigations of processes lead by low-energy secondary electrons, which are produced by a high-energy primary particle, are of particular importance for understanding the radiation damage of a living cell. In this context, a number of both experimental and theoretical results for either a deoxyribose or analogue molecules (tetrahydrofuran – THF, 3-hydroxytetrtahydrofuran, tetrahydrofurfuryl alcohol) have been reported (see [1]). In particular for THF molecule in the gas phase, which has been the object of investigation during the present exchange visit, the recent experimental results include high resolution electron spectroscopy of resonant-enhanced vibrational excitations [2], absolute differential cross sections (DCSs) for elastic electron scattering at incident energies from 20 eV to 300 eV [3] and total cross-section measurements [4]. Moreover, the electron attachment to THF in the gas phase has been recently investigated under EIPAM program at the Institute of Ion Physics, Innsbruck, by measuring yields of different ionic fragments as a function of incident electron energy [5]. Theoretical results on electron interaction with THF have been also reported very recently [6, 7]. The object of the present work was to extend the existing experimental results for THF in gaseous phase to low (below 20 eV) incident electron energies and high (up to 180^{o}) scattering angles, both for elastic and inelastic electron scattering. The obtained results are useful to check recent theoretical calculations and to compare with the solid phase measurements in order to learn how the elementary processes involving electrons change during the transition from isolated particle behavior in a low pressure gas to many body interactions in the condensed phase.

Description of the work carried out during the visit

The cross-beam measurements were performed on a recently built electron spectrometer. The latter includes a monochromator and an energy analyzer, both consisting of two hemispherical electron energy selectors put in a series and fitted with a system of cylindrical zoom lenses and deflectors, a channel electron multiplier as a detector, a magnetic angle-changer allowing electron scattering measurements in the backward direction and a system for relative-flow absolute measurements. The base pressure of about $2x10^{-7}$ mbar is obtained by a diffusion pump. An alternative gas feed to the vacuum chamber is used for checking the influence of the background electron scattering. Data acquisition and control of experimental parameters is performed using an I/O card attached to a PC. The system can automatically switch between several types of measurements (excitation functions, energy loss spectra, constant residual energy spectra). An energy resolution below 100 meV can be easily reached, while angular resolution is about $\pm 2^{o}$. The accessible angular region is from about 20^{o} to 180^{o}. The anhydrous THF was purchased from Aldrich with a declared purity >99.9% and was used after a few freeze-thaw cycles under vacuum. The work carried out consisted of two parts: 1) calibration procedures and testing of the new apparatus, so to obtain the best possible conditions for reliable biomolecule experiments, and 2) measurements on electron interaction with THF molecule.

The test measurements were performed with noble gases (Ar, He) and include cross section measurements in Ar with relative flow method and measurements of energy loss spectra. The incident energy scale was calibrated according to $3p^5 4s^2\ ^2P_{3/2,1/2}$ resonances in elastic electron-Ar scattering (11.098 eV, 172 meV spacing) [8]. The angular scale, both with and without using the magnetic angle-changer, was calibrated by measuring DCSs for elastic electron-Ar scattering in the vicinity of minima. Also, scattered electron intensities in Ar and He have been measured in the whole angular region to find the effective interaction volume corrections. Some of the obtained results are presented in Figure 1.

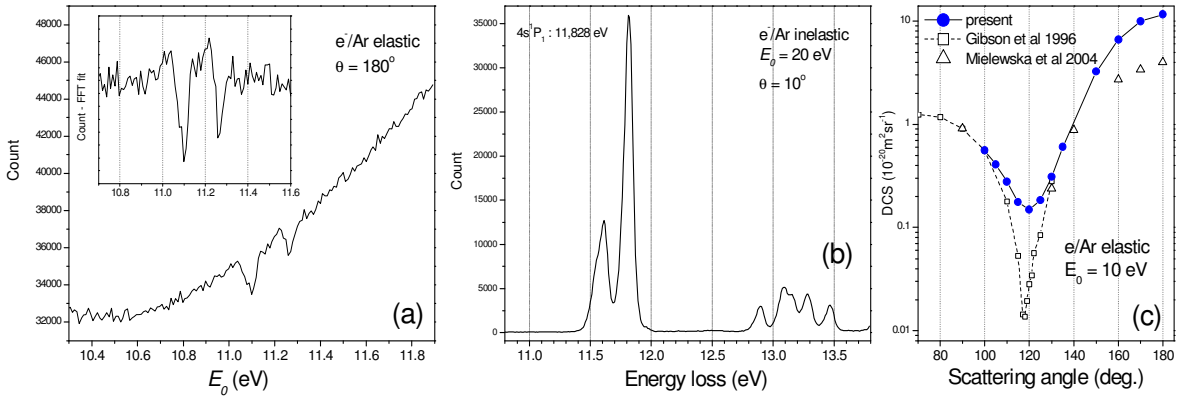

Figure 1. Test measurements for Ar: (a) Elastic scattering intensity as a function of incident electron energy (E_0). (b) Energy loss spectrum of Ar at the incident energy of 20 eV and scattering angle of 10^{o}. (c) DCS for elastic electron scattering by Ar at 10 eV, in the vicinity of the minimum.

Description of the main results obtained

The obtained results include:

a) Absolute DCS for elastic electron scattering from THF at 10 eV, in the angular region from 20° to 180°, in 10° steps. The intensity of the scattered electron current has been measured at the maximum of the elastic peak and relative DCS has been obtained by applying the effective volume corrections using Ar and He together with their known DCSs. The relative DCS has been put on the absolute scale carrying out measurements using the relative-flow method with He as a reference gas, at several scattering angles. The preliminary obtained DCS is presented in Figure 2. The obtained elastic DCS compares well to the previous experimental results at 20 eV [3].

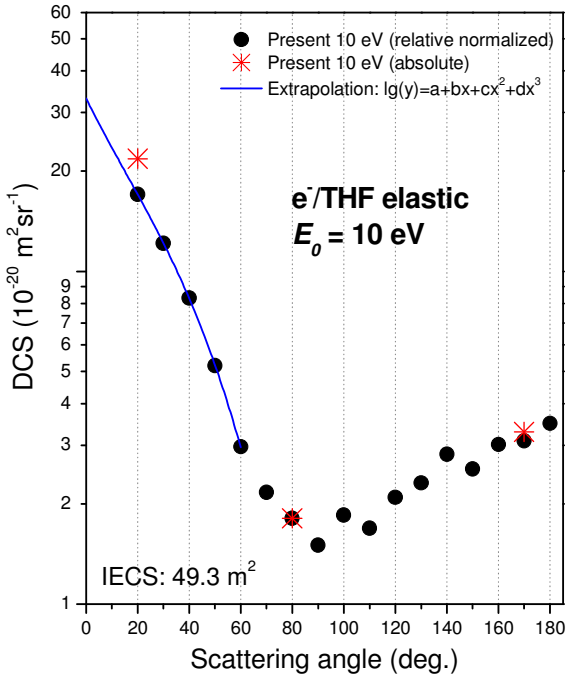

Figure 2. Angular dependence of absolute DCS for elastic electron scattering from THF at the incident energy of 10 eV: *, present absolute measurements obtained by relative-flow method; ●, present relative measurements, normalized at 20° (statistical errors are less then symbol sizes); --, extrapolation of the DCS down to 0°.

b) The integral elastic cross (ICS) section at 10 eV (which is approximately equal to the total cross section (TCS)) has been obtained by integration of the absolute elastic DCS extrapolating the DCS down to 0°. The obtained ICS is equal to 49.3 m^2 and is higher than the TCS of Zecca *et al* [4] (about 35 m^2) indicating that these results underestimate the TCS.

c) Vibrational energy loss spectra, at the incident electron energy of 10 eV and scattering angles from 20° to 180°, in 10° steps. The used energy resolution of about 90 meV did allow to clearly observe a group of vibrational states with energies from 354 meV to 370 meV (-CH2 stretches, see [2]). The obtained spectra agree very well with the existing data [2]. Moreover, the present results extend the energy loss region up to about 1.2 eV. As an

example, the vibrational energy loss spectrum for electron-THF interaction at 10 eV and 30° is presented in Figure 3.

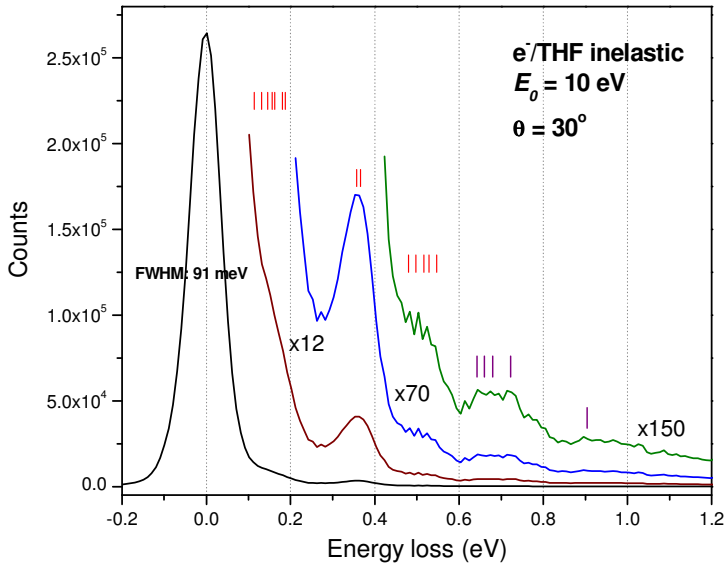

Figure 3. Vibrational energy loss spectrum of THF recorded at incident electron energy of 10 eV and at scattering angle of 30°. The marked vibrational levels are either taken from [2] (red bars) or represent present suggested combination losses (purple bars).

d) Absolute DCSs for the most intense and resolved group of vibrational states (at about 360 meV) are now being obtained from the energy loss spectra measured at 10 eV and in angular range from 20° to 180°. The change of transmission of the analyzer is considered to be negligible in the energy loss region of about 0.5 eV.

e) Elastic electron scattering function for THF at different scattering angles, in the incident energy region from about 5 eV to about 12 eV, where several resonance structures have been predicted by the recent theoretical work [7]. From the first preliminary measurements, the following conclusions can be made: 1) within the statistics of the present measurements (see Figure 4) we are not able to resolve clear resonance structures, 2) if the resonances predicted in [7] exist, they are very week in the elastic channel and thus difficult to identify.

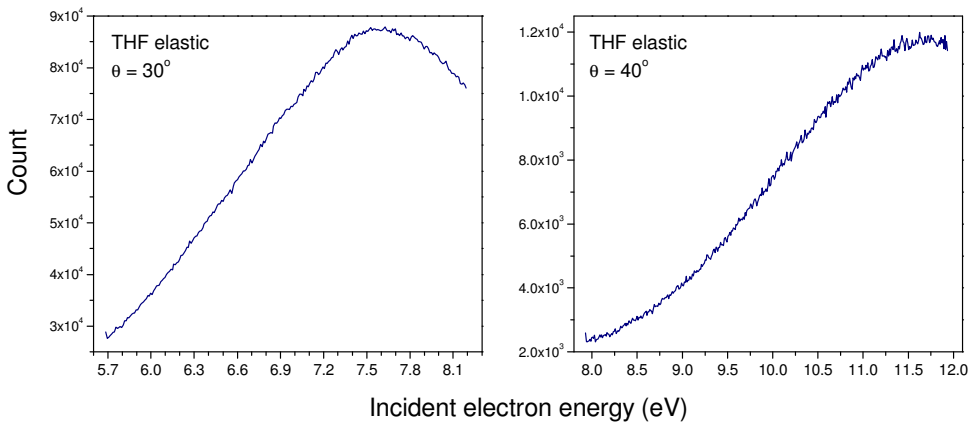

Figure 4. Elastic electron-THF scattering intensity as a function of incident electron energy at scattering angles of 30° and 40°.

Future collaboration with host institution

We expect to continue this collaboration on experimental investigation of electron interaction with molecules of biological interest. The experimental set-up in Gdansk gives possibilities for high-energy resolution measurements of absolute cross-sections at low incident electron energies (below about 30 eV) and in a large angular region (up to 180^o). Complementary to this, experimental system in Belgrade is feasible for fast, high-statistics, low-resolution measurements at high incident electron energies (about 20-500 eV) in the angular region up to about 130^o, in small steps. Also, DCSs can be measured both as a function of scattering angle and incident energy. Therefore, the future collaboration is of interest for both groups.

Projected publications/articles

Part of the obtained results will be presented at forthcoming physics conferences, while at least one article in an international journal is in preparation.

Other comments

In the frame of this EIPAM visit, the grantee A. R. Milosavljević gave a seminar at the Faculty of Applied Physics and Mathematics, Gdansk University of Technology, titled "Electron interaction with DNA deoxyribose analogue molecules".

References

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