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REFERENCE: Short Term Scientific Mission, COST P9
Beneficiary: Aleksandar MILOSAVLJEVIC, Institute of Physics Belgrade
Host: Marie-Jeanne HUBIN-FRANSKIN, Institut de Chimie Sart-Tilman
Period: from 01/06/2004 to 30/06/2004 Place: Liege - 4000 (B)
Reference code: COST-STSM-P9-00204

SCIENTIFIC REPORT

PURPOSE OF VISIT

The purpose of the visit was the exchange of experiences and joint work related to both high-resolution electron energy loss spectroscopy and differential cross section measurements of biomolecules in the gas phase. 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. Finally, the experimental work in the host laboratory as well as meeting and discussion with other colleges involved in COST P9 program, were of great importance for the present work on PhD thesis of the beneficiary A. Milosavljevic.

DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT

The experimental measurements have been performed on the VG-SEELS 400 electron energy loss spectrometer, which consists of an electron gun followed by monochromator, electron energy analyzer and channel electron multiplier as a detector. Elastic and inelastic scattering below 0.5 eV of energy loss, of electrons by gaseous tetrahydrofuran (C_4H_8O), which is the DNA backbone sugar-like analogue molecule were measured at different fixed incident electron energies. The relative elastic differential cross sections as a function of scattering angle in the range from 10° to 110° were obtained for 30, 40, 50 and 60 eV of incident electron energy. Also, the contribution of near zero vibrational excitation to the overall energy loss signal from 0 eV to 0.45 eV was investigated as a function of scattering angle at 30 eV.

Additionally, the investigation of electron-optical system of the VG-SEELS 400 spectrometer was performed with the use of SIMION program. The emphasis was put on the analyzer part of the spectrometer and the input zoom-lens system that projects interaction region into the hemi-spherical analyzer. The investigation of focusing conditions and transmission function of this system should be of use to estimate and elaborate the dependence of the both electron energy loss and impact energy spectra on the electron energy.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

- The first measurements of relative angle dependent differential cross sections for elastic electron scattering by gaseous tetrahydrofuran (THF) molecule, in the angular range from 10° to 110° at several incident electron energies from 30 eV to 60 eV.

- Relative differential cross section for inelastic electron scattering by THF up to 0.45 eV of energy loss, in the angular range from 10° to 110° at 30 eV incident electron energy.
- Focusing characteristics and transmission of the analyzer lens system on the VG-SEELS 400 spectrometer as a function of incident electron energy.

FUTURE COLLABORATION WITH HOST INSTITUTIONS

The future collaboration with host institution will involve further investigation of binary collisions of electrons with gaseous THF molecule as well as with several different molecules that are THF derivates; such are 3-hydroxy tetrahydrofuran and tetrahydrofuranalcol. The measurements should be performed on both apparatus in Liege (high-energy resolution measurements at lower incident energies) and Belgrade (low-energy resolution at higher incident energies and with larger angular range). These will include both angle and energy dependent differential cross sections, as well as investigation of influence of inelastic scattering at lower energies. Also, using the relative-flow technique, the absolute cross sections should be obtained.

PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT FROM THE STSM

Most of the preliminary results that are obtained during this Short Term Scientific Mission will be presented at the 22nd Summer School and International Symposium on the Physics of Ionized Gases (22^{nd} SPIG), 23-27 August 2004, N. P. Tara, Serbia and Montenegro: A. R. Milosavljevic, A. Giuliani, M.-J. Hubin-Franskin and B. P. Marinkovic – poster contribution. The abstract is given in the attachment. Further joint work on these topics in both laboratories should be finalized by joint publications/articles.

Aleksandar Milosavljevic
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Belgrade, 14.07.2004.

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

Execution of this Short Term Scientific Mission has been quite successful. Several publications are in preparation. The host institution has benefited from the large expertise of Aleksandar Milosavljevic in electron optics for the electron spectrometer and data analysis for the differential cross sections.

Prof. Marie-Jeanne Hubin-Franskin
Institut de Chimie Sart-Tilman, Liege

Liege, 15.07.2004.

Elastic Electron Scattering by Tetrahydrofuran

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Abstract. We report preliminary results for elastic and inelastic scattering below 0.5 eV of energy loss, of electrons by gaseous tetrahydrofuran (C_4H_8O), which is the DNA backbone sugar-like analogue molecule. The relative elastic differential cross section (DCS) as a function of scattering angle (10°-110°) is presented at 30 eV impact electron energy. Also, the contribution of near zero vibrational excitation to the overall energy loss signal from 0 eV to 0.45 eV was investigated as a function of scattering angle.

INTRODUCTION

The monomer units of DNA molecule (nucleotides) consist of a 5-carbon sugar (deoxyribose), a nitrogen containing base attached to the sugar and a phosphate group. However, the backbone of the DNA molecule may be seen as a series of tetrahydrofuran (THF) molecules connected by phosphate bonds to which the bases are attached (figure 1). In recent years, it has been emphasized the importance of investigation of electron interaction with molecules whose basic features approximate those found in the deoxyribose backbone of DNA [1, 2]. This could contribute to qualitative estimation of effects linked to chemical and structural changes of cellular DNA connected with radiation damage. To date, there are no data of angular and energy dependence of DCS for electrons elastically scattered by THF. In addition, we investigate the contribution of inelastically scattered electrons to the overall energy loss signal in the range 0 eV to 0.45 eV, as a function of scattering angle. The high-resolution electron energy loss vibrational data of THF for this energy region have been reported recently [1].

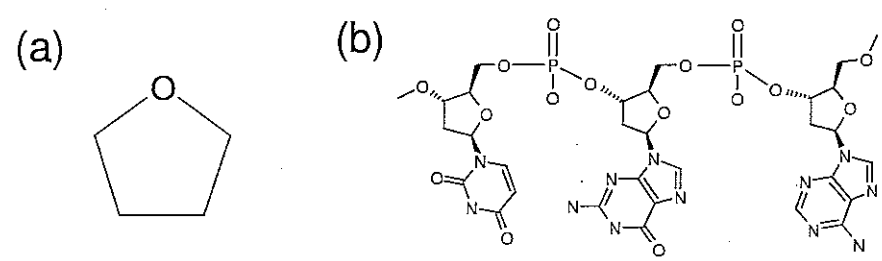

FIGURE 1. Schematic drawing of (a) tetrahydrofuran molecule and (b) short-chain segment of a single-stranded backbone of DNA.

EXPERIMENTAL SETUP

The VG-SEELS 400 electron energy loss spectrometer has been described in detail elsewhere [3]. In short, it consists of an electron gun followed by monochromator, electron energy analyzer and channel electron multiplier as a detector. Both monochromator and analyzer are 150° hemispherical electrostatic type and are fitted with three aperture electrostatic zoom lenses. The effusive molecular beam is formed using the stainless steal needle placed perpendicularly to the incident electron beam. The analyzer can be rotated around the molecular beam in the range –10° to +110°. The angular resolution was investigated earlier [4] and was found to be better than ±2°. The energy loss spectra have been recorded in the constant pass energy mode, with the pass energy of 4 eV and with 8 meV steps. The overall energy resolution was about 45 meV, as measured at the FWHM of the elastic peak. During the acquisition, the retarding and focusing potentials of the analyzer were controlled by the computer. The operating pressure was 1.3 x 10^{-5} mbar and the base pressure was better than 1.0 x 10^{-8} mbar (obtained by cryogenic pumping). For each measurement, the incident beam current was monitored using a Faraday cup. Also, the influence of the effective path length correction was obtained according to elastic DCS for nitrogen, which was measured under the same experimental conditions and compared to existing data [5].

RESULTS AND DISCUSSION

Electron energy loss spectra

A typical electron energy loss spectrum of THF in the region up to 0.45 eV, at the scattering angle of 30° and for impact electron energy of 30 eV is presented in figure 2. The strong elastic peak near zero energy loss possess a slight asymmetry, which is due to the excitation of rotational and vibrational levels that can not be resolved. Some structures in the inelastic part of the spectrum are believed to originate from vibrational excitations and are investigated in detail elsewhere [1].

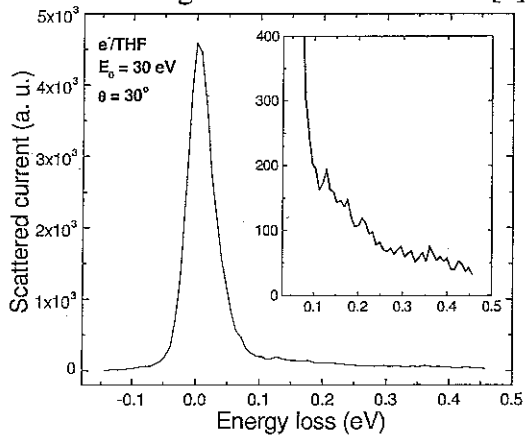

FIGURE 2. Electron energy loss specter of THF recorded at 30 eV and 30° .

Elastic DCS

The relative differential cross section for elastic electron scattering by THF, for 30 eV impact electron energy, is presented in figure 3a. For each scattering angle, the relative DCS was obtained by both integrating the whole quasielastic energy loss peak (up to 0.45 eV) and only by integrating the low-energy part (up to 0 eV). The DCS descends rapidly up to about 90° with the increase of scattering angle. Also, one can see the existence of the minimum at about 90°. Since there are no published data for elastic electron scattering by THF, we can not compare present results with previous ones. However, there is similarity with the behavior of elastic DCS for some other molecular targets at 30 eV impact energy [3, 4].

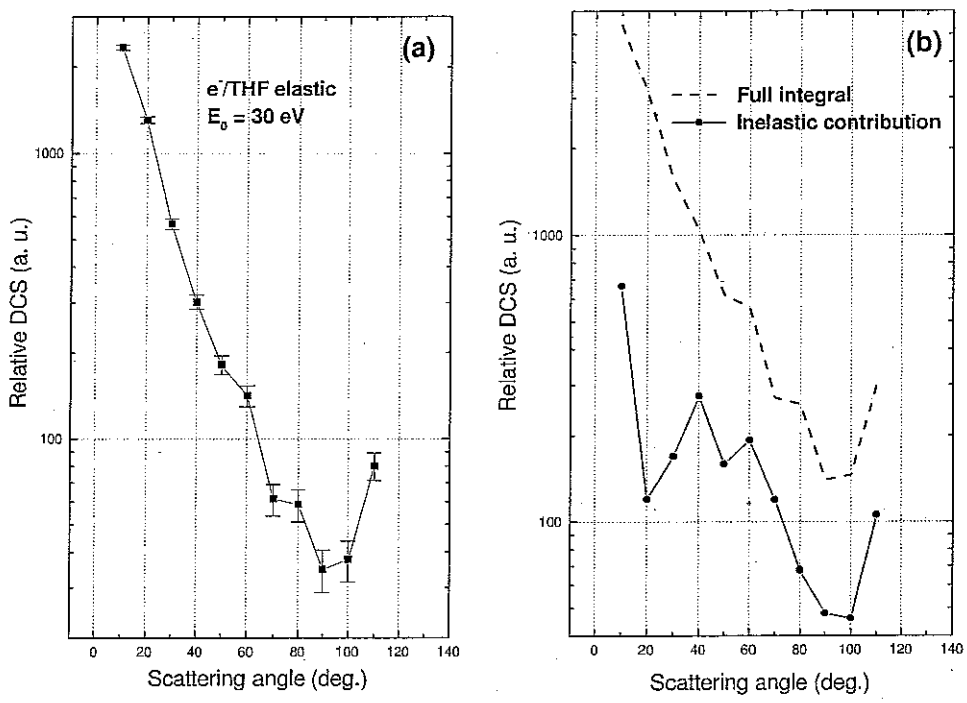

FIGURE 3. (a) Relative differential cross section for elastic electron scattering by THF molecule versus scattering angle at 30 eV impact energy (measured at the maximum of the peak). (b) Inelastic contribution to the integral signal in the range up to 0.45 eV of energy loss as a function of scattering angle at 30 eV impact energy.

Without the influence of inelastic scattering (related to the excitation of rotational and vibrational levels), and supposing the transmission function to be constant in this small energy region, the spectrum around zero energy loss (see figure 2) should be symmetrical. Hence, one can try to estimate the contribution of inelastic scattering (dominantly defined by vibrational excitations) according to the difference between left and right part of the spectrum. The influence of inelastic scattering up to 0.45 eV of electron energy loss to the integral signal, as a function of scattering angle, is presented in figure 3b. One can see the existence of the minimum at about 90°, as for the elastic DCS. However, it is interesting that inelastic angular dependence clearly

reaches the local maximum between 40° and 50°. This could be connected with the strong contribution of the shorter-ranged terms (e. g. polarization, ...), which is again important for the investigation of damage induced to DNA by secondary low-energy electrons [1, 2]. Such kind of behavior has been already observed earlier for other molecules [3, 4].

CONCLUTION

For the first time, the elastic electron scattering by tetrahydrofuran molecule (C_4H_8O) was investigated as a function of angle at fixed impact electron energies. This molecule is a DNA backbone sugar-like analogue and, hence, these results are of importance for the investigation of electron induced DNA damages. The relative DCS for elastic electron-THF scattering is presented for 30 eV impact energy as a function of scattering angle. Also, the contribution of inelastic scattering below 0.45 eV of energy loss was investigated as a function of angle. Further works will include similar measurements for more DNA backbone sugar-like analogues, such as THF derivates.

ACKNOWLEDGMENTS

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