Scientific Report on the EIPAM Exchange Visit

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Reference number: 1260

Dates of visit: 20/11/2006 – 16/12/2006

Title of the project: Investigation of vibrational and electronic excitation of gaseous tetrahydrofuran molecule

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Purpose of the visit

The purpose of the visit was to investigate 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 induced by low-energy secondary electrons, which are produced by high-energy primary particles, 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 [4,5]. Moreover, the electron attachment to THF in the gas phase has been recently investigated by measuring yields of different ionic fragments as a function of incident electron energy [6]. Finally, a number of theoretical results on electron interaction with THF have been reported very recently [7-11]. The object of the present work was to obtain experimental results for THF in gaseous phase for low incident electron energies, below 20 eV and for high scattering angles up to 180^{o}, both for elastic and inelastic electron scattering. The obtained results are important to test the recent theoretical calculations. They are also important for comparison with the solid phase measurements in order to learn how the elementary processes evolve during the transition from isolated particles in a low pressure gas phase 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. This 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 calibration procedures and measurements on electron interaction with THF molecule.

Description of the main results obtained

Elastic scattering

Absolute differential cross sections have been measured for elastic electron scattering from THF in a wide angular range, from 20^o to 180^o, at low incident electron energies ≤20 eV. The aim of these measurements was to extend the existing experimental results [3], both to low energy region and to backward scattering range, which would allow an efficient comparison with the newly reported theoretical data [8-11]. In the measurements the magnetic angle changing technique has been employed to observe the backward scattering of electrons. The angular dependence of the intensity of scattered electron beam has been measured in several overlapping angular regions. The final relative DCSs were obtained by applying effective scattering volume corrections according to benchmark DCSs for He, which were measured under the same experimental conditions and adjusting the head pressures to reproduce the same flow distributions from the needle. The relative DCSs have 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 integral (ICS) and momentum transfer (MTCS) cross sections for elastic scattering have been determined through integration of the measured differential cross sections.

In the measurements special attention has been paid to detect negative–ion resonances predicted in the calculations.

The absolute DCS at the incident electron energy of 20 eV is presented in Figure 1. Present results agree very well with the previous experiment [3], both in DCS shape and on the absolute scale, excluding the DCS at the angle of 110^o which seems to be inaccurate in the previous measurments. Both theoretical curves [9,10] are close to the experimental results, although the calculations of Winstead and McCoy [10] show better agreement both in shape and on the absolute scale. Actually, the latter DCS [10] perfectly agrees at 20 eV with the present measurements except in the angular range from about 40^o-50^o, where the theoretical curve shows a more pronounced shoulder. The large angular range up to 180^o allowed us to obtain accurately MTCS by integrating experimental points. The agreement of the present MTCS at 20 eV with the theory [10] is very good, as shown in Figure 2. Finally, the present ICS compares well with the recent total cross section measurement of Možejko *et al* [5], while the total cross section of Zecca *et al* [4] seems to be somewhat underestimated (see Figure 3).

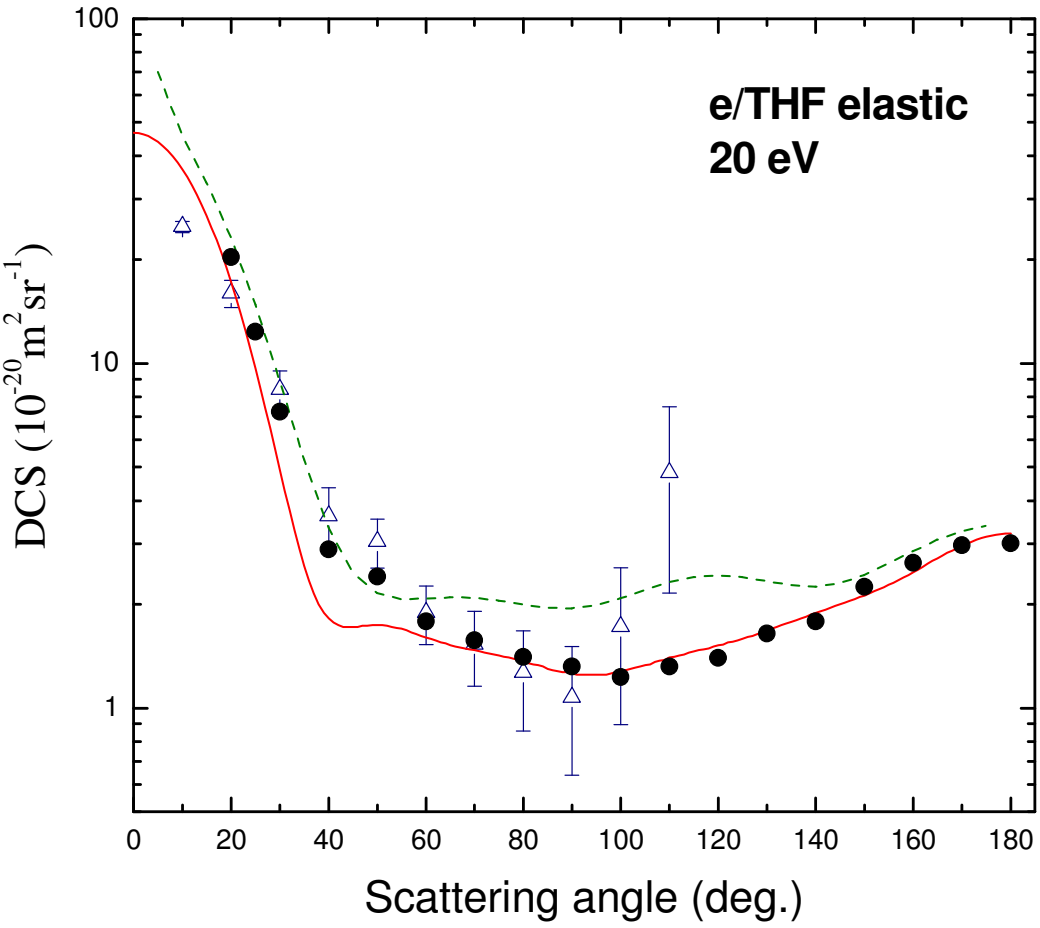

Figure 1. Angular dependence of absolute DCS for elastic electron scattering from THF at the incident energy of 20 eV. Experiment: ●, present results; △, Milosavljević *et al*, 2005 [3]. Theory: --, Trevisan *et al*, 2006 [9]; —, Winstead and McKoy 2006 [10].

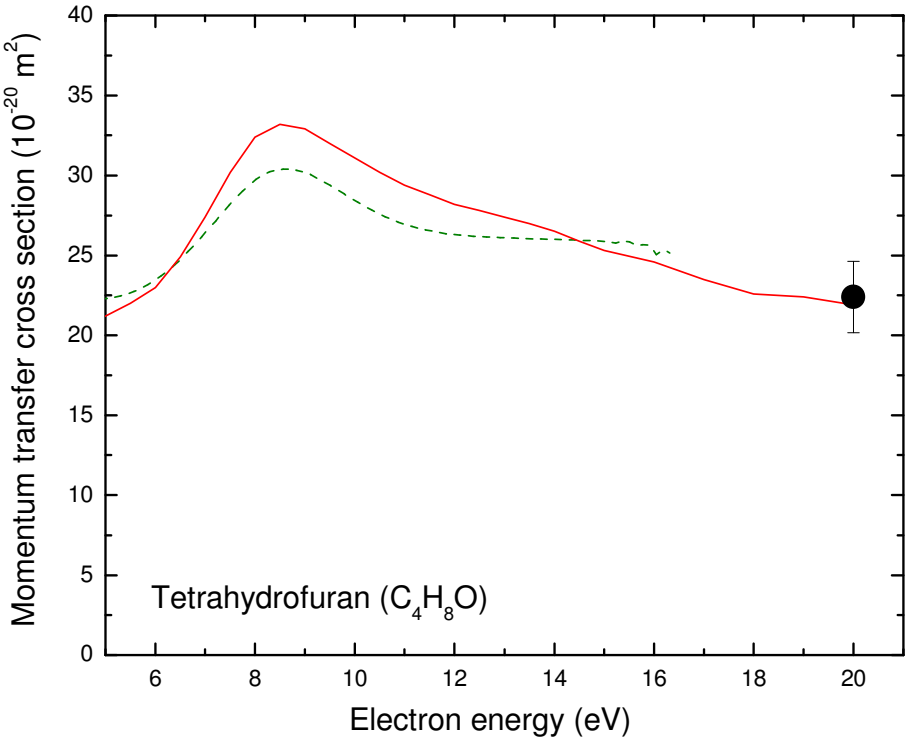

Figure 2. Momentum-transfer cross section for electron collisions with THF. The legend is the same as for Figure 1.

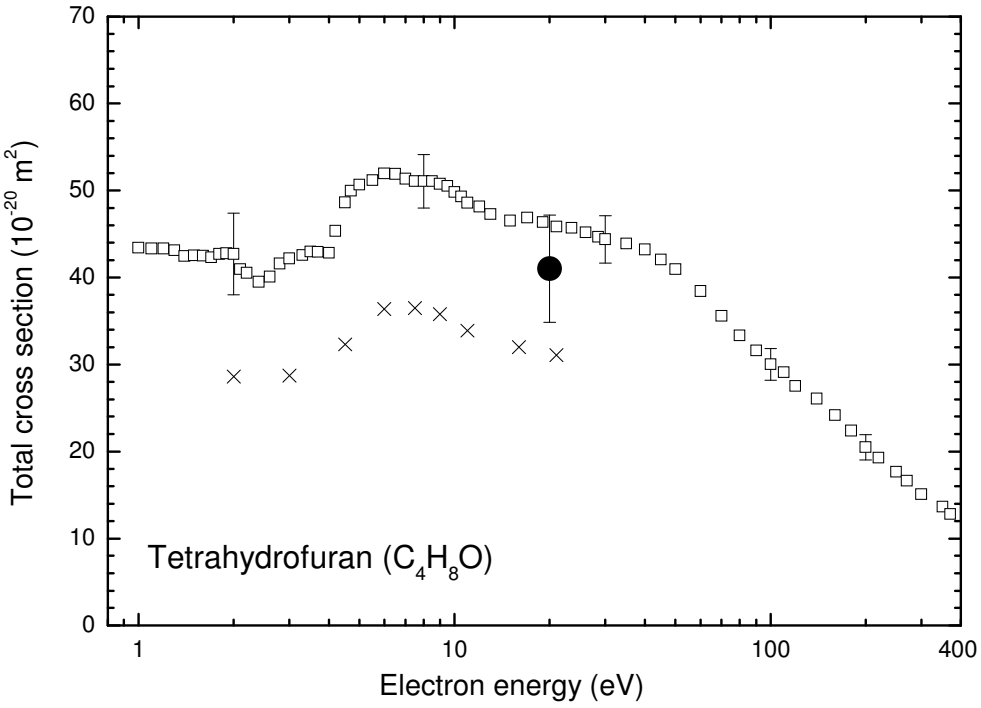

Figure 3. Integral elastic cross section (●, present result) and total cross sections (□, Možejko *et al*, 2006 [5]; ×, Zecca *et al*, 2005 [4]) for electron collisions with THF.

Electronic excitation

The electron energy loss spectra of THF have been reported either at high incident electron energies (~100 eV) and small scattering angles (~2^o) [13], which are the conditions that favor dipole allowed transitions, or at threshold, recorded in a trapped electron spectrometer [14]. The former results [13] are in good agreement with VUV absorption spectrum [14], where the three lowest excitation bands centered at about 6.6, 7.2 and 7.8 eV, has been assigned to excitation of Rydberg states n_o3s, n_o3p and n_o3d. The threshold measurements [14] also reveal a lower triplet state at about 6.3 eV. In the present work, our aim was to investigate the low energy electron impact excitation of the lowest electronic states of THF (4-10 eV residual electron energies) in a large scattering angular region. A preliminary energy loss spectrum at the incident electron energy of 12 eV and the scattering angle of 30^o is presented in Figure 4. Although with lower statistics, the first three excitation bands are resolved. The 3s band shows large contributions of the low lying triplet state.

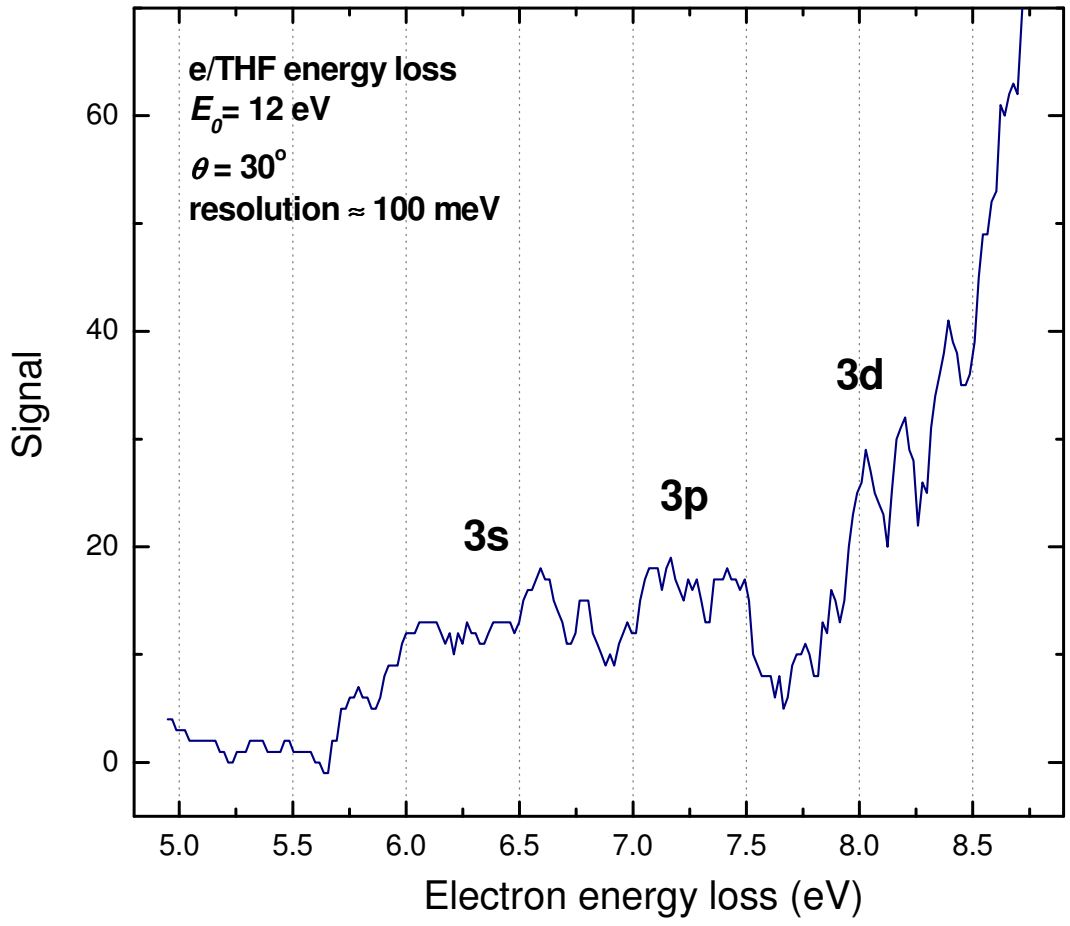

Figure 4. Electron energy loss spectrum of THF obtained at the incident electron energy of 12 eV and the scattering angle of 30^o.

Vibrational excitation

An excitation function obtained for vibrational modes which correspond to the C-H stretching modes (351 meV energy loss), at the scattering angle of 80° is presented in Figure 5. It shows several possible resonant processes in the incident electron energy region from 4.5 eV to 12 eV. Bouchiha *et al* [8] also predicted a number of core-excited resonances in this energy region. According to our knowledge, measurements of the excitation function of this vibrational mode of the gaseous THF has been reported only by Lepage *et al* [2] at 30° showing a resonance process centered at about 8.5 eV. Finally, note that recent measurements of the absolute total cross section for electron collisions with THF [5] also suggest several resonance processes in the energy range from about 4.5 to 10 eV, in a good agreement with the present preliminary result. Further measurements are presently in progress to investigate more accurately resonance positions in the vibrational channels.

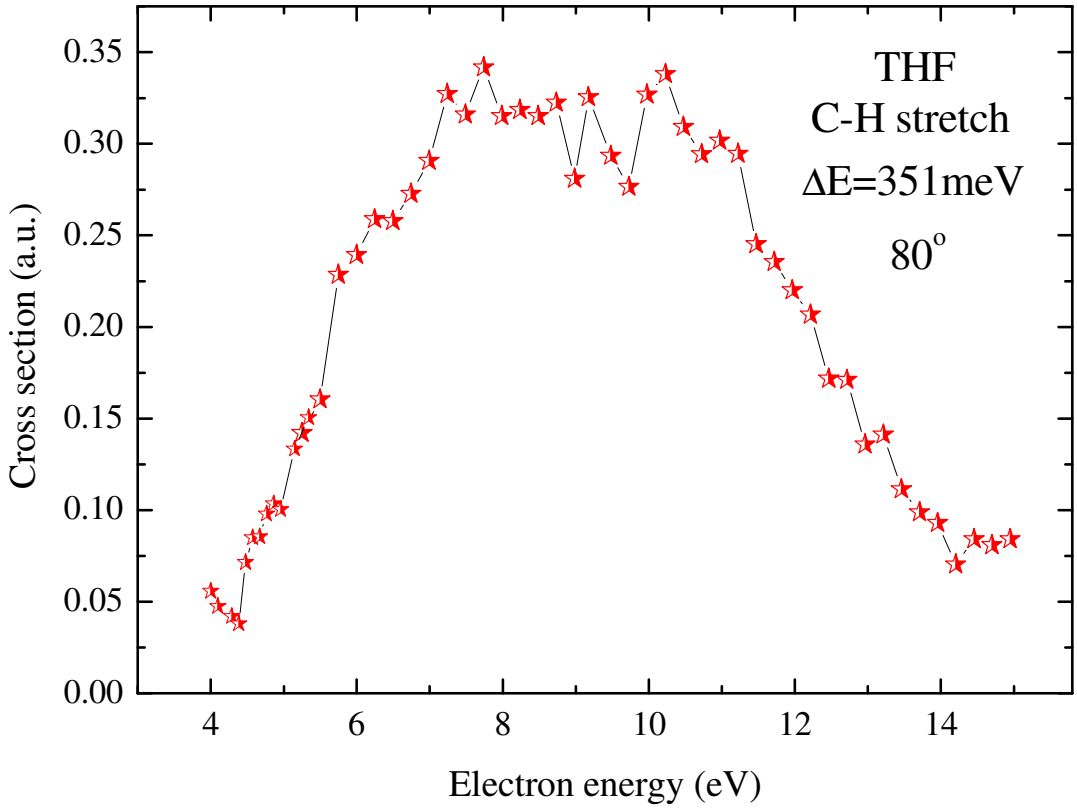

Figure 5. Excitation function of C-H stretching modes of THF (351 meV energy loss), at the scattering angle of 80°.

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

A paper focused to elastic low energy electron scattering from THF is being finalized. Further articles concerning vibrational and electronic excitation are also in preparation.

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