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# Biomolecules From Gas Phase Properties to Reactions relevant in Living Cells

Universitätszentrum Obergurgl (Oetz Valley, near Innsbruck) Austria 24-29 June 2006



EUROPEAN SCIENCE FOUNDATION





A European Science Foundation Research Conference in Partnership with Leopold-Franzens-Universität Innsbruck

# **Biomolecules**

# From Gas Phase Properties to Reactions relevant in Living Cells

Universitätszentrum Obergurgl (Oetz Valley, near Innsbruck), Austria

24 - 29 June 2006

## Chairs

Nigel J. Mason • The Open University, Milton Keynes, UK & Eugen Illenberger • Freie Universität Berlin, Germany

Dear Participants

Welcome to this the first conference held within the ESF high level research conference scheme in partnership with the Austrian Science Fund (SWF) and the Leopold Franzens Universitaet Innsbruck (LFUI).

The scope of the conference ranges from the investigation of gas phase molecules (building blocks of bio-molecules) to the study of molecules under micro-solvation to investigations of larger systems on substrates or in the liquid phase including processes in living cells. The invited lectures address state of the art experimental results including the underlying methods and techniques and progress in theory to describe the complex phenomena. In addition to contributions from established groups, a number of younger colleagues will have the opportunity to present their results in shorter oral contributions.

We welcome you all to what we hope will be an informative conference in a rapidly growing field of interdisciplinary research.

#### Low-energy electron interaction with tetrahydrofuran

### A. R. MILOSAVLJEVIC(1), I. Linert(2), B. Mielewska(2), B. P. Marinkovic(1) and M. Zubek(2)

#### (1) Institute of Physics, 11080 Belgrade, Serbia and Montenegro

(2) Department of Physics of Electronic Phenomena, Gdansk University of Technology,

## 80-952 Gdansk, Poland

We present experimental studies of low-energy electron collisions with tetrahydrofuran (THF) molecules in the gas phase. THF is considered to be the simplest prototype for investigations of electron interactions with deoxyribose molecules and further with the DNA sugar backbone, which are particularly of interest in radiation damage research.

The measurements were performed on a hemispherical electron spectrometer at Gdansk University of Technology. Both, monochromator and electron energy analyzer of the spectrometer incorporate two hemispherical energy selectors arranged in series and are equipped with systems of cylindrical lenses and deflectors. The incident electron beam is crossed at right angle with a target gas beam produced by a stainless still needle. The scattered electrons are detected by a single channel multiplier. The electron analyzer can be rotated around the target gas beam in the angular range from about –100 to 900. The range of accessible scattering angles is further extended up to 1800 by using magnetic angle-changer. The angular scale was calibrated against position of a minimum in the differential cross section (DCS) for elastic electron energy scale was calibrated with respect to positions of the 2P3/2,1/2 resonances in argon. In the present measurements the overall energy resolution of the spectrometer was about 90 meV. The experimental system allows measurements of the absolute DCSs using relative-flow method. The anhydrous THF was purchased from Aldrich with a declared purity >99.9% and was used after a few freeze-thaw cycles under vacuum.

In the present studies, we have measured absolute DCSs for elastic electron scattering by THF at the incident electron energy of 10 eV and in the angular range from  $20^{\circ}$  to  $180^{\circ}$ . The relative DCSs were obtained applying effective scattering volume correction with respect to elastic electron scattering in argon and helium. These relative DCSs were next normalized to absolute values obtained at a few scattering angles by using relative-flow method with helium as a reference gas. From the present absolute DCSs the elastic integral cross section (ICS) is obtained by integration after an extrapolation of the DCSs down to 00. The ICS obtained at 10 eV, which is approximately equal to the total cross section (TCS), appears to be somewhat above the TCS values recently measured by Zecca et al [A. Zecca, C. Perazzoli, M. J. Brunger, J. Phys. B: At. Mol. Opt. Phys. 38, 2079 (2005)]. We have also measured electron energy loss spectra in the energy loss region up to 1.2 eV, at an incident electron energy of 10 eV and at the scattering angles from 200 to 1800. In the spectra, an energy loss peak at 360 meV corresponding to excitation of the vibrational levels of the -CH2 stretch modes [M. Lepage, S. Letarte, M. Michaud, F. Motte-Tollet, M.-J. Hubin-Franskin, D. Roy, L. Sanche, J. Chem. Phys. 109, 5980 (1998)]) is clearly resolved. Using obtained elastic cross sections, absolute DCSs for vibrational excitation of the above levels are obtained in the angular region 20o-180o. We will also present preliminary results of elastic electron scattering from THF at different, fixed scattering angles, in the incident energy region from 5 eV to 12 eV. The aim of these measurements is to observe resonance states which have been recently predicted in their theoretical calculations by Bouchiha et al [D. Bouchiha, J.D. Gorfinkiel, L.G. Caron, L. Sanche, J. Phys. B: At. Mol. Opt. Phys. 39, 975 (2006)].