SCIENTIFIC REPORT

REFERENCE: Short Term Scientific Mission, EIPAM

TITLE: DISSOCIATIVE ELECTRON ATTACHMENT AND ELECTRON IMPACT IONISATION OF FURAN

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PERIOD: from **02.06.2005** to **12.06.2005.**

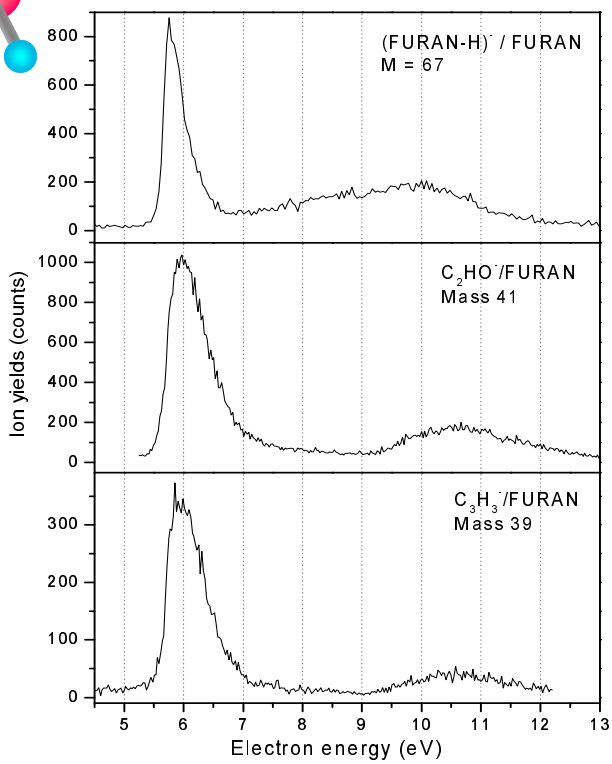
PURPOSE OF THE VISIT

The purpose of the visit was the investigation of inelastic interactions of low energy electrons with furan molecules in gas phase. In the measurements particularly formation of negative ions via (dissociative) electron attachment was investigated. Also electron impact ionization of furan and formation of positive ions were studied.

DESCRIPTION OF THE WORK CARRIED OUT

In the measurements a crossed beam apparatus for high resolution electron attachment and electron impact ionization studies is used [1,2]. It consists of a hemispherical electron monochromator, ion optics, a quadrupole mass filter and a gas inlet system. Negative ions formed by electron attachment to furan molecule are extracted from a collision chamber by a weak electric field and focused into a quadrupole mass filter. The energy scale and the energy resolution for negative ions are calibrated with respect to the resonance at 0 eV for electron attachment to SF_6 (for negative ions) and the ionization threshold of singly charged argon (for positive ions) equal to 15.76eV according to the National Institute of Standards and Technology [3]. The energy resolution is in the range of 100-135meV. Furan vapor (99% min. purity according to the manufacturer Sigma Aldrich) is introduced into the collision region at the base pressure of 3×10^{-6} mbar after several freeze-thaw cycles under vacuum. During the measurements the main chamber was kept at temperature of 85^{o}C.

DESCRIPTION OF THE MAIN RESULTS OBTAINED



Negative Ions

Electron attachment to the furan molecule leads to the formation of negative ions in the energy range from 0 to 14eV. In the mass spectrum the most dominant product is the [Furan – H]$^-$ anion (M = 67amu) but also two lighter fragments of masses M=41 and 39amu are present, that can be assigned to C_2HO^- and $C_3H_3^-$ respectively (Figure 1).

The ion efficiency curves for the observed ions are dominated by a relatively narrow and asymmetric resonance at 6eV followed by a broad structure in higher energy range (7.5-12eV for M=67amu, 9-12eV for M=41 and 39amu). It is worth noting that no zero eV resonance in the energy spectrum was observed. In addition, no parent anion [Furan]$^-$ is observed.

Figure 1. Efficiency curves for negative ions formed by dissociative electron attachment to furan.

Positive Ions

Figure 2 shows the mass spectrum of furan upon electron impact with an electron energy of 70eV. The most abundant ions are $C_3H_3^+$ (M=39amu), formed by loss of CHO, and the parent cation $C_4H_4O^+$ (M=68amu). The spectrum is in good agreement with the mass spectrum published in the NIST data base [3]. For the most abundant ions the ionization efficiency curves near the threshold are measured and the appearance energies are determined (figure 3). The presently determined

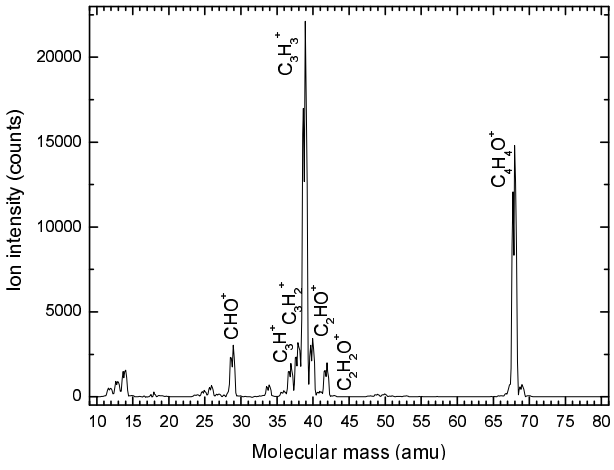


Figure 2. Mass spectrum of furan obtained by 70eV electron impact.

ionization energy agrees well with earlier published values obtained in electron impact experiments. The AE of $C_3H_3^+$ is 12.46eV and is (according to our knowledge) the first result obtained in electron impact experiment and stays in fairly good agreement with those from photoionisation and charge-exchange mass spectrometry.

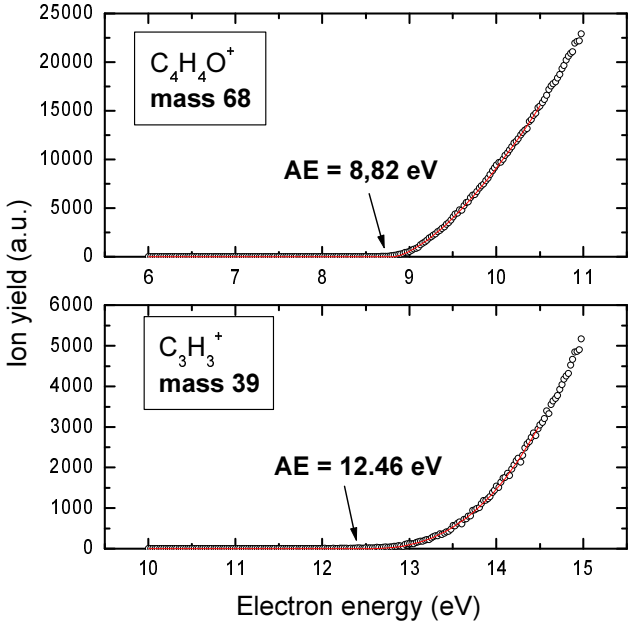


Figure 3. Ionisation efficiency curves near threshold for the formation of furan cations from neutral furan by electron impact.

Refences:

[1] Hanel G.et al. *Int. J. Mass Spectrom.* **205,** 65 (2001),

[2] Denifl S. et al. *J. Chem. Phys.* **120,** 6557 (2004),

[3] NIST chemistry webbook, http://webbook.nist.gov.

FUTURE COLLABORATION WITH HOST INSTITUTION

It is planned to continue the collaboration between our institutions in the area of electron impact spectroscopy, particularly related to biomolecules.

PROJECTED PUBLICATIONS RESULTING FROM THE GRANT

It is planed to publish the above mentioned results in a joined paper in an international journal.

Brygida Mielewska

GDAŃSK, 28.06.2005

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

Herewith I confirm that Dr. Brygida Mielewska successfully worked in the Institute of Ion Physics from June 2nd until June 12th 2005. The obtained results are interesting and this first contact between the participating institutions suggests further collaboration in the future. It was a pleasure to have Dr. Mielewska working in my group.

Innsbruck, June 29th 2005

Paul Scheier