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Research exchange programme for the stay at Berlin Freie Universität by Dr Grzegorz Karwasz, within ESF Electron-Induced Processes in Atoms and Molecules (EIPAM) Programme

Rapport for the exchange grant for the period 24. 01. 2005- 24. 04. 2005

Subject of the exchange:
"Electron-induced negative ion formation in molecules of biological interest"

Purpose of the visit

The main purpose of the visit was to study formation of negative ions and electron- driven reactions in molecules in the gas phase. The aim was to learn innovative techniques used at FU Berlin, in studies of chemical reactions initiated by electron attachment to single molecules and clusters.

Work carried out

The trainee worked essentially on two experiments: initially on electron trochoidal spectrometer for electron attachment to molecules in the gas phase and, mainly, on the experimental set-up for studies of electron attachment and mass spectroscopy of gas-phase clusters.

Some time has been dedicated to test and urgent adjustments of the set-up (diffusion pump, electron spectrometer, mass spectrometer) but majority for measurements of formic acid clusters with several scientific goals. These goals were: the check of preliminary data obtained in ICP-TC on this system, and the systematic search of the electron-scattering resonances in two energy regions - sharp structures below 2 eV, and wide resonances above 5 eV. Mass spectra at given electron energies evidenced the richness of the decay channels, ion-yields at variable electron energies indicate transient-negative ion resonances.

Preliminary studies of the acetic acid, also in fluorinated form were performed (the simplest amino-acid, glycine is based on it). Although negative ions were observed, no desired reaction channels have been reached.

Some research in the field of positron- induced chemistry, based on the experimental data obtained previously were done bye the trainee, with a paper submitted to a summary issue on Electron-Induced Chemistry by European J. Phys. D.

The trainee delivered two seminars at International PhD programme at ICP-TC
"Positrons - an Alternative Probe in Electron Scattering" (28.01.2005)
"Positrons - New Atomic Spectroscopy" (22.04.2005)

Results

Main results was identification of decay channels of transient negative ions of formic acid clusters with 1- 4 monomers. Decay channels vary with the attached electron collision energy. Low energy resonances leading to detachment of one H atom or formation of stable negative ions have been identified. Measurements with deuterated acid allowed to identify the chemical bond being preferentially cut. These results agree with the recent theory [2].

Detailed measurements for electron collision energies up to 15 eV allowed to identify additional decay channels, related to new resonances [2]. These data should allow refinements of the theory, as well. However, decay patterns of formic acid are complex, even for dimers, indicating regrouping of atoms within clusters after the attachment of electron. Some smaller fragments, say with the masses around 110 m.u. can come from regrouping of heavier clusters, like M_4^- but this hypothesis has to be verified.

Preliminary studies of acetic acid clusters were performed. Formation of negatively charged dimers was observed only in atmosphere of oxygen with high partial pressures and at temperatures below 0°C. Trials of reactions with NH_3 gave, for the moment, negative results.

The training result is learning on trochoidal spectrometers with superb energy resolution and new-generation mass spectrometers. Being inserted in the environment of Chemistry is also much acknowledged by the trainee who found it highly complementary to his previous curriculum.

Future plans

Additional 3 month exchange period, completing 6-month stay is planned. Measurements on acetic acid are to be finished in this period and further analysis of formic-acid data to be done. Some convergence with the theoretical works under way at trainee home institution (PAP) is planned.

Publications

Two publications concerning the subject of electron attachment and chemical reactions in formic-acid clusters have been prepared [1, 2], the first one being printed. Two more works, concerning previous subjects have been completed in Berlin and now are accepted for publication [3,4].

[1] Low energy electron driven reactions in single formic acid molecules (HCOOH) and their homogenous clusters, I. Martin, T. Skalicky, J. Langer, H. Abdoul- Carime, G. Karwasz, E. Illenberger, M. Stano and S. Matejcik, Phys. Chem. Chem. Phys. 2005, 7, 2212

[2] Modelling electron-induced processes in "condensed" formic-acid: resonant states of $(HCOOH)_2^-$ at low energies, F. Gianturco, R.R. Lucchese, E. Illenberger, I. Martin, T. Skalicky, J. Langer, G.P. Karwasz, Eur. J. Phys. D, submitted

[3] Positron scattering in helium: virtual - positronium resonances, G.P. Karwasz, D. Pliszka, A. Zecca, R.S. Brusa, Nucl. Instr. Meth. B, accepted

[4] Structural studies of titanium oxide multilayers, G.P. Karwasz, A. Miotello, E. Zomer, R.S. Brusa, B. Kościelska, C. Armellini, A. Kuzmin, Acta Phys. Pol., in print