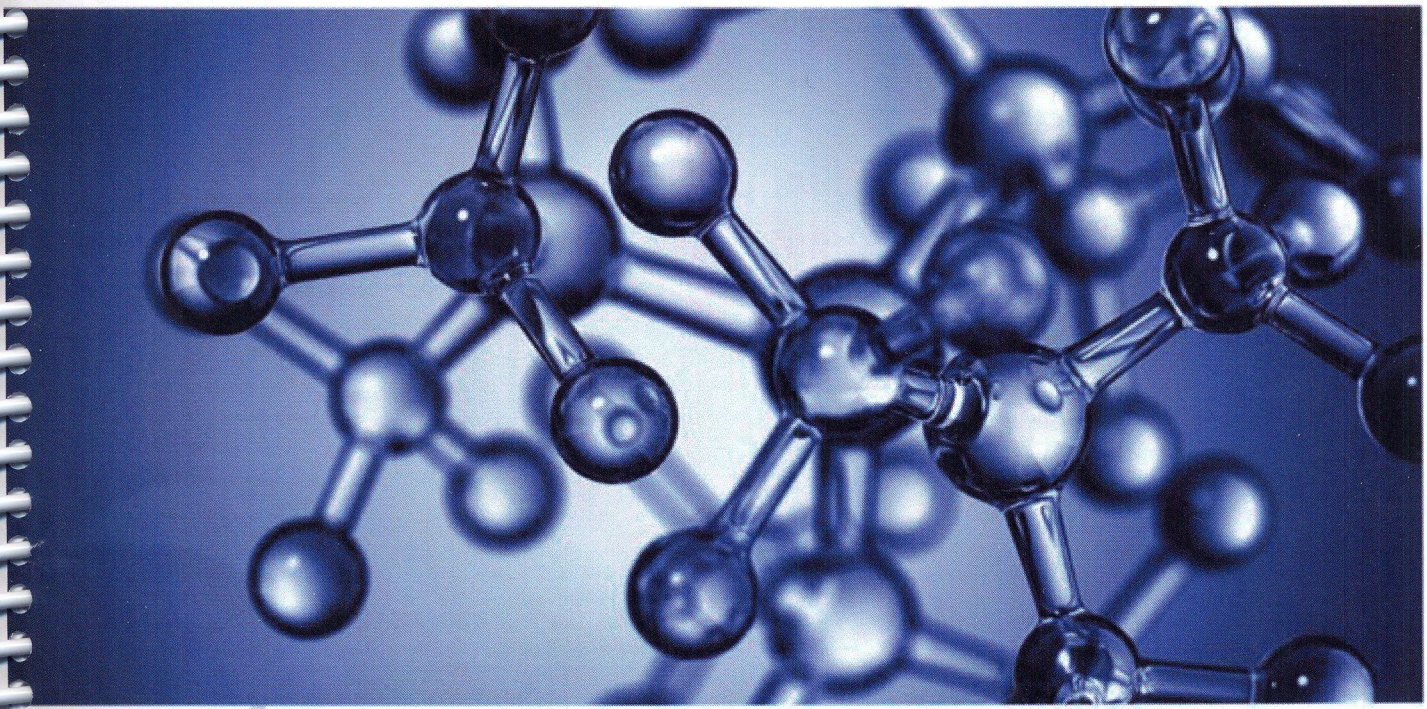
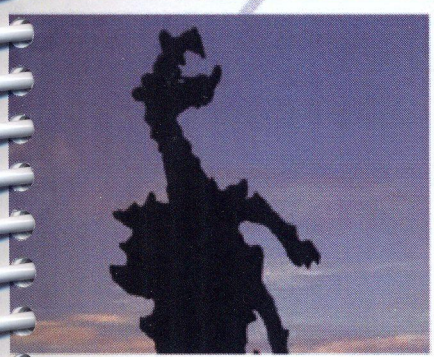
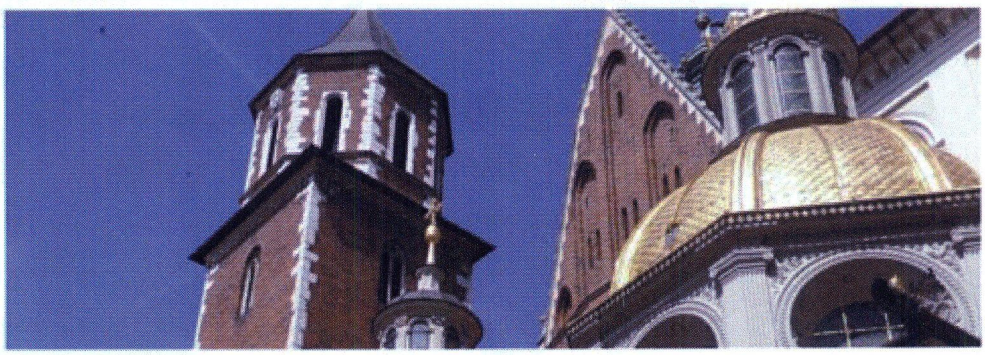
CELINA

cost
EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLO







The 3rd CELINA Meeting

Kraków, May 18-20, 2016

The third Annual Meeting of COST Action CM1301 – Krakow, May 18-20, 2016

is organized by Siedlce University of Natural Sciences and Humaniteis jointly with the Academic Centre for Materials and Nanotechnology of the AGH University of Science and Technology in Krakow:

Organizers:

International Organizing Committee:

Petra Swiderek (University of Bremen, DE)

Cornelis W. Hagen (Delft University of Technology, NL)

Nigel Mason (The Open University, UK)

Janina Kopyra (Siedlce University, PL)

Oddur Ingolfsson (University of Iceland, IS)

Sven Barth (Vienna University of Technology, AT)

Patrik Hoffmann (EMPA Thun, CH)

Ivo Utke (EMPA Thun, CH)

Roser Valenti (University of Frankfurt, DE)

Local Organizing Committee:

Janina Kopyra (Siedlce University)

Aleksandra Szkudlarek (ACMIN)

Katarzyna Berent (ACMIN)

Katarzyna Hnida (ACMIN)

Kamila Kollbek (ACMIN)

Oral contributions

Dissociative electron attachment to benzene chromium tricarbonyl

Jelena Maljković [1*], Paulina Maciejewska [2] and Janina Kopyra [2]

(1) Laboratory for Atomic Collision Processes, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

(2) Siedlce University, Faculty of Sciences, 3 Maja 54, 08-110 Siedlce, Poland

e-mail: jelenam@ipb.ac.rs

We have investigated dissociative electron attachment to benzene chromium tricarbonyl (M = $C_r(C_6H_6)CO_3$). This molecule was in our interest because it is a possible Focused Electron Beam Induced Dissociation (FEBID) precursor. Measurements were performed on experimental setup settled in Siedlce, Poland. Incident electron beam with energy resolution of FWHM ≈ 160 meV (in the present experiment), orthogonally intersects with the molecular beam resulting in dissociation and formation of fragments. The obtained action tandem mass spectra were performed for the energies from 0 eV to 14 eV, with 2 eV step. The compound showed a very rich fragmentation pattern. We have observed the following fragments: $[M - (CO)]^-$ (m/z 186), $[M - (CO)_2]^-$ (m/z 158), $[M - (CO)_3]^-$ (m/z 130), $[M - C_6H_6]^-$ (m/z 136), Cr^- (m/z 52), $[Cr(CO)_2]^-$ (m/z 108) and $[Cr(CO)]^-$ (m/z 80). Energy scan was performed for every fragment mentioned above (some anionic yields are shown in Fig.1). Quite high intensity of C_r^- has been noticed. SF_6 was introduced after every two energy scans, for checking the energy scale calibration.

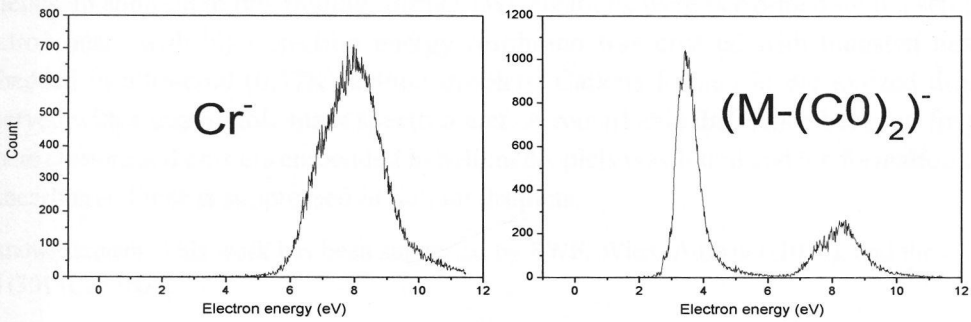


Fig. 1. Ion yield of Cr^- (52 a.m.u) and$(M-(CO)_2)^-$ (158 a.m.u) produced from electron impact on gaseous benzene chromium(0) tricarbonyl.

[1] C. Koenig-Lehmann, J. Kopyra, I. Dabkowska, J. Kočišek and E. Illenbergera, *Phys. Chem. Chem. Phys.* **14** (2008) 6954.

Excited States of $Pt(PF_3)_4$ and Their Role in Focused Electron-Beam Nanofabrication

Matija Zlatar [1,*], Michael Allan [2], and Juraj Fedor [3]

(1) Department of Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000, Belgrade, Republic of Serbia
(2) Departement of Chemistry, University of Fribourg, Fribourg, Switzerland
(3) J. Heyrovský Institute of Physical Chemistry, The Czech Academy of Sciences, Prague, Czech Republic

e-mail: matijaz@chem.bg.ac.rs

Electron-induced chemistry of metal-containing molecules is central in focused electron beam induced deposition (FEBID). While some elementary processes leading to precursor decomposition were quantitatively characterized, *e.g.* electronic excitation by electron impact [1], dissociative electron attachment (DEA) [2], electron-induced chemistry on the surfaces [3], data for neutral dissociation (ND) are missing. Here we provide an indication of how important is the ND channel in the model precursor $Pt(PF_3)_4$, tetrakis(trifluorophosphine)platinum(0).

We have utilized the density functional and time-dependent density functional theory based approaches to characterize ground end excited states for the $Pt(PF_3)_4$. The calculations revealed a number of phenomena, related to the nature of Pt-P bond, that can play a role in the electron-induced chemistry of this compound, *e.g.* a considerable increase of bond dissociation energy with a sequential removal of multiple ligands. The calculated electronically excited states were validated by the comparison with electron energy loss spectra [1]. >From the shape of the potential energy curves, it is concluded that the lowest excited states are dissociative, either directly or, via conical intersections. Taking into account typical electron energy distribution at the FEBID spot reveals that the importance of ND exceeds that of DEA in $Pt(PF_3)_4$. We thus established neutral dissociation as an important, albeit largely neglected, channel for FEBID using $Pt(PF_3)_4$ as a precursor. This conclusion is likely to apply to other precursors as well.

[1] M. Allan, *J. Chem. Phys.* **134** (2011) 204309.
[2] O. May, D. Kubala, M. Allan, *Phys. Chem. Chem. Phys.* **14** (2012) 2979.
[3] K. Landheer, S. G. Rosenberg, L. Bernau, P. Swiderek, I. Utke, C. W. Hagen, D. H. Fairbrother, *J. Phys. Chem. C* **115** (2011) 17452.

Design and performance of an instrument for gas phase electron spectroscopy of trapped molecular ions

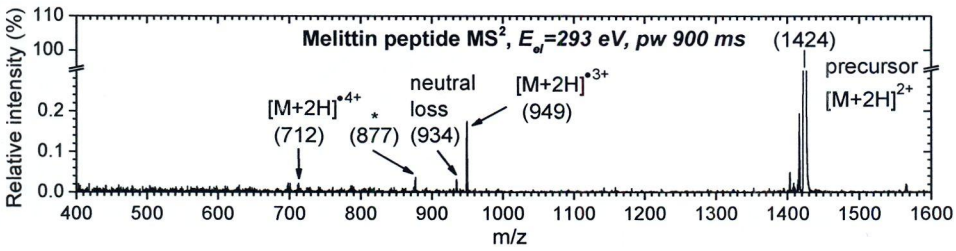
Miloš Lj. Ranković [1,*], Alexandre Giuliani [2,3] and Aleksandar R. Milosavljević [1,2]

(1) Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
(2) SOLEIL, l'Orme des Merisiers, St Aubin, BP48, 91192 Gif sur Yvette Cedex, France
(3) INRA, UAR1008, CEPIA, Rue de la Géraudière, BP 71627, 44316 Nantes, France

e-mail: mrankovic@ipb.ac.rs

The electron interaction with atoms and molecules in the gas phase, has been studied for more than a century [1]. Over the years, electrons are used to probe the fundamental properties of atoms and molecules, such as electronic structure and chemical reactivity. Particularly, inner-shell electron spectroscopy of gas phase molecules, found its application in a wide area of research fields [2].

Recently we have designed a new experimental setup [3], for electron impact tandem mass spectrometry and action spectroscopy of electrosprayed macromolecules, by coupling a focused electron gun with a commercial linear ion trap mass spectrometer. Herein, we discuss the experimental details of this setup and the electron beam tracing simulations performed in SIMION to investigate the propagation of 300 eV energy electrons inside the RF linear quadrupole ion trap. We present the first results of electron-induced dissociation of peptides, as well as possibilities to probe trapped CELINA precursor $SiOEt_4$ by electron impact.



[1] N. J. Mason, *J. Phys. Conf. Ser.*, **565** (2014) 012001.
[2] A. P. Hitchcock, *J. Electron Spectros. Relat. Phenomena*, **112** (2000) 9.
[3] M. Lj. Ranković, A. Giuliani, A. R. Milosavljević, *Appl. Phys. Lett.*, **108 (2016)**064101.