

SEMINÁŘ STUDENTŮ ÚFCH JH 2016



KC AV ČR v Liblicích
10.- 11.5. 2016



Seminář studentů ÚFCH JH 2016

Sborník příspěvků

**ze studentské konference konané
10. - 11. května 2016
v Konferenčním centru AV ČR Liblicích**

Seminar of Students of JHI 2016

Collection of abstracts

**of all lectures given at the student conference
held on 10 -11 May 2016
in Conference Centre of the Academy of Sciences
of the Czech Republic in Liblice chateau**

Seminář studentů ÚFCH JH 2016
Sborník příspěvků ze studentské konference
konané 10. - 11. května 2016
v Konferenčním centru AV ČR Liblicích

Kolektiv autorů

Sestavila: Květa Stejskalová

Vydává: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i. Dolejškova 2155/3,
182 23 Praha 8, Česká republika

Tisk: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i. Dolejškova 2155/3,
182 23 Praha 8

Vydání: první

Náklad: 45 kusů

Místo a rok vydání: Praha, 2016

Publikace neprošla jazykovou úpravou

© Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i.

Seznam prezentujících studentů (28)

Kategorie I (17)

Diplomanti, magistři a zájemci z řad bakalářů (12)

Brandejs Jan

(magistr, MFF UK, školitel J. Pittner)

Guricová Miroslava

(diplomantka, VŠCHT, školitel J. Ludvík)

Jurková Kateřina

(magistr, PřF UK, školitel M. Kalbáč)

Kantnerová Kristýna

(diplomantka, VŠCHT, školitel J. Ludvík)

Knížek Antonín

(bakalář, PřF UK, školitel M. Ferus)

Obluková Michaela

(diplomantka, PřF UK, školitel J. Žabka)

Pastorek Adam

(diplomant, FJFI ČVUT, školitel S. Civiš)

Pižl Martin

(diplomant, VŠCHT, školitel S. Zálíš)

Ráhová Jaroslava

(diplomantka PřF UK, školitel O. Frank)

Sedlecká Lucie

(bakalářka, VŠCHT, školitel M. Hromadová)

Šimaňok Lukáš (bakalář, VŠCHT, stáž u J. Rathouského a R. Žouželky)

Šmídová Daniela

(magistr, VŠCHT, školitel M. Fárník)

Studenti 1. ročníku PGS (5)

Antalík Andrej (školitel J. Pittner)

Grygoryeva Kateřina (školitel M. Fárník)

Hrdlička Vojtěch (školitel T. Navrátil)

Makrlíková Anna (školitel T. Navrátil)

Skalová Štěpánka (školitel T. Navrátil)

Kategorie II (11)

Studenti 2. ročníku PGS (5)

Dostál Michal (školitel Z. Zelinger)

Kasneryk Valeryia (školitel M. Opanasenko)

Křížová Věra (školitel M. Polášek)

Lang Jakub (školitel J. Pittner)

Supíňková Taťána

(školitel M. Kočířík a P. Hrabánek)

Studenti 3. ročníku PGS (4)

Guerra Valentino L. P. (školitel M. Kalbáč)

Melcrová Adéla (školitel M. Hof)

Liška Alan (školitel J. Ludvík)

Pastvová Jana (školitel P. Sazama)

Studenti 4. ročníku PGS (2)

Koukalová Alena (školitel R. Šachl)

Mazur Michal (školitel J. Čejka)

Hodnotící komise:

Martin Srnec (předseda)

Juraj Fedor

Romana Sokolová

Edyta Tabor



SEMINÁŘ STUDENTŮ ÚFCH JH 2016

PROGRAM 1. dne konference - úterý 10.5.2016

Odjezd autobusem z parkoviště před ústavem v 8:30 hodin.

*Předpokládaný příjezd do Konferenčního centra AV ČR v zámku
v Liblicích okolo 9:30 hodiny.*

Čas	Předsedající	Přednášející	Název
9:30-10:15	OBČERSTVENÍ PŘED ZAHÁJENÍM KONFERENCE <i>(káva, nápoje, zákusek - v 1. patře, na ochozu)</i>		
10:20	Zahájení konference „Seminář studentů ÚFCH JH 2016“		
10:30	<u>Michal</u> <u>Mazur</u>	Kristýna KANTNEROVÁ <i>(diplomantka, školitel J. Ludvík) kat. I</i>	EFFECTS OF INTRAMOLECULAR ELECTRON INTERACTIONS OF THREE ISOMERIC BENZENEDIALDEHYDES ON THEIR ELECTROCHEMICAL REDUCTION
10:50		Lukáš ŠIMAŇOK <i>(bakalář, školitel J. Rathouský a R. Žouželka) kat. I</i>	VLIV ROZPOUŠTĚDLA NA VELIKOST VZNIKLÝCH NANOČÁSTIC REDUKCÍ V NEVODNÉM PROSTŘEDÍ TETRAHYDRIDOBORITANEM SODNÝM
11:10		Daniela ŠMÍDOVÁ <i>(magistr, školitel M. Fárník) kat. I</i>	PROCESY VE VODNÍCH NANOČÁSTICÍCH ZA PŘÍTOMNOSTI DUSÍKATÝCH MOLEKUL
11:30		Miroslava GURICOVÁ <i>(diplomantka, školitel J. Ludvík) kat. I</i>	KOMPLEXY PRECHODNÝCH KOVOV S REDOXNE AKTÍVNÝMI LIGANDMI ODVODENÝMI OD VITAMÍNU B6
11:50	PŘESTÁVKA		
12:10	<u>Věra</u> <u>Křížová</u>	Kateřina GRYGORYEVA <i>(I. ročník PGS, školitel M. Fárník) kat. I</i>	HOW TO SEE A SINGLE QUANTUM STATE ROTATIONAL WAVEFUNCTION AND ITS EVOLUTION IN REAL TIME: IMAGING EXPERIMENTS
12:30		Anna MAKRLÍKOVÁ <i>(I. ročník PGS, školitel T. Navrátil) kat. I</i>	DETERMINATION OF TUMOR MARKERS USING SCREEN-PRINTED ELECTRODES
12:50		Jan BRANDEJS <i>(magistr, školitel J. Pittner) kat. I</i>	OPTIMIZING QUANTUM SIMULATIONS AND THE DMRG METHOD
13:10		Vojtěch HRDLIČKA <i>(I. ročník PGS, školitel T. Navrátil) kat. I</i>	HOLLOW FIBRE MICROEXTRACTION AND VOLTAMMETRIC DETECTION OF HOMO VANILLIC AND VANILLYLMANDELIC ACID
13:30	Ukončení dopolední sekce (kat I)		
13:45-15:25	OBĚD (podává se v restauraci v přízemí a v rámci přestávky na oběd si účastníci zajistí UBYTOVÁNÍ v recepci hotelu)		

15:30	<u>Jana</u> <u>Pastvová</u>	Andrej ANTALÍK (<i>I. ročník PGS, školitel J. Pittner</i>) kat. I	COUPLED CLUSTER METHOD WITH SINGLE AND DOUBLE EXCITATIONS TAILORED BY MATRIX PRODUCT STATE WAVE FUNCTIONS
15:50		Štěpánka SKALOVÁ (<i>I. ročník PGS, školitel T. Navrátil</i>) kat. I	DEVELOPMENT OF DNA BIOSENSOR TO STUDY INTERACTIONS OF 2 NITROFLUORENE WITH DNA
16:10		Adam PASTOREK (<i>diplomant, školitel S. Civiš</i>) kat. I	FTIR EMISSION SPECTRA OF NOBLE GASES IN RYDBERG STATES PRODUCED IN DISCHARGE PLASMA
16:30		Lucie SEDLECKÁ (<i>bakalářka, školitel M. Hromadová</i>) kat. I	GUNSHOT RESIDUES ANALYSIS BY MEANS OF ELECTROCHEMICAL METHODS
16:50	PŘESTÁVKA NA KÁVU (<i>1.patro, ochoz</i>)		
17:30	<u>Valeryia</u> <u>Kasneryk</u>	Antonín KNÍŽEK (<i>bakalář, školitel M. Ferus</i>) kat. I	PHOTOCATALYTIC TRANSFORMATION OF NEUTRAL CARBON DIOXIDE-RICH PALEOATMOSPHERE TO REDUCTION GASES ON MINERAL SURFACES
17:50		Jakub LANG (<i>II. ročník PGS, školitel J. Pittner</i>) kat. I	STUDY OF TRIMETHYLENE SYSTEM AND BICYCLOBUTADIENE ISOMERIZATION: INVESTIGATION OF A POSTERIORI USS-D CORRECTION
18:10		Alena KOUKALOVÁ (<i>IV. ročník PGS, školitel R. Šachl</i>) kat. II	BIOPHYSICAL CHARACTERIZATION OF LIPOPEPTIDES INVOLVED IN MEMBRANE FUSION
18:30	Ukončení prvního dne konference VEČEŘE v RESTAURACI - začátek v 18:45		

PROGRAM 2. dne konference - *středa 11.5.2016*

Čas	Předsedající	Přednášející	Název
8:05	Zahájení druhého dne konference - pokračují prezentace studentů kategorie I a II.		
8:10	<u>Alan</u> <u>Liška</u>	Jaroslava ŘÁHOVÁ (<i>magistr, školitel O. Frank</i>) kat. I	PRESTRESS INDUCED GRAPHENE WRINKLING
8:30		Martin PIŽL (<i>diplomant, školitel S. Zálíš</i>) kat. I	VIBRATIONAL SPECTRA OF TRANSITION METALS COMPLEXES CONTAINING LIGANDS DERIVED FROM VITAMIN B6: INTERPRETATION USING DFT METHOD
8:50		Věra KŘÍŽOVÁ (<i>II. ročník PGS, školitel M. Polášek</i>) kat. II	ION-INDUCED IONIZATION AND DISSOCIATION OF ORGANIC MOLECULES BY keV PROJECTILE IONS
9:10		Valeryia KASNERYK (<i>II. ročník PGS, školitel M. Opanasenko</i>) kat. II	UOV GERMANOSILICATE IN THE ADOR STRATEGY. SYNTHESIS OF NEW ZEOLITE IPC-12
9:30	PŘESTÁVKA NA KÁVU (<i>1.patro, ochoz</i>)		
10:00		Kateřina JURKOVÁ (<i>magistr, školitel M. Kalbáč</i>) kat. I	RAMAN SPECTROSCOPY AND SPECTROELECTROCHEMISTRY OF SINGLE-LAYER MOS ₂

10:20	<u>Kristýna</u> <u>Kantnerová</u>	Michaela OBLUKOVÁ (diplomantka, školitel J. Žabka) kat. I	STANOVENÍ NOVÝCH SYNTETICKÝCH DROG V MOČI METODOU LC-MS/MS
10:40		Taťána SUPÍŇKOVÁ (II. ročník PGS, školitel M. Kočířík a P. Hrabánek) kat. I	SYNTHESIS ROUTES TO ZEOLITE SSZ-16 CRYSTALS AND SUPPORTED LAYERS
11:00	PŘESTÁVKA		
11:20	<u>Adéla</u> <u>Melcrová</u>	Michal DOSTÁL (II. ročník PGS, školitel Z. Zelinger) kat. II	PHOTOACOUSTIC DETECTION OF GASES USING MICROMECHANICAL ELEMENTS
11:50		Valentino Libero Pio GUERRA (III. ročník, školitel M. Kalbáč) kat. II	GRAPHENE - PEROVSKITE COMPOSITE, MONOLAYER APPROACH
12:10		Jana PASTVOVÁ (III. ročník PGS, školitel P. Sazama) kat. II	PREPARATION OF HIERARCHICAL MORDENITE ZEOLITES WITH TAILORED TEXTURE AND ACCESSIBILITY OF ACID SITES
12:30	PŘESTÁVKA NA OBĚD (podává se v restauraci od 12:30 do 14 hodin)		
14:00	<u>Jakub</u> <u>Lang</u>	Alan LIŠKA (III. ročník PGS, školitel J. Ludvík) kat. II	CALIX[4]ARENE TETRARADICAL TETRAANION – AN ELECTROCHEMICALLY GENERATED LIGAND
14:20		Adéla MELCROVÁ (III. ročník, školitel M. Hof) kat. II.	INFLUENCE OF CHOLESTEROL ON Ca ²⁺ INTERACTION WITH PHOSPHOLIPID MEMBRANES
14:40		Michal MAZUR (IV. ročník, školitel J. Čejka), kat. II.	SYNTHESIS OF UNFEASIBLE ZEOLITES
15:00-	PŘESTÁVKA NA KÁVU (1.patro, ochoz)		
15:45- 16:15	15:45 - SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ SOUTĚŽNÍ KONFERENCE - V KONFERENCEČNÍM SÁLE UKONČENÍ KONFERENCE		
16:15	Odjezd do Prahy - autobusem z parkoviště u zámku v 16:30 (autobus bude přistaven na 16:15)		





COUPLED CLUSTER METHOD WITH SINGLE AND DOUBLE EXCITATIONS TAILORED BY MATRIX PRODUCT STATE WAVE FUNCTIONS

Mgr. Andrej Antalík

doc. Mgr. Jiří Pittner, Dr. rer. nat., DSc.

We present a method for accurate treatment of strongly correlated systems, which combines the coupled cluster (CC) theory with the density matrix renormalization group (DMRG) method. The connection between the two is carried out utilizing the tailored CC approach of Kinoshita et al.

Firstly, the configuration interaction (CI) coefficients corresponding to single and double excitations within the DMRG active space are computed by efficient contraction of the matrix product state (MPS) matrices. The coefficients are then transformed into CC amplitudes, which are subsequently used to “tailor” a single reference CCSD method. As a result, the DMRG method is responsible for proper description of non-dynamic correlation, while the dynamic correlation is incorporated by means of the CC theory.

We illustrate the method on prominent multi-reference model systems like N_2 or Cr_2 .

References:

J. Gauss, Coupled cluster theory, in *The Encyclopedia of Computational Chemistry*, edited by P. v. R. Schleyer et al., pp. 615-636, Wiley, Chichester, 1998.

S. Szalay et al., *Int. J. Quant. Chem.* **2015**, 115, 1342.

T. Kinoshita, O. Hino, and R. J. Bartlett, *J. Chem. Phys.* **2005**, 123, 074106.



OPTIMIZING QUANTUM SIMULATIONS AND THE DMRG METHOD

Bc. Jan Brandejs

doc. Mgr. Jiří Pittner, Dr. rer.nat, DSc.

“In the year 1992, S. R. White introduced a very powerful numerical method, the density-matrix renormalization group (DMRG). It allows us to determine the physical properties of low-dimensional correlated systems such as quantum spin chains or chains of interacting itinerant electrons to unprecedented accuracy.” [1]

We investigate the quantum information theoretical aspects of simulation of quantum systems on classical computers, in particular how the many-electron strongly correlated wave functions can be most effectively approximated by a lossy compression of quantum information.

For this purpose, we describe the measures of quantum entanglement for the density matrix renormalization group method. We implement the computation of multi-site generalization of mutual information within the DMRG method and investigate entanglement patterns [2] arising from strong electron correlation in chemical systems.

The theoretical conclusions are supported by numerical simulations of molecules exhibiting chemically interesting electronic structure, like e.g. aromatic systems or polyradicals.

In this lecture, I will give a brief talk on principles of the DMRG method. Then I'll explain the quantum informational motivation behind our quantum chemical calculations and present preliminary results.

References:

[1] Szalay, S., Legeza, O.; Tensor product methods and entanglement optimization for ab initio quantum chemistry, *Int. J. Quant. Chem.* **2015**, *115*, 1342-1391.

[2] Barcza, G., Noack, R.M.; Entanglement patterns and generalized correlation functions in quantum many-body systems, *Phys. Rev. B* **2015**, *92* (12), 125-140.



PHOTOACOUSTIC DETECTION OF GASES USING MICROMECHANICAL ELEMENTS

Ing. Michal Dostál

prof. Ing. Zdeněk Zelinger, CSc.

Photoacoustic spectroscopy (PAS) is a method in which the light source energy is converted first sound and then to an electrical signal.¹ This method can be used for quantitative chemical analysis at ultra-low concentrations of gaseous species or samples with low absorption coefficient. These studies deal with two selected modifications of classical photoacoustic methods (employing microphone as pressure wave sensor) oriented towards increased sensitivity, selectivity as well as cost reduction of practically applicable gas sensing systems.

Multilayer graphene (MLG) membrane or cantilever represent one option in order to reach enhanced performance of PAS method. Graphene layers were chosen primarily because of their mechanical properties and the ability to create very thin membrane or cantilever. Several samples of membranes and cantilevers were prepared from highly ordered pyrolytic graphite (HOPG). Such MLG membranes/cantilevers were implemented into experimental setup of PAS and utilised for measuring a pressure wave impulse following the absorption of CO₂-laser pulse in the photoacoustic cell (filled with methanol traces in air)². Amplitude of deformation relevant to these micromechanical components is evaluated using "optical microphone"³ which consists of position sensitive detector responding to movement of reflected He-Ne laser beam.

So called Quartz enhanced photoacoustic spectroscopy (QEPAS).⁴ is another feasible way to achieve sub-ppb level trace gas detection. Moreover, Quantum cascade lasers (QCLs) offer the possibility to use the spectral fingerprints of gas-phase molecules studied and thus to perform highly selective PAS detection in mid-infrared (MIR) region. Case specific design of the photoacoustic cell and experimental setup for the purposes of QCL-QEPAS detection is finally reported within this work.

References:

- ¹ Pao, Yoh-Han (ed.). *Optoacoustic spectroscopy and detection*. New York: *Academic Press*, 1997.
- ² Zelinger, Z., et al. Silicon micro-levers and a multilayer graphene membrane studied via laser photoacoustic detection. *Journal of Sensors and Sensor Systems*, 2015, 4.1: 103.
- ³ Kuusela, Tom; Kauppinen, Jyrki. Photoacoustic gas analysis using interferometric cantilever microphone. *Applied Spectroscopy Reviews*, 2007, 42.5: 443-474.
- ⁴ Kosterev, A. A., et al. QEPAS for chemical analysis of multi-component gas mixtures. *Applied Physics B*, 2010, 101.3: 649-659.



HOW TO SEE A SINGLE QUANTUM STATE ROTATIONAL WAVEFUNCTION AND ITS EVOLUTION IN REAL TIME: IMAGING EXPERIMENTS

Ing. Kateřina Grygoryeva

Mgr. Michal Fárník, Ph.D., DSc.

Velocity map imaging (VMI) is a powerful technique used in various fields of molecular physics and dynamics. In our laboratory, we apply this method to study chemical reactions induced by light irradiation, such as photodissociation. VMI not only enables to detect the selected fragments emerging from the dissociating molecules, it also allows us to record the velocities of the fragments. The magnitude of the velocity reflects the energy released during the process, while the direction speaks about the anisotropy of the photodissociation process. These two properties provide us a detailed insight into the photodissociation.

Using a linearly polarized UV light, the photodissociation maps the molecular rovibrational wavefunction directly onto the H-fragment spatial distribution. In molecular beams, which are usually used in the VMI experiments, molecules in the vibrational ground state are present. However, they populate several rotational J, M states. When such an ensemble is photodissociated, spatial distributions of molecules in different rotational J, M states overlap to give an unresolved spatial distribution. However, the situation will radically differ, if we prepare the molecules in a single rovibrational state.

In our experiments, we were able to excite a single rovibrational transition prior to photodissociation. Thus recording this fragment spatial distribution by the VMI technique provided a direct visualization of the wave function. Besides this, using a pump (IR)-probe (UV) technique we can demonstrate phasing-dephasing due to the coupling between the molecular rotation and the nuclear spin of Cl with a period of 60 ns [1]. This experiment is a beautiful showcase of a simple quantum effect and its dynamical evolution, and is its first real experimental visualization.

Acknowledgement: Grant GACR 14-14082S

References:

[1] D. Sofikitis, L. Rubio-Lago, M.R. Martin, et al., *J. Chem. Phys.* **127**, 1 (2007).



GRAPHENE - PEROVSKITE COMPOSITE, MONOLAYER APPROACH

Valentino Libero Pio Guerra

RNDr. Ing. Martin Kalbáč, Ph. D.

Organic-inorganic hybrid perovskite have been widely used recently for application in the photovoltaic field achieving high performances in very short time compared to the other materials for solar cells (up to 22.1% Power Conversion Efficiency in 4 years)^{1,2}. This fast development however still lacks in some fundamental understanding on the photophysical processes occurring at the interface of perovskite – charge transporting material. During my PhD at University of Salento (Lecce, Italy) I was studying the dynamics of these processes (charge generation, transport, recombination) using spectroscopic and transient techniques like photoinduced absorption (PIA) and transient photovoltage (TPV). To zoom in what is happening at the interfaces I studied the interaction between the charge generating material (perovskite) and charge transporting material in their monolayer form. To do this I have chosen to use as transporting layer the graphene (known 2D material with high conductivity) and a “2D” structure of perovskite.³

In this lecture, I will focus on the approach used to make this composite as a simple junction made by two monolayers (one of graphene and one of perovskite) and its characterization.

References:

1 Henry J. Snaith, *J. Phys. Chem. Lett.*, **2013**, 4 (21), pp 3623–3630

2 NREL chart of the National Center for Photovoltaics, <http://www.nrel.gov/ncpv/>

3 Letian Dou *et al.*, *Science*, **2015**, 349 (6255), 1518-1521



KOMPLEXY PRECHODNÝCH KOVOV S REDOXNE AKTÍVNÝMI LIGANDMI ODVODENÝMI OD VITAMÍNU B6

Bc. Miroslava Guricová

Ing. Irena Hoskovcová, CSs.

Schiffove bázy vznikajú kondenzáciou aldehydu s amínmi. V živých systémoch sú Schiffove bázy medzistupňom transaminačného procesu. Dôležitú úlohu pri tvorbe Schiffových báz zohrávajú ióny ľahkých prechodných kovov. Ako modelové kovy boli vybrané Ni(II), Co(II) a Cu(II).

Študované ligandy boli pripravené zo salicylaldehydu (SAL), pyridoxalu (PL) a amínu taurínu (Tau) a aminokyseliny alanín (Ala). Ligandy PL-Tau, PL-Ala, PLP-Tau, PLP-ala, SAL-Tau boli izolované a charakterizované CHNS analýzou, ^1H NMR, IR a UV-Vis spektroskopiou. Ich správanie bolo sledované elektrochemicky, pomocou cyklickej voltametrie a polarografie. Interakciu ligandov a kovov v roztoku sme sledovali metódou kontinuálnych variácií, určili sme stechiometriu komplexov vznikajúcich v roztoku, na základe čoho sme odvodili pomer reaktantov pri syntéze komplexov. Komplexy boli pripravované templátovou syntézou octanov kovov s neizolovanými ligandmi a bázou KHCO_3 . Komplexy boli izolované a charakterizované CHNS analýzou, IR spektroskopiou, RTG analýzou a cyklickou voltametriadou a polarografiou. V prípade PL-Tau vznikli komplexy $[\text{Ni}(\text{PL-Tau})_2(\text{H}_2\text{O})_2]$ a $[\text{Cu}(\text{PL-Tau})_2(\text{H}_2\text{O})_2]$ so zhodnou štruktúrou, avšak stechiometria izolovaného komplexu je odlišná od stechiometrie komplexu v roztoku.



HOLLOW FIBRE MICROEXTRACTION AND VOLTAMMETRIC DETECTION OF HOMOVANILLIC AND VANILLYLMADELIC ACID

Mgr. Vojtěch Hrdlička

Doc. Dr. Ing. Tomáš Navrátil

Homovanillic acid (HVA) and vanillylmandelic (VMA) acid are end-stage metabolites of dopamine and epinephrine in human body. These compounds are biomarkers of various neurological, metabolic and oncological disorders, e.g. neuroblastoma, the most common extracranial cancer in infants. The determination of HVA and VMA in human fluids is important for clinical applications as well as for large scale pre-emptive screenings.

Hollow fibre microextraction is a relatively new method for biological sample preparation. The hollow fibres are typically made from thin porous polypropylene (pore diameter 0.2 μm). The fibre serves either as a separator between phases (e.g. water/1-octanol) in two phase extraction, or more commonly, as a carrier of a water immiscible liquid membrane. Utilization of liquid membrane in a three-phase system features low consumption of organic phase and possible extraction of ionisable species into aqueous phase. Acidic species are extracted from acidic solution through organic liquid membrane to the basic solution inside the fibre. The aqueous extract is also convenient for subsequent voltammetric detection.

The lecture presents possibilities of HVA and VMA hollow fibre microextraction followed by voltammetric detection. Various aspects of extraction and determination of HVA/VMA in very small volumes or inside the fiber itself will be discussed, including suitable liquid membranes, electrode materials and experimental setup.

References:

Eisenhofer, G.; Kopin I. J.; Goldstein G. S. *Pharm Rev.* **2004**, 56, 331-349.

Monsaingeon, M.; Perel, Y.; Simonnet, G. *Eur J Pediatr.* **2003**, 162, 397-402.

Lee, J. Y.; Lee, H. K.; Rasmussen, K. E. *Anal Chim Acta.* **2008**, 624, 253-268.



RAMAN SPECTROSCOPY AND SPECTROELECTROCHEMISTRY OF SINGLE-LAYER MoS_2

Bc. Kateřina Jurková

RNDr. Ing. Martin Kalbáč, PhD.

Various two dimensional nano-materials have recently attracted plenty of interest. Apart from graphene also various layered dichalcogenides such as MoS_2 are studied for their interesting properties in nano-scale.

MoS_2 layers can be characterized by optical microscopy, Raman spectroscopy and atomic force microscopy (AFM). Especially Raman spectroscopy has proven to be a very effective tool for characterization of various layered materials because it is non-invasive and can provide us with many information concerning the electronic structure of the studied material. Moreover Raman spectroscopy can be rather easily combined with other methods.

The main prospective future application of both graphene and *single-layer* MoS_2 is in electronic devices. Therefore it is necessary to find out more about their behavior in electric field. In this study we report on the investigation of *single* and *few-layers* MoS_2 , which were fabricated by exfoliation from bulk MoS_2 , detected with optical microscopy and characterized with Raman spectroscopy and AFM measurements. We prepared $\text{MoS}_2/\text{CVD-graphene}$ sandwich layers and studied the prepared layers using in-situ Raman spectroelectrochemistry, which allowed us precise and well-controlled doping of carbon materials.



EFFECTS OF INTRAMOLECULAR ELECTRON INTERACTIONS OF THREE ISOMERIC BENZENEDIALDEHYDES ON THEIR ELECTROCHEMICAL REDUCTION

Bc. Kristýna Kantnerová

prof. RNDr. Jiří Ludvík, CSc.

My contribution is dealing with electrochemical reduction of three isomeric benzenedialdehydes – orthophthalaldehyde (OPA), isophthalaldehyde (IPA) and terephthalaldehyde (TPA). These aromatic substances have different electrochemical behaviour due to diverse induction and resonance interactions caused by intramolecular electron communication of both carbonyl groups. In the literature their redox behaviour is described only in aqueous media because OPA is used as derivatization agent in determination of amino acids or as disinfecting solution in the form of aqueous solution.

Its antimicrobial effect is assumed to be due to the interaction with free nucleophilic centers of amino acids built in peptidic chains (nucleophilic groups in side chains of AAs and amino-termini) and of membrane molecules (primary amines, thiols). [1] The disinfecting effect of OPA is generally also explained by reversible hydration including the change between hydrophilic hydrated form (outside or inside a cell) and lipophilic unhydrated form (inside a lipid bilayer) which brings the ability to cross the cell membrane and to interact with the nucleophilic content of the cell (peptides, RNA, DNA) [2]. Therefore OPA can be present also in the non-aqueous environment (lipid bilayers, adipocytes). However, electrochemistry of benzenedialdehydes in non-aqueous aprotic media has not been published yet. To fill this gap, the present work is focused on the investigation of cathodic reduction of benzenedialdehydes in non-aqueous acetonitrile and dimethylformamide and the results are compared with those in aqueous buffered solutions. For comparison the methylated analogues (1,2-diacetylbenzene, 1,3-diacetylbenzene and 1,4-diacetylbenzene) were also studied under the same conditions.

The compounds have been studied using cyclic voltammetry (CV), polarography, coulometry, preparative electrolyses, UV/Vis spectrophotometry, UV/Vis spectro-electrochemistry and electron paramagnetic resonance (EPR) coupled with electrolysis. The attempt to identify products of electrochemical reduction using NMR spectroscopy and HPLC coupled with MS was not fully successful. This work is a part of my diploma thesis at University of Chemistry and Technology, Prague.

References:

[1] Simoes, M. J. *Basic Microbiol.* **2007**, *47*, 230–242.

[2] Zhu, P. C.; Roberts, C. G.; Favero, M. S. *Curr. Org. Chem.* **2005**, *9*, 1155–1166.



UOV GERMANOSILICATE IN THE ADOR STRATEGY. SYNTHESIS OF NEW ZEOLITE IPC-12

Mgr. Valeryia Kasneryk

Dr. Maksym Opanasenko

Zeolites are microporous materials with well-defined structure formed by TO_4 tetrahedra ($T=Si, Al, Ge, \text{etc.}$). These materials are widely applied in heterogenous catalysis, adsorption and separation. Although the millions of zeolite structures were theoretically predicted, just about 230 structures were synthesized up to date, mainly via hydrothermal conditions¹.

In the last few years the *Assembly-Disassembly-Organization-Reassembly* (ADOR) methodology for zeolite synthesis was developed. The ADOR approach was firstly applied for zeolite UTL resulting in the synthesis of a set of new zeolite materials¹⁻³. This work is devoted to the development of the ADOR approach on another germanosilicate – **UOV**.

The tunable *Disassembly* of UOV zeolite was performed under acidic conditions. Following condensation of produced 2D material led to the *Reassembly* and, thus, to the formation of new zeolite material **IPC-12** possessing the same topology of the layers as UOV. The formation of new material was confirmed by the results of theoretical simulation (Fig. 1, left) and TEM analysis (Fig. 1, in the middle and right).

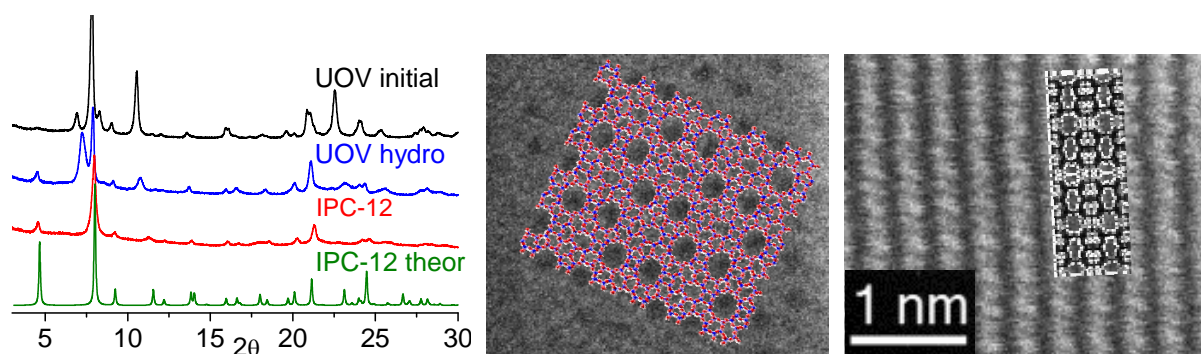


Fig. 1. XRD patterns (left) of parent and hydrolyzed UOV, experimental and theoretically simulated IPC-12; TEM images of IPC-12 in ab (in the middle) and ac (right) projections.

References:

1. Mazur, M., et al, *Nature Chemistry* **2016**, 8, 58–62
2. Verheyen, E., et al, *Nature Mater.* **2012**, 11, 1059–1064
3. Wheatley, P. S., *Angew. Chem. Int. Ed.* **2014**, 53, 1–6



PHOTOCATALYTIC TRANSFORMATION OF NEUTRAL CARBON DIOXIDE-RICH PALEOATMOSPHERE TO REDUCTION GASES ON MINERAL SURFACES

Antonín Knížek

RNDr. Martin Ferus, Ph.D.

Carbon dioxide is one of the most studied gases, as it is relevant to atmospheric chemistry as a greenhouse gas, planetary chemistry, space exploration and mapping and also to the origin of life, where it plays the role of a reaction substrate. However, neutral CO₂-rich atmosphere is supposed to be rather unfriendly environment for the synthesis of biomolecules. Our current study shows that this relatively inert molecule can be readily converted to reactive reduction gases, such as methane and carbon monoxide, which are related to Urey and Miller's original experiments. These conversions take place on mineral surfaces, namely titanium dioxide (anatase) and montmorillonite. The reduction of CO₂ was monitored using the high resolution Fourier-transform infrared spectroscopy of methane, carbon monoxide and carbon dioxide. We further show that an acidic proton can moderate the rate of this conversion and plays a very important role as it directs the reaction routes to various compositions of product mixtures. Moreover, using the high power Prague Asterix Laser System (PALS), we demonstrated that nucleic bases and sugars can be synthesized over mineral surfaces from various mixtures of reduction gases related to CO₂-rich prebiotic atmospheres, such as CH₄, CO, N₂, H₂O or HCHO. These experiments represented possible asteroid impacts on Earth during the Late Heavy Bombardment Era, which, surprisingly, coincides with our first evidence of life on our planet. It then follows that, although indirectly, the photocatalytic reduction of CO₂ may have played a vital role in the process of the creation of life.



BIOPHYSICAL CHARACTERIZATION OF LIPOPEPTIDES INVOLVED IN MEMBRANE FUSION

Mgr. Alena Koukalová

RNDr. Radek Šachl, Ph.D.

Membrane fusion is a key process naturally occurring in cells as it facilitates e.g. delivery of chemicals across biological barriers to specific cellular locations. Intracellular fusion *in vivo* is triggered by the specific interaction of SNARE protein complex forming coiled-coil bundles that brings two membranes into close proximity followed by merging of the membranes (1). Understanding the fusion process is crucial for the development of an efficient and specific system which might be used *in vivo* applications, such as drug delivery technology. The aim of our study is to contribute to the current knowledge using advanced fluorescent confocal microscopic techniques. Therefore, we use reduced system, in which fusion-related proteins are replaced by two complementary synthetic lipopeptides consisting of peptides K₄ [(KIAALKE)₄] or E₄ [(EIAALEK)₄], a flexible polyethylene glycol linker and a cholesterol anchor. Giant unilamellar vesicles (sizes 10 - 50 μm) are used as a biophysical model of the plasma membrane of cells. Our interest is to characterize diffusion properties of both lipopeptides within the membrane, study the aggregation behavior of lipopeptides and describe the interaction of K/E peptide with lipid membranes. The first data show that peptide K tends to aggregate and interact with the membrane more strongly than peptide E. This interaction, however, strongly depends on the membrane lipid composition.

References:

- (1) Calakos, N.; Bennett, MK.; Peterson, KE.; Scheller, RH. *Science*.1994, 263 (5150), 1146-9.



ION-INDUCED IONIZATION AND DISSOCIATION OF ORGANIC MOLECULES BY keV PROJECTILE IONS

Mgr. Věra Křížová

Mgr. Miroslav Polášek, Ph.D.

The keV ion-induced processes in isolated gas-phase atoms and molecules have been a subject of numerous studies in the last few decades. These studies were motivated by an effort to understand molecular mechanisms of radiation damage of biological systems [1], as well as other high-energy ion/molecule processes such as star wind interactions with planetary atmospheres, interstellar clouds and other objects in space [2, 3]. The variety of ions used in these studies was, however, rather limited. Especially in terms of their chemical nature, which covered mostly small atomic cations (H^+ , He^+ , He^{2+} , O^+ , N^+ , etc.) and only a very few simple molecular cations (N_2^+ , O_2^+ , C_{60}^+ , etc.). Moreover, only large scale facilities, like accelerators, have been used for such experiments so far, making these experiments available only to a small number of scientists.

In order to broaden the range of these studies, we measure 5 – 10 keV projectile ion collisions with neutral molecular targets. For that matter, a EI/CI sector type mass spectrometer was modified. The modifications include collision chamber and quadrupole mass analyzer which is to analyze secondary ions stemming from the collisions of projectiles with neutrals. Pressure inside the collision chamber, as well as projectile ion current, are measured absolutely so that we are able to determine collision cross sections for given processes from the secondary ion count rates. The amount of internal energy deposited in secondary ions, as reflected by the extent of their fragmentation, is determined from the acquired mass spectra. Some general trends and selected specific results will be presented.

References:

- [1] G. G. Gomez-Tejedor and M. C. Fuss, *Radiation damage in biomolecular systems* (Springer, New York, 2012).
- [2] J. Postma, S. Bari, R. Hoekstra, A. G. G. M. Tielens, and T. Schlathölter *ApJ* 2010, **708**, 435-444.
- [3] V. Vuitton, R. V. Yelle, and M. J. McEwan, *Icarus* 2007, **191**, 722 – 742.

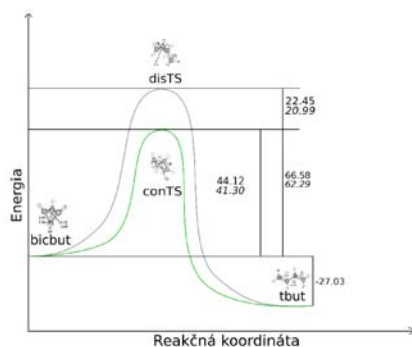


STUDY OF TRIMETHYLENE SYSTEM AND BICYCLOBUTADIENE ISOMERIZATION: INVESTIGATION OF A POSTERIORI USS-D CORRECTION

Mgr. Jakub Lang

Doc. Jiří Pittner *Dr. rer. nat., DSc.*

The single reference coupled cluster (CC) method is one of the most popular methods in quantum chemistry, however its description of systems with high static correlation is rather poor. For example black box coupled cluster methods such as CCSD and CCSD(T) are unable to properly calculate activation barrier of two transition states during the isomerization of bicyclo[1.1.0]butane to buta-1,3-diene.



Another example is trimethylene transition state created during cyclopropane ring opening which exhibits multireference character. It still has not been concluded whether the ground state is singlet or triplet. In these cases, use of multireference methods, which correctly describe static correlation, is necessary.

Unfortunately, some state specific MRCC methods are not size-extensive and to accurately describe the correlation energy a posteriori correction has to be introduced. Until now, such method was Hubac correction for BW-MRCCSD. Recently introduced Universal State Specific (USS) and its diagonal part (USS-D) correction is able to correct this error. Furthermore the USS correction is able to improve calculated correlation energies of other MRCC methods as well.

In my lecture, I will present multireference calculations of these two systems and effect of USS-D correction on results.

References:

- Kinal, A.;Piecuch, P.; *J. Phys. Chem. A* **2007**, *111*, 734-742.
- Lutz, J.J.; *J. Phys. Chem.* **2008**, *995*, 62-71
- Pittner, J. ;Li, X. ; Paldus, J. ; *Mol. Phys*, **2005**, *103*, 2239
- Pittner, J. ; *J. Chem. Phys.* **2003**, *118*, 10876
- Brabec, J.; van Dam, H. J. J.;Pittner, J.; Kowalski, K. *J. Chem. Phys.* 2012, *136*, 124102.



CALIX[4]ARENE TETRARADICAL TETRAANION – AN ELECTROCHEMICALLY GENERATED LIGAND

Mgr. Alan Liška
prof. RNDr. Jiří Ludvík, CSc.

The calixarene skeleton is a popular structural framework in supramolecular chemistry [1], it is itself, however, not electroactive. Hence, the presence of suitable redox probe(s) is necessary for electrochemical investigations, in our case the nitro groups [1-5].

The typical voltammetric reduction mechanism of nitrobenzenes in aprotic media [2] involves reversible radical ion formation followed by irreversible reduction step yielding the corresponding hydroxylamino derivative. The reduction of *cone*-tetranitrocalix [4]arene by first four electrons in two two-electron reversible steps (E_1 , E_2) results in the stable tetraradical tetraanion [3-5] confirmed by EPR spectra.

In the presence of alkali metal ions, a potential shift of E_2 occurs towards less negative potentials while the first one (E_1) remains nearly constant. It is evident that whereas the parent neutral tetranitroderivative does not interact with alkali metal ions, after the electrochemical step new complexes are being formed, i.e. the tetraradical tetraanion generated electrochemically serves as the ligand. The stoichiometry of the complex formation as well as their thermodynamic stability will be discussed in terms of the individual alkali metal ions steric demands and the intensity of electrostatic force effects. In general, they behave as ion pairs with included solvent molecules. The stability constants seem to be higher than in the case of analogical nitrite ion pairs, probably due to a “stereochemical vector” of four definably oriented nitroradical donor groups.

References

- [1] K. Flídrová, A. Liška, J. Ludvík, V. Eigner, P. Lhoták, Fullerene recognition by 5-nitro-11,17,23,29-tetramethylcalix[5]arene, *Tetrahedron Letters* 56 (2015) 1535.
- [2] A. Liška, J. Ludvík, Analýza aromatických nitrosloučenin aneb není nitro jako nitro, *Chem. Listy* 104 (2010) 23.
- [3] A. Liška, P. Vojtíšek, A.J. Fry, J. Ludvík, Electrochemical and Quantum Chemical Investigation of Tetranitrocalix[4]arenes: Molecules with Multiple Redox Centers, *J. Org. Chem.* 78 (2013) 10651.
- [4] A. Liška, M. Rosenkranz, J. Klíma, L. Dunsch, P. Lhoták, J. Ludvík, Formation and proof of stable bi-, tri- and tetraradical polyanions during the electrochemical reduction of *cone*-polynitrocalix[4]arenes. An ESR-UV-VIS spectro-electrochemical study, *Electrochim Acta* 140 (2014) 572.
- [5] J. Ludvík, A. Liška, P. Lhoták, Electrochemical Reduction of Oligo-nitrocalix[4]arenes - Molecules with Multiple Redox Centers. Different Conformations and Variable Shape, *ECS Transactions* 66(26) (2015) 23.

Acknowledgements

The research was supported by grant No. 13-21704S (GAČR), project 798214 (GAUK), and institutional support RVO 61388955.



DETERMINATION OF TUMOR MARKERS USING SCREEN-PRINTED ELECTRODES

Mgr. Anna Makrlíková

Doc. Dr. Ing. Tomáš Navrátil

Determinations of levels of homovanillic acid (HVA), vanillylmandelic acid (VMA), and 5-hydroxyindoleacetic acid (5-HIAA) in urine can be a useful tool for recognition of presence of neuroblastic and carcinoid tumors. Tumor cells correspond to changed metabolism of tryptophan with the release of large amounts of serotonin, which is then metabolized to 5-HIAA. Therefore, the diagnostic test for carcinoid tumors consists in determination of urinary 5-HIAA, the final metabolite of serotonin. All of these acids are usually determined by gas chromatography, gas chromatography-mass spectrometric methods, and high performance liquid chromatography methods.

The electrochemical oxidation of three above mentioned acids at an edge-plane pyrolytic graphite electrode has been tested using differential pulse voltammetry in Britton-Robinson buffer. The acids are electrochemically oxidizable due to the presence of a hydroxyl group on their aromatic system.

Electrochemical measurements were performed using a three electrode system with screen-printed carbon electrodes with a working electrode made from carbon (4 mm diameter), a counter electrode made from carbon and a reference electrode made from silver (DS 110).

Advantage of screen-printing technology consists in its small size (i.e., measuring in small sample volume), fast measurement and in the fact that electrodes are suitable for determination of various organic compounds in biological fluids. Used electrodes are disposed off after one measurement, so there is no problem with their passivation and regeneration.

In my lecture, the results of determination of three tumor biomarkers on screen-printed carbon electrodes in Britton-Robinson buffer will be presented. Results obtained from measurements in buffer will aim to testing these electrodes in human urine.

References:

Lionetto, L.; Lostia, A. M.; Stigliano, A.; Cardelli, P.; Simmaco, M. *Clin. Chim. Acta* **2008**, 398, 53-56.

Renedo, O. D.; Alonso-Lomillo, M. A.; Martinez, M. J. A. *Talanta* **2007**, 73, 202-219.

Ktena, E. *Bachelor thesis*. Charles University, Prague 2014.



SYNTHESIS OF UNFEASIBLE ZEOLITES

Mgr. Michal Mazur

prof. Ing. Jiří Čejka, DrSc.

Conventional zeolites have been recognized as 3D tetrahedrally-connected frameworks however some of them are also known to exist in various 2D layered forms. Recently, the hydrolysis of UTL germanosilicate to layers (IPC-1P) has started the new branch in 2D zeolites chemistry. Modifications of the layered precursor IPC-1P led to discovery of the two novel, 3D zeolites: IPC-4 (PCR) and IPC-2 (OKO). This approach, called ADOR chemistry, is in principle applicable to all layered zeolites [1]. In this contribution authors would like to report the procedure of the synthesis of two new zeolites denoted as IPC-9 and IPC-10 [2] and catalytic properties of ADOR zeolites.

Investigated materials were obtained by reorganization of IPC-1P. Intercalation of proper organic molecules let the layers to organize (e.g. to shift) to the preferable positions. Shifted layers reassemble creating the new zeolites (IPC-9 [Fig.1] and IPC-10) with higher framework energy than well known IPC-4 and IPC-2 topologies. Obtained materials were investigated using XRD, SEM, TEM and adsorption of argon. Structures of the IPC-9 and IPC-10 zeolites were confirmed using Rietveld refinement.

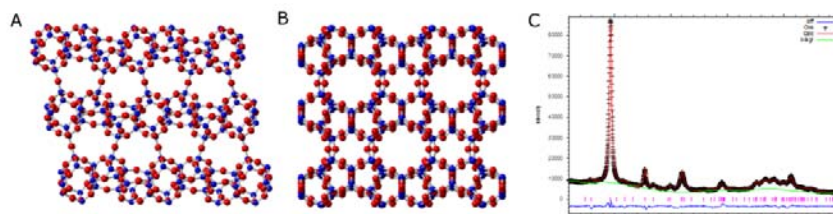


Fig. 1. Structure of IPC-9 zeolite: viewed parallel to the seven-ring channels in the structure (A), parallel to the 10-ring channels (B), the observed and calculated X-ray diffraction patterns after Rietveld refinement (C).

The new zeolites have unprecedented energetics and rare structural features. The presented results show great opportunity for further exploration of this area and the possibility of preparing a whole new class of structures that cannot be accessed by traditional methods of synthesis.

References

- 1) W.J. Roth, P. Nachtigall, R.E. Morris, P.S. Wheatley, V.R. Seymour, S.E. Ashbrook, P. Chlubná, L. Grajciar, M. Položij, A. Zuka, O.V. Shvets, J. Čejka, *Nat. Chem.* **2013** 5, 628.
- 2) M. Mazur, P.S. Wheatley, M. Navarro, W.J. Roth, M. Položij, A. Mayoral, P. Eliášová, P. Nachtigall, J. Čejka, R.E. Morris, *Nat. Chem.* **2016**, 8, 58.



INFLUENCE OF CHOLESTEROL ON Ca^{2+} INTERACTION WITH PHOSPHOLIPID MEMBRANES

Mgr. Adéla Melcrová

Prof. Martin Hof, Dr. rer. nat, DSc.

Ca^{2+} has a major role in many signalling pathways, association of proteins with the plasma membrane or membrane fusion. Ca^{2+} signalling on the inner leaflet of the plasma membrane is known to be localized in lipid rafts and caveolar microdomains rich for sphingolipids and cholesterol [1]. Ca^{2+} signalling on the plasma membrane is likely to be influenced by the presence of cholesterol as this molecule influences binding of membrane-associated proteins [2], it locally organizes the membrane and contributes to its negative curvature [3]. In order to investigate the influence of cholesterol on Ca^{2+} binding to phospholipid bilayers we use the Time-dependent Fluorescence Shift (TDFS) method accompanied by Molecular Dynamics (MD) simulations. The TDFS method allows us to track the changes in local hydration and mobility at Ca^{2+} binding sites upon addition of cholesterol. MD simulations then provide a view at a molecular level. It was already shown that Ca^{2+} binding slows down local mobility in the carbonyl region of a phospholipid bilayer [4]. Experimental results show that the addition of cholesterol even enhances the rigidifying effect of Ca^{2+} on the membrane. The specific interactions between cholesterol and Ca^{2+} ions as well as other macroscopic membrane properties were studied via MD simulations to correctly interpret the observed enhancement.

References:

- [1] Pani, B. and Singh, B. B. Lipid rafts/caveolae as microdomains of calcium signaling., *Cell Calcium*, Jun. 2009, **45**(6), 625–33.
- [2] Zeuschner, D. , Stoorvogel, W. , and Gerke, V. Association of annexin 2 with recycling endosomes requires either calcium- or cholesterol-stabilized membrane domains., *Eur. J. Cell Biol.*, Aug. 2001, **80**(8), 499–507.
- [3] Churchward, M. a , Rogasevskaia, T. , Höfgen, J. , Bau, J. , and Coorssen, J. R. Cholesterol facilitates the native mechanism of Ca^{2+} -triggered membrane fusion., *J. Cell Sci.*, Oct. 2005, **118**(Pt 20), 4833–48.
- [4] Melcrova, A. , Pokorna, S. , Pullanchery, S. , Kohagen, M. , Jurkiewicz, P. , Hof, M. , Jungwirth, P. , Cremer, P. , and Cwiklik, L. The complex nature of calcium cation interactions with phospholipid bilayers, *Sci. Rep.*, Submitted.



STANOVENÍ NOVÝCH SYNTETICKÝCH DROG V MOČI METODOU LC-MS/MS

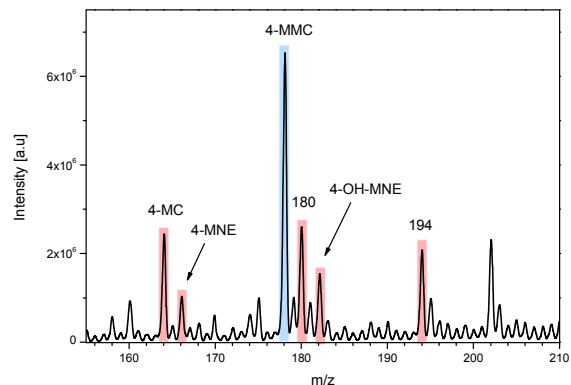
Bc. Michaela Obluková

Mgr. ŽABKA Ján, CSc.

V posledních letech se vedle klasických syntetických drog, jako jsou například kokain, heroin, extáze a další, objevuje řada nových syntetických látek tzv. „Legal Hights“ nebo „New Psychoactive Substances“ (NPS). Tyto látky však nejsou nové z hlediska objevení nebo doby, kdy byly poprvé syntetizovány, ale jsou nové z hlediska výskytu na ilegálním drogovém trhu. Jedná se o syntetické sloučeniny, které projevují značný psychoaktivní efekt, ale nepodléhají kontrole podle mezinárodních úmluv OSN a současně nejsou kontrolovány jako omamné a psychotropní látky [1]. Jsou tedy vyráběny za účelem získání podobných účinků, jako mají drogy nelegální, ale díky jejich odlišné struktuře nejsou uvedeny na seznamu zakázaných látek a jejich užívání je tedy legální. V České republice došlo k rozvoji prodeje NPS v letech 2010 a 2011. NPS byly nabízeny, jak v kamenných obchodech v tzv. Amsterdam shopech, tak i na internetu. NPS byly prodávány jako sběratelské a dárkové předměty, soli do koupele, hnojiva, vonné směsi nebo výzkumné látky. Aby se prodejci vyhnuli trestněprávním nebo správním postihům, byly balení NPS opatřeny varovným nápisem, že výrobky nejsou určeny ke konzumaci [1,2]. Tyto látky se staly velmi populární díky jejich snadné dostupnosti, nízké ceně a legálnímu statusu, díky čemuž mohli zákazníci nabýt dojem, že se jedná o látky bezpečné [1].



Obr.1: Schéma metabolismu mefedronu [3]
o pH3



Obr.2 MS metabolitů mefedronu ve vzorku moče

Mezi významné analytické metody pro analýzu netěkavých a polárních látek, jako je většina drog a jejich metabolitů, se řadí vysoceúčinná kapalinová chromatografie ve spojení s hmotnostní detekcí. Spojení těchto dvou metod významně zvyšuje selektivitu a umožňuje analýzu komponent vzorku ve složitějších maticích.

V této práci bylo metodou LC-MS/MS detekováno stopové množství dostupných standardů syntetických drog. Následně pro vybranou látku, konkrétně mefedron a jeho metabolity (obr. 1), bylo detekováno stopové množství jeho metabolitů v reálném vzorku moči potkana (obr. 2).

Reference

- [1] Grolmusová L, Mravčík V. *Nové syntetické drogy: aktuální situace. Zaostřeno na drogy* 10(5), 1 – 11 (2012)
- [2] Coppola M., Mondola R.: *Synthetic cathinones: Chemistry, pharmacology and toxicology of a new class of designer drugs of abuse marketed as “bath salts” or “plant food”*. Toxicology Letters 211, 144 – 149 (2012)
- [3] Linhart I., Himl M., Židková M., Balíková M., Lhotská E., Páleníček T.: *Metabolic profile of mephedrone: Identification of nor-mephedrone conjugates with dicarboxylic acids as a new type of xenobiotic phase II metabolites*. Toxicology Letters 240, 114 – 121 (2016)



FTIR EMISSION SPECTRA OF NOBLE GASES IN RYDBERG STATES PRODUCED IN DISCHARGE PLASMA

Bc. Adam Pastorek

Prof. RNDr. Svatopluk Civiš, CSc.

Experimental study of atomic spectra of noble gases has nowadays an enormous importance in science. Noble gases are widely used in many discharge techniques where the gas is usually mixed with other molecular substances. Therefore, the knowledge of such atomic spectra is very important not only for calibration and/or diagnostics of these systems. One of the most interesting applications of these laboratory measurements comes from the presence of noble gases in stars which imply the importance of this research for astronomy and astrophysics.

The argon and neon spectra were measured in spectral region from 700 to 7000 cm^{-1} by use of time-resolved Fourier transform infrared spectroscopy in pulsed glow discharge.

In my lecture I will focus on the newly found energy levels and spectral lines of neon and argon as well as the experimental details.

References:

CIVIŠ, Svatopluk a Martin FERUS. Československý časopis pro fyziku: Vysoce rozlišená spektrometrie s Fourierovou transformací a její laboratorní aplikace. 2008, roč. 2008, č. 58, s. 157-164.

KAWAGUCHI, Kentarou, Yoichi HAMA a Shigeki NISHIDA. Time-resolved Fourier transform infrared spectroscopy: Application to pulsed discharges. *Journal of Molecular Spectroscopy*. 2005, vol. 232, issue 1, s. 1-13

PLEŠEK, Jaromír. ÚACH AV ČR. *Geneze prvků*. Praha-Řež

SALOMAN, E. B. Wavelengths, Energy Level Classifications, and Energy Levels for the Spectrum of Neutral Neon. *Journal of Physical and Chemical Reference Data*. 2004, vol. 33, issue 4.



PREPARATION OF HIERARCHICAL MORDENITE ZEOLITES WITH TAILORED TEXTURE AND ACCESSIBILITY OF ACID SITES

Ing. Jana Pastvová

Ing. Petr Sazama, Ph.D.

Mordenite is one of the most important zeolitic structures with a wide range of applications in the petrochemical industry, e. g. applied on a large scale in the hydroisomerization of C_5 - C_6 alkanes. However, the accessibility of the active acid sites in 12MR and 8MR channels is limited by slow diffusion of reactants and products. The aim of this study is to obtain hierarchical mordenite zeolites with different levels of the secondary mesoporosity and targeted concentration of the acid sites with enhanced accessibility.

The micro-mesoporous mordenites were prepared through post-synthesis modifications using sequence of desilication/dealumination steps (Fig. 1) ^{1,2}.

The FTIR spectra of adsorbed n- C_6 provided information on accessibility of OH groups in the microporous channels. After alkaline and acid treatment, the accessibility of OH groups was significantly higher (up to 70%) than of the parent mordenite (50%). Several series of hierarchical mordenites with similar size and volume of mesopores but differing in Si/Al ratio were prepared. The subsequent treatments provided hierarchical mordenites with targeted degree of mesoporosity with external surface area in the ranges 44 – 109 $m^2 \cdot g^{-1}$ and with the targeted concentrations of acid sites.

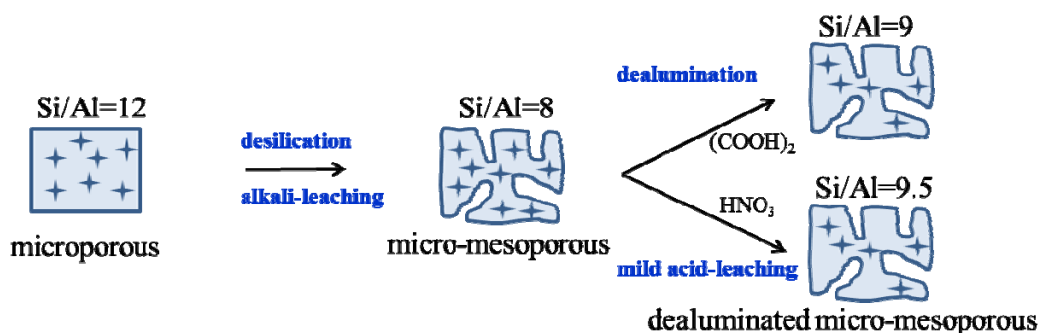
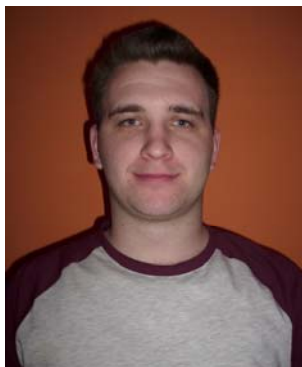


Fig. 1. Schematic illustration of synthesis of micro-mesoporous mordenite zeolites.

References:

- 1) Sazama, P.; Sobalik, Z.; Dedecek, J.; Jakubec, I.; Parvulescu, V.; Bastl, Z.; Rathousky, J.; Jirglova, H. *Angewandte Chemie- International Edition* **2013**, 52, 2038-2041.
- 2) Sazama, P.; Wichterlova, B.; Dedecek, J.; Tvaruzkova, Z.; Musilova, Z.; Palumbo, L.; Sklenak, S.; Gonsiorova, O. *Microporous and Mesoporous Materials* **2011**, 143, 87-96.



VIBRATIONAL SPECTRA OF TRANSITION METALS COMPLEXES CONTAINING LIGANDS DERIVED FROM VITAMIN B6: INTERPRETATION USING DFT METHOD

Bc. Martin Pižl

Ing. Stanislav Záliš, CSc.

Vibrational spectroscopy is one of the important methods for characterization of coordination compounds. Metal complexes containing a ligand derived from vitamin B6 (pyridoxal) were prepared and characterized by IR and Raman spectroscopy. DFT methodology was used for calculation of vibrational frequencies of these complexes. The influence of functional (e.g. BP86, B3LYP, PBE0, M062X and N12) and the effect of diffusion functions within triple- ζ basis set on calculated spectral characteristic was examined. The aim of the work is finding the method which will be in qualitative agreement with the experimental spectra. The influence of anharmonic effects was also tested.



PRESTRESS INDUCED GRAPHENE WRINKLING

Bc. Jaroslava Řáhová

Mgr. Otakar Frank, PhD.

Graphene's unique properties predestines it to be great material for the future use in nanoelectronics. Mechanical deformation is one of the methods to manipulate optoelectronic properties of graphene. However, not many successful experiments have been performed up to date. One particular way to induce changes in the crystal structure is through bending instability, which creates wrinkles in the system. Wrinkles can be the right way to reach the 1D quantum confinement. In our work we report on the formation as well as on the characterisation of wrinkles created on prestrained polymeric substrate.

Graphene sheets were prepared by chemical vapor deposition (CVD) on copper foils. CVD graphene was covered with nitrocellulose film and thereafter transferred onto highly prestretched (50%) polydimethylsiloxane (PDMS) substrate using the common "wet transfer" method. Nitrocellulose coating was dissolved after the transfer using methanol. Gradual stress release of PDMS substrate results in wrinkle formation only in the overlying graphene.

The thus formed graphene wrinkles were characterized by multiple methods. Optical microscopy was used to describe wrinkle formation in-situ during stress release of PDMS substrate. Topography and adhesion were characterized by Atomic Force Microscopy (AFM); the study of mechanical properties of graphene lifted from the substrate (top of the wrinkles) and on the substrate (bottom of the wrinkles) was performed by AFM force curves measurement. Raman spectral mapping was used for quantification of stress levels in the graphene's lattice as well as for charge-transfer doping induced by the transfer polymer residues and/or the substrate. Furthermore, Kelvin Probe Force Microscopy, was used to obtain additional information on the local changes in the surface potential in nanometer scale.

We observe wrinkle formation throughout substrate relaxation as well as tearing of graphene in transversal (i.e. Poisson) direction, at strain levels corresponding to the theoretically predicted ~20% elongation-at-break value. However, the topography of graphene at nanoscale is influenced by the former nitrocellulose coating, too. The amplitude-to-wavelength aspect ratio falls within the interval of 0,25-0,3; the compression level of graphene is in good agreement with the level of substrate contraction. Changes in potential are related to both the graphene-substrate interaction and presence of residual nitrocellulose.



GUNSHOT RESIDUES ANALYSIS BY MEANS OF ELECTROCHEMICAL METHODS

Lucie Sedlecká

Mgr. Magdaléna Hromadová Ph. D.

Gunshot residues (GSR) are organic and inorganic particles originating while shooting from a gun. They belong to a group of criminalistics evidence called trace evidence or micro-traces. Micro-traces are always left at the crime scene and cannot be influenced by the culprit. With modern equipment and new methods the interest in micro-traces has grown, as well as the ability to gain relevant information.

For GSR analysis, forensic laboratories mostly use scanning electron microscopy equipped with energy-dispersive X-ray analyzer (SEM/EDX). The method is time-consuming, requires expensive equipment and an experienced operator. For that reason, other methods of GSR analysis are being developed.

Electroanalysis, specifically differential pulse voltammetry and stripping voltammetry, is quick, easy to realize, exhibits low limits of detection and it is well suited for the analysis of metallic ions included in GSR, such as Pb, Sb, Cu, Zn, Sn.

In my contribution, I will present results of my bachelor thesis I am currently working on. Used cartridges were obtained from the Institute of Criminalistics Prague. Different sampling methods were applied to transfer the GSR into solution. Mercury electrode was used as the working electrode in diverse electrolytes with varying conditions. Analytes were seen at low concentrations using stripping voltammetry, but some problems occurred, which will be discussed. These have to be solved, which will lead to the optimization of the method.

References:

O'Mahony A. M., Wang J.: Electrochemical Detection of Gunshot Residue for Forensic Analysis: A Review.: *Electroanalysis*, **2013**, *25*, 1341–1358

Barek J., Opekar F., Štulík K.: *Elektroanalytická chemie*, Karolinum, **2005**

Schwoeble A.J., Exline D. L.: *Current Methods in Forensic Gunshot Residue Analysis*, CRC Press, **2000**



DEVELOPMENT OF DNA BIOSENSOR TO STUDY INTERACTIONS OF 2-NITROFLUORENE WITH DNA

Mgr. Štěpánka Skalová

Doc. Dr. Ing. Tomáš Navrátil

Nitrated polycyclic hydrocarbons (NPAH) rank among the environmental pollutants. They are produced by incomplete combustion of organic compounds¹. NPAH are highly soluble in lipids and are capable of being absorbed into mammalian organisms from lungs, small intestine and skin². 2-nitrofluorene (2-NF) is considered to be a model representative of these compounds (Fig. 1). 2-NF is known as a potential carcinogen inducing tumours of many organs⁵.

2-NF and its interaction with DNA was examined using the DNA biosensor composed of glassy carbon electrode (GCE) with adsorbed salmon low-molecular-weight DNA by electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and square-wave voltammetry (SWV).

The results of EIS did not show damaging interactions between DNA and 2-NF. However, the results of CV showed intercalation of 2-NF into DNA structure to form the complex 2-NF-DNA. Intercalation of this substance into the DNA structure was also observed using SWV, where intercalation reduced number of electroactive sites and thus the peak heights of adenosine and guanosine were decreased.

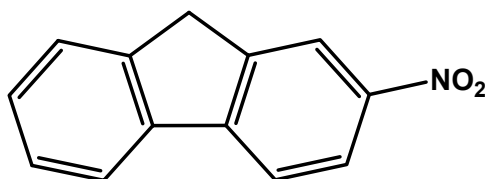


Fig. 1: Structural formula of 2-nitrofluorene (2-NF)

References

1. Wild S. R., Jones K. C.: *Environ. Pollut.* 88, 91 (1995).
2. Wolff R. K., Griffith W. C., Henderson R. F., Hahn F. F., Harkema J. R., Rebar A. H., Eidson A. F., McClellan R. O.: *J. Toxicol. Environ. Health* 27, 123 (1989).
3. Möller L.: *Environ. Health Perspect.* 102, 139 (1994).



SYNTHESIS ROUTES TO ZEOLITE SSZ-16 CRYSTALS AND SUPPORTED LAYERS

Mgr. Tat'ána Supiňková

*RNDr. Milan Kočířík, CSc.
Ing. Pavel Hrabánek, Ph.D.*

There is a strong demand for thermally, mechanically and chemically stable small pore microporous materials. A weakly explored zeolite SSZ-16 is believed to be a promising candidate for applications in catalysis and adsorption or membrane separation of small molecules. This is due to its 3-dimensional channel system, accessible through 8-membered oxygen rings with size 0.36×0.34 nm. The study described in this report represents my contribution to the development of (i) technologically beneficial static *in-situ* hydrothermal synthesis of zeolite SSZ-16 crystals and (ii) seeded synthesis of corresponding supported layers. The substantial progress was achieved in the acceleration and stabilization of zeolite nucleation stage via pre-aging the synthesis solution. Another contribution to the enhancement of synthesis reproducibility was due to optimization of *in-situ* hydrothermal crystallization. This operation was carried out in Teflon-lined stainless steel stationary autoclaves at 160°C , typically for 7 days. A considerable progress was also achieved in the purification of the synthesis product. In total, the products were compact polycrystalline particles, uniform in size throughout the batch, with well developed crystal morphology. The minimum particle size attained via synthesis runs accomplished in this period was about $2.5\ \mu\text{m}$ and product purity was more than 98% by mass of SSZ-16 phase. The SSZ-16 crystals were characterized by SEM, XRD and N_2 adsorption at 77 K. Special attention was paid to two particular problems: (i) removal of template (hexaethylpentane diammonium cation) from the zeolite and evaluation of remaining carbonaceous residues in zeolitic phase and (ii) SSZ-16 seeds formation and their deposition on various solid supports by electrophoretic deposition (EPD).



VLIV ROZPOUŠTĚDLA NA VELIKOST VZNIKLÝCH NANOČÁSTIC REDUKCÍ V NEVODNÉM PROSTŘEDÍ TETRAHYDRIDOBORITANEM SODNÝM..

Lukáš Šimaňok

Mgr. Radek Žouželka

V dnešní době jsou velmi rozvinuty metody syntézy nanočástic stříbra, kterých se hojně využívá jako biocidního prostředku. Tyto metody jsou založeny na redukci kationtů kovů pomocí redukčních činidel, což ovšem do výsledné směsi zanáší množství dalších eventuálně nežádoucích látek.

U stříbrných iontů byly biocidní účinky zjištěny také, nicméně vyšší koncentrace poškozují i tkáň člověka. Z tohoto důvodu není vhodné používat dusičnan stříbrný, což je nejčastější zdroj stříbrných iontů, jakožto velmi dobře rozpustné soli, pro přímou aplikaci jako protekčního materiálu. Také je zde problém fotostability samotného dusičnanu, neboť roztok po aplikaci a interakci se světelným zářením samovolně redukuje a dochází k chemickým změnám.

Během našeho výzkumu jsme se pokoušeli zaměřit na různé metody chemické syntézy nanočástic stříbra a vliv okolních podmínek, jako je teplota a koncentrace reaktantů, na velikost vznikajících částic. Jedním z faktorů udávajícím stabilitu částic je povrchový náboj (zeta potenciál), který lze ovlivnit vhodným rozpouštědlem.

V této práci se zabývám vlivem zvoleného rozpouštědla na stabilitu výsledného systému v závislosti na zvoleném organickém rozpouštědle. Organická rozpouštědla jsou pro práci s nanočásticemi vhodná z důvodu snadnějšího získání pevného podílu ze směsi bez použití metod vyžadujících zvýšení teploty, což vede k destabilizaci vzniklých částic.

References:

Journal of Nanoscience and Nanotechnology Volume 5, Number 2, February 2005, pp. 244-249(6) et al.



PROCESY VE VODNÍCH NANOČÁSTICÍCH ZA PŘÍTOMNOSTI DUSÍKATÝCH MOLEKUL

Bc. Daniela Šmídová

Mgr. Michal Fárník, Ph.D., DSc.

Na povrchu ledových částic polárních stratosférických mraků dochází k heterogenním reakcím, které přispívají k úbytku ozonu. Tyto procesy můžeme experimentálně sledovat na detailní úrovni a zároveň bez zanedbání vlivu okolního prostředí pomocí molekulových klastrů. V experimentu s molekulovými paprsky byly zkoumány jednak samotné vodní nanočástice ale především smíšené klastry složené z vody a dusíkatých molekul (N_2O , NO , NO_2 aj.) [1-4], které jsou významnými polutanty atmosféry. Ke studiu klastrů generovaných supersonickou expanzí byly použity různé metody time-of-flight hmotnostní spektrometrie: elektronová ionizace (EI) v pozitivním i negativním módu a fotoionizace po dopování sodíkem (NaPI). Tato unikátní kombinace uvedených metod představuje nový nástroj pro studium reaktivity hydratovaného elektronu v klastrech [1,2]. Zatímco EI je univerzální a umožňuje ionizovat v principu všechny klastry, pomocí NaPI lze ionizovat pouze klastry s hydratovaným elektronem. Srovnání těchto dvou technik tedy umožňuje určit, zda se solvatovaný elektron v klastru vytvořil nebo zda došlo k jeho reakci s molekulami v klastru. Negativně či pozitivně nabitě fragmenty pozorované v hmotnostních spektrech pak ukazují na možné reakce solvatovaného elektronu v klastrech.

Poděkování: Grant GAČR 15-12386S

Reference:

1. D. Šmídová, J. Lengyel, A. Pysanenko, J. Med, P. Slaviček and M. Fárník: *Reactivity of Hydrated Electron in Finite Size System: Sodium Pickup on Mixed N_2O -Water Nanoparticles*, J. Phys. Chem. Lett. 6 (2015) 2865
2. J. Lengyel, A. Pysanenko, J. Kočišek, V. Poterya, C. Pradzynski, T. Zeuch, P. Slaviček and M. Fárník: *Nucleation of Mixed Nitric Acid-Water Ice Nanoparticles in Molecular Beams that Starts with a HNO_3 Molecule*, J. Phys. Chem. Lett., 3 (2012) 3096
3. J. Lengyel, A. Pysanenko, P. Rubovič and M. Fárník: *Sodium Doping and Reactivity in Pure and Mixed Ice Nanoparticles*, Eur. Phys. J. D 69 (2015) 269
4. J. Lengyel, A. Pysanenko, V. Poterya, J. Kočišek, and M. Fárník: *Extensive water cluster fragmentation after low energy electron ionization*, Chem. Phys. Lett. 612 (2014) 256

SEMINÁŘ STUDENTŮ ÚFCH JH 2016
Konferenční centrum AV ČR v Liblicích
10. - 11. 5. 2016

