

# SEMINÁŘ STUDENTŮ ÚFCH JH

28. - 30. 4. 2014



# 2014



**Zámek  
Liblice**

# **Seminář studentů ÚFCH JH 2014**

## **Sborník příspěvků**

**ze studentské konference konané  
28.-30. dubna 2014  
v Konferenčním centru AV ČR Liblicích**

# **Seminar of Students of JHI 2014**

## **Collection of abstracts**

**of all lectures given at the student conference  
held on 28 -30 April 2014  
in Conference Centre of the Academy of Sciences  
of the Czech Republic in Liblice chateau**

**Seminář studentů ÚFCH JH 2014  
Sborník příspěvků ze studentské konference  
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Kolektiv autorů

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# SEMINÁŘ STUDENTŮ ÚFCH JH 2014

## PROGRAM 1. dne konference - **pondělí 28.4.2014**

**Odjezd autobusem z parkoviště před ústavem ve 14:00 hodin.**

Předpokládaný příjezd do Konferenčního centra AV ČR v zámku  
v Liblicích okolo 15:00 hodiny.

Čas	Předsedající	Přednášející	Název
15:00-15:45	Registrace a ubytování účastníků konference - v recepci zámeckého hotelu		
15:45-16:20	<b>OBČERSTVENÍ PŘED ZAHÁJENÍM KONFERENCE</b> (káva, nápoje, zákusek - v 1. patře, na ochozu)		
16:25	<b>Zahájení konference „Seminář studentů ÚFCH JH 2014“</b> - prezentace studentů z kategorie I. (9 studentů)		
16:30	<b><u>Adéla</u></b> <b><u>FRIDRICHOVÁ</u></b>	Kateřina JURKOVÁ (bakalářské studium, PřF UK; školitel M. Kalbáč) <i>kat I</i>	SPECTROSCOPY AND SPECTROELECTROCHEMISTRY OF MoS <sub>2</sub>
16:50		Miloš VEČEŘA (bakalářské studium, PřF UK; školitel M. Lamač) <i>kat I</i>	POLYMERACE ETHYLENU NA Ti A Zr KOMPLEXECH S CYKLOPENTADIENYL-KETIMIDOVÝMI CHELATUJÍCÍMI LIGANDY
17:10		Daniela ŠMÍDOVÁ (bakalářské studium, VŠCHT Praha, školitel M. Fárník) <i>kat I</i>	EXPERIMENTY S N <sub>2</sub> O A NO NA LEDOVÝCH NANOČÁSTICÍCH
17:30	<b>PŘESTÁVKA</b>		
17:45	<b><u>Radka</u></b> <b><u>METELKOVÁ</u></b>	Michaela OBLUKOVÁ (diplomantka, PřF UK, školitel J. Žabka) <i>kat I</i>	ANALÝZA NOVÝCH SYNTETICKÝCH DROG V LIDSKÉM TĚLE METODOU LC/MS/MS
18:05		Kristýna KANTNEROVÁ (bakalářské studium, školitel J. Ludvík) <i>kat I</i>	REACTIONS OF ORTHOPHTHALALDEHYDE WITH AMINO ACIDS
18:25		Vít SVOBODA (diplomant, VŠCHT Praha, školitel O. Votava) <i>kat I</i>	DVOUTEPLTNÍ ANALÝZA JAKO NÁSTROJ K ROZUZLENÍ KOMPLIKOVANÝCH OVERTONOVÝCH SPEKTER AMONIAKU
18:45	<b>Ukončení prvního dne konference</b>  <b>VEČEŘE v RESTAURACI - začátek v 19:00</b>		

## PROGRAM 2. dne konference - úterý 29.4.2014

Čas	Předsedající	Přednášející	Název
<b>8:25</b>	<b>Zahájení druhého dne konference - pokračují prezentace studentů kategorie I a II.</b>		
8:30	<u>Kateřina</u>  <u>NOVÁKOVÁ</u>	Jana JANOŠCOVÁ (I. ročník PGS, školitel P. Sazama) <b>kat I</b>	SYNTHESIS OF 3D POROUS NANOCARBON WITH DEFINED STRUCTURE
8:50		Alan LIŠKA (I. ročník PGS, školitel J. Ludvík) <b>kat I</b>	ELECTROCHEMICAL REDUCTION OF 1,3-ALT-TETRANITRO-THIACALIX[4]ARENES
9:10		Zuzana KVÍČALOVÁ (I. ročník PGS, školitel M. Cebecauer) <b>kat I</b>	FLUORESCENCE TECHNIQUES TO INVESTIGATE NANOSCALE ORGANISATION OF CELLULAR PLASMA MEMBRANE
<b>Ukončeny prezentace studentů kategorie I. (9 prací)</b>			
<b>9:30</b>	<b>PŘESTÁVKA NA KÁVU</b> (1.patro, ochoz)		
10:00	<u>Jan</u>  <u>PŘECH</u>	Štěpánka LACHMANOVÁ (II. ročník PGS, školitelka M. Hromadová) <b>kat II</b>	SINGLE-MOLECULE CONDUCTANCE MEASUREMENTS OF SELECTED EXPANDED PYRIDINIUM MOLECULES
10:20		Alena KOUKALOVÁ (II. ročník PGS, školitelka J. Humpolíčková) <b>kat II</b>	MEMBRANE ACTIVITY OF PENTAENE MACROLIDE DIDEHYDROROFILAMYCOIN INVESTIGATED ON MODEL LIPID BILAYERS
10:40		Pavla SVRČKOVÁ (III. ročník PGS, školitel M. Fárník) <b>kat II</b>	PHOTODISSOCIATION DYNAMICS - RECONSTRUCTION METHODS
<b>11:00</b>	<b>PŘESTÁVKA</b>		
11:20	<u>Pavla</u>  <u>SVRČKOVÁ</u>	Magda ZLÁMALOVÁ (II. ročník PGS, školitel P. Janda) <b>kat II</b>	OPTIMALIZATION AND CHARACTERIZATION OF POLYMETHYLENE BLUE MODIFIED GRAPHITE ELECTRODE
11:40		Kateřina NOVÁKOVÁ (III. ročník PGS, školitel T. Navrátil) <b>kat II</b>	INFLUENCE OF CHOLESTEROL ON MODEL PHOSPHOLIPID MEMBRANES PROPERTIES
12:00		Michal MAZUR (II. ročník PGS, školitel J. Čejka) <b>kat II</b>	POST-SYNTHESIS MODIFICATIONS OF LAYERED ZEOLITE PRECURSOR IPC-1P
<b>12:20</b>	<b>PŘESTÁVKA NA OBĚD</b> (podává se v restauraci od 12:30)		
14:30	<u>Zuzana</u>  <u>KOMÍNKOVÁ</u>	Regina BRŮHOVÁ - MICHALČÍKOVÁ (II. ročník PGS, školitel P. Španěl) <b>kat II</b>	A SELECTED ION FLOW TUBE, SIFT, STUDY OF REACTIVITY OF IONS DERIVED FROM CARBOXYLIC ACIDS WITH H <sub>2</sub> O
14:50		Jan PŘECH (II. ročník PGS, školitel J. Čejka) <b>kat II</b>	EPOXIDATION OF BULKY ORGANIC MOLECULES OVER ADVANCED TITANOSILICATE CATALYSTS
15:10		Anatolii SPESYVYI (III. ročník PGS, školitel P. Španěl) <b>kat II</b>	SELECTED ION MOBILITY MASS SPECTROMETRY

15:30		Adéla FRIDRICHOVÁ (III. ročník PGS, školitel M. Horáček) <b>kat II</b>	YTTROCENE METHYL COMPLEXES: SYNTHESIS, CHARACTERIZATION, AND ETHYLENE POLYMERIZATION
15:50	<b>PŘESTÁVKA NA KÁVU A ZÁKUSEK</b> (1.patro, ochoz)		
16:20	<b>PREZENTACE STUDENTŮ Z MIMOSOUTĚŽNÍ KATEGORIE "ŠTŘEDOŠKOLÁCI"</b>		
	<b>Květa STEJSKALOVÁ</b>	Květa STEJSKALOVÁ (organizátor popularizačních a vzdělávacích aktivit ústavu) krátce představí stáže studentů Biskupského gymnázia ze Žďáru n. Sázavou v projektu MŠMT "Přírodní a technické obory-výzva pro budoucnost" realizované ve školním roce 2013/2014 ve 4 laboratořích našeho ústavu.	
16:25		Kamila MORIOVÁ (školitel M. Fárník)	Stáž na téma " <b>Optické a laserové experimenty</b> "
16:35		Aneta LAŠTOVIČKOVÁ (školitelka K. Nováková)	Stáž na téma " <b>Studium přenosu biologicky významných látek přes fosfolipidové membrány fyzikálně-chemickými metodami</b> "
16:45		Anna WASSERBAUEROVÁ a O. J.DOLEŽAL (školitel M. Bouša)	Stáže na téma " <b>Příprava a charakterizace pokročilých materiálů pro využití v nových typech baterií</b> "
17:00		Hana PELIKÁNOVÁ (školitelka M. Zlámalová)	Stáž na téma " <b>Moderní fyzikálně chemické metody při přípravě elektrochemických senzorů a jejich charakterizaci</b> "
17:10	Mimokonferenční prezentace (pro zájemce)	<b>Květa STEJSKALOVÁ</b>	Představení vzdělávacích a popularizačních aktivit našeho ústavu v projektu Otevřená věda III (AV ČR) a Tři nástroje (ÚFCH JH) v roce 2013/2014, něco málo o novinkách - letošní akce v harmonogramu VĚDA ZA ŠKOLOU 2014...
ca 18:00	<b>UKONČENÍ DRUHÉHO DNE KONFERENCE</b> <b>VEČEŘE V RESTAURACI OD 18:15 HODIN</b>		

### **PROGRAM 3. dne konference - středa 30.4.2014**

Čas	Předsedající	Přednášející	Název
8:25	<b>Zahájení třetího dne semináře - pokračují prezentace studentů kategorie II.</b>		
8:30	<b>Štěpánka LACHMANOVÁ</b>	Radka METELKOVÁ (III. ročník PGS, školitel J. Ludvík) <b>kat II</b>	INTRAMOLECULAR ELECTRON COMMUNICATION IN BINUCLEAR CHROMIUM FISCHER CARBENE COMPLEXES
8:50		Jakub VIŠŇÁK (II. ročník PGS, školitel J. Pittner) <b>kat II</b>	TRLFS SPECIATION STUDY OF THE $UO_2^{(2+)} - XO_4^{(2-)} - H_2O$ (X = S, SE) SYSTEM COMPARED WITH THEORETICAL QUANTUM-CHEMICAL CALCULATION
9:10		Monika KLUSÁČKOVÁ (III. ročník PGS, školitel P. Janda) <b>kat II</b>	INFLUENCE OF DEPOSITION TECHNIQUES ON ELECTROCATALYTIC ACTIVITY OF WATER- SOLUBLE TETRAPYRIDINOPORPHYRAZINE COMPLEX
9:30		Václav BLECHTA (II. ročník PGS, školitel M. Kalbáč) <b>kat II</b>	GRAPHENE-FIELD-EFFECT-TRANSISTORS
9:50	<b>PŘESTÁVKA NA KÁVU</b> (1.patro, ochoz)		

10:20	<b><u>Michal</u></b> <b><u>MAZUR</u></b>	Zuzana KOMÍNKOVÁ (IV. ročník PGS, školitel M.Kalbáč) <b>kat II</b>	INVESTIGATION OF THE DOPING OF CVD- GRAPHENE IN POLYELECTROLYTE BY RAMAN SPECTROSCOPY
10:40		Marek PEDERZOLI (II. ročník PGS, školitel J. Pittner) <b>kat II</b>	AB INITIO MOLECULAR DYNAMICS WITH NON- ADIABATIC AND SPIN ORBIT EFFECTS APPLICABLE FOR STUDY OF FLUORESCENT PROBES
11:00		Hana KVAPILOVÁ (III. ročník PGS, školitel S. Zálíš) <b>kat II</b>	PHOTOPHYSICAL PROPERTIES OF NEW TUNGSTEN ISONITRILE SENSITIZERS
11:20	<b>Ukončeny prezentace studentů kategorie II. (17 prací)</b>		
<b>11:45 - SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ SOUTĚŽNÍ KONFERENCE - V KONFERENCEM SÁLE</b>			
<b>OBĚD V RESTAURACI od 12:30 hodin</b>			
<b>Odjezd do Prahy - autobusem z parkoviště u zámku ve 14:00</b>			
(Návrat do Prahy k budově ÚFCH JH ca v 15:00 hodin.)			



# Seznam prezentujících studentů (31)

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## Kategorie I (9)

### Diplomanti a zájemci z řad bakalářů (6)

**Jurková Kateřina** (bakalářské studium, PřF UK, stáž u M. Kalbáče)  
**Kantnerová Kristýna** (bakalářské studium, VŠCHT, stáž u J. Ludvíka)  
**Obluková Michaela** (diplomantka, PřF UK, stáž u J. Žabky)  
**Svoboda Vít** (diplomant, FCHI VŠCHT, stáž u O. Votavy)  
**Šmídová Daniela** (bakalářské studium, VŠCHT, stáž u M. Fárníka)  
**Večeřa Miloš** (bakalářské studium, PřF UK, stáž u M. Lamače)

### Studenti 1. ročníku PGS (3)

**Liška Alan** (školitel J. Ludvík)  
**Kvičalová Zuzana** (školitel M. Cebecauer)  
**Janošcová Jana** (školitel P. Sazama)

### Mimosoutěžní kategorie- středoškolská stážistě (5)

**Moriová Kamila** (stáž u M. Fárníka)  
**Laštovičková Aneta** (stáž u K. Novákové)  
**Pelikánová Hana** (stáž u M. Zlámalové)  
**Doležal Ondřej J. a Wasserbauerová Anna** (stáž u M. Bouši)

5 žáků Biskupského gymnázia ze Žďáru nad Sázavou absolvuje své roční stáže v rámci projektu školy "Přírodní a technické obory-výzva pro budoucnost" (v EU programu OPVK, řešitel: kraj Vysočina) v laboratořích ÚFCH JH. Do projektu je ústav zapojen v rámci různých programů svého vzdělávacího a popularizačního projektu Tři nástroje.

## Kategorie II (17)

### Studenti 2. ročníku PGS (9)

**Blechta Václav** (školitel M. Kalbáč)  
**Brůhová Michalčíková Regina** (školitel P. Španěl)  
**Mazur Michal** (školitel J. Čejka)  
**Koukalová Alena** (školitelka J. Humpolíčková)  
**Lachmanová Štěpánka** (školitelka M. Hromadová)  
**Pederzoli Marek** (školitel J. Pittner)  
**Přech Jan** (školitel J. Čejka)  
**Višňák Jakub** (školitel J. Pittner)  
**Zlámalová Magda** (školitel P. Janda)

### Studenti 3. ročníku PGS (7)

**Fridrichová Adéla** (školitel M. Horáček)  
**Klusáčková Monika** (školitel P. Janda)  
**Kvapilová Hana** (školitel S. Záliš)  
**Metelková Radka** (školitel J. Ludvík)  
**Nováková Kateřina** (školitel T. Navrátil)  
**Svrčková Pavla** (školitel M. Fárník)  
**Spesvyvi Anatolii** (školitel P. Španěl)

### Studenti 4. ročníku PGS (1) (nepovinná účast)

**Komínková Zuzana** (školitel M. Kalbáč)

### Hodnotící komise:

**Kseniya Dryahina**  
**Martin Lamač**  
**Martin Srnec**







## GRAPHENE-FIELD-EFFECT-TRANSISTORS

**Mgr. Václav Blechta**

*RNDr. Ing. Martin Kalbáč, Ph.D.*

Graphene is a promising material for future development in nanoelectronics. Field Effect Transistors with graphene channel (GFETs) were fabricated and their features were carefully studied. The GFETs devices exhibited ambipolar transport characteristics with two separated areas of linear  $I_{\text{drain}}(U_{\text{gate}})$  characteristics, where different types of charge carriers were dominating (electron or hole conductivity regimes). The minimal conductivity of GFET devices was shown to be in order of units of  $4e^2/h$  in charge neutrality point (Dirac point). We studied the Dirac point position as a measure of doping level of graphene. Careful investigation of transport characteristics of GFETs enabled us to study electronic properties of graphene and also its interaction with chemicals.

### **References:**

Schwierz, F. *Nature Nanotechnology*. **2010**, 7, 487-496.



## A SELECTED ION FLOW TUBE, SIFT, STUDY OF REACTIVITY OF IONS DERIVED FROM CARBOXYLIC ACIDS WITH H<sub>2</sub>O

**Mgr. Regina Brůhová Michalčíková**

*Prof. RNDr. Patrik Španěl, Dr. rer. nat.*

A selected ion flow tube, SIFT, study has been carried out of the reactions of H<sub>3</sub>O<sup>+</sup>, NO<sup>+</sup> and O<sub>2</sub><sup>+</sup> with four carboxylic acids: formic acid, acetic acid, propionic acid and butyric acid. Ethanol was also included in order to provide data that could facilitate SIFT-MS analyses of formic acid in its presence. The product ion branching ratios of the primary reactions were obtained and compared with the already known values, thus improving the certainty of kinetic data for quantification of these compounds. The primary products of the H<sub>3</sub>O<sup>+</sup> reactions, the protonated molecules MH<sup>+</sup>, and the primary products of the NO<sup>+</sup> reactions, nitrosated (MNO<sup>+</sup>) and dehydroxidated (M-OH)<sup>+</sup> molecules, are observed to react with the molecules of water by three body association. Original data were obtained for the kinetics of these cluster forming reactions. The three body rate constant for the associations of MH<sup>+</sup> with H<sub>2</sub>O in He have been determined in the units of 10<sup>-27</sup> cm<sup>3</sup> s<sup>-1</sup> for formic, acetic, propionic and butyric acids as 1.4, 2.4, 3.8 and 4.9 respectively. The three body rate constant for the associations of MNO<sup>+</sup> with H<sub>2</sub>O in He were obtained in the same units as 2.1, 1.1, 0.15 and 0.7. Results will improve the certainty of identification and accuracy of quantification of SIFT-MS analyses used in medical breath analysis and food science flavour research.

### References:

- Smith, D.; Španěl, P. *Int. J. Mass Spectrom.* **1997**, 167, 375-388.  
Smith, D.; Španěl, P. *Int. J. Mass Spectrom.* **1998**, 172, 137-147.  
Španěl, P.; Smith, D. *Rapid Commun. Mass Spectrom.* **2000**, 14, 1898-1906.  
Smith, D.; Diskin, A.M.; Ji, Y.F.; Španěl, P. *Int. J. Mass Spectrom.* **2001**, 209, 81-97.  
Smith, D.; Španěl, P. *Mass Spectrom. Rev.* **2005**, 24, 661-700.  
Španěl, P.; Dryahina, K.; Smith, D. *Int. J. Mass Spectrom.* **2006**, 249, 230-239.  
Sovová, K.; Dryahina, K.; Španěl, P. *Int. J. Mass Spectrom.* **2011**, 300, 31-38.



# YTROCENE METHYL COMPLEXES: SYNTHESIS, CHARACTERIZATION, AND ETHYLENE POLYMERIZATION

Ing. Adéla Fridrichová

Mgr. Michal Horáček Ph.D.

Alkyl species of group 3 metals have attracted intensive interest for their efficient performance as catalysts in olefin polymerization over past three decades. So far, a large number of monoalkyl group 3 metal complexes supported by various ancillary ligands such as cyclopentadienyls, benzamidates,  $\beta$ -diketiminates, phosphides, crown ethers etc. has been reported. Despite the polymerization activity of such complexes has been limited to ethylene and active polar monomers, whereas the polymerization of higher olefins has remained a challenge.<sup>1,2</sup>

The main goal of the presented work was the synthesis of novel ytrocene methyl complexes containing various substituted cyclopentadienyl ligands. Afterwards, this set of new mixed ytrocene methyl species were tested as homogeneous catalysts for the polymerization of ethylene in the absence of a cocatalyst.

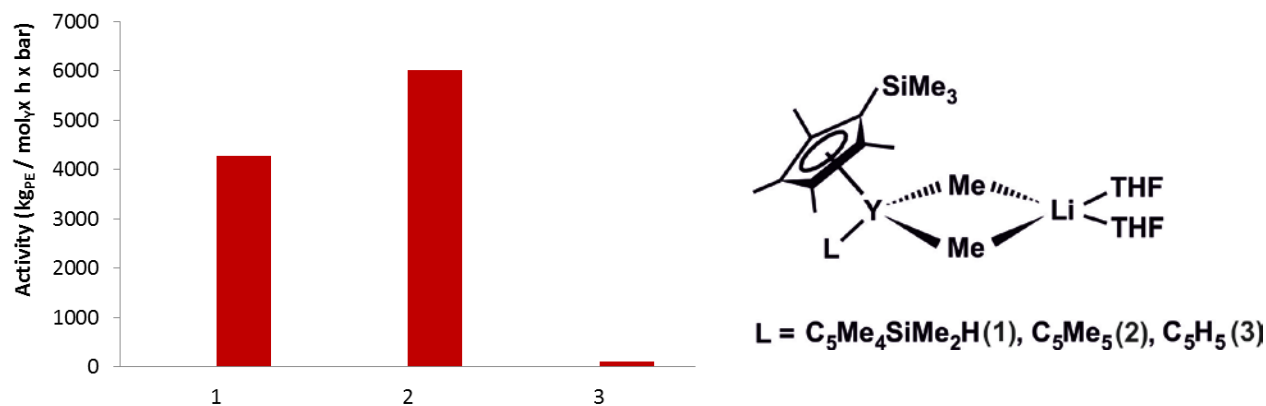


Fig.1. Activities for ethylene polymerization of ytrocene complexes of the type  $(C_5Me_4SiMe_3)Y(L)Me_2Li(THF)_2$  ( $L = C_5Me_4SiMe_2H$  (1),  $C_5Me_5$  (2),  $C_5H_5$  (3)).

This work was financially supported by the Grant Agency of the Czech Republic (Project No. P106/10/0924).

## References:

- <sup>1</sup> Gromada J.; Carpentier J. F. and Mortreux A. *Coord. Chem. Rev.* **2004**, 248, 397.
- <sup>2</sup> Hou Z. and Wakatsuki Y. *Coord. Chem. Rev.* **2002**, 231, 1.



## SYNTHESIS OF 3D POROUS NANOCARBON WITH DEFINED STRUCTURE

Ing. Jana Janošcová

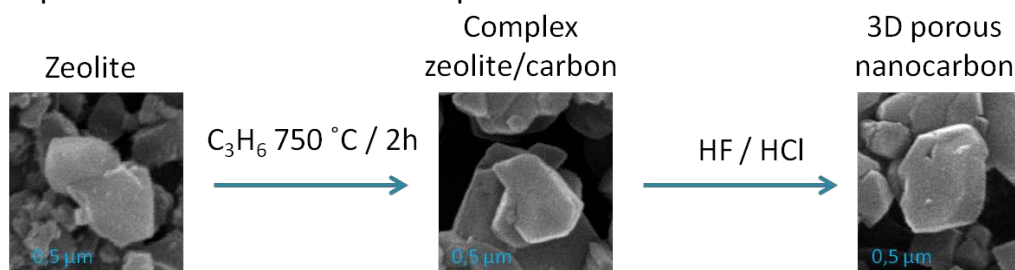
Ing. Petr Sazama, Ph.D.

The microporous and mesoporous carbon materials are interesting for their wide application in electrodes, fuel cells, catalysis, adsorption, gas separation, and water and air purification processes. The properties of carbon materials largely depend on the pore size distribution and surface area<sup>1-3</sup>.

The study aims into synthesis of 3D porous nanocarbon materials with high surface area ( $\geq 2000 \text{ m}^2 \cdot \text{g}^{-1}$ ), and with defined architecture and dimensions of micro-mesoporous structure.

The main effort was centred on synthesis of carbon materials using BEA and Y zeolites as hard templates and the chemical vapour deposition with propylene as a carbon precursor. Synthesis of nanocarbon materials was performed using carbonization of the microporous and micro-mesoporous zeolites in a propylene stream at temperatures from 750 to 850 °C, followed by dissolution of the zeolite framework with HF and HCl acids. Microporous zeolites were employed to obtain 3D porous nanocarbon with unified porous structure formed by an inverse replica of zeolites channel system. Micro-mesoporous zeolites as hard templates were used to shorten the length of micropores in 3D porous nanocarbon and thus enhance mass transport in the defined channel structure. Structure of prepared carbon materials was analysed by using XRD, XPS, SEM and adsorption of N<sub>2</sub>.

In this study, we optimised the synthesis procedure for effective replication of the channel structure of BEA and Y zeolite into carbon providing 3D porous nanocarbon materials with surface area of  $2\ 500 \text{ m}^2 \cdot \text{g}^{-1}$ , and suggested and developed a new synthesis procedure for 3D micro-mesoporous nanocarbon materials.



**Fig.1** Schematic illustration of synthesis of 3D porous nanocarbon materials using Y zeolite as a hard template.

### References:

1. Kyotani, T.; Ma, Z.; Tomita, A.; *Carbon* **2003**, 41, 1451-1459.
2. Lee, J.; Kim, J.; Hyeon, T., *Adv. Mater.* **2006**, 18, 2073–2094.
3. Xu H. et al., *Journal of Catalysis* **2011**, 281, 263–272.



# SPECTROSCOPY AND SPECTROELECTROCHEMISTRY OF MoS<sub>2</sub>

**Kateřina Jurková**

*RNDr. Ing. Martin Kalbáč, Ph. D.*

Recently, a lot of attention has been paid to graphene and MoS<sub>2</sub> – both 2-D materials with interesting properties. Graphene and MoS<sub>2</sub> have potential use in opto- and nanoelectronics. Nevertheless, before this comes true proper understanding their electronic properties is needed. Since Raman spectroscopy provide us with quite a lot of information about the electronic structure, it represents a powerful tool to investigate these materials.

In this study we report on *single* and *few-layers* MoS<sub>2</sub>, which were fabricated by exfoliation from bulk MoS<sub>2</sub>, detected with optical microscopy and characterized with Raman spectroscopy and AFM measurements. In addition we prepared MoS<sub>2</sub>/CVD-graphene sandwich layers and studied the interactions of MoS<sub>2</sub> with doped CVD graphene using in-situ Raman spectroelectrochemistry.



# REACTIONS OF ORTHOPHTHALALDEHYDE WITH AMINO ACIDS

Kristýna Kantnerová

prof. RNDr. Jiří Ludvík, CSc.

Reactions of orthophthalaldehyde (OPA) with nucleophiles are used in analytical and biologically significant reactions for many years [1, 2]. Besides the analytical method for determination of amino acids, the solution of OPA is broadly applied in hospitals as a disinfecting agent for surgery instruments made from plastics. In the literature, there are several different protocols concerning the composition of the active solutions with different timing of the use. This situation is a consequence of the fact that the mechanisms are not understood [3] and therefore the processes could not be optimized.

OPA as a dialdehyde is a molecule with two communicating redox centers. The ortho-position of the two carbonyls enable intramolecular cyclization of intermediates, hence its reactivity with nucleophiles offers a number of structural and stoichiometric possibilities. In addition to this, hydration of the original structure plays a crucial role, since H<sub>2</sub>O is, in fact, the most abundant nucleophile in the system. Nevertheless, for the above mentioned use, the reaction of OPA with amines and particularly with amino acids is the most important. Due to the reducibility of carbonyl groups and their nitrogen analogues, the electrochemical approach is favorable for this mechanistic investigation.

Besides the hydration/dehydration studies, the first series of experiments were focused on the reaction of OPA with aliphatic amino acids: eight simple amino acids with only one  $\alpha$ -amino group (glycine, alanine, leucine, isoleucine, valine, norvaline, aminobutyric and aminoisobutyric acid), one ester preventing zwitterionic equilibrium (glycine ethyl ester) and lysine with two amino groups. Polarography and spectrometry were the main used techniques. Measurements were done in two phosphate buffers (pH 7,90 and 11,20) with pH above and below the pK<sub>a</sub> of amino groups in used amino acids.

In contrast to the literature [3, 4], it was found out that the antecedent hydration of orthophthalaldehyde is necessary for its further reaction with amines. The kinetics of the reaction of OPA with amino acids measured electrochemically and using the UV/Vis spectra was evaluated, discussed and compared with alkyl amines. The products were identified and two main surprising results were achieved: a) the reactive species is not OPA in dialdehydic form but its (mono)hydrated form; b) amino acids and amines with quaternary  $\alpha$ -carbon (e.g. aminoisobutyric acid) exhibit negligible reactivity with OPA.

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## INFLUENCE OF DEPOSITION TECHNIQUES ON ELECTROCATALYTIC ACTIVITY OF WATER-SOLUBLE TETRAPYRIDINOPORPHYRAZINE COMPLEX

**Mgr. Monika Klusáčková**

*Ing. Pavel Janda, CSc.*

The rich and reversible redox behaviour of metallophthalocyanines allows them to serve as mediators in many electron transfer reactions. Our interest has been focused on water-soluble complex  $N,N',N'',N'''$ -tetramethyltetra-3,4-pyridinoporphyrazinocobalt (CoTmt-3,4-ppa), which form insoluble electrically conducting films on the electrode surface.

We have studied the influence of deposition technique and type of used electrode to electrocatalytic activity of CoTmt-3,4-ppa with respect to analyte. Ethylene and propylene were employed as model gaseous analytes. Adsorption, electrochemical deposition and spincoating on highly ordered pyrolytic graphite (HOPG) and annealed gold (Au111) were characterized by cyclic voltammetry. The electrochemical behavior was completed by *in situ* backscattering VIS spectroscopy and *ex situ* atomic force microscopy.

We have confirmed that electrocatalytic properties of CoTmtppa exposed to model gases depends on the deposition method as well as the type of used electrode.

### Acknowledgements

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## INVESTIGATION OF THE DOPING OF CVD-GRAPHENE IN POLYELECTROLYTE BY RAMAN SPECTROSCOPY

**Mgr. Zuzana Komínková**

*RNDr. Martin Kalbáč, Ph.D.*

Raman spectroscopy is a sensitive characterization tool widely used to study graphene samples due to the strong resonant enhancement of the Raman signal. It provides information about number of layers, doping, defects, and stress in graphene.

The important Raman active bands are the tangential displacement mode (TG, G) and the high frequency, two phonon mode (G', 2D). The D band is also found in some graphene samples, which indicates presence of defects as in ordinary graphite.

In-situ Raman spectroelectrochemistry is a well-established method to study the electronic structure of carbon nanostructures. Electrochemistry allows precise and well-controlled doping of carbon materials. The change in electrochemical potential leads to a shift of the Fermi level which is reflected in a change of the Raman spectra.

Raman spectroscopy and in-situ Raman spectroelectrochemistry have been applied to study chemical vapor deposition grown graphene coated with layers of different types of polyelectrolytes.<sup>1,2</sup> A new electrolyte system based on a combination of liquid electrolyte and a protective polyelectrolyte layer, allowed strong doping of the graphene. The change of the Raman intensity of the G band with increasing applied electrode potential will be also discussed.

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## MEMBRANE ACTIVITY OF PENTAENE MACROLIDE DIDEHYDROROFAMYCOIN INVESTIGATED ON MODEL LIPID BILAYERS

**Mgr. Alena Koukalová**

*Mgr. Jana Humpolíčková, Ph.D.*

Recently isolated member of a polyene macrolide family didehydroroflomycoin (DDHR) was shown to have an antibacterial and antifungal activity. Mechanism of its action however has not been investigated so far. Antibiotics from this family are of amphiphilic nature, which renders them membrane active and consequently it is the membrane where their biological action is localized and it is the membrane composition and its physical properties that helps the particular compound identify the target organism. In this work, we use model lipid membranes of giant unilamellar vesicles (GUVs) for a systematic study of the DDHR action. In parallel the experiments are carried out for Filipin III and Amphotericin B, other members of the family and the behavior observed for DDHR is given to the context of the two heavily studied compounds. The study shows that DDHR possesses two different mechanisms of membrane disruption and that their involvement is subjected to the presence of cholesterol.

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## PHOTOPHYSICAL PROPERTIES OF NEW TUNGSTEN ISONITRILE SENSITIZERS

Ing. Hana Kvapilová

*Ing. Stanislav Záliš, CSc.*

W(0) hexakis arylisonitrile complexes  $[W(CNAr)_6]$  are promising photosensitizers. They absorb strongly in the visible region and depending on the aryl residue Ar, their excited state lifetimes range between 10–300 ns. Moreover, they have been found to possess strong photoreducing properties. Such visible light-absorbing photoreductants are used in inorganic and organic synthesis and they are sought after as the key components in devices for the production of solar fuels.

In this work we focus on electronic properties of complexes with 2,6-dimethylphenyl and 2,6-diisopropylphenyl residues in place of the Ar substituent. Their excited-state structure, electron density distribution and relaxation dynamics were studied using UV-Vis absorption, emission spectroscopy and time-resolved infrared (TRIR) spectroscopy. The experimental results were explained with aid of theoretical calculations using the DFT and TDDFT method with PCM solvent correction.

The calculated energies, intensities and shifts of the visible and infrared spectra well reproduce the experimental observations. The DFT calculations help to describe the excited-state behavior of the studied complexes. Two stable conformers of  $[W(CNAr)_6]$  were found and spectral variations caused by the conformational changes were explained.

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## FLUORESCENCE TECHNIQUES TO INVESTIGATE NANOSCALE ORGANISATION OF CELLULAR PLASMA MEMBRANE

**Mgr. Zuzana Kvíčalová**

*Marek Cebecauer, PhD.*

The plasma membrane is important for proper function and survival of cells. Exact organisation of its components, especially membrane proteins, contributes to a number of vital processes such as cellular metabolism, adhesion and signalling.

Current dramatic of fluorescence single-molecule localisation microscopy techniques enable localising membrane proteins with previously unreachable precision of 20 to 50 nm.

Proteins can be randomly distributed or clustered in cellular membranes. We use localisation microscopy and image data processing to achieve high-resolution distribution maps of wild-type CD4 and its mutants on the surface of resting T cells. Clustering is further determined by statistical methods such as Ripley K-function and Gettis-Franklin or pair-correlation analyses. Comparing clustering parameters determined for wild-type CD4 and its variants allows us to determine structural elements of CD4 molecule responsible for its precise membrane localisation.

We have also employed dual-colour localisation microscopy to characterise the impact of transmembrane domain (TMD) on distribution of membrane proteins. Cross-correlation and co-localisation (Manders) analyses are used to determine relative distribution of two membrane proteins, which can co-localise, segregate or have independent (random) distribution in the plasma membrane. We expect to observe the formation of protein-specific clusters (segregation) determined by their TMD. Random or co-localised distribution would indicate no or minor impact of TMD.

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# SINGLE-MOLECULE CONDUCTANCE MEASUREMENTS OF SELECTED EXPANDED PYRIDINIUM MOLECULES

Mgr. Štěpánka Lachmanová

Mgr. Magdaléna Hromadová Ph. D.

The miniaturisation of the electronic components more or less continues due to the trends predicted by the Moore's law. Nevertheless, the limit of this precondition is approaching because of the minimal achievable dimension of the metallic components. One of the possible ways how to reach smaller size of the electronic parts is the usage of the specialized molecules [1]. Among the promising molecules rank the extended and expanded pyridinium derivatives.

In this work, we have studied the single-molecule conductance of the selected expanded branched pyridinium cations 2',6'-diphenyl-[4,1':4',4''-terpyridin]-1'-ium (1) and 9-(pyridin-4-yl)benzo[*c*]benzo[1,2]quinolizino[3,4,5,6-*ija*][1,6]naphthyridin-15-ium (2) (structures in figure below) by STM-controlled break junction (STM-BJ) method in mesitylene. In this measurement the molecule forms a bridge between two gold electrodes, which are connected to a power source. It is possible that even a single molecule closes the circuit. Expanded branched pyridinium molecules make the connection between the electrodes by the specific interaction of their terminal nitrogen atoms with gold. The success rate of creating such connections is relatively low and the results have to be reached by use of statistical methods.

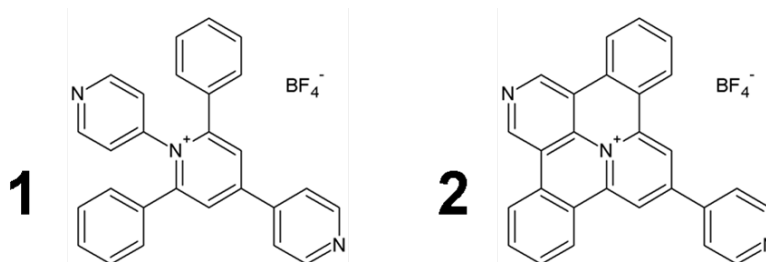


Fig. 1: Studied molecules

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## Acknowledgement:

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# ELECTROCHEMICAL REDUCTION OF 1,3-ALT-TETRANITRO- THIACALIX[4]ARENES

Mgr. Alan Liška

Prof. RNDr. Jiří Ludvík, CSc.

Calixarene skeleton is a stable supramolecular frame which is electrochemically not reducible. Suitable substitution on the upper and lower rim, eventually structure modification or introduction of heteroatoms lead to unusual and surprising properties of this system. Easily reducible nitro group was proved to be a suitable substituent (redox probe) enabling electrochemical investigations [1].

Generally, calix[4]arenes can exist in four conformations: *cone*, *partially cone*, *1,2-* and *1,3-alternating*. One of many principal questions is, whether (and how) the electrochemical response reflects the conformation of the compound. As an example, a comparative study of two (*cone*- and *1,3-alt*-) dinitrocalix[4]arenes is presented.

In thiacalix[4]arenes (Fig. 1) four aromatic units are connected by sulphur atoms (instead of methylene bridges). The present contribution is focused on a series of *1,3-alt*-tetranitrothiacalix[4]arenes with different substitution on the lower rim. Their cathodic reduction in aprotic media (DMF) starts with two 2-electron reversible processes which correspond to the presence of two different couples of equivalent nitro groups. This result proves that this seemingly circular molecule must exist in a pinched form, The full reversibility points to the fact that the four-electron reduction intermediate involves four equivalent non-communicating nitro radical anions. This stable tetradical tetraanion is then reduced by 12 electrons (one broad wave or two separated steps) to yield the corresponding tetrahydroxylamino derivative. The lower-rim substitution does not play a significant role in reduction mechanism.

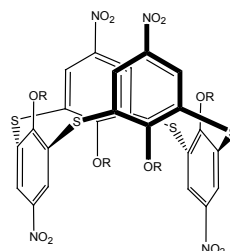


Fig. 1

**Acknowledgement:** This work was supported by the GACR grant No. 13-21704S and institutional support RVO: 61388955. The authors thank prof. Pavel Lhoták for granting the compounds.

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## POST-SYNTHESIS MODIFICATIONS OF LAYERED ZEOLITE PRECURSOR IPC-1P

**Mgr. Michal Mazur**

*Prof. Ing. Jiří Čejka, DrSc.*

Zeolites are crystalline aluminosilicates with well-defined, 3D structures having pores and cavities of molecular dimensions. Some of them are known to form 2D layered precursors providing many opportunities to design new zeolitic materials <sup>[1]</sup>. Recently, the 'top-down' conversion of germanosilicate UTL into the lamellar precursor (IPC-1P) has been described <sup>[2]</sup>. Very rich chemistry of this material provides various possibilities of post-synthesis modifications, especially towards new zeolites (PCR, OKO) <sup>[3]</sup> and more accessible zeolite-like structures.

Modifications like intercalation, stabilization and pillaring were applied on IPC-1P. Pillaring demonstrated the ability to adjust the interlamellar space and to control pore volume choosing appropriately intercalated precursor. The pillaring of IPC-1P samples intercalated with  $C_nH_{2n+1}N(CH_3)_3OH$  ( $n = 8 - 18$ ) leads to mesoporous materials with narrow pore size distribution in the range 2.5 – 3.5 nm. Pillared materials (IPC-1PI) exhibit BET areas in the range of 497-1006 m<sup>2</sup>/g <sup>[4]</sup>.

The use of different silanes (e.g. diethoxydimethylsilane) as linkers made possible to stabilize IPC-1P layers to obtain the IPC-2 (OKO) zeolite and more expanded structures. Textural and structural properties of the obtained materials were investigated using XRD, SEM and adsorption of Ar and N<sub>2</sub>.

The study shows that introducing of appropriate organics in between the layers of IPC-1P is determining step in producing new zeolitic architectures with variable textural properties, which are potential catalysts for transformation of bulky molecules.

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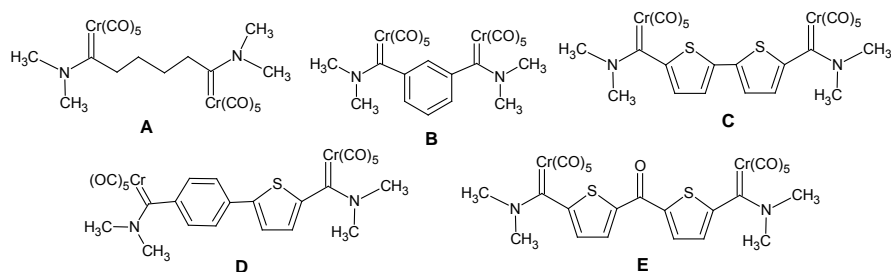
# INTRAMOLECULAR ELECTRON COMMUNICATION IN BINUCLEAR CHROMIUM FISCHER CARBENE COMPLEXES

Ing. Radka Metelková

prof. RNDr. Jiří Ludvík, CSc.

Bimetallic chromium(0) aminocarbene complexes are molecules with multiple redox centers: two reducible aminocarbene moieties and two oxidizable coordinated chromium atoms. The molecules include different bridging group between the centers (see the figure) influencing the intramolecular electron communication (delocalization). The electrochemical studies of such "molecular conductivity" are related to the research concerning organometallic molecular wires and their models<sup>1</sup>.

In our previous research of aminocarbene "mono" chromium complexes it was found that according to the structure, the aminocarbene moiety is able to form more or less delocalized system with the substituent on the carbene carbon<sup>2,3</sup>. In the presented series of binuclear complexes, this substituent serves as a bridging unit mediating the electronic communication within the molecule. Electrochemical oxidation is quasi-reversible and involves oxidation of the chromium atom with a follow-up reaction of carbonyl ligands loss. Electrochemical reduction is irreversible and involves splitting of the carbene bond accompanied by dimerization of the organic part. The intramolecular electron communication manifests itself as two separated oxidation (or reduction) responses of the two oxidation (reduction) centers. The negligible separation of peaks was observed for complex A while the highest peak separation was observed for complex C. It was found also that the solvent plays an important role. Complexes C, D and E are the most stable according to UV-Vis measurement in acetonitrile.



## Acknowledgement:

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# INFLUENCE OF CHOLESTEROL ON MODEL PHOSPHOLIPID MEMBRANES PROPERTIES

**Ing. Kateřina Nováková**

*Assoc. Prof. Dr. Ing. Tomáš Navrátil*

Biological membranes represent a nature barrier. Various types of model phospholipid membranes (PLMs) are utilized for elucidation and characterization of processes realized on real membranes. Model PLMs were formed in pores of a polycarbonate substrates which are suitable for study of mechanism of transporting processes and properties of biological membranes<sup>1,2</sup>. These model membranes are usually composed of simple phospholipids, especially 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine was used. Cholesterol was added to model PLMs to simulate the properties of real biological membranes<sup>3,4</sup>.

The PLMs and the transporting processes were characterized by electrochemical methods (electrochemical impedance spectroscopy (EIS) and voltammetry) as well as non-electrochemical methods (optical microscopy, atomic force microscopy (AFM), electrospray ionization mass spectrometry (ESI-MS)).

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## *Acknowledgments*

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## ANALÝZA NOVÝCH SYNTETICKÝCH DROG V LIDSKÉM TĚLE METODOU LC/MS/MS

**Bc. Michaela Obluková \*\*\***

*Mgr. Ján Žabka, CSc.*

V posledních letech se na trhu s drogami objevují stále nové syntetické psychoaktivní látky, které napodobují účinky ilegálních drog. Snaha výrobců těchto látek je obejít seznam zákonem zakázaných látek a vyrobit substanci, která na tomto seznamu nefiguruje. Tyto látky jsou volně distribuované prostřednictvím internetu nebo jsou dostupné v tzv. SmartShopech. Syntetické drogy zahrnují syntetické kanabinoidy, deriváty katinonu a další. Riziko užívání těchto látek spočívá v tom, že nejsou dostatečně prozkoumány jejich účinky, toxicita, interakční vlastnosti a jejich detekce. Principiální problém těchto látek spočívá v neúčinnosti současných metod toxikologického screeningu biologického materiálu z důvodu velkého množství jednotlivých derivátů [1].

Cílem práce je metodou LC/MS/MS detekovat stopové množství syntetických drog v reálném vzorku [2]. Budu se zabývat optimalizací podmínek pro tvorbu prekurzorových iontů, jejich fragmentů pro standardy syntetických drog i jejich metabolity. Získané výsledky této studie budou následně aplikovány při analýze reálných vzorků.

Ve své prezentaci představím předběžnou studii detekce standardů těchto látek a jejich vlastností.

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# **AB INITIO MOLECULAR DYNAMICS WITH NON-ADIABATIC AND SPIN ORBIT EFFECTS APPLICABLE FOR STUDY OF FLUORESCENT PROBES**

**Ing. Marek Pederzoli, MSc**

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

Ab initio non-adiabatic molecular dynamics is a relatively new and modern approach for describing the time evolution and time-dependent properties of molecular systems, which cannot be described employing neither simple force field methods nor quantum chemical methods limited by the Born-Oppenheimer approximation. This approach is particularly needed for study of phenomena involving fluorescence and photochemistry in general, where excited states and crossings between potential energy surfaces are essential.

In some photochemical reactions, transitions may even occur between states of different spin multiplicity, which is known as inter-system crossing. Even though inter-system crossings are usually associated with the presence of heavy atoms, they were recently shown to play a dominant role even in certain light-atom molecules.

To account for inter-system crossings, the relativistic spin-orbit interaction needs to be taken into account. We have implemented a method for inclusion of spin-orbit couplings into the Newton X package in the context of Tully's version of surface hopping dynamics.

We tested our implementation on a model system, IBr, and we will soon be able to apply this approach to simulations of bigger systems including fluorescent probes in bio-membranes employing the quantum mechanics/molecular mechanics (QM/MM) method.

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## EPOXIDATION OF BULKY ORGANIC MOLECULES OVER ADVANCED TITANOSILICATE CATALYSTS

Ing. Jan Přeč

Prof. Ing. Jiří Čejka, DrSc.

TS-1 is currently a catalyst of choice for epoxidation of C=C double bonds. However, the access of bulky substrates like terpenes to the active sites is restricted due to its narrow pores (5.5 Å). One of the solutions is preparation of large-pore titanosilicates<sup>1</sup>. Another approach is the application of hierarchical materials (possessing micro and mesopores) or layered materials (having large external surface area) as catalysts represents one of the solutions how to overcome the diffusion problems.

Different types of hierarchical TS-1 were prepared by desilication and secondary templating. In addition, layered TS-1 was prepared according to Ryoo protocol<sup>2</sup>. Subsequent pillaring treatment (using silicon (IV) ethoxide and titanium (IV) butoxide) introduce pure silica or a mixture of silica and TiO<sub>2</sub> (Si-Ti-pillared TS-1) pillars to keep the crystalline layers apart and enhance the accessibility of the active sites. Furthermore, Ti-MCM-36 material<sup>3</sup> was prepared. The titanosilicates were characterized using DR-UV/Vis spectroscopy, X-ray powder diffraction analysis, nitrogen adsorption analysis at -196°C, and SEM-EDX spectroscopy.

The materials were studied in epoxidation of substituted norbornenes, verbenol and cyclooctene with hydrogen peroxide as the oxidant at 60°C with alkene/catalyst mass ratio 10 and alkene/H<sub>2</sub>O<sub>2</sub> molar ratio 2 in acetonitrile. Standard TS-1 was used as a benchmark.

The highest yield of norbornene oxide was achieved using Ti-MCM-36 and Si-Ti-pillared TS-1 (7.6% resp. 7.4% after 3 h) while standard TS-1 gave the epoxide yield only 0.8 %. Similarly, in epoxidation of cyclooctene, yield of 9.7% was obtained using Si-Ti-pillared TS-1 after 3.5 h contrary to the yield of 2.8% using standard TS-1. On the other hand, verbenol underwent rapid epoxidation over layered TS-1 (yield 41% after 3 h) but the pillared materials underwent fast deactivation (Si-Ti-pillared TS-1) or their performance was low (Ti-MCM-36: yield 11% after 3 h) in comparison to the layered TS-1. We assume the high reactivity of verbenol to electron rich nature of its double bond.

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## EXPERIMENTY S N<sub>2</sub>O A NO NA LĚDOVÝCH NANOČÁSTICÍCH

Daniela Šmídová

*Mgr. Michal Fárník, Ph.D., DSc.*

Oxidy dusíku se účastní mnoha důležitých dějů v atmosféře (vznik ozonové díry, kyselé deště, skleníkový efekt aj.). Na povrchu polárních stratosférických mraků, které jsou tvořeny ledovými nanočásticemi, dochází k heterogenním reakcím přispívajícím k úbytku ozonu. V laboratorních podmínkách lze tyto nanočástice napodobit vodními klastry, což nám umožní detailní studium těchto procesů.

Ve zdroji molekulových paprsků obsahujícím vodní páru byly supersonickou expanzí čistého N<sub>y</sub>O (N<sub>2</sub>O a NO) nebo 5% směsi 5 N<sub>y</sub>O v argonu generovány smíšené klastry. Pomocí time-of-flight hmotnostní spektrometrie jsme detekovali velké množství fragmentů vzniklých elektronovou ionizací klastrů. Sledovali jsme vliv expanzních podmínek na tvorbu klastrů a jejich intenzitu po ionizaci. Potvrdili jsme, že je preferována tvorba ionů obsahujících lichý počet molekul NO. Při expanzi N<sub>2</sub>O se kromě (H<sub>2</sub>O)<sub>N</sub>H<sup>+</sup> série vyskytuje i (H<sub>2</sub>O)<sub>N</sub><sup>+</sup>, což je pravděpodobně způsobeno podobnými hodnotami ionizačních potenciálů N<sub>2</sub>O (12,89 eV) a H<sub>2</sub>O (12,62 eV).

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**Poděkování:** Projekt GAČR 14-08937S



## SELECTED ION MOBILITY MASS SPECTROMETRY

Mgr. Anatolii Spesyvyi

*prof. RNDr. Patrik Španěl, Dr. rer.nat.*

Selected ion flow tube mass spectrometry (SIFT-MS) is an analytical technique for real time qualification and quantification of a great variety of organic and non-organic volatile compounds with concentrations down to the part per billion by volume.

SIFT-MS technique is based on ion-molecule reactions in the flow tube between selected ions and neutrals from the sample. Products of these reactions are detected by quadrupole mass filter. But there is often situation for organic compounds when product ions have equal mass while their molecule structures are different. In order to separate them, an electrical field could be used as the ion mobility depends on the geometry and size of the molecular ion.

It is proposed to extend SIFT-MS with an ion mobility stage and thus to develop selected ion mobility mass spectrometry technique (SIM-MS). In my presentation, the theory of ion mobility in drift fields and the first results of the construction of new instrument for SIM-MS will be presented.

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# DVOUTEPLTNÍ ANALÝZA JAKO NÁSTROJ K ROZUZLENÍ KOMPLIKOVANÝCH OVERTONOVÝCH SPEKTER AMONIAKU

**Bc. Vít Svoboda**

*Mgr. Ondřej Votava, Ph. D.*

Amoniak je oblíbenou molekulou v oboru molekulové spektroskopie již řadu let. Je tomu tak ze dvou hlavních důvodů. Zaprvé hraje důležitou roli v zemské atmosféře, atmosférách planet a měsíců Sluneční soustavy, ale i v průmyslové sféře. Zadruhé figuruje jako prototypická molekula využívaná pro testování precizních teoretických modelů. Oba dva zmíněné důvody vyžadují kvalitní experimentální data získaná pomocí vysoce rozlišené spektroskopie. Spektrum amoniaku v blízké infračervené oblasti (NIR) je značně komplikované přítomností řady overtonových a kombinačních pásů, proto i přes velké experimentální úsilí není NIR spektrum amoniaku úplně přiřazeno.

V naší práci se zabýváme spektrální oblastí okolo 1,5  $\mu\text{m}$ , kde se nacházejí první overtóny a kombinační pásy N-H vibrací amoniaku. Ve spektru je dále přítomna řada poruch spojených s interakcí mezi rotací a vibrací molekuly. Navíc molekula amoniaku má nízkou inverzní bariéru, proto dochází k překlápění molekuly mezi dvěma rovnovážnými pyramidálními geometriemi. To v důsledku komplikuje spektra přítomností inverzního štěpení čar do dubletů. Všechny tyto poruchy vedou k problémům při experimentální práci a při teoretických výpočtech.

V předkládané práci bude demonstrováno vůbec první použití metody dvouteplotní analýzy vycházející čistě ze spekter změřených v supersonické expanzi. Bude diskutováno, jak je možné využít kvalitní teoretické predikce a kvalitní experimentální data pro získání důležitých spektroskopických informací, které jsou jinak velmi těžko získatelná z klasických experimentů ve statických kyvetách. Bude diskutována relevantnost empirického přiřazení založeného na dvouteplotní analýze pro jednotlivé rotačně-vibrační linie a následná validace těchto přiřazení pomocí výpočtu kombinačních diferencí (GSCDs). Na závěr bude diskutováno přiřazení vibračního stavu pro sedm nejsilnějších spektrálních pásů v dané oblasti a jeho kritické srovnání s předešlými pracemi.

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Yurchenko S. N., Barber R. J., Tennyson J., *Mon. Not. R. Astr. Soc.* **2011**, 413, 1828-1834.

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## PHOTODISSOCIATION DYNAMICS - RECONSTRUCTION METHODS

**Mgr. Pavla Svrčková**

*Mgr. Michal Fárník Ph.D. DSc.*

We examine the photodissociation dynamics using velocity map imaging method [1]. This method is very convenient because the images of photofragments contain the complete information about the dynamics of the photodissociation process. In the experiment we record the image, which is projection of a three-dimensional (3-D) velocity distribution onto a two-dimensional (2-D) detector. After that we need to extract all the information contained in the image: the kinetic energy and angular distribution of the photofragments. For that we can use some reconstruction methods.

We have available three reconstruction programs for evaluation experimental data (Image Manipulation, DaVis, Basex) using following reconstruction methods: Abel inversion, Hankel inversion, Iterative inversion and Basis set expansion. My task is to evaluate the suitability of these methods for our experiments. I test various optional parameters in each method and I compare these results for finding the optimal reconstruction method with optimal settings.

Acknowledgement: Grant No. 301614

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## TRLFS SPECIATION STUDY OF THE $\text{UO}_2^{(2+)} - \text{XO}_4^{(2-)} - \text{H}_2\text{O}$ (X = S, SE) SYSTEM COMPARED WITH THEORETICAL QUANTUM-CHEMICAL CALCULATION

Ing., Mgr. Jakub Višňák

*Mgr. Jiří Pittner Dr. rer. nat.*

Chemical properties of water solutions of U(VI) and  $\text{XO}_4^{2-}$  (X=S, Se) at low pH (<4) in temperature range 5-70°C are important objects of both experimental and theoretical studies because of their importance in geochemical modelling (i.e. uranium mining process, safety studies of radioactive waste repositories).

Spectrofotometric and TRLFS measurements of solutions mentioned above revealed estimations of stability constants of several complex species of general formula  $[\text{U}^{\text{VI}}\text{O}_2(\text{OH})_n(\text{XO}_4)_m(\text{H}_2\text{O})_p]^{2-n-2m}$ , present in solutions. (by multilinear analysis – PCA and PARAFAC). Experimental part of the work was done on The Department of Nuclear chemistry, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague in collaboration with Mgr. Aleš Vetešník, PhD.

Experimentally obtained stability constants were compared with quantum-chemical calculations – DFT/B3-LYP (scalar relativistic effects treated by pseudopotential ECP, in collaboration with Ing. Lukáš Sobek), four component all-electron *ab initio* calculation based on Dirac equation (with both Dirac-Coulomb and Dirac-Coulomb-Breit hamiltonians) and DFT calculations derived from the previously mentioned *ab initio*. Other possible relativistic quantum-chemical methods are discussed.

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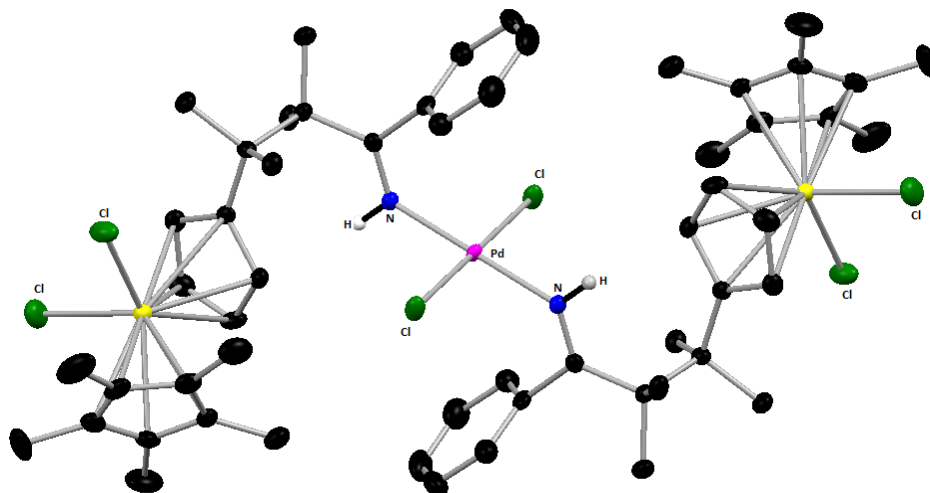
# POLYMERACE ETHYLENU NA Ti A Zr KOMPLEXECH S CYKLOPENTADIENYL- KETIMIDOVÝMI CHELATUJÍCÍMI LIGANDY

Miloš Večeřa

RNDr. Martin Lamač, Ph.D.

Metalocenové komplexů prvků 4. skupiny jsou v současné době studovány pro jejich různá potenciální uplatnění. Mohly by sloužit jako látky s cytostatickými účinky v medicíně,<sup>1</sup> fotokatalyzátory pro rozklad vody<sup>2</sup> a především pak jako katalyzátory Ziegler-Nattaova typu pro polymerace olefinů.<sup>3</sup> Na základě rozdílných ligandů, použitých kovů, olefinů či jejich směsí se liší jejich katalytická aktivita pro daný typ polymerace. Speciálním typem jsou tzv. CGC (constrained geometry complex) komplexy. Tyto komplexy se ukázaly jako vynikající katalyzátory kopolymerací ethylenů s  $\alpha$ -olefiny s vysokou aktivitou, která bývá vysvětlována výrazným obnažením aktivního centra díky geometrii uvedených ligandů.<sup>4</sup>

V naší práci se věnujeme přípravě a charakterizaci metalocenových a polosendvičových komplexů s hybridními Cp-ketimidovými ligandy. Tyto komplexy testujeme v polymeračních reakcích a studujeme jejich reaktivitu s Lewisovými či Brønstedovými kyselinami. Jako Lewisovské kyseliny mohou vystupovat i různé kovové fragmenty (viz obrázek).



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## OPTIMALIZATION AND CHARACTERIZATION OF POLYMETHYLENE BLUE MODIFIED GRAPHITE ELECTRODE

Mgr. Magda Zlámlová

Ing. Pavel Janda, CSc.

Electropolymerization is an effective way of the electrode surface modification. Electro-synthesized polymers exhibit some unique behavior that the corresponding monomers do not always display.

The electrocatalytic activity of poly(methylene blue) (pMB) in the presence of some biologically active compounds has been reported in several studies<sup>1-3</sup>. Cyclic voltammetry of methylene blue (MB) in aqueous solution leads to the formation of stable conductive polymer film on the solid electrode surface. It has been already published that basic solutions are optimal media for the polymerization of MB<sup>4</sup> and electrochemical properties of electrodeposited polymer film are affected by solid electrode substrate<sup>5</sup>.

The aim of our work is to design new electrode system which combines auspicious electrochemical properties of pMB and advantages of highly oriented pyrolytic graphite (HOPG). We have optimized the conditions of electropolymerization and characterized the properties of pMB/HOPG electrode. The modified electrode exhibits electrocatalytic activity towards SH<sup>-</sup> group. Our findings will be utilized for development of new potentiometric or amperometric sensor.

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