



SEMINÁŘ STUDENTŮ ÚFCH JH 2011

Konferenční centrum
AV ČR v Liblicích
11. - 13. 4. 2011



Seminář studentů ÚFCH JH 2011

Sborník příspěvků

**ze studentské konference konané
11.-13. dubna 2011
v Konferenčním centru AV ČR Liblicích**

Seminar of Students of JHI 2011

Collection of abstracts

**of all lectures given at the student conference
held on 11 -13 April 2011
in Conference Centre of the Academy of Sciences
of the Czech Republic in Liblice chateau**

**Seminář studentů ÚFCH JH 2011
Sborník příspěvků ze studentské konference
konané 11.-13. dubna 2011
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Kolektiv autorů

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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: 75 kusů

Místo a rok vydání: Praha, 2011

Publikace neprošla jazykovou úpravou

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ISBN 978-80-87351-11-6

SEMINÁŘ STUDENTŮ ÚFCH JH 2011

PROGRAM 1. dne konference - **Pondělí 11.4.2011**

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

Předpokládaný příjezd do Konferenčního centra AV ČR v zámku
v Liblicích v 15:00 (15:30) hodin.

Čas	Předsedající	Přednášející	Název
15:15 – 16:40	Registrace a ubytování účastníků konference Občerstvení před zahájením konference <i>(od 15:45 hodin: káva, nápoje, sendvič)</i>		
16:45	Zahájení konference „Seminář studentů ÚFCH JH 2011“ - prezentace studenta z mimosoutěžní kategorie a studentů kategorie I.		
16:55	<u>Květa</u> <u>STEJSKALOVÁ</u>	Jan BOHUSLAV <i>(středoškolský stážista SOČ, šk. P.Janda) mimosoutěžní kategorie</i>	NANOČÁSTICOVÁ ELEKTRODA: NANOMORFOLOGIE A ELEKTROCHEMIE
17:10	<u>Libor</u> <u>VEIS</u>	Tomáš HODÍK <i>(bakalářské studium VŠCHT Praha školitel M.Lamač a J.Pinkas) kat I</i>	SYNTÉZA A ZAKOTVENÍ POLO-SENDVIČOVÝCH KOMPLEXŮ TITANU NA MODIFIKOVANOU SILIKU
17:30		Monika KLUSÁČKOVÁ <i>(diplomantka PřF UK, školitel P. Janda) kat I</i>	REAKCE PŘENOSU NÁBOJE V PYRIDIN-PORFYRAZINÁTOVÉM FILMU PRO VYUŽITÍ V ELEKTROCHEMICKÉM SENZORU
17:50		Helena DRAGONOVÁ <i>(bakalářské studium, LF UK Plzeň; šk. P.Hrabánek) kat I</i>	SYNTHESIS OPTIMIZATION AND ADVANCED CHARACTERIZATION OF ZEOLITE SSZ-16 (AFX)
18:10	PŘESTÁVKA		
18:20	<u>Věra</u> <u>MANSFELDOVÁ</u>	Marie KOLÁŘOVÁ <i>(diplomantka PřF UK, školitel A. Benda) kat I</i>	DYNAMIC SATURATION OPTICAL MICROSCOPY USING REVERSIBLY PHOTOSWITCHABLE FLUORESCENT PROTEINS
18:40		Pavel KOŠŤÁL <i>(bakalářské studium MFF UK; šk. M. Fárník) kat I</i>	MONTE – CARLO SIMULATION OF PHOTODISSOCIATION SPECTRA FROM MOLECULAR BEAM EXPERIMENT
19:00		Hana KVAPILOVÁ <i>(diplomantka VŠCHT Praha školitel S. Zális) kat I</i>	DFT CALCULATIONS OF TRANSITION METAL AMINOCARBENE COMPLEXES – CORRELATION BETWEEN EXPERIMENT AND THEORY
19:20		Šárka POKORNÁ <i>(II. ročník PGS, školitel M. Hof) kat I</i>	SPECIFIC ION INTERACTION WITH POSITIVELY CHARGED PHOSPHOLIPID BILAYERS
19:40	Ukončení prvního dne konference VEČEŘE v RESTAURACI - začátek v 19:45		

PROGRAM 2. dne konference - úterý 12.4.2010

Čas	Předsedající	Přednášející	Název
8:30	Zahájení druhého dne konference - prezentace studentů kategorie I a II.		
8:30	<u>Petr KUBELÍK</u>	Petr JELÍNEK (<i>I. ročník PGS, školitel S.Civiš</i>) kat I	NOVĚ IDENTIFIKOVANÉ ATOMÁRNÍ LINIE VE SLUNEČNÍM SPEKTRU
8:50		Štěpánka LACHMANOVÁ (<i>diplomantka PŘF UK, školitelka M. Hromadová</i>) kat I	KATALYTICKÉ A REDUKČNÍ VLASTNOSTI ORGANOMETALICKÉHO KOMPLEXU RUTHENIA VE VOLNÉ FORMĚ A PO JEHO NAVÁZÁNÍ NA PAPAİN
9:10		Pavla CHLUBNÁ (<i>I. ročník PGS, školitel J.Čejka</i>) kat I	THE POST-SYNTHESIS TRANSFORMATION OF B-UTL INTO A LAMELLAR ZEOLITE WITH MODIFIABLE STRUCTURE
9:30		Jozef LENGYEL (<i>diplomant STU Bratislava; šk. M. Fárnik</i>) kat I	FORMATION AND PHOTODISSOCIATION OF $(\text{HNO}_3)_m \cdot (\text{H}_2\text{O})_n$ CLUSTERS IN MOLECULAR BEAMS
9:50	PŘESTÁVKA NA KÁVU A ZÁKUSEK		
10:20	<u>Martin FERUS</u>	Zuzana KOMÍNKOVÁ (<i>I. ročník PGS, školitel M.Kalbáč</i>) kat I	REMOVING SINGLE-WALLED CARBON NANOTUBES FROM MIXTURE OF SINGLE- AND DOUBLE-WALLED CARBON NANOTUBES USING REACTION WITH LITHIUM
10:40		Jan SUCHÁNEK (<i>I. ročník PGS, školitel Z. Zelinger</i>) kat I	EXPERIMENTÁLNÍ SPEKTROSKOPICKÉ STUDIE NANOČÁSTIC KVANTOVÝCH TEČEK
11:00		Milan BOUŠA (<i>I. ročník PGS, školitel L. Kavan a O. Frank</i>) kat I	DEVELOPMENT OF CAPACITIES IN CATHODE OLIVINE/CARBON COMPOSITE MATERIALS
11:20		Jana PAVLATOVÁ (<i>I. ročník PGS, školitel J.Čejka</i>) kat I	ACYLAČNÍ REAKCE DERIVÁTŮ DRUHÉ TŘÍDY BENZENU NA ZEOLITECH
11:40	PŘESTÁVKA		
11:50	<u>Barbora ŠUSTROVÁ</u>	Jaroslav KOČIŠEK (<i>I. ročník PGS, školitel M.Fárnik</i>) kat I	SCIENCE FROM PHOTOGRAPHY ? PHOTODISSOCIATION OF HB_r IN RARE GAS CLUSTERS
12:10		Elizaveta KUZNETSOVA (<i>PGS zahraniční host, školitel P.Krtil</i>) kat I	OXYGEN EVOLUTION ON IRIDIUM BASED OXIDES
12:30		Hana LIPŠOVÁ (<i>I. ročník PGS, školitel J.Jlrkovský</i>) kat I	FOTOCHEMICKÁ METODA DEKONTAMINACE PODZEMNÍCH VOD V REAKTIVNÍ CHEMICKÉ BARIÉŘE
PŘESTÁVKA NA OBĚD (OBĚD SE PODÁVÁ V RESTAURACI OD 13:00)			
14:30	<u>Lukáš SOBEK</u>	Jakub PASTVA (<i>I. ročník PGS, školitel J.Čejka</i>) kat I	PREPARATION AND CHARACTERIZATION OF NEW MATERIALS FOR METATHESIS
14:50		Barbora LÁSKOVÁ (<i>I. ročník PGS, školitel L.Kavan</i>) kat I	ELECTROCHEMICAL AND SPECTROELECTRO-CHEMICAL BEHAVIOR OF (001)-ORIENTED ANATASE TiO_2 NANOSHEETS

15:10		Tushar R. SHINDE (<i>I. ročník PGS, školitel H. Balcar</i>) kat I	HOVEYDA-GRUBBS TYPE METATHESIS CATALYST IMMOBILIZED ON MESOPOROUS MOLECULAR SIEVES
15:30		Šárka RAMEŠOVÁ (<i>diplomantka PŘF UK, školitelka R.Skolová</i>) kat I	ELEKTROCHEMICKÉ STUDIUM DEGRADACE PŘÍRODNÍCH BARVIV
15:50	PŘESTÁVKA NA KÁVU A ZÁKUSEK		
16:20	Ludmila ŠIMKOVÁ	Aleš HAVLÍK (<i>II. ročník PGS, školitel M Horáček</i>) kat II	ELECTRON DEFICIENT IV.B GROUP TRANSITION METAL COMPLEXES CONTAINING STABILIZING N-CHELATE FORMING LIGANDS AND A CYCLOPENTADIENYL RING
16:40		Tomáš STEINBERGER (<i>II. ročník PGS, školitel M. Hof</i>) kat II	FLUORESCENCE CROSS-CORRELATION SPECTROSCOPY AS A TOOL FOR STUDY OF ANTIMICROBIAL ACTIVITY OF PEPTIDES
17:00		Barbora ŠUSTROVÁ (<i>III. ročník, šk. -konzultant V. Mareček</i>) kat II	SOME WAYS OF MODIFICATION OF POLY-CRYSTALLINE GOLD ELECTRODES BY THIOLATED COMPOUNDS
17:20		Lukáš SOBEK (<i>III. ročník, školitel J.Pittner</i>) kat II	A STUDY OF INDOLE AND PRODANE EXCITED STATES WITH QM/MM MODELLING OF PRODANE EMBEDDING IN DOPC BILAYER
17:40	UKONČENÍ DRUHÉHO DNE KONFERENCE. <u>VEČEŘE</u> V RESTAURACI OD <u>18:00</u> HODIN		
17:45-18:00	Pro zájemce - mimokonferenční prezentace	Květa STEJSKALOVÁ	Na téma "Od popularizace vědy ke vzdělávání a zase zpět, tj. od vzdělávání k popularizaci"; stručně o zapojení ÚFCH JH do programu mezinárodního Roku chemie 2011

PROGRAM 3. dne konference - Středa 13.4.2010

Čas	Předsedající	Přednášející	Název
8:30	Zahájení třetího dne semináře - prezentace studentů kategorie II.		
8:30	Martin ŠTEFL	Ludmila ŠIMKOVÁ (<i>III. ročník, šk. J.Ludvík</i>) kat II	ELECTROCHEMICAL AND SPECTROMETRIC STUDY OF 2,2-DINITROETHENE-1,1-DIAMINE IN APROTIC SOLVENTS
8:50		Libor VEIS (<i>III. ročník, školitel J. Pittner</i>) kat II	QUANTUM CHEMISTRY ON QUANTUM COMPUTERS
9:10		Kristýna SOVOVÁ (<i>II. ročník PGS, školitel P. Španěl</i>) kat II	REAL-TIME SIFT-MS DETECTION OF VOLATILE FORMS OF SELENIUM RELEASED BY PLANTS
9:30		Martin FERUS (<i>III. ročník, školitel S. Civiš</i>) kat II	FORMAMIDE CHEMISTRY AND PREBIOTIC SYNTHESIS
9:50	PŘESTÁVKA NA KÁVU A ZÁKUSEK		

10:30	<u>Milan ONČÁK</u>	Milan MAŠÁT (IV.ročník, šk. O. Votava) kat II	CRDS MEASUREMENT DATA AQUISITION IN SUPERSONIC EXPANSION
10:50		Petr KLEIN (II. ročník PGS, školitel J. Dědeček) kat II	MULTI-NUCLEAR MAS NMR STUDY OF EXTRA-FRAMEWORK CATION SITING IN SILICON RICH ZEOLITES
11:10		Věra MANSFELDOVÁ (III. ročník, školitel-konzultant P.Janda) kat II	PHthalocyanine MODIFIED HOPG ELECTRODES FOR ELECTROCHEMICAL SENSORS
11:30	PŘESTÁVKA		
11:45	<u>Milan MAŠÁT</u>	Petr KUBELÍK (III. ročník, školitel S. Civiš) kat II	CHEMICAL MODELLING AND DISCHARGE PLASMA CHEMISTRY
12:05		Milan ONČÁK (III. roč., šk. P.Slaviček a M.Fárník) kat II	SOLVATED ELECTRON EXPLORED BY METHODS OF THEORETICAL CHEMISTRY: FROM GAS PHASE CLUSTERS TO BULK
12:25		Martin ŠTEFL (III. ročník, školitel M. Hof) kat II	FLUORESCENCE STUDY OF MEMBRANE RAFTS FORMATION USING CHOLERA TOXIN PROTEIN
12:45	UKONČENÍ PREZENTACÍ A CELÉ KONFERENCE		
SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ			
13:15 14:30	OBĚD V RESTAURACI od 13:15 hodin Odjezd do Prahy - autobusem z parkoviště u zámku ve 14:30 <i>(Návrat do Prahy k budově ÚFCH JH do 16:00 hodin.)</i>		



Seznam prezentujících studentů (37)

Kategorie I (22)

Diplomanti a zájemci z řad bakalářů (9)

Dragounová Helena (bakalářské st. 2.r., LF UK
Plzeň, stáž u P. Hrabánka)
Hodík Tomáš (bakalářské studium 1.r., VŠCHT, stáž
u M. Lamače a J. Pinkase)
Klusáčková Monika (diplomantka PřF UK, školitel
P. Janda)
Kolářová Marie (diplomantka PřF UK, školitel
A. Benda)
Košťál Pavel (bakalářské studium 3.r., MFF UK,
stáž u M. Fárníka)
Kvapilová Hana (diplomantka, VŠCHT, školitel
S. Zálíš)
Lachmanová Štěpánka (diplomantka PřF UK,
školitel M. Hromadová)
Lengyel Jozef (diplomant, STU Bratislava, školitel
M. Fárník)
Ramešová Šárka (diplomantka PřF UK, školitel R.
Sokolová)

Středoškolský stážista – nesoutěžní kategorie

Bohuslav Jan – student 3. ročníku Gymnázia PORG
v Praze 8 představí svou středoškolskou odbornou
činnost (SOČ) v rámci stáže u Ing. Pavla Jandy, CSc.
ve vzdělávacím a popularizačním projektu ÚFCH JH
s názvem Tři nástroje.

Studenti 1. ročníku PGS (12)

Bouša Milan (školitel L. Kavan)
Chlubná Pavla (školitel J. Čejka)
Jelínek Petr (školitel S. Civiš)
Kočišek Jaroslav ((PGS studium v rámci EU
projektu ICONIC, školitel M. Fárník)
Komínková Zuzana (školitel M. Kalbáč)
Kuznetsova Elizaveta (PGS stáž v rámci EU
projektu ELCAT, školitel P. Krtil)
Lásková Barbora (školitel L. Kavan)
Lipšová Hana (2. školitel J. Jirkovský)
Pastva Jakub (školitel J. Čejka)
Pavlatová Jana (školitel J. Čejka)
Shinde Tushar Raghunath (školitel H. Balcar)
Suchánek Jan (školitel Z. Zelinger)

Kategorie II (15)

Studenti 2. ročníku PGS (5)

Havlík Aleš (školitel M. Horáček)
Klein Petr (školitel J. Dědeček)
Pokorná Šárka (školitel M. Hof)
Sovová Kristýna (školitel P. Španěl)
Steinberger Tomáš (školitel M. Hof)

Studenti 3. ročníku PGS (9)

Ferus Martin (školitel S. Civiš)
Kubelík Petr (školitel S. Civiš)
Mansfeldová Věra (2. školitel P. Janda)
Ončák Milan (školitel P. Slavíček,
2. školitel M. Fárník)
Sobek Lukáš (školitel J. Pittner)
Šimková Ludmila (školitel J. Ludvík)
Šustrová Barbora (školitel V. Mareček)
Štefl Martin (školitel M. Hof)
Veis Libor (školitel J. Pittner)

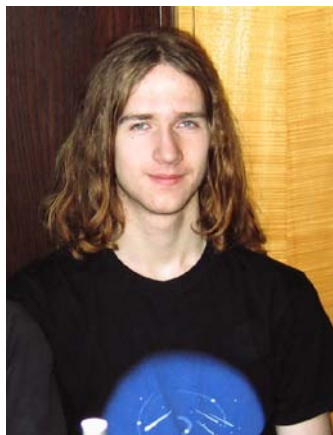
Možnost prezentovat se naposledy mají i studenti 4.ročníku PGS (nepovinně)

Mašát Milan (školitel O. Votava)

Hodnotící komise

Svatopluk Civiš
Michal Horáček
Magdalena Hromadová





NANOČÁSTICOVÁ ELEKTRODA: NANOMORFOLOGIE A ELEKTROCHEMIE

Jan Bohuslav***

Ing. Pavel Janda, CSc.

Nanočásticová elektroda byla připravena napařením niklu na monokrystalický substrát – vysoce orientovaný grafit (HOPG). Nikl patří mezi katalyticky aktivní kovy, které se účastní různých procesů v chemické syntéze, především v hydrogenačních procesech. Nikl rovněž nachází uplatnění v bateriích a v palivových článcích, proto je v poslední době intenzivně zkoumán s ohledem na možné využití v alternativních zdrojích energie.

Pole niklových nanočástic deponovaných na inertním vodivém substrátu slouží jako model dobře definované nanočásticové elektrody, jejíž vlastnosti lze ovlivňovat množstvím a velikostí nanočástic deponovaného kovu.

Morfologie nanočásticové elektrody v závislosti na množství deponovaného niklu byla zkoumána metodou mikroskopie atomárních sil. Elektrochemické chování a stabilita nanočástic deponovaných na HOPG byla studována v alkalickém prostředí (1 M KOH) metodou cyklické voltametrie.

*** účastník mimosoutěžní kategorie; ,středoškolský student-stážista představí svou práci realizovanou v rámci vzdělávacího a popularizačního projektu ÚFCH JH s názvem Tři nástroje



DEVELOPMENT OF CAPACITIES IN CATHODE OLIVINE/CARBON COMPOSITE MATERIALS

Mgr. Milan Bouša

Mgr. Otakar Frank, Ph. D.

Prof. RNDr. Ladislav KAVAN, DSc.

Lithium-ion batteries are widely used as power sources in many devices and are expected as a source of energy in electric vehicles. Electrochemical qualities of lithium-ion batteries depend on variable factors like physical and chemical properties of electrode materials. However, it is necessary to prepare safe materials with low cost but with sufficient power/energy density.

In this work we used mainly nanocrystalline LiFePO_4 olivine-type material (LFP) as the cathode material because of its low-cost, stability and availability. To improve the conductivity and charge transfer in the active electrode material, some form of sp^2 -hybridized carbon should be added. In the presented study we compare carbon nanotubes, conductive carbon black and few-layer graphene oxide (FLGO) as the additive to olivine material. Various voltametric and amperometric measurements were performed to investigate the influence of the carbon material on the reversibility, cycle stability and capacity of the prepared electrodes.

The composite of LFP and FLGO shows an intriguing evolution of capacities during the electrochemical cycling. To elucidate the observed behavior, Raman and IR spectroscopy were used for the characterization of the structural changes in the graphene oxide induced by electrochemical charge/discharge processes.



SYNTHESIS OPTIMIZATION AND ADVANCED CHARACTERIZATION OF ZEOLITE SSZ-16 (AFX)

Helena Dragounová

Ing. Pavel Hrabánek, Ph.D.

RNDr. Milan Kočířík, CSc.

Small pore high silica zeolite SSZ-16 with 8-membered oxygen rings belongs to AFX zeolite framework type. SSZ-16 consists of three-dimensional pore network and is isotopic with SAPO-56 and MAPSO-56. The channel size of SSZ-16 (0.34 nm x 0.36 nm) is attractive for separations, where molecular sieving effect can be exploited. Zeolite SSZ-16 has been also considered for catalytic reduction of NO_x [1]. Zeolite SSZ-16 was hydrothermally synthesized inside Teflon lined autoclaves. Duration of crystallization was substantially reduced from 35 to 7 days for synthesis mixtures that were aged for 7 days at room temperature under vigorous mixing in polypropylene vessels. The optimization of synthesis mixture composition was done by (i) replacement of fumed silica by colloidal silica to accelerate formation of precursor particles in synthesis solutions, (ii) ultrasonication and/or centrifugation of aged synthesis mixtures before hydrothermal crystallization, (iii) microfiltration of aged synthesis mixtures. The aim of optimization was to promote growth of SSZ-16 crystals instead of SSZ-16 shell particles with amorphous core. Zeolite SSZ-16 samples were characterized with X-ray diffraction, Scanning Electron Microscopy and physical adsorption of gases (nitrogen, argon).

Reference:

[1] Fickel, D.W.; Lobo, R.F., *J. Phys. Chem. C* **2010**, *114*, 1633-1640.



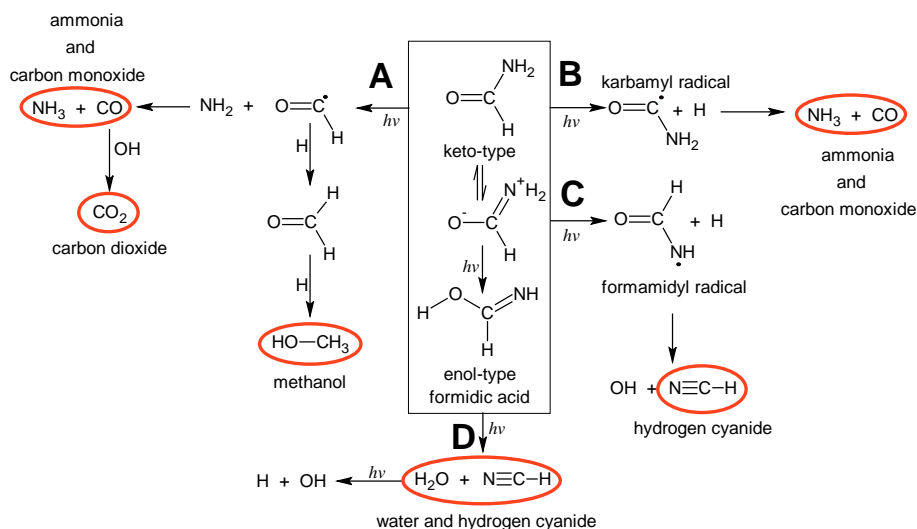
FORMAMIDE CHEMISTRY AND PREBIOTIC SYNTHESIS

RNDr. Martin Ferus

Doc. RNDr. Svatopluk Civiš, CSc.

Formamide (HCONH_2) provides a chemical frame potentially affording all the monomeric components necessary for the formation of nucleic polymers. Simpler small molecules composed of only three different types of atoms such as hydrogen cyanide are, in principle, endowed with similarly high prebiotic potential as proposed by Oró, Saladino and other authors. Understanding of formamide decomposition chemistry plays a key role in the research of amino acids and nucleic bases formation.

High resolution FT-IR spectroscopy was used for the analysis of gaseous decomposition products of formamide molecule in three different systems: High energy LIDB plasma, glow discharge and UV photodissociation. High energy LIDB plasma experiment is intended for the simulation of the high-density-energy event, glow discharge simulates lighting in the upper atmosphere and UV experiment simulates the photochemistry of the lower atmosphere of the Earth and terrestrial planets. Simulation of the reaction-dynamics was performed for the estimation of the main reaction pathways of formamide dissociation and simple molecular and radical fragments formation. A scheme of the photodissociation process is depicted.





ELECTRON DEFICIENT IV.B GROUP TRANSITION METAL COMPLEXES CONTAINING STABILIZING N-CHELATE FORMING LIGANDS AND A CYCLOPENTADIENYL RING

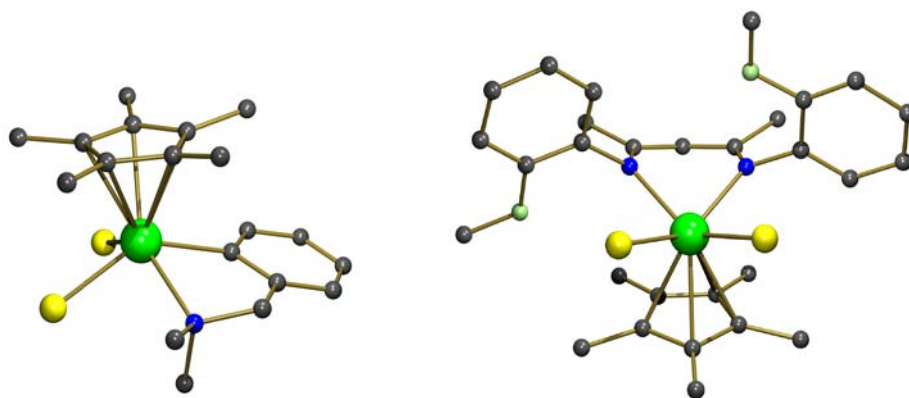
Ing. Aleš Havlík

Mgr. Michal Horáček, Ph.D.

Our interest has been directed to a combination of cyclopentadienyl ligand with a ligand containing a weak neutral additional donor site in strongly electrophilic early transition metal complexes.

The aim of my work is to prepare new Ti, Zr and Hf complexes containing highly-methylated cyclopentadienyl ring and N,N-dimethylbenzylamine or bifunctional beta-diketiminato.

A series of corresponding pentamethyl- and tetramethyl-substituted metallocene trichlorides (η^5 -C₅Me₅)MCl₃ and (η^5 -C₅HMe₄)MCl₃ (M = Ti, Zr, Hf) have been used as a starting material for reaction with one equivalent of lithium salt of N,N-dimethylbenzylamine or beta-diketiminato, respectively. The new complexes containing N,N-dimethylbenzylamine or beta-diketiminato have been synthesized in high yield. All compounds were characterized by spectroscopic methods. Molecular structures of the most of the products have been determined by X-ray crystallography. Reactivity of prepared metallocene complexes is under investigation and will be discussed.





SYNTÉZA A ZAKOTVENÍ POLO-SENDVIČOVÝCH KOMPLEXŮ TITANU NA MODIFIKOVANOU SILIKU

Tomáš Hodík

Mgr. Jiří Pinkas, Ph.D.

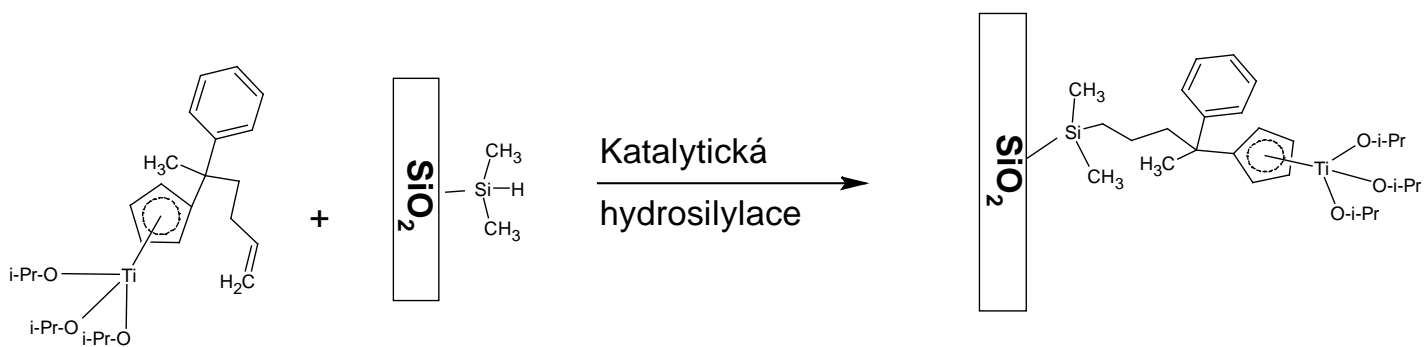
Mgr. Martin Lamač, Ph.D.

Hex-1-en je významnou průmyslovou surovinou při výrobě kopolymerů; (např. LLDPE – lineární nízkohustotní polyetylen, používaný na výrobu potravinářských folií). Hex-1-en je možno vyrábět trimerizací ethyleny, která je katalyzována směsí polo-sendvičového titaničitého komplexu a methylaluminoxanu ($(\eta^5\text{-C}_5\text{H}_4\text{CMe}_2\text{Ph})\text{TiCl}_3$ / MAO).

Nevýhodou daného systému je vysoká spotřeba drahého kokatalyzátoru (MAO), který je používán ve velkém molárním nadbytku vzhledem ke komplexu. Jednou z možností jak snížit množství kokatalyzátoru je použití titaničitého komplexu zakotveného na vhodný nosič.

Naším cílem bylo připravit nový polo-sendvičový titaničitý komplex mající cyklopentadienylový kruh substituovaný 1-methyl-1-fenylpent-4-enylovou skupinou. Visící alkenylovou skupinu je možno využít k zakotvení titaničitého komplexu na různé nosiče modifikované SiH skupinou (silika modifikovaná SiMe_2H) pomocí hydrosilylační reakce (viz schema).

V mém příspěvku bude blíže objasněna příprava a charakterizace homogenních titaničitých komplexů a pokus o jejich zakotvení na vhodné nosiče.



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THE POST-SYNTHESIS TRANSFORMATION OF B-UTL INTO A LAMELLAR ZEOLITE WITH MODIFIABLE STRUCTURE

Mgr. Pavla Chlubná

Prof. Ing. Jiří Čejka, DrSc.

Zeolites have attracted a lot of industrial and research interest as adsorbents, ion exchangers and mainly as selective heterogeneous catalysts, e.g. in petroleum refining. Traditionally the frameworks of zeolites are manifested as continuous in 3-D produced by direct synthesis. B-UTL is the example of zeolite which is possible to transform by post-synthetic modifications into a lamellar (2D) form with a preservation of the initially present dense layers.

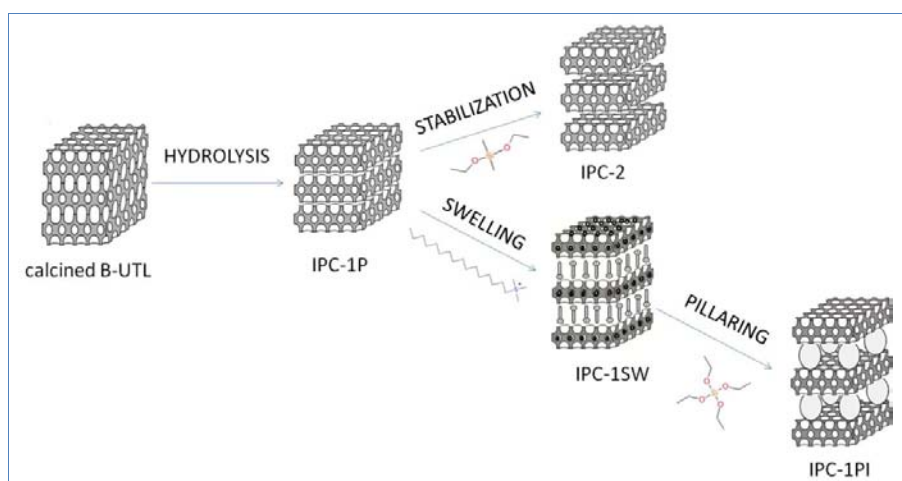


Fig. 1 - The scheme of hydrolysis of B-UTL and the subsequent treatments

UTL is a germanosilicate with attractive large pore system combining 14-ring pores intersecting with 12-rings [1]. The 3D structure of B-UTL (Si/Ge~2, $\text{BO}_{1.5}$ molar content 0-0.11) was post-synthetically transformed (via hydrolysis) into a lamellar product. The structure is further modifiable by using various treatments like swelling, pillaring and stabilization (Fig. 1) previously developed for investigation of layered zeolite precursors, like MCM-22P [2,3].

The individual steps of various treatments with B-UTL will be presented to explain their influence on the structure. X-ray powder diffraction (XRD) was used to follow the changes after the treatments in combination with TEM and nitrogen sorption measurements.

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NOVĚ IDENTIFIKOVANÉ ATOMÁRNÍ LINIE VE SLUNEČNÍM SPEKTRU

Mgr. Petr Jelínek

Doc. RNDr. Svatopluk Civiš, CSc.

Časově rozlišená infračervená spektrometrie s Fourierovou transformací byla použita pro pozorování emise vznikající po ozařování různých kovových terčů pulzním nanosekundovým ArF ($\lambda = 193 \text{ nm}$) laserem. Vysoko-frekvenční laser s výstupní energií 3 – 11 mJ v jednom pulzu byl fokusován na rotující kovový terč umístěný ve vakuové komoře (průměrný tlak $2 \cdot 10^{-4}$ bar). Infračervená emisní spektra byla pozorována ve spektrální oblasti $1200 - 8000 \text{ cm}^{-1}$ s časovým profilem ukazujícím maximální intenzitu emise v 1. – 60. μs po výstřelu laseru.

Takto experimentálně získaná spektra byla porovnána s atomárními liniemi ve slunečním spektru.

Atomární linie slunečního spektra byly v oblasti $1200 - 8000 \text{ cm}^{-1}$ dosud identifikovány pouze na základě výpočtů a predikcí z ultrafialové a viditelné části spektra. Srovnání takto určených linií s výsledky experimentálně získanými v naší laboratoři vedlo u některých atomárních linií slunečního spektra k potvrzení jejich správné identifikace a u některých k opravě jejich identifikace.

Literatura:

Civiš, S. et al. *Time-resolved Fourier-transform infrared emission spectroscopy of Ag in the (1300-3600)-cm(-1) region: Transitions involving f and g states and oscillator strengths*. Physical review A. 2010. **82**:2. 022502/1-022502/16.

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MULTI-NUCLEAR MAS NMR STUDY OF EXTRA-FRAMEWORK CATION SITING IN SILICON RICH ZEOLITES

Ing. Petr Klein

Mgr. Jiří Dědeček, CSc.

Zeolites (crystalline microporous aluminosilicates) represent the widest group of industrial catalysts. Recently, attention is focused on silicon-rich zeolites due to their stability and specific properties of metal ion species in these matrices. Extra-framework cation balancing the negative charge of AlO_4^- tetrahedra represent catalytically active sites for many important reactions. Recently, it was shown that Al siting in silicon-rich zeolites is not random and can be controlled by conditions of zeolite synthesis [1]. Thus, analysis of cation siting and geometry in silicon-rich matrices is essential to understand their properties and to rational design of catalysts. Determining cation siting using diffraction methods in silicon-rich zeolites is rather limited due to the low concentration of metal ions in these matrices. Therefore, a different method for characterizing cation distribution in silicon-rich matrices is highly demanded. High-resolution NMR spectroscopy reveals to be a promising tool for this purpose. Application of this approach was tested on the analysis of Li and Na ion siting.

^{23}Na and ^7Li MAS NMR spectra of dehydrated Na and Li-exchanged ferrierite and ZSM-5 zeolites were collected using a Bruker Avance 500 MHz (11.7 T) Wide Bore spectrometer using 4 mm o.d. ZrO_2 rotors with a rotation speed of 11 kHz and a high-power decoupling pulse sequence.

According to ab initio calculations and ^7Li MAS NMR experiment, ^7Li shielding in cationic sites is not affected by the vicinity of a second Li ion balancing a second Al atom of the Al-O-(Si-O) $_2$ -Al sequence in the framework. Thus, lithium ions monitored by ^7Li MAS NMR can serve as a probe of the aluminium siting in zeolites with isolated aluminium atoms or with Al-O-(Si-O) $_2$ -Al sequences. The siting of Li ions in extra-framework sites in a set of ferrierites with different framework Al content and prepared under different conditions was investigated and compared with results of ^{23}Na MAS NMR study of Na siting in extra-framework sites in these matrices and with previous results of ^{27}Al MAS NMR study of Al siting in these frameworks.

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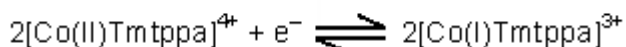


REAKCE PŘENOSU NÁBOJE V PYRIDIN-PORFYRAZINÁTOVÉM FILMU PRO VYUŽITÍ V ELEKTROCHEMICKÉM SENZORU

Bc. Monika Klusáčková

Ing. Pavel Janda, CSc.

Tato práce se zabývá reakcí přenosu náboje na tenké vrstvě filmu tetramethyltetra-3,4-pyridinoporfyrazino kobaltu (CoTmtppa) deponovaného na povrchu vysoce orientovaného pyrolytického grafitu (high oriented pyrolytic graphite = HOPG). Ve vodě rozpustný Co(II)Tmtppa prochází jednoelektronovou redukcí centrálního kovu a přechází na nerozpustný vodivý film Co(I)Tmtppa [1], jehož bylo využito pro modifikaci povrchu elektrody. Film CoTmtppa byl vyloučen na basální rovině HOPG dvěma způsoby: adsorpcí [2] a elektrochemickou depozicí [3]. Byl zjištěn posun redox potenciálu odpovídajícího reakci [4]:



což ukazuje na odlišný mechanismus imobilizace CoTmtppa v obou případech. Průběh depozice, stabilita filmu deponovaného na elektrodě byla zkoumána reflexní spektroskopii v průběhu cyklické voltametrie. Elektrochemické chování takto modifikované elektrody bylo charakterizováno cyklickou voltametrií. K zobrazení nanomorfologie deponovaného filmu a k určení jeho tloušťky bylo použito techniky mikroskopie atomárních sil (AFM). Elektroda modifikovaná filmem porfyrazinu byla studovaná pro použití v elektrochemickém senzoru.

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SCIENCE FROM PHOTOGRAPHY ? PHOTODISSOCIATION OF HBr IN RARE GAS CLUSTERS

Mgr. Jaroslav Kočišek

Mgr. Michal Fárník, Ph.D.

Imaging detection technique is based on photographic acquisition of experimental data. Despite the artistic character of the experimental work, the technique combined with velocity mapping [1] give us one of the most powerful experimental tools to study photodissociation dynamics. Our newly constructed experimental setup AIM (Apparatus for IMaging) is combining the techniques with pulsed molecular beam in unusual perpendicular configuration. The innovative approach brings more light and sufficiently more information on our images in comparison to traditional beam to detector configuration.

Photodissociation, the reaction where the molecule absorbs the light quanta resulting in fragmentation to neutral products, is of high importance in a variety of processes from the cosmos, through atmosphere to our everyday life. Of the special interest are processes in the atmosphere involving the UV photons and halogen-hydrates in cluster environment [2]. The well known photodissociation reaction of HBr with UV photons (243nm) [3] was our first choice to test the AIM setup. We obtained the HBr photodissociation fragment kinetic energies in good agreement with the theory and previous studies. The experiments in clusters reveal new features, clearly identifying the HBr-Rg cluster structure as HBr caged in the huge Rg cluster.

The talk will introduce the experimental setup and its advantages. The range of information, we can obtain from the images, will be presented on recent HBr results. The scientific conclusions will be shared in an audience friendly manner.

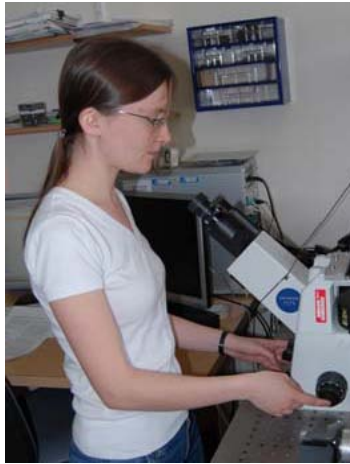
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Acknowledgement:

This project was supported by grant GAČR 203/09/0422.



DYNAMIC SATURATION OPTICAL MICROSCOPY USING REVERSIBLY PHOTOSWITCHABLE FLUORESCENT PROTEINS

Bc. Marie Kolářová

Mgr. Aleš Benda, Ph.D.

Fluorescence microscopy is an essential technique for live cell imaging. One of its drawbacks is a rather low diffraction limited spatial resolution, which is described by Abbe diffraction law. Therefore, in the last decade a lot of new methods improving resolution were developed. One of them is dynamic saturation optical microscopy^{1,2} (DSOM) that is based on spatial monitoring of transition kinetics between bright and dark states of fluorophores. The dark state is possible to obtain for example by using reversibly photoswitchable fluorescent proteins such as Dronpa³ and its mutants. These proteins undergo reversible transition from fluorescent to nonfluorescent state after irradiation by blue and ultraviolet light. In my work I focus on employing the kinetics of controllable photoswitching of Dronpa in improving the overall image quality, including the spatial resolution. The experiments were performed on yeasts expressing selected proteins labelled with Dronpa. First we confirmed that photoswitching appears on millisecond time scale. Secondly we optimized experimental conditions by studying dependence of switching rate on laser intensities and on excitation wavelength. Using the optimal experimental conditions we obtained a DSOM image having two times better spatial resolution than classical scanning confocal microscope. Moreover, fluorescence signal out of focal plane was suppressed as well as autofluorescence from nonswitchable fluorescent compounds, leading to sharper images.

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REMOVING SINGLE-WALLED CARBON NANOTUBES FROM MIXTURE OF SINGLE- AND DOUBLE-WALLED CARBON NANOTUBES USING REACTION WITH LITHIUM

Mgr. Zuzana Komínková

RNDr. Martin Kalbáč, Ph.D.

We investigated mixture of single-walled carbon nanotubes (SWCNTs) and double-walled carbon nanotubes (DWCNTs) after reaction with lithium and subsequent thermal treatment. Due to chemical reaction with lithium we achieved the removing of SWCNTs from mixture and we obtained sample containing DWCNTs only. The Li treated samples were examined by electrochemical doping using in-situ Raman spectroelectrochemistry. In Raman spectrum we focused on the radial breathing modes (RBMs), whose intensity decrease rate provided information about present SWCNTs or DWCNTs in mixture. Then sample with DWCNTs were treated by annealing at 450°C in helium and argon. Annealing caused decrease of defects in carbon lattice, which was identified by a decreasing intensity of the disorder induced mode (D) in Raman spectrum. Because doping nanotubes causes reduction intensity in Raman spectrum, in-situ Raman spectroelectrochemistry was used to verify removing SWCNTs from the mixture. In-situ Raman spectroelectrochemistry caused re-doping annealed sample. Nevertheless, in the Raman spectrum the RBMs of SWCNTs were not appeared and thereby was confirmed succesfull removal of SWCNTs.



MONTE – CARLO SIMULATION OF PHOTODISSOCIATION SPECTRA FROM MOLECULAR BEAM EXPERIMENT

Pavel Košťál

Mgr. Michal Fárník, Ph. D.

The elementary processes in clusters such as the photodissociation of molecules are investigated in our laboratory. The clusters provide a finite size environment (microsolvation) in which processes can be investigated at the molecular level in analogy with the macroscopic systems [1]. The studied systems range from atmospheric clusters, which play an important role in the stratospheric ozone depletion, to clusters relevant to biophysics.

In the photodissociation experiment, the kinetic energy spectra of a fragment are measured. The evaluation of these spectra involves computer simulation of the photodissociation process in an experiment using Monte-Carlo method and fitting of experimental data with the simulated spectra [2]. A complex computer program for the data evaluation will be introduced.

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Acknowledgement:

This project was supported by grant GAČR 203/09/0422



CHEMICAL MODELLING AND DISCHARGE PLASMA CHEMISTRY

Mgr. Petr Kubelík

Doc. RNDr. Svatopluk Civiš, CSc.

Plasma chemistry has been intensively studied for several decades. During this period great advance has been achieved in general research as well as in many technical applications. Nowadays plasma chemistry is widely applied in electronic devices fabrication, material surface modification, gas lasers design and many others. Despite of the rapid development of this science many plasma chemical systems are still not understood and many have not been studied yet.

In our laboratory the low temperature plasma is experimentally studied by time-resolved FT spectroscopy with high spectral resolution. This method provides direct information about the time development of the plasma chemistry after the pulse discharge excitation of the reaction mixture. Proper interpretation of the obtained data requires application of the suitable numerical model of the plasma behavior.

For this purpose a computational system is developed. The main goal of this study is to obtain a system suitable for the interpretation of FT experimental data. Such system should incorporate and describe all necessary elementary processes occurred in plasma and use appropriate computational approaches.

The applied modeling approach was tested on different chemical systems: BrCN/He discharge, CH₄/He discharge etc. To study these chemical systems is interesting not only for the detail understanding of the fundamental plasma chemistry processes but also for simulation of the high energy events like the impacts of the comets or extraterrestrial bodies into the planetary atmospheres.



OXYGEN EVOLUTION ON IRIDIUM BASED OXIDES

Mgr. Elizaveta Kuznetsova

Ing. Petr Krtil, CSc.

The need for a new energy carrier is well established and there is no doubt that the world current use of hydrocarbons as a primary energy source is not sustainable. That is why alternative energy sources need to be investigated, such as those based on renewable energy.

Hydrogen is attractive as an energy carrier, and many established ways of producing and utilizing hydrogen exist. Hydrogen production by water electrolysis is expected to play an important role in a possible future hydrogen energy system. However, also in the shorter term, water electrolysis is also important in a number of applications, such as food industries or for hydrogen makeup for hydrogen-cooled turbo-generators.

The power losses in water electrolysis are associated with the oxygen evolution reaction (OER) at the anode, both in the traditional alkaline electrolyzers and more recent polymer-electrolyte membrane (PEM) electrolyzers. Conducting oxides such as iridium or ruthenium oxides are good anodic catalysts for PEM systems (1).

Ruthenium oxide is a well studied OER catalyst (2). At present work the structure and electrochemical properties of iridium-based mixed oxides (with doping elements – Ni, Zn, Co) were studied.

Structural characterization of catalysts was performed by XRD, SEM and EXAFS methods. Local environment of iridium atoms in iridium-based mixed oxides was found.

Catalytic properties of material were studied by classical electrochemical methods.

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DFT CALCULATIONS OF TRANSITION METAL AMINOCARBENE COMPLEXES – CORRELATION BETWEEN EXPERIMENT AND THEORY

Bc. Hana Kvapilová

Ing. Stanislav Záliš, CSc.

Fischer-type transition metal aminocarbene complexes have been widely used in organic synthesis, both as reactants and catalysts. Recently, the redox behavior of these compounds has been studied by means of electrochemistry and it has been shown that there are two separated redox centres¹. While the reduction centre is located mainly on the carbene carbon, oxidation takes place on the central metal.

Investigation has been done on a series of aminocarbenes of Cr and Fe with general formula $(CO)_nM=C(NMe_2)(4-R-Ph)$, n being 5 and 4 for Cr and Fe, respectively. Instead of the methyl, chelating allyl group was also used, thus forming analogous series of chelated complexes with one less CO ligand. Effects of the central metal, phenyl group substitution and presence of the chelate ring have been explored. For comparison, binuclear phenyl-bridged complex of Cr was added into the study.

To support explanations of the observed results we have performed calculations by density functional theory method (DFT). B3LYP hybrid functional was used with 6-31g* double- ζ basis set and solvent effect was described by polarizable continuum model (PCM). To ensure reliability of the presented model, correlations between calculated and experimental data have been done. Theoretical and measured Raman spectra have been compared and experimental redox potentials were correlated with calculated free energies. So far the data have shown to be in a good agreement.

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KATALYTICKÉ A REDUKČNÍ VLASTNOSTI ORGANOMETALICKÉHO KOMPLEXU RUTHENIA VE VOLNÉ FORMĚ A PO JEHO NAVÁZÁNÍ NA PAPAİN

Bc. Štěpánka Lachmanová

Mgr. Magdaléna Hromadová Ph. D.

Papain (EC 3.4.22.2) patří mezi cysteinové endopeptidasy, které katalyzují hydrolýzu peptidových vazeb proteinů. Na volnou sulfhydrylovou skupinu cysteinu Cys25 v aktivním centru papainu může být kovalentně navázán organometalický komplex $[\eta\text{-}6\text{-C}_6\text{H}_5(\text{CH}_2)_2\text{NHCO}(\text{CH}_2)\text{Cl}]\text{Ru}(\text{N}^{\wedge}\text{N})\text{Cl}]\text{Cl}$, ($\text{N}^{\wedge}\text{N}$) = 1,10-fenanthrolin (TB11), který má schopnost katalyzovat přenos vodíku při hydrogenaci ketonů a iminů nebo Dielsovu-Alderovu reakci. [1,2]

Redoxní vlastnosti komplexu TB11 ve volné formě i po jeho kovalentním navázání na papain byly studovány za použití voltametrických a polarografických měření. Průběh cyklických voltamogramů redukce TB11 ve vodném prostředí naznačuje katalytické uvolňování vodíku. Byl navržen katalytický cyklus, který se v zásadních krocích shoduje s katalytickým cyklem v případě redukce $[(\text{RhCl}(\eta\text{-}5\text{-C}_5(\text{CH}_3)_5)(\text{bpy}))](\text{PF}_6)$, bpy = 2,2'-bipyridine. [3]

Modifikovaný papain se redukuje v adsorbovaném stavu, proto byla pro studium přenosu elektronu použita fázově rozlišená AC voltametrie. Získané AC voltamogramy vykazují signál katalytického vylučování vodíku nejen pro volný TB11, ale i pro jím modifikovaný protein. Studie byla doplněna výsledky elektrochemické impedanční spektroskopie pro dané systémy.

Tento výzkum byl finančně podpořen grantem GACR 203/08/1157 a GAAV IAA400400802.

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ELECTROCHEMICAL AND SPECTROELECTROCHEMICAL BEHAVIOR OF (001)-ORIENTED ANATASE TiO₂ NANOSHEETS

Mgr. Lásková Barbora

Prof. RNDr. Ladislav Kavan, DSc.

Nanocrystalline TiO₂ anatase electrodes exhibit promising performance in Li-ion batteries and photoelectrochemical solar cells¹. The dominating face in TiO₂ anatase is (101) face followed by (100) and (001) faces. Since comparative studies of anatase (101) or (001) faces on macroscopic single-crystal electrodes confirmed higher activity of the (001) face for Li insertion², our aim was to carry out analogous study for polycrystalline material too.

The electrochemical and spectroelectrochemical behavior of polycrystalline TiO₂ anatase with a predominant (001) face was studied and compared to a reference anatase material with dominating (101) face³. Li insertion is facilitated on the (001) anatase as evidenced by voltammetric and chronoamperometric diffusion coefficients and rate constants. This can be due to more open structure of the anatase lattice in the direction parallel to the *c*-axis. UV/Vis spectroelectrochemistry at potentials between 0 and -1.4V was used to determine the flatband potential and proved its negative shift for (001) anatase as compared to (101) one. This different band energetic is obviously the reason for larger open circuit voltage of the solar cell employing (001) anatase electrode as a photoanode.

Acknowledgement:

This work was supported by the Academy of Sciences of the Czech Republic (contract KAN 200100801).

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FORMATION AND PHOTODISSOCIATION OF $(\text{HNO}_3)_m \cdot (\text{H}_2\text{O})_n$ CLUSTERS IN MOLECULAR BEAMS

Ing. Jozef Lengyel

Mgr. Michal Fárník, Ph.D.

Hydrogen halides and nitrogen compounds are a key intermediate species in the atmospheric chemistry. Photochemistry of these species on ice particles in polar stratospheric clouds (PSC) plays a key role in the ozone depletion. Therefore the UV photochemistry of hydrogen halides (e.g., HCl, HBr, HI) on ice nanoparticles has recently received quite some attention in our laboratory [1-3].

The PSCs can be composed either of pure ice nanoparticles or the mixed water/nitric acid ice particles. Therefore the next step in our studies is to investigate the photochemistry in $(\text{HNO}_3)_m \cdot (\text{H}_2\text{O})_n$ clusters. The photolysis of pure HNO_3 has been extensively investigated in the laboratory under bulk and beam conditions [4].

In our experiment the $(\text{HNO}_3)_m \cdot (\text{H}_2\text{O})_n$ clusters are prepared by supersonic expansion in a molecular beam in vacuum. As the first step we characterize the generated clusters by a mass spectrometric analysis. Next, we intend to investigate the photolysis of HNO_3 molecules in the clusters by UV lasers. Finally, we plan to deposit the hydrogen halide molecules on the $\text{HNO}_3/\text{H}_2\text{O}$ ice nanoparticles and study their photochemistry, thus mimicking in laboratory the UV induced processes in the stratosphere. The preliminary results of these experiments will be presented at the conference.

Acknowledgement:

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FOTOCHEMICKÁ METODA DEKONTAMINACE PODZEMNÍCH VOD V REAKTIVNÍ CHEMICKÉ BARIÉŘE

Mgr. Hana Lipšová

RNDr. J. V. Datel, PhD.

RNDr. J. Jirkovský, CSc.

Cílem práce je přispět k řešení problematiky kontaminovaných podzemních vod v oblastech starých ekologických zátěží. K dekontaminaci se využívá tzv. reaktivní chemická bariéra, v níž aktivním čisticím procesem je fotochemicky indukovaná oxidativní mineralizace rozpuštěných organických škodlivin. Součástí je jednak prozkoumání a výběr vhodných kontaminovaných lokalit a jednak vývoj a aplikaci fotochemické metody čištění zamořených podzemních vod.

Na základě údajů o přírodních poměrech a rozsazích znečištění byly pro možnou aplikaci reaktivní chemické bariéry vybrány čtyři vhodné lokality. Ze zvažovaných možností byla nakonec jako nejvhodnější zvolena průmyslová oblast v blízkosti Ostravy, nacházející se na terasách řeky Odry. Hydrogeologicky se jedná o vysoce propustný kolektor. Lokalita je znečištěna hlavně aromatickými uhlovodíky a dalšími organickými sloučeninami, jakož i anorganickými kontaminanty, zejména ionty síranovými a amonnými.

Na odebraných vzorcích znečištěných podzemních vod byla prokázána použitelnost nové fotochemické metody k úplnému odstranění organických kontaminantů. Metoda je založena na přímé fotolýze peroxidu vodíku intenzivním krátkovlnným ultrafialovým zářením, vedoucí ke vzniku hydroxylových radikálů. Ty následně atakují přítomné organické molekuly a indukují tak jejich postupnou oxidativní degradaci. Nakonec dochází k úplné mineralizaci, tj. k přeměně všech organických látek na konečné anorganické produkty, jimiž jsou oxid uhličitý, voda a odpovídající minerální kyseliny.

Pro laboratorní pokusy a praktické testy byly použity dvě různé verze speciálního průtokového fotoreaktoru. Základem konstrukce je křemenná trubice obklopená rtuťovými výbojkami, emitujícími dominantně ultrafialové záření o vlnové délce 254 nm. Před vstupem do fotoreaktoru je do čištěné vody kontinuálně dávkován peroxid vodíku. Pracovní podmínky fotoreaktoru byly optimalizovány pro dané složení a koncentrace znečišťujících organických látek.

Při vývoji fotochemické metody byly jako modelové organické kontaminanty zvoleny 4-chlorfenol a 2-butoxyethanol. Průběh jejich fotoindukované degradace a oxidativní mineralizace byl sledován metodami UV/VIS absorpční spektrofotometrie, kapalinové chromatografie s absorpční a fluorescenční detekcí a stanovením obsahu celkového organického uhlíku. Za obdobných podmínek byly provedeny i testy s reálnou kontaminovanou podzemní vodou. Změřená reakční rychlost fotoindukované mineralizace organických škodlivin byla dostatečná pro použití této fotochemické metody v rámci konceptu reaktivních chemických bariér.

V současné době se práce zaměřují na konstrukci a testování zvětšené poloprovodní verze fotoreaktoru. Pracovní podmínky se optimalizují z ohledem na jeho budoucí praktické nasazení v rámci sanační jednotky budované na lokalitě v Ostravě.

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PHTHALOCYANINE MODIFIED HOPG ELECTRODES FOR ELECTROCHEMICAL SENSORS

Mgr. Věra Mansfeldová

Ing. Pavel Janda CSc.

Electrodes modified by phthalocyanines have been widely studied due to their numerous applications in electrocatalysis such as in O_2 reduction [1], sulphide [2] or cysteine [3] oxidation. In our work we have investigated electrochemical behaviour of new synthesized phthalocyanine with covalently bonded C_{60} molecule [Fig. 1 A] and compared to cobalt tetra-n-pentoxophthalocyanine [Fig. 1 B] to consider how fullerene influences phthalocyanine stability and electrocatalytic properties in detection of sulphides and sulphide derivatives by phthalocyanine mediated oxidation and how detection is influenced by oxygen.

Due to differences in various techniques of preparation phthalocyanine-modified carbon electrodes, we have performed a comparative study on the influence of different pretreatment methods on the course of electrochemical detection of sulphide compounds. Dependence of the electrode properties on the phthalocyanine-layer thickness and nanomorphology was studied by cyclic voltammetry, backscattering spectroelectrochemistry and atomic force microscopy.

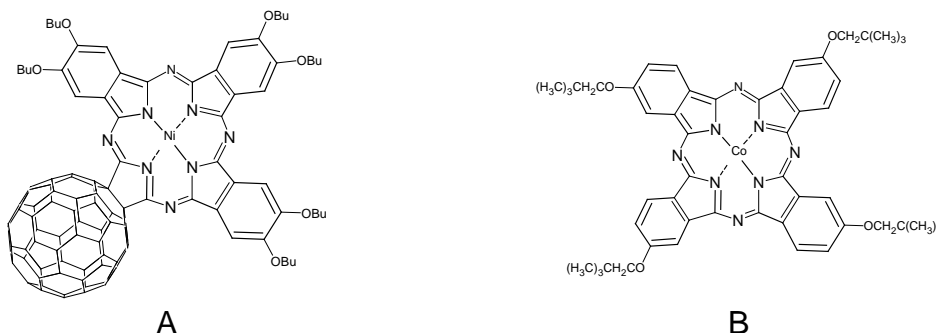


Fig. 1 Structure of nickel hexabutylphthalocyanine- C_{60} [A] and cobalt tetra-n-pentoxophthalocyanine [B].

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CRDS MEASUREMENT DATA ACQUISITION IN SUPERSONIC EXPANSION

Mgr. Milan Mašát

Mgr. Ondřej Votava, PhD.

In our research we focus on the spectroscopy of molecules with atmospheric relevance in the near IR spectral region. Analysis of spectra in this spectral region is difficult, because even simple polyatomic molecules such as CH_4 have extremely congested spectra at room temperature. Cooling the sample puts larger number of molecules into ground rotational state, suppressing some spectral lines, and thus simplifying spectra interpretation. With assigned ground state energies one can move further to higher temperatures.

In our experiment we use supersonic expansion for the cooling. This method is extremely useful to reach desired temperatures, but typical concentrations and absorption path length are low, which limits sensitivity in direct absorption detection. Multipass setting effectively multiplies absorption length and so improves detection capabilities but there are several limitations of this technique in the slit nozzle geometry.

An alternative technique that effectively increases the absorption sensitivity is the cavity ringdown spectrometry. This method, which was recently implemented into our experiment, enhances the signal to noise ratio significantly. The effective increase of the absorption path is typically by a factor of several thousands. This theoretical limit for sensitivity improvement is hard to achieve because of various technical difficulties

Effective coupling of the cavity ringdown detection with the pulsed supersonic beams is however challenging, both from the point of experiment design and data acquisition techniques. In this contribution I will outline the difficulties accompanying with synchronising the ringdown events and nozzle opening and describe our strategies for achieving reliable and effective data collection.

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SOLVATED ELECTRON EXPLORED BY METHODS OF THEORETICAL CHEMISTRY: FROM GAS PHASE CLUSTERS TO BULK

Ing. Milan Ončák

Doc. RNDr. Petr Slavíček, Ph.D.

Mgr. Michal Fárník, Ph.D.

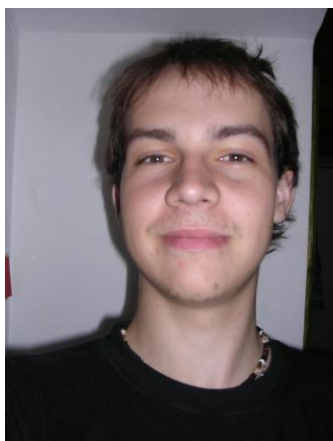
Hydrated electron is a short living (ps time scale) intermediate which potentially play an important role in radiation chemistry, biophysics or atmospheric chemistry. Structure of the solvated electron is a matter of some controversy: Does it reside in a cavity within water or is the electron delocalized on the water molecules? Or is it even represented by some other structure, e.g. H_3O radical in water? In the present contribution, we simulate measurable properties for various forms of solvated electron, following their transition from small clusters to bulk.

In the first part of my talk, I will present our studies on solvated electron formed by doping a sodium atom on small solvent clusters ($\text{Na}(\text{H}_2\text{O})_n$, $\text{Na}(\text{NH}_3)_n$, $\text{Na}(\text{CH}_3\text{OH})_n$). Here, the $\text{Na}^+ \dots \text{e}^-$ ion pair is formed; it can be either solvent separated or contact ion pair. By comparison with the experimental photoelectron spectra, we are able to analyze not only structure of the solvated electron (solvent separated vs. contact ion) but also to some extent characterize temperature of the cluster.

In the second part, I will argue that different types of solvated electron in bulk water can emerge within different routes of its preparation. We have explored formation of solvated electron via charge transfer to solvent process or within water photodissociation. In the latter case, H_3O transient species (equal to $\text{H}_3\text{O}^+ \dots \text{e}^-$ ion pair) is formed. We have calculated properties of different types of solvated electrons and compare them with available experiments. We have also studied the dynamics of the solvated electron species using methods of non-adiabatic dynamics.

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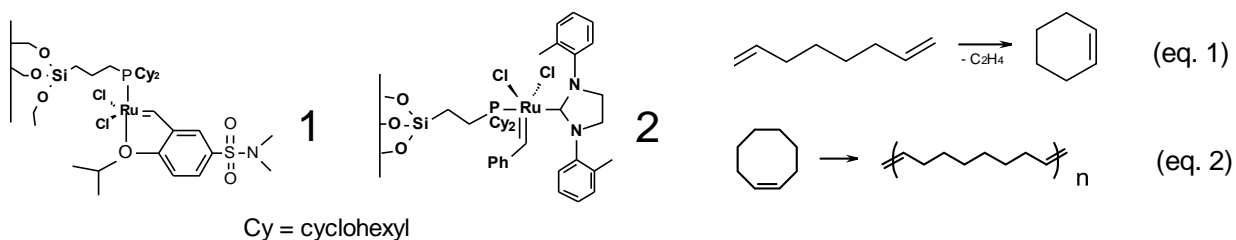
PREPARATION AND CHARACTERIZATION OF NEW MATERIALS FOR METATHESIS

Mgr. Jakub Pastva

Prof. Ing. Jiří Čejka, DrSc.
RNDr. Hynek Balcar, CSc.

Olefin metathesis has become one of the most important chemical reactions and is now extremely useful having numerous applications in fine chemical synthesis¹. Ruthenium catalysts are widely used due to their high efficiency and tolerance to a variety of functional groups in substrate molecules. Mesoporous molecular sieves are siliceous materials with well-defined regular architecture, large surface areas, large void volumes and narrow pore size distribution of mesopores. They are used as excellent supports for different catalysts. Immobilization of soluble metathesis catalysts on siliceous molecular sieve SBA-15 provides heterogeneous metathesis catalysts with high efficiency and low metal leaching.

Two new heterogeneous metathesis catalysts **1** - **2** have been prepared by immobilization of commercial Grubbs 2nd and Hoveyda-Grubbs 1st generation catalysts on the surface of mesoporous molecular sieve SBA-15 ($S_{\text{BET}} = 688 \text{ m}^2/\text{g}$, $V = 1,1 \text{ cm}^3/\text{g}$, $d = 6,9 \text{ nm}$), modified with linkers containing dicyclohexylphosphine.



The catalysts exhibited a high activity and selectivity in ring-closing metathesis (eq. 1) of 1,7-octadiene (98 % conversion and 100 % selectivity for **1**, 120 min, 80 °C, Ru:DEDAM = 1:250) and ring opening metathesis polymerization (eq. 2) of cyclooctene (high molar weight polymer in 74 % yield) as the model reactions. Filtration tests proved that the activity of the catalyst **1** is bound to the solid phase. Catalyst **1** was successfully reused 3 times (RCM of 1,7-octadiene) and exhibited very low Ru leaching (only 0.11 % of the original content of Ru in catalyst, which represents 5.57 ppm of Ru in the product).

References:

¹ Grubbs R.H., (Ed.), *Handbook of Metathesis*, Wiley-VCH, Weinheim, **2003**.



ACYLAČNÍ REAKCE DERIVÁTŮ DRUHÉ TŘÍDY BENZENU NA ZEOLITECH

Mgr. Jana Pavlatová

Prof. Ing. Jiří Čejka, DrSc.

Zeolity a molekulová síta jsou hojně zkoumanou skupinou heterogenních katalyzátorů. V posledních letech je pozorován značný nárůst reakcí, ve kterých lze tyto katalyzátory použít, a to především ke zvýšení selektivit a výtěžků.

Acylační reakce představují klíčový stupeň syntézy aromatických ketonů, které jsou významnými meziprodukty při syntéze speciálních chemikálií jako jsou léčiva, barviva, vonné a chuťové látky aj. Acylace patří mezi elektrofilní substituce a je katalyzována Brønstedovými a Lewisovými kyselinami. Obecně se pro acylační reakce nejčastěji používají zeolity s třírozměrnou kanálovou strukturou (zeolity Beta a USY), které poskytují nejvyšší konverze.

Byly zkoumány acylační reakce derivátů druhé třídy benzenu (benzonitril a benzaldehyd) s chloridy a anhydridy karboxylových kyselin na zeolitech. Katalyzátory se lišily jak strukturou (1D, 2D nebo 3D), tak rozměry vstupních oken do kanálové struktury zeolitu.

Katalytické testy byly prováděny v kapalně fázi za atmosférického tlaku a za teploty 150 °C na přístroji StarFish. Reakční směsi byly analyzovány plynovou chromatografií s hmotnostní detekcí.

Bylo zjištěno, že s rostoucí délkou řetězce činidla roste konverze acylační reakce benzaldehydu. Nejvyšších konverzí bylo dosaženo v reakci benzaldehydu s hexanoylchloridem resp. hexahydridem (63 resp. 65 %). Ze zeolitů Beta lišících se poměrem Si/Al byly nejvyšší konverze benzaldehydu pozorovány na zeolitu Beta 37. Hlavními produkty reakcí jsou příslušné chloroestery a diestery.

Konverze acylačních reakcí benzonitrilu s rostoucí velikostí činidla klesá od acetylchloridu k benzoylchloridu, resp. od acetanhydridu k benzanhydridu. Nejvyšší konverze bylo dosaženo v reakci benzonitrilu s acetylchloridem (40 %) na zeolitu Beta 37. Selektivita reakcí k příslušným imidům karboxylových kyselin byla ve všech případech 100 %.

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SPECIFIC ION INTERACTION WITH POSITIVELY CHARGED PHOSPHOLIPID BILAYERS

Mgr. Šárka Pokorná

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

In 1888 Franz Hofmeister published one of the seven papers from the series 'Zur Lehre von der Wirkung der Salze' (about the science of the effect of salts), where he described his observation, that the different monovalent ions have different effect on the hen-egg white protein precipitation and ordered them into a row according to their ability to precipitate the protein. This is nowadays known as a Hofmeister series. Since this time number of similar phenomena was observed, but the mechanism of this so called Hofmeister effect is still not fully understood.

In my lecture I'd like to speak about influence of some ions representing partial Hofmeister series on positively charged phospholipid membranes. We used large unilamellar vesicles composed from positively charged DOTAP and zwitterionic DOPC in few different ratios as a model system and the influence of few cations (Na^+ , K^+ , NH_4^+ , TMA^+ and TBA^+) and anions (Cl^- , Br^- , F^- , ClO_4^-) was measured.

Experimental data were measured by fluorescent solvent relaxation technique. In this method the fluorescent decays for a series of different wavelength are measured and the time resolved emission spectra (TRES) are reconstructed. From TRES two parameter can be obtained, the total spectral shift and mean solvent relaxation time which reflect the environment polarity and membrane mobility, respectively.

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ELEKTROCHEMICKÉ STUDIUM DEGRADACE PŘÍRODNÍCH BARVIV

Bc. Šárka Ramešová

Mgr. Romana Sokolová, Dr.

Předmětem práce je studium oxidace flavonoidů, které se používaly již od počátku 16. století jako přírodní barviva pro barvení tapisérií a dalších uměleckých děl. Jejich zástupci jsou quercetin, luteolin a apigenin, které se vyskytují v bylinách (smetanka lékařská, srpice barvířská) a stromech (dub černý) pocházejících ze Severní Ameriky. Působením vnějších vlivů a procesů stárnutí se originální barva, ale i samotný textilní materiál, často mění.

Byla studována oxidace quercetinu ve vodném prostředí pomocí elektrochemických metod. Bylo zjištěno, že přenos elektronu je spřažen s přenosem vodíkových iontů, a byl navržen mechanismus oxidace quercetinu. Hlavním oxidačním produktem je 2-(3',4'-dihydroxybenzoyl)-2,4,6-trihydroxybenzofuran-3(2H)-on, který vzniká hydroxylací nestálého meziprojektu. Pomocí separačních analytických metod LC-MS a HPLC-DAD bylo sledováno zastoupení produktů oxidace quercetinu také za přítomnosti vzdušného kyslíku. K posouzení vlivu přítomnosti vodíkových iontů na mechanismus oxidace je nezbytná znalost disociační konstanty. Studium vlivu kyslíku na absorpční spektrum ukázalo, že spektrofotometrické stanovení hodnoty disociační konstanty je nezbytné provádět v inertní atmosféře. Tím lze vysvětlit výrazně rozdílné hodnoty pK_1 nalezené v literatuře.

Poděkování: Tento výzkum byl finančně podporován z projektu GAČR 203/09/1607.

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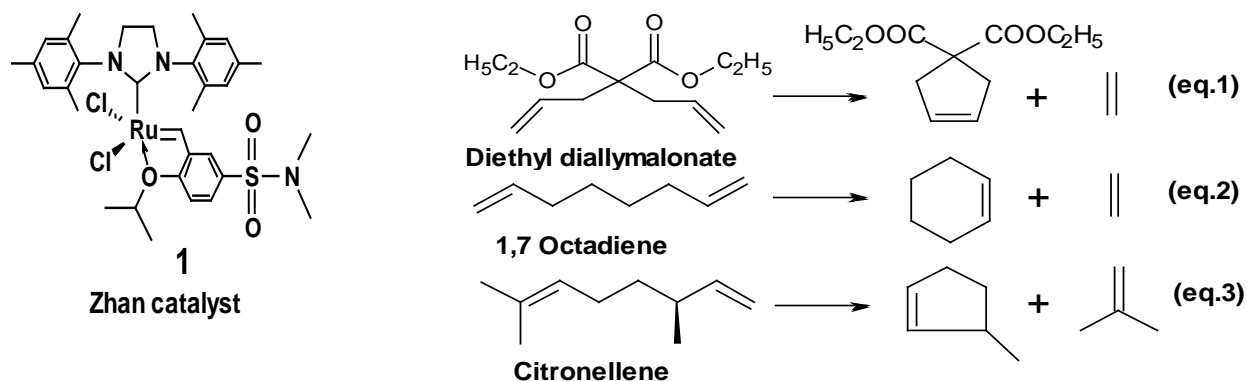
HOVEYDA-GRUBBS TYPE METATHESIS CATALYST IMMOBILIZED ON MESOPOROUS MOLECULAR SIEVES

Tushar Shinde

RNDr. Balcar Hynek, CSc.

The Ru - alkylidene complexes (Grubbs and Hoveyda-Grubbs catalysts) are the most active and frequently used metathesis catalysts. Their high tolerance to the heteroatoms in substrate molecules made them an important tool in organic synthesis. The immobilization of these complexes on solid supports attracts attention, because it opens a possibility for easy catalyst - product separation and catalyst reusing [1].

The aim of this contribution is to report new hybrid catalysts prepared by the immobilization of complex 1 on mesoporous molecular sieves of different architecture and pore size (d in nm): SBA-15 large pore (d = 11.1), SBA-15 (d = 6.8), MCM-41 (d = 4.0), conventional SiO₂ (d = 4.5) and MCM-48 (d = 6.0) via direct interaction of 1 with the surface of molecular sieves. These catalysts (1 wt. % Ru) exhibited high activity and selectivity in ring-closing metathesis (RCM) of diethyl diallylmalonate (DEDAM) and 1,7-octadiene (eqs.1 and 2) [2]. In RCM of citronellene (eq.3), metathesis of 1,9-decadiene and 1-decene, the catalytic activity was found to increase with increasing pore size of the catalyst. As 1 was attached to the sieve surface by non-covalent interactions, the Ru leaching depends on the polarity of solvent as well as substrate used. The highest leaching was found for RCM of DEDAM in CH₂Cl₂ (14 % with respect to the original content of Ru) and negligible leaching for RCM of 1,7-octadiene in cyclohexane. (0.04%). This dependence confines the practical importance of these catalysts to non-polar substrates. Hence, a new way for immobilizing 1 by the covalent bond has been developed very recently, which consists of exchange of Cl ligands in 1 for Me₃SiO ones and subsequent reaction with surface OH groups.



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ELECTROCHEMICAL AND SPECTROMETRIC STUDY OF 2,2-DINITROETHENE-1,1-DIAMINE IN APROTIC SOLVENTS

Mgr. Ludmila Šimková

Doc. RNDr. Jiří Ludvík, CSc.

2,2-Dinitroethene-1,1-diamine, $(\text{H}_2\text{N})_2\text{C}=\text{C}(\text{NO}_2)_2$ (FOX-7) is a recently developed [1,2] and broadly tested energetic material with significant potential for application due to its high detonation energy and velocity (about 5000 J/g and 8800 m/s, respectively) and simultaneously low impact and friction sensitivity and high temperature of ignition (over 220°C). Its chemical and physical properties have been recently extensively reviewed [3].

Besides the above applicability, this molecule is one of the most interesting molecules with multiple redox centres. The structure is remarkable due to the combination of two geminal easily reducible nitro-groups in the neighbourhood of two strongly electron donating amino-groups. This combination represents a typical case of “push-pull” system allowing also intramolecular electron transfer. Due to this fact, one should not expect that the functional groups would retain their original redox properties and therefore a new conjugated system with new electronic qualities should be considered.

Generally, explosion is based on thermally initiated intramolecular redox reactions. Recently it has been found [4] that also electrochemical reduction in aqueous solutions is able to start a chain of intramolecular redox processes leading to gaseous products analogously like during explosion. This comparison and the elucidation of the involved mechanism is the next aim of this work.

After the studies in aqueous solutions, the present experimental activity is focussed to reductive degradation of FOX-7 in aprotic media. Whereas the reduction of two nitro-groups in AN or in DMF should involve 8 electrons, only two one-electron reversible steps were observed up to – 2,9 V indicating the presence of radical intermediates. During the exhaustive electrolysis the solution changes its colour, therefore the UV-VIS spectra are continuously recorded and simultaneously the proportion of products is analyzed using HPLC/MS. The total consumption of electrons is dependent on applied potential. The obtained products are characterized and identified by mass spectrometry. The presence of small amount of moisture has little effect to the reduction process, but the addition of acetic acid dramatically changes the mechanism.

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A STUDY OF INDOLE AND PRODANE EXCITED STATES WITH QM/MM MODELLING OF PRODANE EMBEDDING IN DOPC BILAYER

Ing. Lukáš Sobek

Mgr. Jiří Pittner Dr. rer. nat.

In our theoretical research we have aimed our attention to two organic molecules routinely used in the biochemistry as fluorescent dyes : indole (2,3-benzopyrrole) and PRODANE (6-propionyl-2-N,N-dimethyl-ainonaphthalene) .

In the case of the indole, we have finished earlier computations by working on potential energy profiles along the NH-bond stretch which were computed by a means of the coordinate-driven minimum-energy-path approach: for a given value of bond distance ranging from 0.9 to 2.3Å while all remaining intramolecular coordinates were optimized with CASSCF analytical gradient. We came to the conclusion, that energetic gap between HPEs of S_0 and S_1 -states are very close together for bond distances in the interval from 1.85 to 1.93Å and that is why we performed a conical intersection optimisation. Computations have been performed at CASSCF level.

In the case of PRODANE there recently took place spectroscopic measurements which should be now interpreted with theoretical approaches. Among other problems, our group (L.Cwiklik, Sobek and J.Pittner) made the calculations of geometric parameters of one of two more stable conformers and electrical charge distribution in the molecular frame of the PRODANE and the alteration of these parameters under excitation of the system. We have also computed PRODANE absorption and emission spectra. Methods DFT and TDDFT have been employed.

We plan to perform modelling a more complex task inspired with the work of [1] calculating the PRODANE embedding (statistical distribution of the geometry and vertical coordination) in the 1,2-di-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine (DOPC) bilayer [2] and its alteration by the PRODANE excitation.

The calculations have been worked out by NEWTON-X, COLUMBUS and TURBOMOLE programs.

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REAL-TIME SIFT-MS DETECTION OF VOLATILE FORMS OF SELENIUM RELEASED BY PLANTS

Mgr. Kristýna Sovová

RNDr. Patrik Španěl Dr. rer. nat.

Selected Ion Flow tube Mass Spectrometry, SIFT-MS, allows a real time detection and quantification of trace amounts of gases including vapours of volatile organic compounds present in ambient humid air. This technique was previously mainly used for analyses of compounds present in human breath. However, it has a potential to be used in other areas of interdisciplinary research including plant physiology with the ultimate aims of mechanisms involved in use of plants for decontamination of polluted soil. The initial results in this area are presented.

SIFT-MS was used to study gaseous volatile products of selenium originating in the process of so called phytovolatilization. Selenium is essential for many organisms but in higher concentration can be toxic. The toxicity of selenium in higher concentration is due to its similarity to sulphur, which leads to a replacement of sulphur by Se in proteins. One way how to remove selenium contamination from water or soil is the application of phytoremediation techniques, specifically phytovolatilization¹. Phytovolatilization uses green plants to take up and assimilate selenate or selenite using sulphur transporters and enzymes from soil and transform them into a



volatile form of DMSe (dimethyl selenide)², which is 500 to 700 times less toxic to rats than the other inorganic forms³. These plants, which accumulate or volatilize selenium, can be used for selenium phytoremediation and/or as an enriched source of food.

We have investigated a method for quantitative and real-time measurements of DMSe released by plants and we are also looking for other types of volatile forms of selenium such H_2Se , CH_3SeH or $(CH_3)_2Se_2$.

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FLUORESCENCE CROSS-CORRELATION SPECTROSCOPY AS A TOOL FOR STUDY OF ANTIMICROBIAL ACTIVITY OF PEPTIDES

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Fluorescence cross-correlation spectroscopy (FCCS) is a method based on ideas of fluorescence correlation spectroscopy (FCS) which monitors the fluorescence intensity fluctuations of single labeled molecules moving in and out of a fixed illuminated volume. Interpretation of FCS data is based on a statistical autocorrelation analysis of the time scale of fluctuations.

By contrast, FCCS measures the temporal fluorescence fluctuations coming from two differently labeled molecules diffusing through a small sample volume. Afterwards, the measured fluctuations are evaluated by cross-correlation analysis of the fluorescence signals from separate detection channels. By this way the information of the dynamics of the dual-labeled molecules is extracted. FCCS is used as a tool for the characterization of diffusion coefficients, binding constants, kinetic rates of binding, and determining molecular interactions in solutions and cells.

At first we used FCCS to measure double labeled large unilamellar vesicles (LUV), there should be highest achievable positive correlation. The second step was measurement with a mixture of vesicles which are labeled with two dyes but every vesicle only by one type of the dye. There should not be cross-correlation, because they move independently of each other. If there is some cross-correlation, it means that there is imperfect separation of fluorescence from the two dyes. In the third step we used mixture of two differently labeled vesicles with vesicles which were labeled with both dyes.

In the last series of experiment we tried to measure vesicles which were labeled with one dye and has the other type of dye in inside solution. After interaction between this vesicles with membrane active peptides, there should be measured some leakage of inside dyes induced by pore forming peptide.

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EXPERIMENTÁLNÍ SPEKTROSKOPICKÉ STUDIE NANOČÁSTIC KVANTOVÝCH TEČEK

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Kvantové tečky (QD) mají vlastnosti luminiscentních polovodičových nanokrystalů. Jedná se o unikátní spektrální vlastnosti jako je široký absorpční pás, úzká, symetrická a intenzivní emise se závislostí na velikosti částic, nebo například resistance proti fotovybělování. Právě možnost cíleně laditelné emise patří mezi nejatraktivnější vlastnosti kvantových teček, které umožňují široké aplikační využití v různých oblastech. Schopnost přenést absorbovanou energii na jinou látku lze využít například k excitaci fotosenzitizéru ve fotodynamické terapii – léčebné metodě využívané při léčbě nádorů. Využívá se zde přenosu energie z excitovaných tripletních stavů fotosenzitizéru na molekuly kyslíku a následného generování reaktivního singletního kyslíku [1], [2].

Ve svém příspěvku se budu zabývat generováním singletního kyslíku kvantovými tečkami v závislosti na jejich velikosti a struktuře. Singletní kyslík emituje na vlnové délce 1270 nm, čehož se využívá pro jeho měření. Byly studovány dva druhy kvantových teček různých velikostí (CdSe, CdS). Porovnáním naměřených signálů studované látky (QD) a tetrafenylporfyrinu (TPP) jako reference byly získány kvantové výtěžky procesu. K excitaci vzorku byl použit excimerový laser emitující na vlnové délce 308 nm, emise byla detekována pomocí detektoru s filtrem propouštějícím na vlnové délce 1270 nm. Měření byly vždy dva signály – vzorek, který obsahoval rozpuštěný kyslík, a vzorek nasycený argonem. Pro ověření, zda nedochází během měření k poškození vzorku, byla měřena UV/vis absorpční spektra před měřením, po měření a po nasycení vzorku.

Cílem této práce je charakterizace kvantových teček a jejich interakcí s velkými (bio)molekulami, tzn. změny jejich optických vlastností studované pomocí laserové spektroskopie. Dané téma nabízí do budoucnosti širokou škálu možných experimentů a tedy i interpretací získaných výsledků.

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SOME WAYS OF MODIFICATION OF POLYCRYSTALLINE GOLD ELECTRODES BY THIOLATED COMPOUNDS

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Surface modification of metal electrodes provides one of the most elegant approaches to optimizing many electrochemical analyses or designing ion-selective electrodes (ISE). The main aim of our work is utilization of ligand molecules to modify a gold electrode surface and to use this system for monitoring differences in the electrochemical properties in the presence of various ions.

The principle of modification consists of covalent bonding between the gold electrode surface and the –SH functional groups of the ligand molecules. There are two principal ways of the gold surface modification. The self-assembly process is most common, the modifying molecules are adsorbed on the metal surface without any applied potential, but the process takes several hours. On the other hand, the modifying process can be rapid under a potential applied.

This study compares the modification processes with two types of organothiols, namely, that with thiolated calix[4]arene containing 4 –SH groups located on the lower rim, and that represented by a linear chain undecanethiol. The processes of modification were optimized, the different ways of modification were compared (those with or without an applied potential) and the properties of the modifier layer were described.

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FLUORESCENCE STUDY OF MEMBRANE RAFTS FORMATION USING CHOLERA TOXIN PROTEIN

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Pro. Dr. Martin Hof, DSc.

Knowledge of lateral compartmentalization of cell membranes is crucial in lipid science. According to the latest observations, the membrane consists of rigid regions (usually called rafts or ordered phase) and surrounding fluid phase (disordered phase). The mechanism of raft formation has been and still is a key question. There are discussed two processes of rafts creation so far, in which a) the ordered phase is created in one step by collapsing of raft lipids into the raft phase or b) pre-existed nano- or microdomains are merged into the raft structure [1, 2]. Since the size of latter mentioned is under the microscope resolution (< 200 nm), study of domains is very demanding.

Because of the rigid structure of raft phase, there is limited amount of fluorescence dyes situated in there. Thus, cholera toxin B (CTx) subunit is often used as a raft marker, because of specific interaction with GM₁ ganglioside located in ordered phase.

Here, I will be presenting original data supporting the idea of existence of microscopically unresolvable raft domains. All the data were observed on the model membrane system, giant unilamellar vesicles (GUVs) [3], with different lipid compositions. Using diffusion times determined by z-scan FCS approach, we are able to observe CTx clustering and, thus, creation of small, rigid microdomains in visually clear disordered phase. Similar behavior has been also confirmed by Förster Resonance Energy Transfer. Such observations clearly indicate that membrane rafts are formed from pre-existing structures.

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QUANTUM CHEMISTRY ON QUANTUM COMPUTERS

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Quantum computers have a potential to change computer science completely. In fact, not only the computer science. Quantum chemistry could in principle benefit from them as well, for example by an efficient solution of many-body Hamiltonian eigenvalue problem [1]. As was shown in the seminal work by Aspuru-Guzik et. al. [2], quantum computers, if available, would be able to perform the full configuration interaction (FCI) energy calculations with only a polynomial scaling, in contrast to conventional computers where FCI scales exponentially.

The lecture will summarize our work in the field of interconnection of quantum chemistry and quantum computing. I will present the improved version of the quantum full configuration interaction (QFCI) method which uses the iterative phase estimation algorithm [3] and its application to non-relativistic as well as relativistic configuration interaction (CI) energy calculations.

As far as non-relativistic CI calculations are concerned, simulations (on a conventional computer) of QFCI calculations of the four lowest lying electronic states of methylene molecule (CH_2), which exhibit a multireference character were performed [4]. It has been shown that with a suitably chosen initial state of the quantum register, one is able to achieve the probability amplification regime of the iterative phase estimation even for nearly dissociated molecule. For the case of relativistic CI calculations, Kramers-restricted CI calculations employing the QFCI algorithm have been applied to the spin-orbit coupling in the SbH molecule.

Last but not least, I will speak about possible use of genetic algorithms in the design of quantum circuits for QFCI calculations.

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**Seminář studentů ÚFCH JH 2011
Sborník příspěvků ze studentské konference
konané 11.-13. dubna 2011
v Konferenčním centru AV ČR v Liblicích**

Kolektiv autorů

Sestavila: Květa Stejskalová

Vydává: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i.

Dolejškova 2155/3, 182 23 Praha, Česká republika

Tisk: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i.

Dolejškova 2155/3, 182 23 Praha

Vydání: první

Náklad: 75 kusů

Místo a rok vydání: Praha, 2011

Publikace neprošla jazykovou úpravou.

SEMINÁŘ STUDENTŮ ÚFCH JH 2011
Konferenční centrum AV ČR v Liblicích
11. - 13. 4. 2011

