



SEMINÁŘ STUDENTŮ ÚFCH JH **2013**



Konferenční centrum
AV ČR v Liblicích
24. - 26. 4. 2013

Seminář studentů ÚFCH JH 2013

Sborník příspěvků

**ze studentské konference konané
24.-26. dubna 2013
v Konferenčním centru AV ČR Liblicích**

Seminar of Students of JHI 2013

Collection of abstracts

**of all lectures given at the student conference
held on 24 -26 April 2013
in Conference Centre of the Academy of Sciences
of the Czech Republic in Liblice chateau**

**Seminář studentů ÚFCH JH 2013
Sborník příspěvků ze studentské konference
konané 24.-26. dubna 2013
v Konferenčním centru AV ČR Liblicích**

Kolektiv autorů

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SEMINÁŘ STUDENTŮ ÚFCH JH 2013

PROGRAM 1. dne konference - **středa 24.4.2013**

Odjezd autobusem z parkoviště před ústavem ve 13:00 hodin.

Předpokládaný příjezd do Konferenčního centra AV ČR v zámku
v Liblicích okolo 14:00 hodiny.

Čas	Předsedající	Přednášející	Název
14:00-15:25		Registrace a ubytování účastníků konference - v recepci <u>Od 15 hodin - občerstvení před zahájením konference</u> (káva, nápoje, zákusek - v 1. patře)	
15:25		Zahájení konference „Seminář studentů ÚFCH JH 2013“ - prezentace studentů z kategorie I.	
15:30	<u>Adéla</u> <u>FRIDRICHOVÁ</u>	Jakub LANG (<i>magisterské studium, PřF UK, školitel J. Pittner</i>) kat I	AN AB INITIO INVESTIGATION OF THE ISOMERIZATION OF BICYCLOBUTANE: DESCRIPTION OF THE CONROTATORY AND DISROTATORY STATES
15:50		Roman NEBEL (<i>bakalářské studium, VŠCHT Praha školitel P. Krtil</i>) kat I	VYSOKOTLAKÁ SYNTÉZA FLUORESCENTNÍCH A KATALYTICKY AKTIVNÍCH SULFIDŮ
16:10		Michaela RYBÁROVÁ (<i>magisterské studium, FBMI ČVUT, školitel P. Španěl</i>) kat I	VÝVOJ METOD EXTRAKCE TĚKAVÝCH LÁTEK Z BIOLOGICKÝCH VZORKŮ
16:30		Jan BOHUSLAV (<i>bakalářské studium, VŠCHT Praha školitelé P.Janda a H.Tarábková</i>) kat I	NANOČÁSTICOVÁ ELEKTRODA: ELEKTROCHEMICKÉ A NANOMORFOLOGICKÉ VLASTNOSTI NI/HOPG ELEKTRODY PŘIPRAVENÉ RŮZNÝMI METODAMI DEPONOVÁNÍ
16:50	PŘESTÁVKA		
17:00	<u>Milan</u> <u>BOUŠA</u>	Miloš VEČEŘA (<i>bakalářské studium, PřF UK; školitel M. Lamač</i>) kat I	SYNTÉZA KOMPLEXŮ PRVKŮ 4. SKUPINY S CYKLOPENTADIENYL-KETIMIDOVÝMI CHELATUJÍCÍMI LIGANDY
17:20		Kateřina JURKOVÁ (<i>bakalářské studium, PřF UK, školitel M.Kalbáč</i>) kat I	SINGLE-LAYER MOS2 AND ITS INTERACTION WITH GRAPHENE
17:40		Pavel KOŠTÁL (<i>bakalářské studium MFF UK; šk. M. Fárník</i>) kat I	STUDIUM DYNAMIKY FOTODISOCIACE ZOBRAZOVACÍ METODOU IMAGING
18:00	PŘESTÁVKA		
18:10	<u>Pavla</u> <u>CHLUBNÁ</u>	Tomáš HODÍK (<i>bakalářské studium, VŠCHT Praha školitel J. Pinkas</i>) kat I	SWEET TITANOCENES AND FERROCENES
18:30		Vít SVOBODA (<i>bakalářské studium, VŠCHT Praha, školitel O.Votava</i>) kat I	OVERTONOVÁ SPEKTROSKOPIE V SUPERSONICKÝCH EXPANZÍCH
18.50		Jakub VIŠŇÁK (<i>I. ročník PGS, PřF UK, školitel J. Pittner</i>) kat I	AB INITIO VIBRATIONAL TRANSITION CALCULATION BY THE NOMO/CI METHOD ON A SIMULATED QUANTUM COMPUTER

19:10		Alan LIŠKA (magisterské studium, PřF UK, školitel J. Ludvík) kat I	ELECTROCHEMICAL REDUCTION OF STRUCTURALLY MODIFIED POLYNITROCALIX[4]ARENES
19:30	Ukončení prvního dne konference		
	VEČEŘE v RESTAURACI - začátek v 19:30		

PROGRAM 2. dne konference - čtvrtek 25.4.2013

Čas	Předsedající	Přednášející	Název
8:25	Zahájení druhého dne konference - pokračují prezentace studentů kategorie I a II.		
8:30	<u>Barbora</u> LÁSKOVÁ	Matej ŠVAŇA (magisterské studium, PřF UK, školitel J. Pittner) kat I	STUDY OF DIRADICALS BY EXPLICITLY CORRELATED MULTIREFERENCE COUPLED CLUSTER METHODS
8:50		Jakub EDERER (magisterské studium, PřF UK, školitel P. Janda) kat I	MULTIKOMPONENTNÍ ANALÝZA VZORKU POUŽITÍM VÍCEELEKTRODOVÉHO SYSTÉMU
9:10		Štěpánka LACHMANOVÁ (I. ročník PGS, PřF UK, školitelka M. Hromadová) kat I	REDUCTION OF SELECTED BRANCHED EXPANDED PYRIDINIUM CATIONS
9:30		Martina PARISOVÁ (I. ročník PGS, PřF UK, šk. T. Navrátil) kat I	CHARACTERIZATION OF BIOLOGICAL MEMBRANE
9:50	PŘESTÁVKA NA KÁVU A ZÁKUSEK		
10:20	<u>Radka</u> METELKOVÁ	Magda ZLÁMALOVÁ (I. ročník PGS, PřF UK, šk. P. Janda) kat I	ELEKTROCHEMICKÝ SENZOR S ELEKTRODOU MODIFIKOVANOU POLYMERNÍ METHYLENOVOU MODŘÍ PRO STANOVENÍ SULFANU
10:40		Martin RAJMON (magisterské studium, FBMI ČVUT, školitel Z. Bastl) kat I	NOVÁ SKUPINA FUNKČNÍCH MOLEKULÁRNÍCH STRUKTUR NA BÁZI CARBORAN THIOLŮ
11:00		Monika REMZOVÁ (I. ročník PGS, školitel J. Rathouský) kat I	MODIFIED SILICATE GELS FOR THE CONSOLIDATION OF WEATHERED HISTORICAL MATERIALS
11:20		Michal MAZUR (I. ročník PGS, školitel J. Čejka) kat I	INTERCALATION CHEMISTRY OF LAYERED ZEOLITE PRECURSOR IPC-1P
11:40	PŘESTÁVKA		
11:50	<u>Jan</u> SUCHÁNEK	Václav BLECHTA (I. ročník PGS, školitel M. Kalbáč) kat I	STUDY OF GRAPHENE'S PROPERTIES AND ITS SENSOR APPLICATIONS
12:10		Marek PEDERZOLI (I. ročník PGS, PřF UK, šk. J. Pittner) kat I	TOWARDS ACCURATE AB INITIO SIMULATIONS OF FLUORESCENT PROBES
12:30		Jan PŘECH (I. ročník PGS, školitel J. Čejka) kat I	SYNTHESIS AND PROPERTIES OF GERMANOSILICATE AND TITANOSILICATE FORMS OF CIT-5 ZEOLITE

-----		Ukončeny prezentace studentů kategorie I. (22 prací)	
12:50		Monika KLUSÁČKOVÁ (II. ročník PGS,, školitel P. Janda) kat II	ELECTROCATALYTIC OXIDATION OF UNSATURATED HYDROCARBONS MEDIATED BY PHTHALOCYANINE DERIVATE
13:10	PŘESTÁVKA NA OBĚD (PODÁVÁ SE V RESTAURACI OD 13:15)		
14:45	Zuzana KOMÍNKOVÁ	Adéla FRIDRICHOVÁ (II. ročník PGS, školitel M. Horáček) kat II	YTTROCENE COMPLEXES CONTAINING VARIOUSLY SUBSTITUTED CYCLOPENTADIENYL LIGANDS: SYNTHESIS, CHARACTERIZATION AND REACTIVITY
15:05		Marie OLŠINOVÁ (II. ročník PGS, školitel M. Cebecauer) kat II	EFFECT OF INTEGRAL PEPTIDES ON MODEL MEMBRANES
15:25		Pavla SVRČKOVÁ (II. ročník PGS, školitel M. Fárník) kat II	CHLOROBENZENE - MASS SPECTRA, PHOTODISSOCIATION DYNAMICS
15:45		Kateřina NOVÁKOVÁ (II. ročník PGS, školitel T. Navrátil) kat II	APPLICATION OF COPPER SOLID AMALGAM ELECTRODE FOR DETERMINATION OF DITHIOCARBAMATE FUNGICIDE
16:05	PŘESTÁVKA NA KÁVU A ZÁKUSEK		
16:45	Jakub PASTVA	Sabina PETRÁŠOVÁ (II. ročník PGS, školitel H. Balcar) kat II	POLYMER NETWORKS DERIVED FROM ETHYNYLPYRIDINES
17:05		Radek ŽOUŽELKA (II. ročník PGS, školitel J. Rathouský) kat II	THE TOXICITY OF SILVER NANOPARTICLES TO SCENEDESMUS QUADRICAUDA AND CHLORELLA VULGARIS
17:25		Radka METELKOVÁ (II. ročník PGS, školitel J. Ludvík) kat II	SPECTRO-ELECTROCHEMICAL STUDY OF CHROMIUM AMINOCARBENE REDUCTION MECHANISM
17:45		Hana KVAPILOVÁ (II. ročník PGS, školitel S. Zálšíš) kat II	VARIATION OF PHOTOPHYSICAL PROPERTIES OF [REX(CO) ₃ (DIIMINE)] ^{N+} COMPLEXES BY MODIFICATION OF THE DIIMINE LIGAND: DFT AND TRIR STUDY
18:05	UKONČENÍ DRUHÉHO DNE KONFERENCE. VEČEŘE V RESTAURACI OD 18:30 HODIN		
18:05 - 18:30	Pro zájemce - mimokonferenční prezentace	Květa STEJSKALOVÁ	<i>Představení vzdělávacích a popularizačních aktivit našeho ústavu v projektu Tři nástroje v roce 2012/2013, něco málo o novinkách - programy našich workshopů pro žáky ZŠ a j. akce pro ostatní cílové skupiny...</i>

PROGRAM 3. dne konference - pátek 26.4.2013

Čas	Předsedající	Přednášející	Název
8:25	Zahájení třetího dne semináře - pokračují prezentace studentů kategorie II.		
8:30		Zuzana KOMÍNKOVÁ (III. ročník PGS, školitel M. Kalbáč) kat II	RAMAN SPECTROSCOPY STRONGLY DOPED CVD-GRAPHENE

8:50	<u>Petr</u> <u>POSPÍŠIL</u>	Jan SUCHÁNEK (III. ročník PGS, školitel Z. Zelinger) kat II	INTERACTION OF QUANTUM DOTS WITH ORGANIC MOLECULES
9:10		Barbora LÁSKOVÁ (III. ročník PGS, školitel L. Kavan) kat II	PSEUDOCAPACITIVE CONTRIBUTION TO THE TOTAL LITHIUM-ION STORAGE IN TiO ₂ (B)
9:30		Jakub PASTVA (III. ročník PGS, školitel J. Čejka) kat II	MESOPOROUS MOLECULAR SIEVES: MATERIALS FOR HETEROGENEOUS METATHESIS CATALYSTS AS WELL AS CO ₂ ADSORPTION
9:50	PŘESTÁVKA NA KÁVU A ZÁKUSEK		
10:30	<u>Hana</u> <u>KVAPILOVÁ</u>	Petr POSPÍŠIL (III. ročník PGS, školitel M. Hof) kat II	QUENCHING OF BADAN BY TRYPTOPHAN CAUSED BY PHOTON INDUCED ELECTRON TRANSFER IN MODEL MICELLAR SYSTEM
10:50		Ana SANTIDRIÁN (III. ročník PGS, školitel M. Kalbáč) kat II	PURIFICATION AND CHARACTERIZATION OF SINGLE WALL CARBON NANOTUBES
11:10		Tushar R. SHINDE (III. ročník PGS, školitel H. Balcar) kat II	RUTHENIUM CATALYSTS FOR METATHESIS AND ETHENOLYSIS OF CARDANOL
11:30	PŘESTÁVKA		
11:45	<u>Pavla</u> <u>SVRČKOVÁ</u>	Jaroslav KOČIŠEK (III. ročník PGS, školitel M. Fárník) kat II	MOLECULAR BEAM EXPERIMENTS RELEVANT FOR THE FORMATION OF POLAR STRATOSPHERIC CLOUDS
12:05		Pavla CHLUBNÁ (III. ročník PGS, školitel J. Čejka) kat II	NEW ZEOLITES PREPARED BY POST-SYNTHESIS METHODS
12:25		Milan BOUŠA (III. ročník PGS, školitel L. Kavan a O. Frank) kat II	RAMAN AND X-RAY PHOTOELECTRON SPECTROSCOPIC CHARACTERIZATION OF GRAPHENE OXIDE ELECTROCHEMICAL REDUCTION
12:45	Ukončeny prezentace studentů kategorie II. (19 prací)		
13:15 - SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ SOUTĚŽNÍ KONFERENCE - V KONFERENCEČNÍM SÁLE			
OBĚD V RESTAURACI od 13:30 hodin			
Odjezd do Prahy - autobusem z parkoviště u zámku ve 14:45			
(Návrat do Prahy k budově ÚFCH JH ca v 16:00 hodin.)			



Seznam prezentujících studentů (41)

Kategorie I (22)

Diplomanti a studenti magisterského studia a zájemci z řad bakalářů (13)

Bohuslav Jan (bakalářské studium, VŠCHT, stáž u P.Jandy a H. Tarábkové)
Ederer Jakub (magisterské studium, PřF UK, stáž u P.Jandy)
Hodík Tomáš (bakalářské studium, VŠCHT, stáž u J. Pinkase)
Jurková Kateřina (bakalářské studium, PřF UK, stáž u M.Kalbáče)
Košťál Pavel (magisterské studium, MFF UK, stáž u M. Fárníka)
Lang Jakub (magisterské studium, PřF UK, stáž u J.Pittnera)
Liška Alan (magisterské studium, PřF UK, stáž u J. Ludvíka)
Nebel Roman (bakalářské studium, VŠCHT, stáž u P. Krtily)
Rajmon Martin (magisterské studium, FBMI ČVUT, stáž u Z.Bastla)
Rybářová Michaela (magisterské studium, FBMI ČVUT, u stáž P.Španěla)
Svoboda Vít (bakalářské studium, VŠCHT, stáž u O. Votavy)
Švaňa Matej (magisterské studium, PřF UK, stáž u J.Pittnera)
Večeřa Miloš (bakalářské studiu., PřF UK, stáž u M. Lamače)

Studenti 1. ročníku PGS (9)

Blechta Václav (školitel M. Kalbáč)
Lachmanová Štěpánka (školitel M. Hromadová)
Mazur Michal (školitel J. Čejka)
Parisová Martina (školitel T. Navrátil)
Pederzoli Marek (školitel J. Pittner)
Přech Jan (školitel J. Čejka)
Remzová Monika (školitel J. Rathouský)
Višňák Jakub (školitel J. Pittner)
Zlámalová Magda (školitel P. Janda)

Kategorie II (19)

Studenti 2. ročníku PGS (9)

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)
Olšinová Marie (školitel M. Cebecauer)
Petrášová Sabina (školitel H. Balcar)
Svrčková Pavla (školitel M. Fárník)
Žouželka Radek (školitel J. Rathouský)

Studenti 3. ročníku PGS (10)

Bouša Milan (školitel L. Kavan)
Chlubná Pavla (školitel J. Čejka)
Kočišek Jaroslav (školitel M. Fárník)
Komínková Zuzana (školitel M. Kalbáč)
Lásková Barbora (školitel L. Kavan)
Pastva Jakub (školitel J. Čejka)
Pospíšil Petr (školitel M. Hof)
Santidrián Ana (školitel M. Kalbáč)
Shinde Tushar Raghunath (školitel H. Balcar)
Suchánek Jan (školitel Z. Zelinger)

Hodnotící komise:

Roman Čurík
Otakar Frank
Petr Sazama
Romana Sokolová





STUDY OF GRAPHENE'S PROPERTIES AND ITS SENSOR APPLICATIONS

Mgr. Václav Blechta

RNDr. Ing. Martin Kalbáč Ph. D.

Graphene is a monolayer of carbon atoms that can be viewed as an individual atomic plane extracted from graphite [1]. Due to its unique structure, graphene exhibits extraordinary physical properties, which have potential to employ graphene in many applications [2]. This novel nanomaterial has been studied experimentally and theoretically by many authors since its discovery in 2004. In 2007 graphene-based field effect transistor device was successfully used for detection of individual gas molecule [3].

Our graphene is synthesized by chemical vapor deposition, then transferred onto silicon/silicon-oxide substrate and after other treatment graphene is contacted by metal electrodes. Raman spectroscopy, optical microscopy and atomic force microscopy are used for characterization of synthesized graphene. Graphene solution-gated field effect transistor (SG-FET) shows ambipolar transport characteristics, which is slightly modified while graphene is doped; SG-FET with graphene channel is a promising candidate for chemical sensor. In this presentation graphene's structure and basic properties are briefly introduced, graphene solution-gated field effect transistor device is defined and obtained results are shown.

References:

[1] Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A. *Science* **2004**, 306, 666-669.

[2] Huang, X.; Yin, Z. Y.; Wu, S. X.; Qi, X. Y.; He, Q. Y.; Zhang, Q. C.; Yan, Q. Y.; Boey, F.; Zhang, H. *Small* **2011**, 7, 1876-1902.

[3] Schedin, F.; Geim, A. K.; Morozov, S. V.; Hill, E. W.; Blake, P.; Katsnelson, M. I.; Novoselov, K. S. *Natural Materials* **2007**, 6, 652-655.



**NANOČÁSTICOVÁ ELEKTRODA:
ELEKTROCHEMICKÉ A NANOMORFOLOGICKÉ
VLASTNOSTI Ni/HOPG ELEKTRODY PŘIPRAVENÉ
RŮZNÝMI METODAMI DEPONOVÁNÍ**

Jan Bohuslav

*Ing. Pavel Janda, CSc.
RNDr. Hana Tarábková, PhD.*

Elektroda byla připravena depozicí nanočástic niklu, resp. oxidu a hydroxidu niklu na bazální rovinu vysoce orientovaného pyrolytického grafitu (HOPG) sloužícího jako kolektor. K deponování bylo využito technik: UHV-napařování, spin-coatingu a sprejování vodné suspenze $\text{Ni}(\text{OH})_2$. Práce porovnává různými technikami deponovaný $\text{Ni}(\text{OH})_2$ z hlediska nanomorfologie a její změny (AFM) a reakce přenosu náboje (voltametrie). Napařováním a ablací ve vakuu nebo v inertním plynu (Ar) lze získat niklové nanočástice, které se teprve na povrchu HOPG oxidují na oxid resp. oxohydroxid $\text{Ni}(\text{II})$, nanášením suspenze $\text{Ni}(\text{OH})_2$ spin-coatingem a sprejem jsou na povrchu imobilizovány přímo nano-lamely $\text{Ni}(\text{OH})_2$. Proces lze finalizovat kalcinací.

Niklové nanočástice deponované na inertním vodivém substrátu slouží jako model nanočásticové elektrody s možným uplatněním ve zdrojích proudu.



RAMAN AND X-RAY PHOTOELECTRON SPECTROSCOPIC CHARACTERIZATION OF GRAPHENE OXIDE ELECTROCHEMICAL REDUCTION

Mgr. Milan Bouša

Mgr. Otakar Frank, Ph. D.

Prof. RNDr. Ladislav KAVAN, DSc.

Previously we reported on an effect of a spontaneous electrochemical activation during the electrochemical cycling of a few-layered graphene oxide (FLGO) performing as a conductive additive to a nanocrystalline LiFePO_4 olivine. Based on electrochemical, IR and Raman studies we suggested that a gradual in-situ reduction of FLGO is responsible for this activation.

We studied the reduction of FLGO and graphene nanoplatelets during electrochemical cycling. Using in-situ Raman spectroelectrochemistry we found out the redox processes are reversible for graphene nanoplatelets and irreversible for graphene oxide. Hence, the primary degree of oxidation has an influence on the initial reduction process. Our X-ray photoelectron spectroscopy measurements show a preferential removal of carboxy and hydroxy functional groups initially present in FLGO structure, while most of the epoxy groups remain present in the material. Furthermore, the behavior of a pristine FLGO electrode was studied during redox processes and measured throughout alternating long-time reduction, oxidation and at open circuit potential (relaxation). The acquired data show a certain degree of reversibility even in the redox behavior of FLGO, which is, however, switched to a completely different pattern after crossing a distinct reduction degree.

Acknowledgements. This work was supported by FP7-Energy-2010-FET project Molesol (Contract No. 256617).



MULTIKOMPONENTNÍ ANALÝZA VZORKU POUŽITÍM VÍCEELEKTRODOVÉHO SYSTÉMU

Bc. Jakub Ederer

RNDr. Karel Nesměrák, Ph.D.

Ing. Pavel Janda, CSc.

Při analýze vzorku, který obsahuje více analytů je selektivita jedné elektrody v rámci směsi mnohdy nedostatečná. Proto je výhodnější využití systému tvořeného větším počtem elektrod, které poskytují více informací o analyzovaném vzorku. Selektivita takového systému je vzájemně posunuta a je vyšší než selektivita při použití jednotlivých elektrod individuálně. V tomto systému bude použita metoda cyklické voltametrie v tříelektrodovém uspořádání na pevných elektrodách z různých materiálů (Au, Pt, HOPG, Pt, amalgámové elektrody). Získaná a parametricky zpracovaná data budou použita pro vytvoření tzv. „finger-rintu“ analytu.

Pro tento účel byly zvoleny dvě organické kyseliny, s cyklem ve své molekule. Kávová kyselina, u níž byly prokázány antioxidační, antimutagenní a antikarcinogenní účinky [2]. Askorbová kyselina, která je běžně používané konzervační činidlo používané během výroby a skladování vín, jejímž vlivem dochází k oxidativnímu hnědnutí bílých vín [1]. Zvolené kyseliny byly prozatím analyzovány v modelovém roztoku.

References:

[1] Lopes, P.; Drinkine, J.; Saucier, C.; Glories, Y. *Anal. Chim. Acta.* **2006**, 555, 242–245.

[2] Fracesetti, D.; Lawrence, N.; Tredoux, A. G. J.; Tirelli, A.; Nieuwoudt, H. H.; Du Toit, W. J. *Food Chemistry*, **2011**, 128, 1136–1142.



YTTROCENE COMPLEXES CONTAINING VARIOUSLY SUBSTITUTED CYCLOPENTADIENYL LIGANDS: SYNTHESIS, CHARACTERIZATION AND REACTIVITY

Ing. Adéla Fridrichová

Mgr. Michal Horáček Ph.D.

The interest in the chemistry of group 3 metals and organolanthanide compounds has increased recently because these complexes exhibit an enormous potential in homogeneous catalysis. Alkyl and hydride species, Cp^*_2LnR ($\text{Cp}^* = \eta^5\text{-C}_5\text{Me}_5$; Ln = Sc, Y, La, Ce, Nd, Sm, Lu; R = $\text{CH}(\text{SiMe}_3)_2$, Me, H) have been shown to be active in selective C-C bond formation and C-H/C-X bond activation. Typical examples are found in transformations of olefins (oligo/polymerization, hydrogenation, hydroboration, hydrosilylation, amino-olefin hydroamination/cyclization) and alkynes (oligomerization, hydrogenation, and hydroamination/cyclization) [1,2].

The aim of the presented work was the synthesis and characterization of a set of new mixed yttrocene complexes of the type $(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Y}(\text{L})(\mu\text{-Cl})_2\text{M}(\text{THF})_2$ (L = C_5H_5 , C_5Me_5 , $\text{C}_5\text{Me}_4\text{SiMe}_2\text{H}$, $\text{C}_5\text{Me}_4\text{CH}_2\text{Ph}$; M = Li, K) prepared by stepwise treatment of the tetrahydrofuran adduct $\text{YCl}_3 \cdot 3.5\text{THF}$ with one equivalent of $\text{Li}(\text{C}_5\text{Me}_4\text{SiMe}_3)$ and corresponding lithium or potassium salt of the second Cp-ring (L). Subsequently, methylation reactions of these complexes using MeLi was investigated.

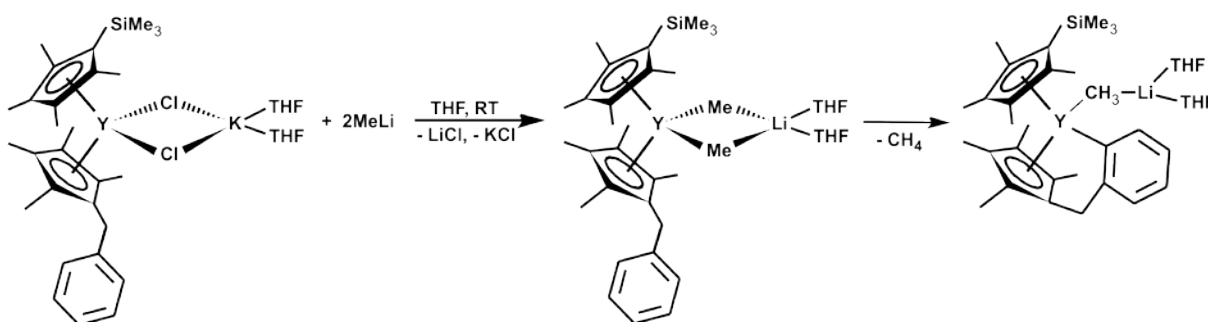


Fig. Methylation of yttrocene complex $(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Y}(\text{C}_5\text{Me}_4\text{CH}_2\text{Ph})(\mu\text{-Cl})_2\text{K}(\text{THF})_2$.

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SWEET TITANOCENES AND FERROCENES

Tomáš Hodík

Mgr. Jiří Pinkas, Ph. D.

The discovery of cytotoxic activity of *cis*-diamminedichloroplatinum(II) in 1965 initiated investigation of cytotoxic properties of other transition metal (Ti, Fe, Ru, Zr etc). Similar motif of cisplatin with titanocene dichloride caused the interest about it early 80's. It was the first non-platin potential cytostatic which entered clinical trials, however it is relatively low anticancer activity and nephrotoxicity precludes further testing. During last decade was discovered that substitution at cyclopentadienyl ring caused higher anticancer activity, less toxicity etc.

The aim of our work has been synthesis of organometallic compounds derived from titanium and iron which are substituted by *D*-xylose, *D*-ribose etc. at cyclopentadienyl ring. We assume that presence of a carbohydrates moiety at a metallocene periphery may reduce toxicity, improve solubility and allow selective transport into cancer cell.

In my contribution synthesis and characterization of prepared substituted titanocene and ferrocene compounds will be discussed. Cytotoxic activity of selected compounds will be presented too.

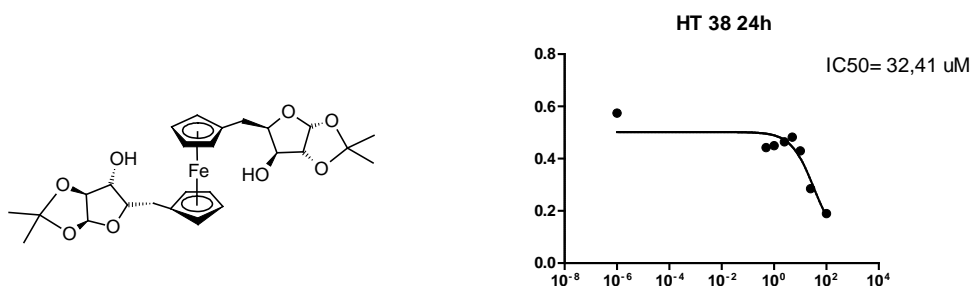


Fig. 1: Structure of ferrocene bearing *D*-xylose and graph showing dependence its activity on concentration (IC₅₀ = concentration of the active substance which lead to reduction of amount of cancer cell to half)

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NEW ZEOLITES PREPARED BY POST-SYNTHESIS METHODS

Mgr. Pavla Chlubná

Prof. Ing. Jiří Čejka, DrSc.

Zeolites are traditionally 3D-framework microporous crystalline aluminosilicates with a wide range of applications¹. Recently, the group of zeolites has been expanded by the development of 2D zeolites prepared through the “bottom-up” (direct) synthesis as so called zeolite precursors, e.g. MCM-22P². These 2D mono-layer materials can be post-synthetically modified into materials with improved textural properties.

It was lately discovered that germanosilicate UTL undergoes structural changes in acid environment where D4R units are removed and only UTL layers remain³. This “top-down” synthesis produces a new lamellar material IPC-1P and offers a new attitude in the synthesis of zeolitic materials. It is possible to expand the interlayer space by treatments like swelling and pillaring, similarly like in the case of MCM-22P⁴, or we can organize the layers and reconnect them again. Choosing and controlling of the linkers used for reassembling give us the tool for preparation of materials with predictable structures, like zeolites IPC-2 and IPC-4 (IZA code PCR). They preserve the UTL-like layers but differ in new linkers between them and also in pore sizes (Fig. 1).

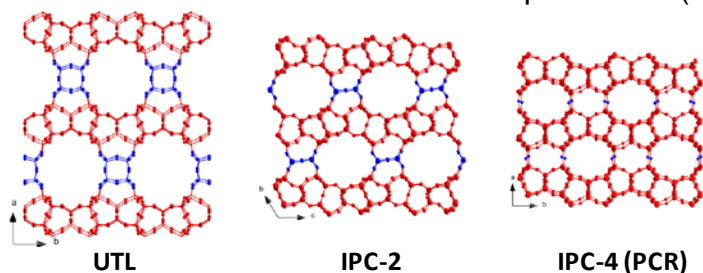


Fig. 1 The structures of UTL, IPC-2 and IPC-4. The layer topology (in red) is common to all three materials which differ in sized linkers (in blue).

The novel strategy called ADOR (assembly-disassembly-organization-reassembly) offers new possibilities in the synthesis of zeolitic materials. There are some application limitations like chemical composition of the parent zeolite or presence of D4R units, however, it has been already applied on other germanosilicates (IWW, IWR) with first promising results.

We would like to acknowledge Grant Agency of the Czech Republic (P106/12/G015) for the financial support.

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SINGLE-LAYER MOS₂ AND ITS INTERACTION WITH GRAPHENE

Kateřina Jurková

RNDr. Ing. Martin Kalbáč., Ph. D.

Various two dimensional nano-materials have recently attracted plenty of interest due to their physical and electrical properties. Since its discovery in 2004, a lot of attention has been focussed on graphene, one atom thick layer of carbon atoms packed with hexagonal lattice. Apart graphene, also its analogues such as MoS₂ have got into the centre of interest. [1]

Single layer MoS₂ was initially prepared by mechanical exfoliation which is still the most effective method for its preparation. Though other various methods have been developed, optical microscopy, Raman spectroscopy and atomic force microscopy (AFM) are the most effective methods for identification the thickness of both graphene and MoS₂ layers. [2] [3]

Proper understanding to electrical properties of these materials is essential for their potential future application in nano-electronics. [4] One of the things in which we are interested in our laboratory is the investigation of spectroelectrochemical properties of these materials.

The content of my lecture will be a brief characterization of single layer (SL) MoS₂ by AFM and Raman spectroscopy and its interaction with CVD graphene.

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ELECTROCATALYTIC OXIDATION OF UNSATURATED HYDROCARBONS MEDIATED BY PHTHALOCYANINE DERIVATE

Mgr. Monika Klusáčková

Ing. Pavel Janda, CSc.

Unsaturated hydrocarbons as ethylene and propylene are not only gases of considerable industrial significance but also typical air pollutants that are produced in global quantities. These gases have high photochemical reactivity and may form photochemical smog with possible impact on a global scale. Therefore the monitoring of hydrocarbons is critical for quality of environment [1, 2].

The oxidation of ethylene and propylene was studied on basal plane of highly ordered pyrolytic graphite (HOPG) electrode with deposited thin layer Co-phthalocyanine derivate as a mediator and in aqueous buffer phosphate solution as an electrolyte. Cyclic voltammetry, backscattering VIS spectroscopy and atomic force microscopy were utilized. The choice of tetrapyridinoporphyrazines as a mediator was given by its redox properties, ability to form low soluble, electrically conducting film on the electrode surface [3, 4]. Our interest has been focused on conditions for electrocatalytic oxidation of these molecules on modified electrode.

Acknowledgements

This work was financially supported by the Research project MSM0021620857 of the Ministry of Education, Youth, and Sports of the Czech Republic, by grant project SVV267215 of Charles University of Prague, by Grant Agency of the Academy of Sciences of the Czech Republic (Contract IAA 400400804) and by the EC 7th FP project ORION (Contract No. NMP-229036).

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MOLECULAR BEAM EXPERIMENTS RELEVANT FOR THE FORMATION OF POLAR STRATOSPHERIC CLOUDS

Mgr. Jaroslav Kočišek

Mgr. Michal Fárník, DSc.

Results of two independent experimental studies [1, 2] are presented, which could illuminate the processes leading to the formation of ice particles in the Polar Stratospheric Clouds (PSCs). PSCs serve as an important catalysts of the ozone depletion cycle. Two types of PSC particles are present in the Stratosphere: $\text{HNO}_3/\text{H}_2\text{O}$ ices in the type Ia PSCs and pure water ices in the type II PSCs. In the molecular beam experiments, these particles could be mimicked by large mixed $\text{HNO}_3/\text{H}_2\text{O}$ clusters and pure H_2O clusters, respectively.

At first we explore the formation of the type Ia PSCs. Experiments combining the Na pickup technique followed by the UV photoionization and the precise electron ionization mass spectroscopy demonstrate the importance of nitric acid in the clustering process [1]. We show that the mixed $\text{HNO}_3/\text{H}_2\text{O}$ clusters in the supersonic expansions are exclusively formed by the water freezing on the HNO_3 condensation core. In the atmosphere, condensation is explained to process by the nucleation of H_2O on the sulphuric acid core. Our observation shows that nucleation on the HNO_3 core can be effective at low temperature and the direct channel can significantly contribute to the PSC Ia particle formation.

In the second experiment we focus on the adsorption of additional molecules on the large water clusters. The experiment combining the pickup technique with the precise velocity measurement [2] shows that the water clusters interact with adsorbing molecules via dipole interactions. The observation leads to significantly higher values of adsorption cross sections in the comparison to the generally used geometrical ones.

Both studies show that the formation of PSCs is significantly faster than expected, what can have impact on the future ozone level predictions.

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RAMAN SPECTROSCOPY STRONGLY DOPED CVD-GRAPHENE

Mgr. Zuzana Komínková

RNDr. Ing. Martin Kalbáč, Ph.D.

Raman spectroscopy is sensitive characterization method for carbon-based materials such as graphene, carbon nanotubes or peapods due to the strong resonant enhancement of the Raman signal.

The Raman spectra from sp^2 nano-carbons are composed of first-order and higher-order Raman modes, as well as disorder-induced features. The important Raman active bands, which appear in Raman spectra of all graphene-based materials, are the tangential displacement mode (TG, G) and the high frequency, two phonon mode (G' , 2D). In some graphene sample, the D band is also found and is believed to indicate the presence of defects as in ordinary graphite.

Well-established method to study the electronic structure of carbon nanostructures is in-situ Raman spectroelectrochemistry. 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 Raman spectra.

Raman spectroscopy and in-situ Raman spectroelectrochemistry have been applied to study chemical vapor-deposition-grown graphene coated with layers of polyelectrolytes. In our study we focused on analyzing the change of the Raman shift and the Raman intensity of the G and G' bands as a function of the electrode potential. Due to polyelectrolyte coating a strong doping level could be achieved. The intensity of the G' band decreases with increasing magnitude of the electrode potential, but the G band exhibits a more complex behavior. An anomalous increase in the intensity of the G band at both high positive and negative potentials has been observed.

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STUDIUM DYNAMIKY FOTODISOCIACE ZOBRAZOVACÍ METODOU IMAGING

Pavel Košťál

Mgr. Michal Fárník Ph.D.

Při studiu dynamiky elementárních chemických reakcí je klíčové současně měřit rozdělení rychlostí produktů chemických reakcí a zároveň jejich úhlové rozdělení. Určení vnitřní energie a rychlostí všech produktů reakce je použito ke studiu molekulárních reakcí, procesů přenosu energie a fotodisociace [1]. K tomuto účelu se využívá iontové zobrazování, díky kterému určíme trojrozměrné rozdělení rychlostí vybraného stavu zvoleného produktu reakce. Navíc, když se omezíme pouze na fotodisociaci, při které se uvolní právě dva fragmenty, lze ze zákona zachování energie a hybnosti určit vnitřní stav druhého produktu.

Iontové zobrazování [2] je experimentální metoda pro měření směru a velikostí rychlostí vzniklých produktů po fotodisociaci [3] či po chemické reakci. Tato technika používá dvoudimenzionální, pozičně senzitivní detektor k záznamu pozice příletu vzniklého produktu.

V přednášce bude představena fotodisociace systémů obsahující chlor jako například CH_3Cl , freony apod., které jsou atmosféricky relevantní systém, protože se podílejí na tvorbě ozónové díry.

Poděkování:

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VARIATION OF PHOTOPHYSICAL PROPERTIES OF $[\text{ReX}(\text{CO})_3(\text{DIIMINE})]^{n+}$ COMPLEXES BY MODIFICATION OF THE DIIMINE LIGAND: DFT AND TRIR STUDY

Ing. Hana Kvapilová

Ing. Stanislav Záliš, CSc.

Photophysical behavior of Re(I) tricarbonyl diimine complexes $[\text{ReX}(\text{CO})_3(\text{diimine})]^{n+}$ strongly depends on the coordination sphere. Character of the lowest lying excited states and their relative energies, properties and reactivity can be controlled by variations of the ligand structure and/or the medium. In this talk complexes with a halide atom in place of the ligand X and with various types of diimine ligands will be described. Excited states participating in the ultra-fast intersystem crossings (~ps time scale) of these molecules were studied using femtosecond infrared spectroscopy experiments, so called time-resolved IR spectroscopy (TRIR). In this method, shifts of CO stretching frequencies point to the character of excited states and the time development of the spectra indicates kinetic behavior.

In order to understand the character and dynamics of optically excited states, DFT calculations were performed on these systems. The theoretical model employed hybrid functionals with triple- ζ polarized basis sets and PCM solvent correction. Optimized excited-state geometry was calculated for the lowest singlet and triplet states by the unrestricted Kohn-Sham (UKS) or time dependent DFT (TDDFT) approach. Calculations of vibrational frequencies were performed on harmonic level and also with anharmonic correction using generalized second-order vibrational perturbation (GVPT2) model. The calculated shifts of CO stretching frequencies well reproduce experimentally measured TRIR spectra and help to describe the excited-state behavior of these compounds.

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REDUCTION OF SELECTED BRANCHED EXPANDED PYRIDINIUM CATIONS

Mgr. Štěpánka Lachmanová

Mgr. Magdaléna Hromadová, Ph.D.

The Branched expanded pyridinium molecules are among the most extensively studied compounds because of their redox properties. Their characteristics depend strongly on the structure of the molecule. [1, 2]

In this work we have studied the redox properties of four expanded pyridinium cations (their structures are shown in Fig. 1) by various electrochemical methods with the emphasis put on the redox processes of the electron transfer. Although the structures of the studied molecules seem to be quite similar, the process of their reduction is completely different. The compounds 1-*N*-methyl-2,4,6-triphenylpyridinium (**A**) and 1',3',5'-trimethyl-2,4,6-triphenyl-1,4'-bipyridine-1,1'-dium (**B**) were reduced in two separate one-electron transfer steps. 1'-methyl-2,4,6-triphenyl-1,4'-bipyridine-1,1'-dium (**C**) and 1',3,5-trimethyl-2,4,6-triphenyl-1,4'-bipyridine-1,1'-dium (**D**) accept two electrons too, but in a single two-electron transfer. This contribution describes the determination of the heterogeneous rate constants for the compounds **A** to **D**.

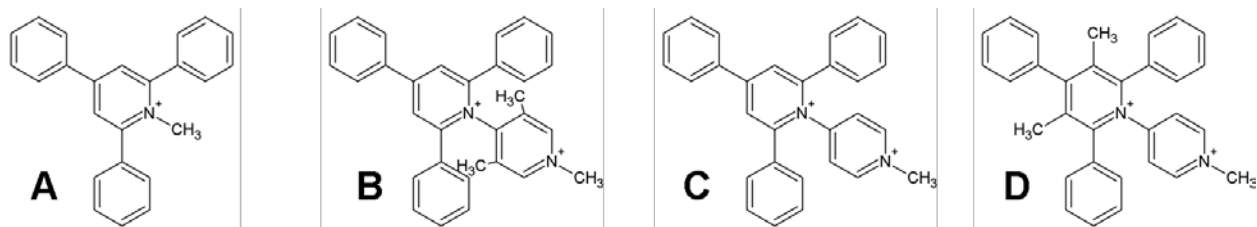


Fig. 1: Studied molecules

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Acknowledgement:

This work was supported by the Academy of Sciences of the Czech Republic (M200401202).



AN AB INITIO INVESTIGATION OF THE ISOMERIZATION OF BICYCLOBUTANE: DESCRIPTION OF THE CONROTATORY AND DISROTATORY STATES

Bc. Jakub Lang

Mgr. Jiří Pittner Dr. rer. nat.

Standard quantum chemical methods are able to calculate the activation barrier of the isomerization of bicyclo[1.1.0]butane to Buta-1,3-diene in excellent agreement with the experimental values. However, the single-reference methods fail in situations where static correlation is important. One of such situations is a transition state of the disrotatory pathway channel, which exhibits a strong biradical character. To account for a static correlation it is necessary to apply multireference methods such as Multiconfiguration self consistent field (MCSCF), multireference configuration interaction, and multireference Coupled Clusters (CC) methods.

In my lecture, the results of calculations performed with multireference wave function methods, in particular using the multireference CC methods developed in our group, will be presented.

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PSEUDOCAPACITIVE CONTRIBUTION TO THE TOTAL LITHIUM-ION STORAGE IN $\text{TiO}_2(\text{B})$

Mgr. Lásková Barbora

Prof. RNDr. Ladislav Kavan, DSc.

RNDr. Markéta Zúkalová, Ph. D.

TiO_2 belongs to widely studied semiconducting metal oxides. Tetragonal modification of titanium dioxide (anatase) and monoclinic one ($\text{TiO}_2(\text{B})$) are both attractive for applications in Li-ion batteries, however, $\text{TiO}_2(\text{B})$ shows more facile Li^+ insertion in comparison with that in anatase. The total stored charge in these materials can be separated into charge associated with capacitive processes and charge corresponding to diffusion-controlled insertion processes. The analysis of cyclic voltammograms of $\text{TiO}_2(\text{B})$ and anatase using the previously published method¹ can give us more detailed information about different charging mechanisms of these materials and explains the facilitated Li^+ insertion in $\text{TiO}_2(\text{B})$. The pseudocapacitive contribution to the total stored charge was determined for both types of materials. The difference of 30% was found between capacitive contributions in $\text{TiO}_2(\text{B})$ and in reference anatase materials (C240, P90). Deconvolution of cyclic voltammograms also indicates different capacitive contributions of the two particular voltammetric peaks of $\text{TiO}_2(\text{B})$.

References:

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Acknowledgement:

This work was supported by the Grant Agency of the Czech Republic (contract No. 13-07724S and P108/12/0814).



ELECTROCHEMICAL REDUCTION OF STRUCTURALLY MODIFIED POLYNITROCALIX[4]ARENES

Bc. Alan Liška

Prof. RNDr. Jiří Ludvík, CSc.

Calixarene skeleton is a stable supramolecular frame which is electrochemically inactive. Suitable substitution on the upper and lower rim, eventually structure modification or introduction of heteroatoms lead to unusual and surprising properties of this system.

The nitro substituents on the upper rim make the molecule reducible. Presence of one, two, three or four nitro groups in the same molecule provokes principal questions: What is the intramolecular electronic interaction between them? Are they reduced simultaneously or stepwisely? What are the respective intermediates in aprotic media?

The electrochemical study revealed that reduction of the tetranitrocalix[4]arenes starts with two 2-electron reversible waves corresponding to the presence of two different couples of equivalent nitro groups. This result reflects well the finding of the X-ray structural analysis, that the "calix" in fact, is not circular, but pinched with a strong " π -stacking" of the opposite benzene rings. The full reversibility points to the fact that the four-electron intermediate involves four equivalent non-communicating nitro radical anions. This stable tetraanion tetraradical is then able to be reduced by a following broad 12-electron wave, yielding the tetrahydroxylamino derivative. Product of total reduction - the tetraamino derivative - can be used for introduction of other functional groups and prolongation of the pendant chains.

The partial or full reduction of these molecules opens the possibility of an electron-transfer induced change in geometry of the parent calixarene, moreover, the reduced nitrogroups can serve as ligands enabling complex formation or host-guest interaction. Both UV-Vis-NIR spectroelectrochemical measurements (IFW Dresden) of pure compounds and complexation experiments with alkali metal cations were performed and the results discussed.

The recently synthesized new derivatives with nitro groups in *meta*-positions and with bridging sulfur atoms are promising as surface active species being able to modify the electrode.

The experimental findings were correlated with quantum chemical calculations and discussed.



INTERCALATION CHEMISTRY OF LAYERED ZEOLITE PRECURSOR IPC-1P

Mgr. Michal Mazur

Prof. Ing. Jiří Čejka, DrSc.

The discovery of two-dimensional layered zeolites opened many opportunities to design new structures and zeolite architectures^{[1],[2]}. One of the recent breakthroughs in this area has been the conversion of the UTL zeolite into a lamellar precursor (IPC-1P)^[3]. The change is attributed to the degradation of Ge-containing double four rings (D4R) connecting the 'UTL'/IPC-1P layers.

Post-synthesis modification of IPC-1P afforded variety of structures like swollen, pillared and stabilized. Remarkably, it also produced previously unknown zeolites IPC-2 and PCR (IPC-4). These zeolites were synthesized via newly proposed synthetic mechanism ADOR (A – assembly, D – disassembly, O – organization, R – reassembly). The ADOR approach is believed to be a general strategy that will lead to the preparation of new zeolites.

We investigated the intercalation chemistry of IPC-1P with various organic compounds. We look for possibility of obtaining additional, more expanded materials with preserved 'UTL' layers.

X-ray powder patterns proved that various organic agents can expand IPC-1P layers with different distances between them. Calcination of the intercalated IPC-1P leads to materials similar to IPC-4 or IPC-2 zeolites but also some solids with unknown structure. Selected materials were pillared with tetraethyl orthosilicate to fix the separation of layers permanently. Obtained materials were characterized using XRD, SEM and adsorption of nitrogen. Post-intercalation pillaring showed promise in producing new, larger pore materials.

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SPECTRO-ELECTROCHEMICAL STUDY OF CHROMIUM AMINOCARBENE REDUCTION MECHANISM

Ing. Radka Metelková

Prof. RNDr. Jiří Ludvík, CSc.

Fischer type aminocarbene complexes are widely used in various organic syntheses but they are also a promising material in redox catalysis. Nevertheless, for such use the redox mechanism needs to be investigated.

Our previous studies dealt with influence of various substitutions in aminocarbene complexes on their redox behaviour ^[1]. Recently, a detail study of their reduction mechanism is carried on by means of electrochemical and spectroelectrochemical methods.

Reduction mechanism was investigated on a series of chromium aminocarbene complexes substituted by a heterocycle: $[(CO)_5Cr=C(NMe_2)het]$, where het=2-(resp.3-furyl, 2-(resp.3-)thienyl), 2-N(CH₃)pyrrole]. Cyclic voltammetry(CV) on various electrode materials was used for distinguishing the mechanism but further research was needed, so we did bulk electrolysis together with reduction products identification by mass spectroscopy (MS).

Reduction (CV) of the whole series proceeds in a similar way: irreversible electrode reduction is followed by a chemical reaction. The spectroelectrochemical study has shown that follow-up reaction is dimerization of carbene carbon part of the original molecule. The resulting dimer is able to form three isomers so the real product of the reaction needs to be distinguished. NMR spectroscopy was thus used as a confirmation of MS results and identification of the product isomer.

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VYSOKOTLAKÁ SYNTÉZA FLUORESCENTNÍCH A KATALYTICKY AKTIVNÍCH SULFIDŮ

Roman Nebel

Ing. Petr Krtil CSc.

Syntéza nekonvenčních materiálů s definovanými vlastnostmi je jedním z určujících trendů současného materiálového výzkumu. Praktický vývoj nových materiálů využívá dvou základních strategií, „racionálního designu“ nebo kombinatorického postupu. První strategie je založena na detailním pochopení fyzikálně chemické podstaty funkčnosti materiálu, která umožňuje teoretický předvýběr perspektivních struktur a jejich cílenou syntézu, druhá možná strategie využívá systematického průzkumu existujících fází a jejich následné charakterizace.

Tento přístup je aplikovatelný na jakýkoliv typ materiálů a jeho praktická využitelnost je omezena pouze dostupností jednotlivých fází. Potenciál kombinatorického přístupu lze výrazně zvýšit, pokud je experimentu přístupna oblast metastabilních fází. Syntéza za vysokých teplot a tlaků (750 – 1000°C, 0,6 – 5 GPa) představuje preparativní postup, spadající do této strategie, vhodný k cílené modifikaci elektronové struktury pevných látek.

Příspěvek bude zaměřen na demonstraci tohoto syntetického postupu na případech ternárních a kvartérních sulfidů v systémech Ca-Zn-S, Sr-Zn-S, Ca-Ba-Zn-S, Sr-Si-S, Sr-Zn-Si-S. Podrobně bude diskutována zejména aplikace difrakčních a mikroskopických technik při identifikaci reakčních produktů.



APPLICATION OF COPPER SOLID AMALGAM ELECTRODE FOR DETERMINATION OF DITHIOCARBAMATE FUNGICIDE

Ing. Kateřina Nováková

Assoc. Prof. Dr. Ing. Tomáš Navrátil

Thiram belongs to the widely used protective dimethyldithiocarbamate fungicides. This compound is used for control of many fungal diseases in cropping fruits, vegetables and ornamentals. Thiram is hazardous to the environment. The main problem of this dithiocarbamate pesticide in soils is based on its persistence^{1,2}. Thiram is irritating to the eyes, skin, and respiratory tract. Thiram creates complexes with copper. These interactions can have the effect on its toxicity^{3,4}.

The voltammetric behavior of thiram was studied by differential pulse voltammetry (DPV) and cyclic voltammetry (CV) at polished (p-CuSAE) and mercury meniscus-modified (m-CuSAE) copper solid amalgam electrode with inner diameter 1.5 mm. The optimum conditions for DPV determination of this fungicide were received in Britton-Robinson buffer. The reaction mechanism was studied using CV and elimination voltammetry with linear scan (EVLS). DPV with optimized parameters was used for determination of thiram in analyzed solutions. The limits of detection were calculated as 16 nmol L^{-1} ($t_{\text{acc}} = 100 \text{ s}$) for m-CuSAE and 23 nmol L^{-1} ($t_{\text{acc}} = 60 \text{ s}$) for p-CuSAE. The proposed method was tested in real sample solutions.

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EFFECT OF INTEGRAL PEPTIDES ON MODEL MEMBRANES

Mgr. Marie Olšinová

Mgr. Marek Cebecauer, Ph.D.

Biological membranes are essential parts of the cell that separate outer and inner space in or around the cell. Membranes consist of a mixture of lipids and integral and peripheral proteins. Protein localisation and function is influenced by the surrounding lipid and protein environment. Transmembrane domains (TMD) of proteins mediate the closest contact with lipids. In this study, we tested how mutual interactions of lipids and proteins influence membrane organisation. Proteins are represented by synthetic peptide derived from the TMD and proximal amino-acid residues of LAT protein, and by WALP. WALP is an artificial peptide frequently used in biophysical studies¹ as typical TMD of plasma membrane protein. Model membranes (giant unilamellar vesicles; GUVs) were prepared using low melting temperature lipid DOPC, cholesterol and peptide. Changes in diffusion of fluorescently-labelled lipid in the absence or presence of TMD peptides and cholesterol were monitored by z-scan² fluorescence correlation spectroscopy. Increased content of both, cholesterol and peptide reduced lipid diffusion rates. Decrease in lipid mobility is probably caused by several effects such as changes in bilayer thickness due to cholesterol presence³, membrane crowding⁴ or lipid-peptide interaction. We are currently investigating the impact of the latter two effects.

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CHARACTERIZATION OF BIOLOGICAL MEMBRANE

Mgr. Martina Parisová

Assoc. Prof. Dr. Ing. Tomáš Navrátil

Biological membranes are very complex structures which separate intracellular space of cells from external space and ensure different processes important for life of cells. Because real biological membranes are very complicated, suitable model systems with similar properties have been introduced (e.g., [1, 2]). For these purposes, large unilamellar liposomes (LUVs) have been used. Biological membranes are formed from amphipathic molecules – phospholipids. Composition of liposomes is very similar to biological membranes, because their basic structure is formed from phospholipids too. This is one of the reasons why liposomes are used as models of artificial cell membranes. This contribution deals with preparation and with characterization of artificial liposomes. They can be used for investigation of heavy metal transport across biological membranes [3, 4]. Liposomes were prepared by a hydration method and their properties in presence and absence of cadmium ions were studied voltammetrically by glassy carbon electrode. Size of liposomes was determined using dynamic light scattering.

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MESOPOROUS MOLECULAR SIEVES: MATERIALS FOR HETEROGENEOUS METATHESIS CATALYSTS AS WELL AS CO₂ ADSORPTION

Mgr. Jakub Pastva

Prof. Ing. Jiří Čejka, DrSc.

RNDr. Hynek Balcar, CSc., Ing. Arnošt Zukal, CSc.

Siliceous mesoporous molecular sieves are relatively new material with regular structures, high surface areas (even more than 1000 m²/g), high void volumes (up to 1.5 cm³/g), and pore size in mesoporous region (diameter from 2 nm to 50 nm) with narrow pore size distribution. Due to these exceptional properties, mesoporous sieves have great potential in many catalysis, separation and adsorption¹. Olefin metathesis has become a powerful tool in organic synthesis and is now extremely useful having numerous applications in fine chemical synthesis. In adsorption field, control of the CO₂ emission has become serious and challenging topic. One of the options for the removal of CO₂ is adsorption on suitable solid adsorbents. Among the large number of such materials, mesoporous magnesium oxide has been studied as a plausible adsorbent for carbon dioxide mainly because of its lower energy requirement for regeneration.

Heterogeneous catalysts have been prepared by immobilization of commercial Hoveyda-Grubbs 1st generation catalyst on siliceous mesoporous molecular sieve of different pore size and architecture modified with linkers containing dicyclohexylphosphine (PCy₂) groups. These catalysts show low Ru leaching and can be used repeatedly. Activity of the catalysts was tested in the ring closing metathesis of various substrates².

Magnesia–alumina have been applied for the pillaring of the layered precursor of zeolite MCM-22. Calcination of pillared materials has led to new varieties of MCM-36 type zeolite. The carbon dioxide isotherms on prepared samples reveal that their adsorption properties are decisively influenced by the type of pillaring agent used. The comparison of starting MCM-22, siliceous MCM-36 and modified samples MCM-36/MgO·Al₂O₃ (A) and (B) has shown that impregnation of MgO into the pillars of MCM-36 enhances adsorption capacity in the region of equilibrium pressures lower than 10 kPa due to the strong interaction of CO₂ molecules with MgO.

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TOWARDS ACCURATE *AB INITIO* SIMULATIONS OF FLUORESCENT PROBES

Bc. Marek Pederzoli, MSc

Mgr. Jiří Pittner Dr. rer. nat., DSc.

The use of fluorescent probes in biochemical and biophysical research is very well established and the number of their applications is constantly growing due to their high versatility, sensitivity and quantitative capabilities. Among many other uses, fluorescent probes are employed for localization of biomolecules in cellular systems, monitoring transport of molecules through membranes, identifying conformational changes of proteins and studying biochemical processes in vivo.

Two of the main challenges for an accurate simulation of photochemical processes involving fluorescent probes are: i) precise calculation of the potential energy surfaces of the probe ii) description of interactions of the fluorescent probe with a complex system like a bio-membrane.

The potential energy surfaces of fluorescent probes are complicated by the presence of conical intersections and avoided crossings, which enable non-radiative transitions. In some photochemical reactions, the non-radiative transitions may even occur between states of different spin multiplicity. These so-called inter-system crossings are usually associated with the presence of heavy atoms, but recently they were 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 are presently implementing a method for inclusion of spin-orbit couplings into the Newton X package in the context of Tully's version of surface hopping dynamics.

In order to describe the interaction of the fluorescent probe with the system, we employ the quantum mechanics/molecular mechanics (QM/MM) method. The use of this approach is demonstrated on the example of prodan molecule in water. The newly developed interface of Newton X with Gromacs will enable us to perform simulations of fluorescent probes in bio-membranes.

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QUENCHING OF BADAN BY TRYPTOPHAN CAUSED BY PHOTON INDUCED ELECTRON TRANSFER IN MODEL MICELLAR SYSTEM

Mgr. Petr Pospíšil

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

The fluorescence environment-sensitive dyes are extensively used in the protein science. Detection of the conformational changes, studying of the protein-protein interaction, protein-membrane interaction and in fact, a number of biosensing approaches are often based on following the changes in fluorescence signal of these fluorophores. One of the classical solvatochromic probes is Badan, a relatively small thiol-reactive Prodan analogue. This probe can be covalently attached to the cysteine moiety possessing a defined location within the protein scaffold.

It was proposed that Badan could be quenched by tryptophan via photoinduced electron transfer (PET) as suggested for a large number of different dyes (Doose, 2009). The implication for PET between Badan and Tryptophan has already been mentioned in work by (Tsalkova, 2007) nevertheless, up to our knowledge no systematic study on this issue has been published so far. We therefore decided to map the quenching mechanism of Badan in a model micellar system containing tryptophan.

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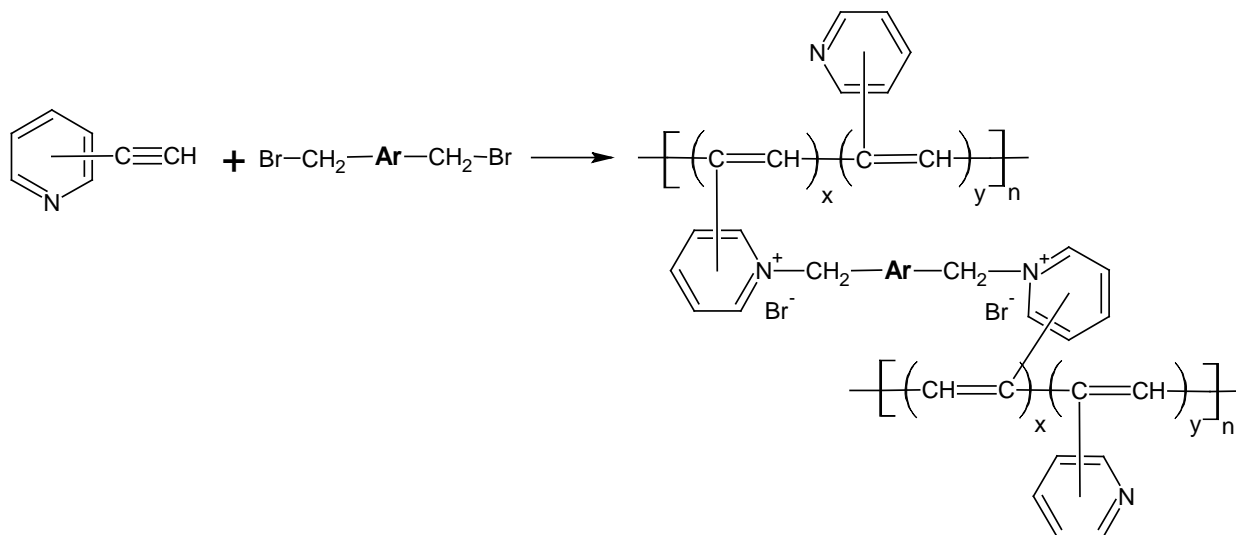
POLYMER NETWORKS DERIVED FROM ETHYNYLPYRIDINES

Mgr. Sabina Petrášová

RNDr. Hynek Balcar, CSc.

Doc. RNDr. Jan Sedláček, Dr.

Spontaneous quaternization polymerization of ethynylpyridines (EPy) known as the reaction yielding linear polyacetylenes [1] was modified so that the insoluble polymer networks resulted as the products (Scheme 1). Modification consisted in the application of bifunctional quaternizing agents of the bis(bromomethyl)arene (BBMA) type. Networks contained polyacetylene chains substituted by pyridyl and pyridiniumyl units. The latter units were quaternized by BBMAs that served as inter-chains linkers. Prepared networks were found active in CO₂ capture performed at near to ambient temperature. The influence of (i) the structure of EPy and BBMA and (ii) EPy to BBMA ratio on the properties of networks will be discussed.



Scheme 1

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SYNTHESIS AND PROPERTIES OF GERMANOSILICATE AND TITANOSILICATE FORMS OF CIT-5 ZEOLITE

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CIT-5 zeolite (IZA code: CFI) is an extra-large pore zeolite with one-dimensional 14 ring pores. These are accessible even for bulky molecules. Therefore, with incorporation of proper active sites, it could represent a valuable catalyst. The CIT-5 structure was prepared as a pure silica and with incorporated boron, gallium and aluminium¹ but neither as a germanosilicate and nor as titanosilicate.

CIT-5 has chains of “V” assembled 4-rings in its structure and it crystallizes into thin plate shaped crystals. Therefore we expect it might be possible to prepare its lamellar form in a similar way to conversion of UTL zeolite into IPC-1P.² Germanium in the structure (which is preferentially incorporated into 4-rings in the UTL) is crucial for this conversion. CIT-5 titanosilicate form could represent a useful catalyst for epoxidation of double bonds in bulky molecules used in perfumery and pharmacy.

Titanium and germanium containing CIT-5 structures were successfully prepared by direct synthesis using Cab-O-Sil and titanium (IV) butoxide or germanium oxide mixtures respectively in the presence of LiOH with N-methylspartheinium hydroxide as a structure directing agent. Application of different ratios of silicon and titanium source led to a group of samples with Si/Ti ratio as low as 42 (according to EDX measurement). Germanium containing CIT-5 was prepared as pure germanosilicate and as a germanium-aluminosilicate with initial ratio Al/Ge 1. The influence of the amount of heteroelement on the synthesis will be discussed. Crystalline phases following the formation of CIT-5 zeolite were also identified from the XRD patterns.

The catalytic activity of the titanosilicate samples was tested on selective epoxidation reaction of 1-octene, cyclooctene and α -pinene with hydrogen peroxide as an oxidant. The results were compared with standard TS-1 zeolite.

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NOVÁ SKUPINA FUNKČNÍCH MOLEKULÁRNÍCH STRUKTUR NA BÁZI CARBORAN- THIOLŮ

Martin Rajmon

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Molekulární uspořádané vrstvy na površích kovů jsou zajímavou a prakticky důležitou oblastí výzkumu vzhledem k jejich uplatnění v chemickém průmyslu, medicíně, v mikroelektronice, při zhotovení biokompatibilních materiálů, biosenzorů, jejich potenciálnímu využití pro distribuci léčiv v živých organismech aj. Nejvíce zkoumanými a využívanými strukturami v oblasti povrchových molekulárních uspořádaných vrstev jsou lineární alkylthioly vázané nejčastěji k povrchu zlata. Jejich nevýhodou je však m.j. jejich nestabilita spočívající v postupné degradaci při expozici na vzduchu.

Cílem tohoto příspěvku je představit nové, stabilnější a perspektivní uspořádané molekulární vrstvy na bázi thiolů karboranů a jejich derivátů chemisorbovaných na površích zlata a stříbra. V příspěvku jsou uvedeny příprava a výsledky studia stability a čistoty výchozích povrchů zlatých vrstev připravených metodou PVD a použitých pro imobilizaci molekul, příprava uspořádaných molekulárních vrstev sloučenin 1-SH-1,12-C₂B₁₀H₁₁, 1-SH-12-COOH-1,12-C₂B₁₀H₁₀, 2-(SH)₂-1,2-C₂B₁₀H₁₀ a 9,12-(SH)₂-1,2-C₂B₁₀H₁₀ adsorpcí z roztoku a výsledky jejich charakterizace metodou fotoelektronové spektroskopie. Byla měřena a numericky zpracována fotoelektronová spektra S 2p, B 1s, C 1s, O 1s a Au 4f (Ag 3d) fotoelektronů. Ze spekter byla vypočítána stechiometrie povrchových vrstev a určen způsob vazby molekul k povrchu kovu. Získané výsledky jsou důležité pro optimalizaci podmínek přípravy těchto vrstev.

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MODIFIED SILICATE GELS FOR THE CONSOLIDATION OF WEATHERED HISTORICAL MATERIALS

M.Sc. Monika Remzová

Ing. Jiří Rathouský, CSc.

Silicon alkoxides, such as silicon ethoxide or its oligomers are excellent consolidants for the weathered silicate materials. Their soft point is the cracking of formed gels due to the syneresis and residual drying stress leading to their decreased mechanical strength, and certain incompatibility of their physical properties with those of the stone.

The shrinkage and cracking of the gel can be reduced by the formation of mesopores within the gels or by the modification with particles. Mesopores could be created by adding a template, such as amphiphilic polymers or other surfactants, to the sol and removing it after the rigid mineral structure has been formed. By adding particles of oxides to the alkoxide sols composites are formed after the hydrolysis and polymerization, which exhibit microstructure of particulate systems and are distinct from the polymeric gels without particles.

We have aimed at two systems, namely at particle and particle-pore modified gels. Both approaches have provided materials with improved mechanical properties. Cracking of layers about 5mm in thickness due to drying is reduced owing to the presence of nanoparticles 10 to 20 nm in size. The polymers or surfactants added to the sol improve the elasticity of the formed gel which also reduced cracking. After their removal mesopores are formed. The physical properties of the modified gels are therefore much closer to those of the historical materials in comparison with purely polymeric non-porous gels.

VÝVOJ METOD EXTRAKCE TĚKAVÝCH LÁTEK Z BIOLOGICKÝCH VZORKŮ

Bc. Michaela Rybárová

Prof. RNDr. ŠPANĚL Patrik, Dr. rer. nat.

Poměrně novou a atraktivní metodou klinické diagnostiky je analýza dechu. Její výhody spočívají zejména v neinvazivnosti metody. Podstatou analýzy dechu je kvantifikace metabolitů v dechu, jenž mohou indikovat určitá onemocnění. Jelikož se tyto metabolity vyskytují v koncentracích v řádech ppm (a menších), lze je analyzovat pouze nejmodernějšími analytickými metodami, jako je například SIFT-MS (Selected ion flow tube mass spectrometry, respektive hmotnostní spektrometrie v proudové trubici s vybranými ionty). Optimálně by se měl dech analyzovat pomocí SIFT-MS v reálném čase, avšak ne vždy je to možné. Cílem tohoto experimentu je proto vyvinout metodu a zařízení pro odběr biologického vzorku tak, aby jej bylo možné analyzovat později v laboratoři.

Během laboratorního výzkumu byl zvolen sorbent vhodný pro metodu odběru vzorku dechu a jeho pozdější analýzu. Sorbent byl vložen do tzv. sorpční trubičky, která je určena k odběru plyných biologických vzorků pomocí čerpadla. Prostřednictvím vhodně zvoleného sorbentu dojde k zachycení zkoumaných analytů na trubičce. Analyt je dále ze sorpční trubičky uvolněn, v tomto případě pomocí termální desorpce, a analyzován metodou SIFT-MS. Mezi zkoumané sorbenty byly zvoleny tři druhy sorbentů - polymerní sorbent Tenax TA a uhlíkaté sorbenty Carbopack C a aktivní uhlí.



PURIFICATION AND CHARACTERIZATION OF SINGLE WALL CARBON NANOTUBES

Ana Santidrián García

RNDr. Ing. Martin KALBÁČ, Ph.D.

As prepared carbon nanotubes (CNTs) are usually accompanied by carbonaceous or metallic impurities, so purification is essential. Recent studies showed that steam is able to remove the amorphous carbon and the graphitic shells coating the metal particles present in as-made CNTs without changing the tubular structure or inducing defects or functional groups. Steam is also used to open and shorter carbon nanotubes. We use steam purification following the process by Thermogravimetric analysis. Our efforts are focus on the improvement of this technique looking for the optimizing set up and conditions.

As well as steam purification, it was shown that magnetic filtration followed by oxidation is a powerful tool for purification. Our idea is to combine the steam purification and magnetic filtration to obtain a reduction in the ferromagnetic catalyst content, to remove amorphous carbon and graphitic particles without damaging the structure of carbon nanotubes.

Spectroscopy (Near Infrared, Raman), Raman Spectroelectrochemistry, and Thermogravimetric Analysis were used to analyze samples, mainly to evaluate purification steps, trying to analyze the different diameter distribution in the steps and the defects present in the CNTs samples.

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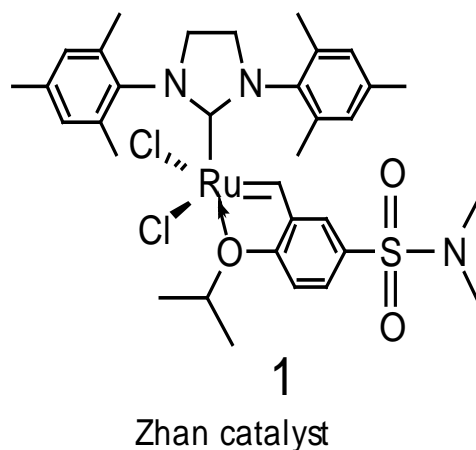
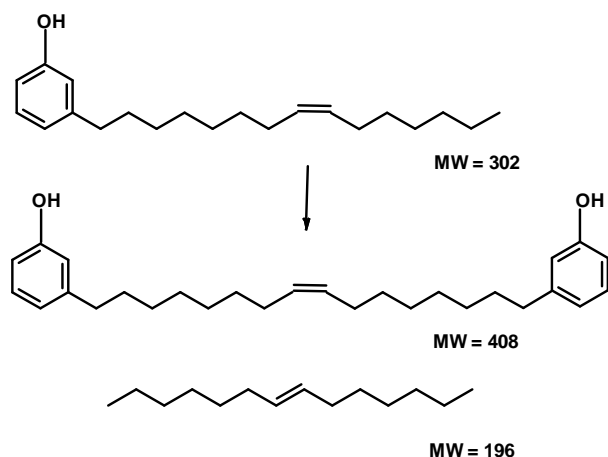
RUTHENIUM CATALYSTS FOR METATHESIS AND ETHENOLYSIS OF CARDANOL

Tushar Shinde

RNDr. Balcar Hynek, CSc.

The Ru - alkylidene complexes (Grubbs and Hoveyda-Grubbs catalysts) belong to 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.^[1]

The aim of this contribution is to report the application of Ru catalysts {1 and 1 immobilized on SBA-15 (d = 6.8 nm)}, in metathesis of cardanol. Cardanol is the phenolic substrate which can be obtained by decarboxylation of anacardic acid, the main component of Cashew Nut Shell Liquid (CNSL). Cardanol is worth to study because firstly it's a natural product (i.e. renewable source of chemicals) and secondly CNSL are produced in large quantity but it is little known about chemical transformation of cardanol by metathesis. The given catalysts have proved to be active in cardanol metathesis even without protecting OH groups. Cardanol ethenolysis (cross metathesis with ethylene) proceeded with nearly 100% conversion with high selectivity under mild conditions (room temperature and 3 bar ethylene pressure).



As the catalyst 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 in the reaction.^[2] The Ru leaching was found for ethenolysis of cardanol in toluene (2.5 % with respect to the original content of Ru).

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INTERACTION OF QUANTUM DOTS WITH ORGANIC MOLECULES

Ing. Jan Suchánek

Doc. Ing. Zdeněk Zelinger, CSc.

Quantum dots (QD's) are fluorescent nanoparticles with many useful size dependent properties. The most known QD's are semiconductor nanocrystals (e.g. CdS, CdSe) [1]. The very interesting QDs based on other materials (carbon, boron nitride QD's) were reported recently [2, 3]. The interaction of these nanoparticles with organic dyes has large impact to different fields like photovoltaics, bioimaging, photodynamic therapy (PDT) and sensors.

The studies of the formation of self-assemblies between CdSe 520 (~2,5 nm) quantum dots (QD's) and Zn phthalocyanines (Pc) and azaphthalocyanines (AzaPc), respectively were an aim of my previous work. The photophysical properties of these assemblies were studied using both steady-state and time-resolved luminescence/absorption spectroscopy. The formation of the self-assemblies was accompanied by a blue shift of the Q - band of the dyes and by quenching of the CdSe QDs luminescence.

This work is focused on the interaction of differently sized CdSe (CdSe 520, size ~ 2,5 nm and CdSe 640, size ~ 6,5 nm) quantum dots with Pc and AzaPc, respectively. The comparison of both studies provided a controlled spectral analysis. A selection of different sizes of QDs allowed tuning of the spectral overlap between CdSe QD's luminescence and dye absorption. Any Forster resonance energy transfer to the dye wasn't observed, in spite of the luminescence emission of CdSe 640 matches the Q-bands of studied Pc's and the luminescence of CdSe 640 was quenched upon interaction. The quenching mechanism was attributed to the photoinduced electron transfer between CdSe and Pc.

The further studies were targeted the comparison of semiconductor QD's with new class of QD's – graphene quantum dots (GQD). The interaction of GQD with porphyrins is studied by absorption and luminescence spectroscopy. Small bathochromic shift of the Soret band of TMPyP porphyrin and quenching of fluorescence lifetime of TMPyP porphyrin were observed.

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STUDY OF DIRADICALS BY EXPLICITLY CORRELATED MULTIREFERENCE COUPLED CLUSTER METHODS

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One of the most often used approaches of computational chemistry nowadays is the single reference coupled cluster (CC). In specific, the coupled cluster singles doubles (CCSD) method has found a widespread use for its well balanced ratio between cost and accuracy. Nowadays, also the perturbative triples coupled cluster method (CCSD(T)) is gaining popularity.

There are cases, however, where the single-determinantal approach does not perform so excellently. Examples include open-shell systems such as carbenes, transition metal atoms, biradicals and excited states in general. The difficulties arise because of the degeneracy or quasi-degeneracy of the reference Slater determinants.

One of the possible cures to tackle these complications is to use the multi reference (MR) methods. These, however, introduce a new level of complexity into the calculations. In order to lower the computational cost of such an approach, explicit correlation (the F12 methods) is used.

In my lecture, I will be talking about the multireference Brillouin-Wigner coupled cluster method with perturbative triples and explicit correlation (MR BWCCSD(T)-F12), which is being developed in our group.

I will focus on the results of calculations performed on the Bergmann reaction, with a possibility of discussing one another biradical system.

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OVERTONOVÁ SPEKTROSKOPIE V SUPERSONICKÝCH EXPANZÍCH

Vít Svoboda

Mgr. Ondřej Votava PhD.

Spektroskopie s vysokým rozlišením v plynné fázi je vhodnou experimentální technikou umožňující studium vibračně-rotačních stavů molekul. Pomocí této techniky je například možné studovat zemskou atmosféru, ale i atmosféry planet Sluneční soustavy. Vibrační spektra molekul za pokojové teploty dosahují značné složitosti díky populaci vyšších rotačních stavů. Při použití expanze plynu supersonickou tryskou do vakua dochází k výraznému ochlazení molekul, což vede ke zjednodušení měřených spekter.

Cílem práce je studium overtonových a kombinačních vibračních pásů N-H vazeb amoniaku v blízké infračervené oblasti pomocí vysoce rozlišené absorpční spektroskopie, konkrétně v oblasti $6600\text{--}6900\text{ cm}^{-1}$. Pomocí spektrálních metod byly nejdříve charakterizovány podmínky expanze a následně byly identifikovány spektrální linie s nízkým rotačním kvantovým číslem J s využitím dvouteplotní analýzy pro empirické přiřazení rotačních kvantových čísel. Je diskutován vliv nukleární spinové statistiky na populaci rotačních stavů a na charakter měřených spekter. Bude diskutována souvislost práce s teoretickými předpověďmi spekter [1] a s nejaktuálnější publikovanou experimentální prací [2]. Součástí práce je kromě spektroskopických měření i vývoj a charakterizace používaných laserů, konkrétně SAF (Single Angled Facet) laserových čipů umožňujících přeladění přes širokou spektrální oblast 450 cm^{-1} .

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CHLOROBENZENE - MASS SPECTRA, PHOTODISSOCIATION DYNAMICS

Mgr. Pavla Svrčková

Mgr. Michal Fárník Ph.D. DSc.

Chlorobenzene is one of the molecules, which is located in atmosphere and it assists in creating the ozone hole. The gas acts as a source of ClO, which helps in the breakdown of stratospheric ozone. Therefore understanding chlorobenzene photochemistry is essential for overall understanding of the processes in the stratosphere.

We carried out an initial exploratory measurements of the chlorobenzene and mixed chlorobenzene-water clusters. Chlorobenzene in a reservoir in the source chamber is heated and expanded in a carrier gas (He, Ar) through a nozzle into a vacuum. The generated clusters are electron ionized and detected by a reflectron time-of-flight (RTOF) mass spectrometer [1].

In the next stage, we examine the photodissociation dynamics of chlorobenzene using velocity map imaging method [2]. This method is very convenient because the images of photofragments contain the complete information about the kinetic energy and angular distribution.

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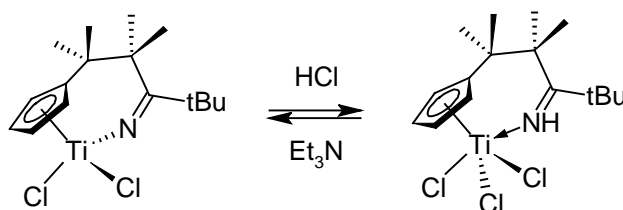
SYNTÉZA KOMPLEXŮ PRVKŮ 4. SKUPINY S CYKLOPENTADIENYL- KETIMIDOVÝMI CHELATUJÍCÍMI LIGANDY

Miloš Večeřa

RNDr. Martin Lamač, Ph.D.

Koordinační sloučeniny prvků 4. skupiny s cyklopentadienylem (Cp) jakožto η^5 -ligandem byly v minulosti intenzivně studovány jako katalyzátory pro polymeraci olefinů.¹ Byly připraveny různě modifikované tzv. sendvičové i polosendvičové komplexy (tj. s jedním či dvěma Cp ligandy). Příkladem jsou tzv. CGC (constrained geometry complex) komplexy, jež mají na Cp připojen substituent nesoucí nejčastěji amidovou funkční skupinu, která je také vázána na kovové centrum. Tyto komplexy se ukázaly jako vynikající katalyzátory kopolymerací ethylenu s α -olefiny s vysokou aktivitou, která bývá vysvětlována výrazným obnažením aktivního centra díky geometrii uvedených ligandů.² Obdobně jsou pro polymerace zajímavé i komplexy kombinující Cp a ketimidové ligandy.³

V naší práci se věnujeme přípravě sendvičových a polosendvičových komplexů s hybridními Cp-ketimidovými ligandy. Vycházíme z námi dříve připravené lithné soli Cp s pendantní nitrilovou skupinou, na které provádíme alkylaci. Produktem je dilithná sůl, která s příslušnými kovovými prekurzory poskytuje metallocenové komplexy. Ty poté charakterizujeme spektrálními nebo difrakčními metodami a studujeme jejich katalytické vlastnosti a reakce s Lewisovými či Brønstedovými kyselinami.



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AB INITIO VIBRATIONAL TRANSITION CALCULATION BY THE NOMO/CI METHOD ON A SIMULATED QUANTUM COMPUTER

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Mgr. Jiří Pittner Dr. rer. nat.

Ab initio quantum chemical calculations of molecular properties done on classical computers demand large computation resources (time, memory). For the full configuration interaction (FCI), which gives the most precise results within given set of molecular orbitals (and which is the only truly reliable method in many cases), computational resources scale exponentially with the number of molecular orbitals (size of the molecule). Quantum computers are able to give the same results in polynomial time [1]. In other words – quantum computers can simulate quantum systems efficiently [2].

For the vibrational transitions computation the above mentioned reduction of asymptotic complexity of quantum (full) configuration interaction (QCI as algorithm for quantum computer), when compared to FCI calculation (done on classical computer), calls for NOMO/CI method (which treats electrons and nuclei explicitly on equal footing and goes beyond the adiabatic approximation [3]). In this way, vibrational states are obtained directly, rather than by introducing the potential energy surface(s) and subsequently performing a nuclear-motion calculation.

The lecture presents results of NOMO/CI hamiltonian eigenvalue estimation by the Iterative Phase Estimation Algorithm (IPEA, part of the QCI [4]), simulated on a classical computer, as a demonstration of possibility to directly compute energy of rotationless vibrational 0-1 transition in several isotopomers of the hydrogen molecule (H_2 , HD, HT, ...) on (future) quantum computers.

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ELEKTROCHEMICKÝ SENZOR S ELEKTRODOU MODIFIKOVANOU POLYMERNÍ METHYLENOVOU MODŘÍ PRO STANOVENÍ SULFANU

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Sulfan, plyn známý pro svou vysokou toxicitu, je v posledních letech zkoumán jako přirozená endogenní látka se slibnými terapeutickými účinky [1]. Velmi nízká fyziologická koncentrace sulfanu i potencionální terapeutická koncentrace si žádají vývoj vhodnějších analytických metod s důrazem na jejich citlivost a selektivitu.

Ke stanovení sulfanu jsou v poslední době hojně vyvíjeny metody využívající elektrod modifikovaných vhodným redoxním mediátorem, jež řeší problémy čistých pevných elektrod, jako jsou nízká citlivost, pomalý přenos elektronů, nízká elektrokatalytická aktivita, oscilace proudů či nutnost vysokého přepětí na elektrodě.

Fenothiazinové barvivo methylenová modř je využívána nejen ve spektrometrickém stanovení sulfidů, ale v posledních letech právě jako mediátor elektronového přenosu v elektrochemii [2].

Elektropolymerizací methylenové modři vzniká na povrchu pevných elektrod vodivý polymerní film vykazující elektrokatalytickou aktivitu při oxidaci sulfidů, thiolů a dalších sirných sloučenin [3]. Díky silné adhezi polymeru k elektrodovému povrchu je film stabilní rovněž v široké škále pH [4].

Práce prezentuje studii vrstvy polymerní methylenové modři a elektrochemickou detekci sulfidových aniontů ve vodném prostředí metodou cyklické voltametrie na elektrodě, která je tvořená bazální rovinou vysoce orientovaného pyrolytického grafitu (HOPG) modifikovanou polymerní methylenovou modří.

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THE TOXICITY OF SILVER NANOPARTICLES TO SCENEDESMUS QUADRICAUDA AND CHLORELLA VULGARIS

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Silver nanoparticles were prepared via reduction of $[\text{Ag}(\text{NH}_3)_2]$ cation by various saccharides or by sodium borohydride. Three monosaccharides (glucose, galactose and xylose) and two disaccharides (maltose and lactose) were used. The syntheses produced very small particles about 5-100 nm in size with narrow size distributions. The use of disaccharides yields smaller particles than using monosaccharides. The smallest silver nanoparticles with an average size of 5 nm with a narrow size distribution as determined by DLS were prepared using sodium borohydride. The maximum of the UV-VIS absorption spectrum depends on the particle size; being red shifted with increasing particles size.

The smallest nanoparticles of about 5 nm exhibit the highest toxicity to algae *Scenedesmus quadricauda* and *Chlorella vulgaris*, EC 50 being 1 mg/L. The toxicity of the 5 nm particles to *S. quadricauda* is even higher than that of silver cations at the same concentration. *C. vulgaris* is more vulnerable than *S. quadricauda* and is effectively killed by substantially larger particles (40-100 nm) at low concentration of about 2-4 mg/L. The toxicity of silver nanoparticles can be associated with their size and their oxidation to the silver ions. For *S. quadricauda* there is a linear correlation between the size of nanoparticles and their biocidal efficiency. Testing the biocidal performance was carried out at the Department of Water Technology and Environmental Engineering of the Institute of Chemical Technology Prague.

