SEMINÁŘ STUDENTŮ ÚFCH JH 2017

Konferenční centrum
AV ČR v Liblicích
9. - 10. 5. 2017

Seminář studentů ÚFCH JH 2017

Sborník příspěvků

ze studentské konference konané
9. - 10. května 2017
v Konferenčním centru AV ČR Liblicích

Seminar of Students of JHI 2017

Collection of abstracts

of all lectures given at the student conference
held on 9-10 May 2017
in Conference Centre of the Academy of Sciences
of the Czech Republic in Liblice chateau

Seminář studentů ÚFCH JH 2017
Sborník příspěvků ze studentské konference
konané 9 - 10. května 2017
v Konferenčním centru AV ČR Liblicích

Kolektiv autorů
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SEMINÁŘ STUDENTŮ ÚFCH JH 2017

PROGRAM 1. dne konference - úterý 9.5.2017

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

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

May 9, 2017 - Departure from parking place (in front of the JHI building) - 8:30

Čas	Předsedající	Přednášející	Název
9:30 - 10:20	Ubytování - v recepci po příjezdu. **OBČERSTVENÍ PŘED ZAHÁJENÍM KONFERENCE** *(káva, nápoje, zákusek - v 1. patře, na ochozu)* *Coffee break*		
10:25	**Zahájení konference „Seminář studentů ÚFCH JH 2017“** *Annual conference "Seminar of Students JHI 2017"*		
10:30	***Věra Křížová***	Martin PIŽL *(I. ročník PGS, školitel S. Záliš)* ***kat. I***	EXCITED STATES OF BINUCLEAR IRIDIUM COMPLEX: EXPERIMENTAL AND DFT STUDY
10:50		Michaela OBLUKOVÁ *(I. ročník PGS, školitel J.Žabka)* ***kat. I***	STUDY OF METABOLISM OF SYNTHETIC CANNABINOIDS. OPTIMIZATION OF METHODS FOR TOXICOLOGICAL DETECTION
11:10		Young ZHOU¨ *(I. ročník PGS, školitel M. Opanasenko)* ***kat. I***	ISOMORPHOUSLY SUBSTITUTED ISORETICULAR ZEOLITES WITH UTL TOPOLOGY
11:30		Adam PASTOREK *(diplomant, školitel S. Civiš)* ***kat. I***	A STUDY ON SYNTHESIS OF BIOGENIC MOLECULES FORMATION BY THE EFFECTS OF GAMMA IONISING RADIATION
11:50	**PŘESTÁVKA** *Break*		
12:10	***Jakub Lang***	Roman NEBEL *(I. ročník PGS, školitel P. Krtil)* ***kat. I***	EFFECT OF TIO_2 (ANATASE) SURFACE STRUCTURE ON SELECTIVITY OF PHOTO-ELECTROCHEMICAL WATER OXIDATION
12:30		Antonín KNÍŽEK *(magisterské studium, školitel M. Ferus)* ***kat. I***	PHOTOCATALYTIC TRANSFORMATION OF PLANETARY ATMOSPHERES IN CONNECTION TO EXOPLANETS, MARS AND EARLY EARTH
12:50		Lea ASSIES *(diplomantka, školitel M. Kalbáč)* ***kat. I***	PHOTOLITHOGRAPHY AND SELF ASSEMBLY FOR MOLECULAR ELECTRONICS
13:10		Dávid HVIZDOŠ *(I. ročník PGS, školitel R. Čurík)* ***kat. I***	DISSOCIATIVE RECOMBINATION OF H_2^+ : A COMPARISON OF THEORETICAL METHODS
13:30 - 15:00	**OBĚD** *(Lunch at the restaurant- 13:30)* *(podává se v restauraci v přízemí a v rámci přestávky na oběd si účastníci zajistí UBYTOVÁNÍ v recepci hotelu, pokud se neubytovali ráno po příjezdu)*		
15:00	***Anna Makrlíková***	Jan BRANDEJS *(I. ročník PGS, školitel L. Veis)* ***kat. I***	ENTANGLEMENT-BASED METHODS IN COMPUTATIONAL QUANTUM CHEMISTRY
15:20		Mariia LEMISHKA *(I. ročník PGS, školitel J. Dědeček)* ***kat. I***	DETERMINATION OF NICKEL SPECIES IN FERRIERITES USING FTIR AND UV-VIS SPECTROSCOPY

15:40		Wasif Baig MIRZA (*I. ročník PGS, školitel J. Pittner*) ***kat. I***	SIMULATION OF ABSORBTION AND EMISSION SPECTRA OF LAURDAN IN PHOSPHOLIPID LAYER SYSTEMS
16:00		Eduard JEŠKO (*I. ročník PGS, školitel M. Hof*) ***kat. I***	NEURODEGENERATIVE AMYLOIDOSES AND PROTEIN-MEMBRANE INTERACTIONS:MOLECULAR INSIGHTS INTO MEMBRANE MEDIATED PROTEIN OLIGOMERISATIONIONS
16:20-16:40	**PŘESTÁVKA** *Break*		
16:40	***Valeryia Kasneryk***	David DUNLOP (bakalář, *školitel M. Lamač*) ***kat. I***	KATIONTOVÉ ORGANOKOVOVÉ KOMPLEXY JAKO PREKURZORY REAKTIVNÍCH LEWISOVSKÝCH PÁRŮ
17:00		Jana HRNČÍŘOVÁ (bakalářka, *školitel M. Ferus*) ***kat. I***	TERMOLÝZA FORMAMIDU V PŘÍTOMNOSTI JÍLŮ: VZNIK NUKLEOVÝCH BÁZÍ A DALŠÍCH STAVEBNÍCH KAMENŮ ŽIVOTA
17:20		Andrej ANTALÍK *(II. ročník PGS, školitel J. Pittner)* ***kat. II***	THE INTRICATE CASE OF TETRAMETHYLENEETHANE
17:40	**Ukončení prvního dne konference** **VEČEŘE v RESTAURACI - začátek v 18:00** *(Dinner at the restaurant- 18:00)*		

PROGRAM 2. dne konference - středa 10.5.2017

Čas	**Předsedající**	**Přednášející**	**Název**
9:00	**Zahájení druhého dne konference - pokračují prezentace studentů kategorie I a II.**		
9:10	***Taťána Supiňková***	Alan LIŠKA (*IV. ročník PGS, školitel J. Ludvík*) ***kat. II***	STEREOELECTROCHEMISTRY OF CALIXARENES
9:30		Valeryia KASNERYK (*III. ročník PGS, školitel M. Opanasenko*) ***kat. II***	HOW DOES POST-SYNTHESIS INCORPORATION OF ALUMINUM PROCEED IN UOV GERMANOSILICATE FRAMEWORK?
9:50		Jakub LANG (*III. ročník PGS, školitel J. Pittner*) ***kat. II***	USS CORRECTED MRCC-LPNO STUDY OF CYCLOPROPANE ISOMERIZATION
10:10		Anna MAKRLÍKOVÁ (*II. ročník PGS, školitel T. Navrátil*) ***kat. II***	OPTIMIZATION OF CONDITIONS FOR VOLTAMMETRIC DETECTION OF TUMOR BIOMARKER 5-HYDROXYINDOLE-3-ACETIC ACID USING FLOW INJECTION ANALYSIS
10:30 - 10:50	**PŘESTÁVKA** *Break*		
10:50	***Alan Liška***	Ján SABÓ (bakalář, *školitel M. Cebecauer*) ***kat. I***	PEPTIDE ANALYTICS IN SOLUTION AND VESICLES BY LIQUID CHROMATOGRAPHY FOLLOWED BY MASS SPECTROMETRY
11:10		Taťána SUPIŇKOVÁ (*III. ročník PGS, školitel M. Kočiřík*) ***kat.I I***	INSIGHT INTO CHEMISTRY OF STRUCTURE DIRECTING AGENTS IN RELATION TO PREPARATION OF SSZ-16 ZEOLITE

11:30		Vojtěch HRDLIČKA *(II. ročník PGS, školitel T. Navrátil)* ***kat. II***	HOLLOW FIBRE LIQUID-PHASE MICROEXTRACTION OF CATECHOLAMINE BASED BIOMARKERS
12:00	**PŘESTÁVKA NA OBĚD** *(podává se v restauraci od 12:00 do 14 hodin)* *(Lunch at the restaurant - 12:00)*		
14:00	***Andrej*** ***Antalík***	Michal DOSTÁL *(III. ročník PGS, školitel Z. Zelinger)* ***kat. II***	TOWARDS QUARTZ ENHANCED PHOTOACOUSTIC SPECTROSCOPY OF ACETONITRILE
14:20		Věra KŘÍŽOVÁ *(III. ročník PGS, školitel M. Polášek)* ***kat. II***	ION-INDUCED IONIZATION AND DISSOCIATION OF SIMPLE ORGANIC MOLECULES BY SELECTED KEV PROJECTILE IONS
14:40		Valentino Libero Pio GUERRA *(III. ročník, školitel M. Kalbáč)* ***kat. II***	SELECTIVE GROWTH OF HYBRID PEROVSKITES ON GRAPHENE
15:00 - 15:30	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** *(1.patro, ochoz)* *Coffee break*		
15:30- 16:00	**15:30 - SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ SOUTĚŽNÍ KONFERENCE - V KONFERENČNÍM SÁLE** **UKONČENÍ KONFERENCE** *Closing ceremony - Results announcement (in conference hall)*		
16:15	**Odjezd do Prahy -** *autobusem z parkoviště u zámku* ***v 16:15*** *(autobus bude přistaven na 16:00 hodin)* ***Departure from parking place (in front of the chateau) - 16:00 -16:15***		

Seznam prezentujících studentů (25)

Kategorie I (15)

Diplomanti. magistři a zájemci z řad bakalářů (6)

Assies Lea
(diplomantka, školitel M. Kalbáč)
Dunlop David
(bakalář, PřF UK, školitel M. Lamač)
Hrnčířová Jana
(bakalářka, PřF UK, školitel M. Ferus)
Knížek Antonín
(magisterské studium, PřF UK, školitel M. Ferus)
Pastorek Adam
(diplomant, FJFI ČVUT, školitel S. Civiš)
Sabó Ján
(bakalář, PřF UK, školitel M. Cebecauer)

Studenti 1. ročníku PGS (9)

Brandejs Jan *(školitel J. Pittner)*

Hvizdoš Dávid *(školitel R. Čurík)*

Ješko Eduard *(školitel M. Hof)*

Lemishka Mariia (*školitel J. Dědeček)*

Mirza Wasif Baig *(školitel J. Pittner)*

Nebel Roman (*školitel P. Krtil)*

Obluková Michaela *(školitel J. Žabka)*

Pižl Martin *(školitel S. Záliš)*

Zhou Young *(školitel M. Opanasenko)*

Kategorie II (10)

Studenti 2. ročníku PGS (3)

Antalík Andrej (*školitel J. Pittner)*

Hrdlička Vojtěch (*školitel T. Navrátil)*

Makrlíková Anna *(školitel T. Navrátil)*

Studenti 3. ročníku PGS (6)

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

Dostál Michal (*školitel Z. Zelinger)*

Kasneryk Valeryia (*školitel M. Opanasenko)*

Křížová Věra (*školitel M. Polášek)*

Lang Jakub (*školitel J. Pittner)*

Supiňková Taťána (*školitel M. Kočiřík)*

Studenti 4. ročníku PGS (1)

Liška Alan *(školitel J. Ludvík)*

Hodnotící komise:

Michal Fárník
Martin Lamač
Eva Krupičková - Pluhařová
Jiří Pittner

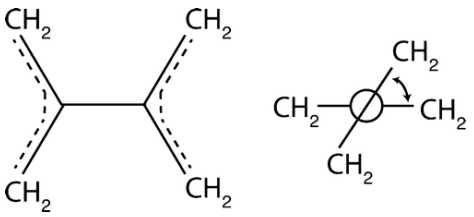
THE INTRICATE CASE OF TETRAMETHYLENEETHANE

Mgr. Andrej Antalík

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

Tetramethyleneethane (TME), the simplest disjoint non-Kekulé diradical, often serves as a model of more complicated disjoint diradicals. Although the system might seem simple, correct calculation of its electronic structure poses a very challenging problem. It has been shown that to accurately describe its potential energy surface with respect to rotation around the central carbon-carbon bond, one has to employ methods with excellent treatment of both static and dynamic correlation combined with large enough basis sets [1].

In this study, we follow the work of Pozun et al [1]. We provide a new benchmark using the full configuration interaction quantum Monte Carlo (FCIQMC) method, which agrees well with experimental data. These data are then used as a reference to test the methods developed in our group, namely Mukherjee's MRCC [2] and DMRG-TCCSD [3].



References:

[1] Z. D. Pozun, X. Su, K. D. Jordan, *J. Am. Chem. Soc.*, **2013**, 135, 13862

[2] D. I. Lyakh, M. Musiał, V. F. Lotrich, R. J. Bartlett, *Chem. Rev.*, **2012**, *112,* 182

[3] L. Veis, A. Antalík, J. Brabec, F. Neese, Ö. Legeza, J. Pittner, *J. Phys. Chem. Lett.*, **2016**, 7, 4072

PHOTOLITHOGRAPHY AND SELF-ASSEMBLY FOR MOLECULAR ELECTRONICS

Lea Assies

RNDr. Ing. Martin Kalbáč, Ph. D.

Conjugated polymers containing extended π-systems are of big interest because they can be doped into electrically (semi)conducting state.[1] Due to properties such as flexibility and good processability in solution they seem to have large potential for (opto)electronic and electrochemical devices.[2]

Polymers containing imine-bonds, such as polyimines and polyazines, are particularly promising because they offer advantages due to the dynamic covalent character of the C=N linkage, such as self-healing, error-repair and thermodynamic control.[3, 4]

The goal of the project is the synthesis of polyimines and polyazines with long aliphatic side-chains that selectively assemble in organized monolayers on graphene. For this purpose monomers have been synthesized and the reaction conditions optimized. Conditions optimization and proof-of-principle experiments have been performed with commercial analogues. The polymers have been deposited on graphene by spin- and dip-coating and then compared with layers polymerized directly on the surface (on-surface reaction). Using photolithography, patterned graphene has been prepared and used as a confined 2D space in which the polymerization can take place. Setting the spatial boundaries should promote directionality of the polymerization and thus lead to maximally ordered polymers on the surface with periodic assembly over a long distance, similarly to the small molecule physisorption on graphite governed by the free energy of adsorption, i.e. both the adsorption enthalpy and entropy loss on adsorption.[5]

References:

1 Hauer, C. R.; King, G. S.; McCool, E. L.; Euler, W. B.; Ferrara, J. D.; Youngs, W. J. *J. Am. Chem. Soc*. **1987**, *109*(19), 5760-5765.

2 Fallahi, A.; Alahbakhshi, M.; Mohajerani, E.; Afshar Taromi, F.; Mohebbi, A. R.; Shahinpoor, M. *J. Phys. Chem. C.* **2015**, *119*(23), 13144-13152.

3 Rowan, S. J.; Cantrill, S. J.; Cousins, G. R. L.; Sanders, J. K. M.; Stoddart, J. F. *Angew. Chem. Int. Ed.* **2002**, *41* (6), 898–952.

4 Belowich, M. E.; Stoddart, J. F. *Chem. Soc. Rev.* **2012**, *41* (6), 2003–2024.

5 Ciesielski, A.; El Garah, M.; Haar, S.; Kovaříček, P.; Lehn, J.-M.; Samorì, P. *Nat. Chem.* **2014**, *6* (11), 1017–1023.

ENTANGLEMENT-BASED METHODS IN COMPUTATIONAL QUANTUM CHEMISTRY

Mgr. Jan Brandejs

RNDr. Libor Veis, Ph.D.

Concepts of the quantum information theory (QIT) like *mutual information*, *entanglement entropy* and *Schmidt decomposition* have proven themselves powerful tools for the treatment of strongly correlated (multi-reference) systems. These terms form the basis of entanglement-based tensor network approaches, one of those being the famous *density matrix renormalization group* (DMRG) method.

In the first part of my talk, I will show how can the “clever” manipulation of entanglement help to boost the performance of the quantum chemical DMRG method through the underlying *local basis optimization* [1]. Results on extended systems (graphene nanoribbons) as well as transition metal complexes will be presented.

Secondly, I will talk about the entanglement analysis of a chemical bond, another promising application of QIT [2]. Entanglement measures in fact allow us to describe the nature of complex chemical bonds where nontrivial quantum phenomena play an essential role, such as the electron-deficient bonds. Our most recent focus was on neutral zero-valent s-block complexes with strong multiple bonding, with electron-deficient bond between C-Be-C atoms [3]. Last but not least, I will also mention an application in solid state physics, namely the SU(4) Hubbard model [4].

References:

[1] C. Krumnow, L. Veis, Ö. Legeza, and J. Eisert; Fermionic orbital optimisation in tensor network states, *Phys. Rev. Lett.* **2016** *117*, 210402.

[2] S. Szalay, G. Barcza, T. Szilvási, L. Veis, and Ö. Legeza; The correlation theory of the chemical bond, *arxiv:1605.06919*

[3] M. Arrowsmith, H. Braunschweig et. Al.; Neutral zero-valent s-block complexes with strong multiple bonding, *Nature Chemistry.* **2016**, 8, 890–894.

[4] G. Barcza, R. M. Noack, J. Sólyom, and Ö. Legeza; Entanglement patterns and generalized correlation functions in quantum many-body systems, *Phys. Rev. B.* **2015**, *92*, 125140.

TOWARDS QUARTZ ENHANCED PHOTOACOUSTIC SPECTROSCOPY OF ACETONITRILE

Ing. Michal Dostál

prof. Ing. Zdeněk Zelinger, CSc.

Methyl cyanide (acetonitrile, CH_3CN) is strongly prolate (A>>B) symmetric top molecule, which has been a subject of numerous spectroscopic studies. From the practical point of view this molecule is of importance as a marker of explosive compounds such as trinitrotoluene (TNT) and hexogen (RDX)[1], or it can be released into the atmosphere during combustion of biomass[2].

Previously, relatively long absorption pass (employing multi-reflection or cavity-enhanced setup) were used for recording infrared CH_3CN spectra thus limiting implementation for gas sensing applications[3].

Quartz enhanced photoacoustic spectroscopy (QEPAS) enables rapid and highly sensitive detection of trace gas concentrations, when using quartz tuning fork (QTF) with a high Q-factor[4]. Tunable quantum cascade laser (QCL) covering several acetonitrile rovibrational lines around 936 cm^{-1} was employed in this study as an excitation source for QEPAS analysis.

Recent progress in QCL-QEPAS setup development as performed in our lab is reported here. Firstly, resonant frequencies of low-cost commercially available tuning forks and their response to external sound waves were determined. Beam profile of the QCL was optimized using appropriate infrared focusing optics. Furthermore, QEPAS cell design and construction was modified in order to minimize the free volume of gas sample within the cell thus to limit the radiation loss due to absorption along the optical path. It can be concluded, that feasible parameters of the QCL-QEPAS setup were achieved promising for gas-phase acetonitrile detection at trace levels.

References:

[1] T. Osborn, S. Kaimal, W. Burns, A.R. Ford, S.W. Reeve, Spectral signatures for volatile impurities in TNT and RDX based explosives, (n.d.). doi:10.1117/12.777844.

[2] R. Holzinger, J. Williams, G. Salisbury, T. Kï Upfel, M. De Reus, M. Traub, P.J. Crutzen, J. Lelieveld, Oxygenated compounds in aged biomass burning plumes over the Eastern Mediterranean: evidence for strong secondary production of methanol and acetone, Atmos. Chem. Phys. 5 (2005) 39–46. www.atmos-chem-phys.org/acp/5/39/ (accessed April 18, 2017).

[3] H.S.P. Müller, B.J. Drouin, J.C. Pearson, Rotational spectra of isotopic species of methyl cyanide, CH 3 CN, in their ground vibrational states up to terahertz frequencies, A&A. 506 (2009) 1487–1499. doi:10.1051/0004-6361/200912932.

[4] A.A. Kosterev, Y.A. Bakhirkin, R.F. Curl, F.K. Tittel, Quartz-enhanced photoacoustic spectroscopy, Opt. Lett. 27 (2002) 1902. doi:10.1364/OL.27.001902.

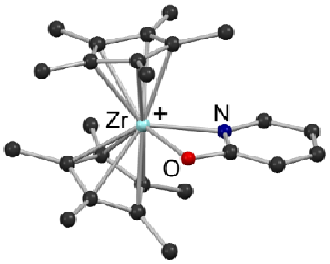
KATIONTOVÉ ORGANOKOVOVÉ KOMPLEXY JAKO PREKURZORY REAKTIVNÍCH LEWISOVSKÝCH PÁRŮ

David Dunlop

RNDr. Martin Lamač Ph.D.

Koncept frustrovaných Lewisovských párů byl popsán na systémech obsahujících boranovou skupinu $–B(C_6F_5)_2$ a stericky náročnou fosfinovou skupinu. Hlavním poznatkem byla schopnost systému reverzibilně aktivovat molekulu vodíku, která byla dosud pro prvky hlavních skupin nevídaná.[1] Bráněná tvorba aduktu kyselina-báze umožňuje i aktivaci řady dalších substrátů, zejména malých molekul, například CO, NO a CO_2, ale i vazeb C-O cyklických etherů, B-H vazeb boranů, či C=C vazeb nenasycených uhlovodíků.[2] Koncept byl dále rozšířen za využití rozmanitých kombinací bází a kyselin, mimo jiné také komplexů přechodných kovů.[3,4]

V současné době se zabýváme přípravou intra- i intermolekulárních systémů Lewisovských párů obsahujících kationtové metalocenové komplexy prvků 3. a 4. skupiny, jmenovitě Y, Zr a Hf, a studiem jejich reaktivity. Coby báze byly v případě Zr a Hf využity deriváty pyridinu (viz obrázek), pro Y rozmanitě substituované fosfiny. Reaktivita charakteristická pro FLP byla prozatím pozorována u aduktu yttrocenium-fosfin, kdy docházelo např. k aktivaci C-Cl vazeb či inzerci CO_2. V současnosti se pokoušíme izolovat a charakterizovat produkty reakcí studovaných systémů s dalšími substráty.



Tato práce vzniká s podporou GAČR (č. grantu 17-05838S).

Zdroje:

1. Welch G. C., Juan R. R. S., Mazura J. D., Stephan D. W.: *Science* **2006**, *314*, 1124

2. Review: Stephan D. W., Erker G.: *Angew. Chem. Int. Ed.* **2015**, *54*, 6400

3. Xu X., Kehr G., Daniliuc C. G., Erker G.: *J. Am. Chem. Soc.* **2011**, *133*, 18463

4. Flynn S. F., Metters O. J., Manners L., Wass D. F.: *Organometallics* **2016**, *35*, 847

SELECTIVE GROWTH OF HYBRID PEROVSKITES ON GRAPHENE

Valentino Libero Pio Guerra

RNDr. Ing. Martin Kalbáč, Ph. D.

Perovskite materials came into focus of investigation for electroluminescence application due to their low trap density, high charge mobility, narrow photoluminescence emission and adjustable band-gap.[1,2] To meet the potential, methods and protocols for optimization of critical features and parameters need to be developed specifically involving the increase of radiative recombination efficiency, spatially resolved patterning and electrical contacts fabrication. The intrinsic HPs low exciton binding energy represents a great advantage for PV applications but it could be a serious limitation for the achievement of high EL efficiencies in LEDs. In fact, the reported values of a few meV for $MAPbI_3$ could hinder radiative recombination of loosely bound charges populating the active layer, even though a low exciton binding energy promotes a good charge transport through the film, a further fundamental condition for efficient light emitting devices. To solve the issue, excitons could be spatially confined by reducing the dimensionality of the materials forcing holes and electrons to recombine in a highly efficient radiative process. Layered perovskites, in fact, show very large exciton binding energies (above hundreds of meV)**Chyba! Záložka není definována.** originating from the very different dielectric constant between the two counterparts and from the reduced symmetry.

During the part of my PhD here in Prague, 2D layered halide perovskite as highly luminescent materials were designed and synthesized, foreseeing future applications in LED. In this lecture, a process of selective perovskite growth on graphene serving as contacting electrodes is described. Investigating a series of 2D layered hybrid organic halide perovskites, a non-covalent graphene functionalization has been found to provide high selectivity and spatial resolution of the perovskite film formation.

References:

[1] Filip, M. R., Eperon, G. E., Snaith, H. J. & Giustino, F. “Steric engineering of metal-halide perovskites with tunable optical band gaps”, *Nat. Commun.*, **2014**, 5, 5757.

[2] S. Colella, M. Mazzeo, A. Rizzo, G. Gigli, and A. Listorti ,“The Bright Side of Perovskites,” *J. Phys. Chem. Lett.*, **2016**, 7 (21), pp 4322–4334.

HOLLOW FIBRE LIQUID-PHASE MICROEXTRACTION OF CATECHOLAMINE BASED BIOMARKERS

Mgr. Vojtěch Hrdlička

Doc. Dr. Ing. Tomáš Navrátil

Catecholamine metabolites, in particular homovanillic acid (HVA) and vanillylmandelic (VMA) are widely used biomarkers either for various oncological, metabolic and neurological disorders, either for monitoring of treatment or as a tool for pre-emptive screening tests.

Three phase liquid/liquid/liquid microextraction with porous polypropylene as a liquid membrane carrier was used for preconcentration of HVA and VMA. Both HVA and VMA were extracted from acidic donor solution to basic acceptor solution through the water-immiscible liquid membranes. Following liquid-membranes were tested: dodecane, phenyldecane, 1-octanole, dihexyl ethere, isoamyl benzoate and propyl benzoate. Highest enrichment factors obtained after 30 minutes of extraction were 30 for HVA using 1-octanole and 2.6 for VMA using propyl benzoate.

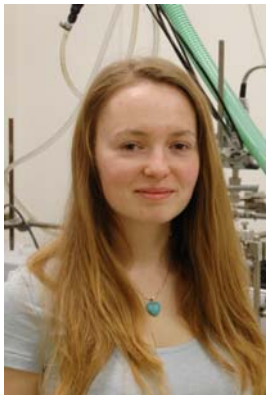
For determination of HVA and VMA in a 10 µl hollow-fibre extract, cathodically pretreated boron doped diamond electrode was used, with LOD = 1.2 µmol/l and standard error of 5.9% (n=10) in a miniaturized three-electrode arrangement. Using this method, HVA and VMA can be determined simultaneously, even in the presence of uric and ascorbic acid.

References:

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

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

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



TERMOLÝZA FORMAMIDU V PŘÍTOMNOSTI JÍLŮ: VZNIK NUKLEOVÝCH BÁZÍ A DALŠÍCH STAVEBNÍCH KAMENŮ ŽIVOTA

Jana Hrnčířová

RNDr. Martin Ferus, Ph.D

Otázkou původu života na zemi či ve vesmíru se lidstvo zabývá již od nepaměti. Na počátku dvacátého století nahradila metafyzický přístup vysvětlující Božím zásahem vznik života i základních stavebních kamenů biogenních látek, jako jsou aminokyseliny, báze a cukry, Oparinova teorie o syntéze těchto chemikálií z abiogenní směsi molekulárních plynů a následné formování živých struktur v tzv. koacervátech.[1] Syntézu aminokyselin následně potvrdily experimenty Millera a Ureye, [2] některé nukleové báze byly připraveny např. v experimentech Ferrise a Oróa.[3] Zejména téma jednoduchého vzniku nukleových bází se stalo základním rozporem mezi představami evolučních a molekulárních biologů a chemiků. Z biologického pohledu se zdá vysoce pravděpodobné, že prvotní živé struktury byly založeny na sebereplikující entitě ribonukleové kyseliny (RNA). Z chemického hlediska se však jevila syntéza nukleových bází značně problematická, takže favorizovány byly modely živých struktur založené na aminokyselinách. To však odporuje základnímu dogmatu molekulární biologie, které postuluje výhradně jednosměrnou transkripci sekvence bází nukleové kyseliny do sekvence aminokyselin. V našich experimentech navazujeme na představu jednoduchého vzniku nukleových bází z molekuly formamidu za prebiotických podmínek. Směs formamidu s různými druhy všudypřítomných minerálů, v tomto případě řady jílů, byla vystavena teplotě 160^{o} C v přítomnosti hoblin železného meteoritu. Cílem bylo zjistit, zda železný meteorit, jemuž jsou v pracích biochemika Sutherlanda[4] přisuzovány významné pozitivní účinky na vznik nukleových bází, nemá spíše opačný efekt pozorovaný v celé řadě našich předchozích prací. Ukázalo se, že meteorit skutečně spíše potlačuje vznik základních biomolekul. Nicméně jestliže je železo interkalováno v jílu, výtěžnost reakcí roste. Lze předpokládat, že pakliže bylo prostředí rané Země bohaté na železo, které bylo působením eroze interkalováno do porézních materiálů (tak jako je to např. v případě dnešního Marsu), mohly být katalytickým účinkem takových minerálů zefektivněny syntetické reakce vedoucí ke vzniku nukleových bází. Tyto pochody mohly být prvním krokem při tvorbě složitějších biogenních látek, nezbytných pro samotný vznik života na naší planetě. To se možná také stalo na povrchu železných jílů.

References:

[1] Oparin A.I.: Произхождение жизни. M. Московский рабочий, Москва 1924. Vyšlo v nakladatelství Naše vojsko, titul Vznik a vývoj života, Praha 1950, překlad Karel Pátek.
[2] Miller, S. L.; Urey, H. C. *Science* **1959**, 3370, 245
[3] McCollom: Miller-Urey and beyond... *Annu.Rev.Earth.Planet.Sci.* **2013**, 41, 207.
[4] Sutherland, J.: The Origin of Life-Out of Blue. *Angew.Chem.* **2016**, 55, 104.

DISSOCIATIVE RECOMBINATION OF H_2^+ : A COMPARISON OF THEORETICAL METHODS

Mgr. Dávid Hvizdoš

Mgr. Roman Čurík, Ph.D.

Dissociative recombination (DR) - the neutralization of molecular ions by interaction with electrons followed by dissociative breakup – is a very important but complicated process of molecular plasma dynamics. Due to the presence of a long-range coulombic interaction, exact models of this phenomenon are quite hard to work with, so when calculating DR cross sections, approximative methods are used instead and exact results exist for only a handful of the simplest cases.

One such approximative approach is to take the well-established frame transformation [1] method commonly used to model rovibrationally inelastic collisions of electrons with neutral molecules and adapt it to the case of DR. This has been done for the case of H_2^+, H_3^+, LiH^+, HeH^+, NO_2^+ and $LiHe^+$, using Siegert states for the nuclear vibrational basis. All the previous studies that employ this method use several non-trivial intuitive or ad-hoc assumptions to obtain their final results and the validity of their use could be called into question. The goal of the present project is to provide theoretical and numerical evidence confirming or disproving these assumptions. In my lecture I will present how the results of the aforementioned approximative method hold up when compared with results from an exact model [2].

References:

[1] E.S. Chang and U. Fano. Theory of electron-molecule collisions by frame transformations. Physical Review A, 6(1):173–185, 1972.

[2] K Houfek, TN Rescigno, and CW McCurdy. Numerically solvable model for resonant collisions ofelectrons with diatomic molecules. Physical Review A, 73(3), MAR 2006.

NEURODEGENERATIVE AMYLOIDOSES AND PROTEIN-MEMBRANE INTERACTIONS: MOLECULAR INSIGHTS INTO MEMBRANE MEDIATED PROTEIN OLIGOMERISATIONIONS

Mgr. Eduard Ješko

Prof. Martin Hof, Dr. DSc.

Aberrant aggregation of amyloidogenic proteins is implicated in the onset and progression of the neurodegenerative Alzheimer's (AD), Parkinson's and Prion diseases. The molecular factors responsible for these incurable diseases are largely unknown. Several theories propose links between disease development and membrane interactions of amyloidogenic proteins. Characterisation of these protein/membrane interactions and the understanding of their biological significance is still incomplete.

Our work focuses on obtaining molecular insights regarding the interaction of amyloidogenic proteins and membranes, and the catalysis of oligomerisation. Particular aspects under study will be the influence of gangliosides sugar chemistry and sphingomyelin derivatives on the interaction with amyloid proteins (beta-amyloid, Prion protein) and the characterisation of the formed oligomeric structures. The experimental work is performed on model membrane systems using state-of-the-art advanced fluorescence spectroscopy and microscopy at the single molecule level.

In my lecture mainly an introduction to this topic will be presented.

References:

[1] M. Amaro, R. Sachl, G. Aydogan, I. I. Mikhalyov, R. Vácha, and M. Hof, "GM1 Ganglioside Inhibits β-Amyloid Oligomerization Induced by Sphingomyelin," Angew. Chemie Int. Ed.,vol. 55, no. 32, pp. 9411–9415, Aug. **2016**.

[2] K. L. Viola and W. L. Klein, "Amyloid β oligomers in Alzheimer's disease pathogenesis, treatment, and diagnosis," Acta Neuropathol., vol. 129, no. 2, pp. 183–206, Feb. **2015**.

[3] K. Yanagisawa, "GM1 ganglioside and Alzheimer's disease," Glycoconj. J., vol. 32, no. 3–4,pp. 87–91, May **2015**.

[4] G. Wu, Z.-H. Lu, N. Kulkarni, and R. W. Ledeen, "Deficiency of ganglioside GM1 correlates with Parkinson's disease in mice and humans.," J. Neurosci. Res., vol. 90, no. 10, pp.1997–2008, **2012**.

[5] N. Sanghera, B. E. F. S. Correia, J. R. S. Correia, C. Ludwig, S. Agarwal, H. K. Nakamura, K. Kuwata, E. Samain, A. C. Gill, B. B. Bonev, and T. J. T. Pinheiro, "Deciphering the molecular details for the binding of the prion protein to main ganglioside GM1 of neuronal membranes.," Chem. Biol., vol. 18, no. 11, pp. 1422–31, Nov. **2011**.

HOW DOES POST-SYNTHESIS INCORPORATION OF ALUMINUM PROCEED IN UOV GERMANOSILICATE FRAMEWORK?

Mgr. Valeryia Kasneryk

Dr. Maksym Opanasenko

Zeolites are microporous materials with well-defined structure formed by TO_4 tetrahedra (where T=Si, Al, Ge, etc). These materials are widely applied in heterogeneous catalysis, adsorption and separation. At the present time, germanosilicate class of zeolites attracted a lot of attention because of their unique structure properties. Their frameworks can be described as Si-rich layers connected by double four rings (D4Rs) preferentially occupied by Ge atoms. This phenomenon in combination with hydrolytic instability of Si–O–Ge and Ge–O–Ge bonds was perfectly exploited for formation of transport pores in the frameworks [1]. Moreover, the germanium leaching combined with incorporation of aluminum can be used for that purpose, which can allow not only to form mesopores but also to generate acid centers in germanosilicates.

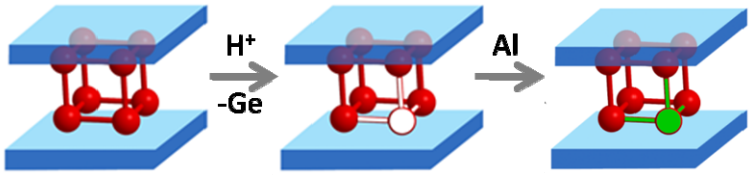


Fig. 1. Scheme of two-step alumination process

We studied the influence of conditions of post-synthesis alumination (temperature and duration) and the chemical composition of parent germanosilicate zeolite UOV on textural and acidic properties. Treatment of UOV (Si/Ge = 0.5-1.5) zeolites with aqueous $Al(NO_3)_3$ solution led to the formation of both strong Brønsted and Lewis acid sites and an increasing fraction of micro- and mesopores in framework. Investigation of the time effect showed multi-stage of the process of alumination (Fig.1). Thus, at the first step of alumination we observed the acidic hydrolysis of Ge-rich D4Rs and leaching of Ge from the framework. And with prolongation of the experiment time Al atoms get into the zeolite pores and start to incorporate and heal up the defects formed at the beginning. The increasing temperature of alumination from 80 to 175 °C resulted in a slight increase in the concentration of acid sites formed for both Si-rich and Si-poor samples.

References:

1. Kasneryk V. I.; Shamzhy M. V.; Opanasenko M. V.; Čejka J. J., *J. Energy Chem*. **2016**, *25*, Issue 2, 318-326.

PHOTOCATALYTIC TRANSFORMATION OF PLANETARY ATMOSPHERES IN CONNECTION TO EXOPLANETS, MARS AND EARLY EARTH

Bc. Antonín Knížek

RNDr. Martin Ferus,, Ph.D.
Prof. RNDr. Svatopluk Civiš, CSc.

We have explored significance of carbon dioxide photocatalytic reduction to methane and carbon monoxide for the chemistry of planetary atmospheres. In particular, we have focused on the formation of methane on Mars and under conditions of early Earth.

Photoinduced synthesis of methane and carbon monoxide has been studied over acidic anatase and montmorillonite surfaces upon 365 nm UV irradiation. This photocatalytic experiment grossly represents the Martian atmosphere. Reaction kinetics of the process has been monitored by means of high-resolution infrared spectroscopy and the rate constants, external quantum efficiencies and effectiveness of the reduction process were compared with the seasonal variation of methane in the Martian atmosphere. This comparison provides a clue for the possible mechanism of abiotic methane production on the surface on the Red planet.

This reduction may also help understand the atmospheric reprocessing on early Earth and contribute to the discussion on the reduction/oxidation state of the initial atmosphere. Also, a model mixture of a planetary atmosphere obtained in such way may be reprocessed in the likeness of the Miller Urey experiment in electric discharge or laser shock wave plasma. Using gas chromatography-mass spectrometry after derivatization of the samples, nucleic acid bases have been detected in experiments simulating impact shock wave reprocessing of CO-CH_4-N_2 atmosphere over acidic montmorillonite and anatase. In conclusion, we reconstructed a complete pathway leading from a neutral carbon dioxide rich atmosphere (produced for instance by regular volcanic outgassing) via reactive reduced gases (CH_4 + CO + N_2 or NH_3) to fundamental building blocks of the RNA-World, i.e. to nucleobases, but also to glycine and urea. Furthermore, we have demonstrated that such chemistry leading to the synthesis of nucleobases can be observed in the famous Miller-Urey experiment, which pioneered modern research on the molecular origins of life. The actual relevance of the original research in this field was later questioned, because the gas mixture used in their research was considered too reducing and nucleases have not yet been observed among products. We show here that not only can the atmosphere be transformed, but also that nucleic acid bases can be detected, when modern day sensitive analytical techniques are employed.

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

Mgr. Věra Křížová

Mgr. Miroslav Polášek, Ph.D.

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

In this study the effects of mass, charge and chemical structure of a projectile ion on the ionization cross section and the amount of internal energy deposited in nascent secondary ions are investigated using a modified sector type mass spectrometer.

The modifications include collision chamber and quadrupole mass analyzer which is to analyze secondary ions stemming from the collisions of projectiles with neutrals. Pressure inside the collision chamber, as well as projectile ion current, are measured absolutely so that we are able to determine collision cross sections for given processes from the secondary ion count rates. The amount of internal energy deposited in secondary ions, as reflected by the extent of their fragmentation, is determined from the acquired mass spectra. Some general trends and selected specific results will be presented.

References:

[1] G. G. Gomez-Tejedor and M. C. Fuss, *Radiation damage in biomolecular systems* (Springer, New York, 2012).

[2] J. Postma, S. Bari, R. Hoekstra, A. G. G. M. Tielens, and T. Schlathölter *ApJ* 2010, **708,** 435-444.

[3] V. Vuitton, R. V. Yelle, and M. J. McEwan, *Icarus* 2007, **191**, 722 – 742.

USS CORRECTED MRCC-LPNO STUDY OF CYCLOPROPANE ISOMERIZATION

Mgr. Jakub Lang

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

The single reference coupled cluster (CC) method is one of the most popular methods in quantum chemistry, however its description of systems with a large amount of static correlation is rather poor. For example black box coupled cluster methods such as CCSD and CCSD(T) are unable to properly calculate a trimethylene state created during cyclopropare ring opening which exhibits multireference character. It still has not been concluded whether the ground state is singlet or triplet[1]. In these cases, use of multireference methods, which correctly describe static correlation, is necessary [2].

Unfortunately, some state specific MRCC methods are not size-extensive and to accurately describe the correlation energy a posteriori correction has to be introduced. Until now, such method was Hubac correction for BW-MRCCSD [2]. Recently introduced Universal State Specific (USS) and its diagonal part (USS-D) correction is able to correct this error [3]. Furthermore, the USS correction is able to improve calculated correlation energies of other MRCC methods as well [3].

Yet, all these canonical methods are not feasible for large scale computations of big systems. For example, the scaling of CCSD(T) method is N^7, where N is number of orbitals. Due to this, better scaling is highly desired. One of the newest approaches which are able to scale almost linearly is Local Pair Natural Orbitals method. With this method, we are able to calculate systems as large as carotene with an unparalleled precision [4].

In my lecture, I will present multireference calculations of these two systems and effect of USS correction on canonical and LPNO methods [5].

References:

[1] Kinal, A.;Piecuch, P.; *J. Phys. Chem. A* **2007**, *111, 734-742.*
[2] *Pittner, J. ; J. Chem. Phys.* ***2003****, 118, 10876.*
[3] Brabec, J.; van Dam, H. J. J.;Pittner, J.; Kowalski, K.; *J. Chem. Phys.* **2012**, *136*, 124102.
[4] Demel, O.;Pittner, J.; *J. Chem. Phys.* **2015**, 11, 3104-3114.
[5] Lang. J.; Svana. M.; et al.; *Mol. Phys.* **2017** (accepted for publication).

DETERMINATION OF NICKEL SPECIES IN FERRIERITES USING FTIR AND UV-VIS SPECTROSCOPY

Mariia Lemishka

RNDr. Jiří Dědeček, DSc.

Zeolites, a class of microporous crystalline aluminosilicate materials, are widely used in many industrial applications related to catalysis, adsorption and separation due to their high thermal/hydrothermal stability, strong acidity, well-defined microporosity and shape selectivity[1]. Zeolites exchanged with transition metal ions provide active sites for catalysing a variety of important reactions, particularly redox catalysis. It has recently been shown that ferrierite is a highly active catalyst for important reactions, especially in its H-form for the isomerisation of n-butene to isobutene, and in its transition metal cation-exchanged forms (Co^{2+}, Mn^{2+}, Ni^{2+}) for the abatement of N_2O and NO_x with hydrocarbons[2]. Among the factors controlling catalytic activity, a fundamental role is played not only by the zeolite topology, but also by the type of cation, its location and coordination[3]. The essential role of cations in above reactions is connected with this location, siting, coordination and distances in zeolite frameworks.

Nickel-exchanged ferrierites were prepared by ion exchange NH_4-FER (Si/Al 8.5) with aqueous $Ni(NO_3)_2*6H_2O$ solutions. The serie of Ni-FERs with Ni loading ranging form 0.5 to 2.0 wt. % was prepared to check the influence of Ni content on the formation of various Ni species in FER. The structural analysis of Ni-FER was performed using UV-Vis, FTIR spectroscopies.

Concluding, the combination of UV-Vis and FTIR spectra of skeletal vibrations can provide information on the type of Ni species in FER and can serve as a base for characterization of Ni^{2+} in other Si-rich zeolites.

References:

[1]Teng Xue, Huaping Liu, Yi Meng Wang. RSC Adv. **2015**, 5, 12131-12138.

[2] Dalconi, M. C.; Cruciani, G.; Alberti, A.; Ciambelli, P.; Rapacciuolo, M. T. Micropor. Mesopor. Mat. **2000**, 39, 423-430.

[3] Sobalik Z.; Tvaruzkova Z.; Wichterlova B. J. Phys. Chem. **1998**, 102, 1077-1085.

STEREOELECTROCHEMISTRY OF CALIXARENES

Mgr. Alan Liška

prof. RNDr. Jiří Ludvík, CSc.

Calixarene skeleton is a stable framework, very popular in nowadays supramolecular chemistry [1], which is, however, electrochemically inactive. For this reason, a suitable substituent ("redox probe") must be introduced in order to enable studying the system by means of electrochemical methods.

Whereas the determination of the molecular structure in solid phase can be perfectly accomplished using x-ray structure analysis, the shape, conformation, dynamic behavior and other structure parameters of molecules in solution is difficult to study. Calixarenes have complicated structure with many degrees of freedom. Nevertheless, detailed interpretation of electrochemical data appeared to be a useful and novel approach to experimental investigations of actual 3D characteristics of calixarenes in solution. Until now, relationships between the structural types / parameters listed below and the corresponding electrochemical responses have been studied and formulated - "stereoelectrochemistry":

a) the conformation: *cone-* / *paco-* / *1,2- and 1,3-alt-* [2,3];
b) type of bridging units: methylene / thia / oxa / sulphone [4];
c) type of the redox probe: nitro / nitroso / carbonyl (aldehydic and ketonic) / oxime / nitrile / sulphonyl / ferrocenyl [2-5];
d) position of the redox probe(s), their mutual intramolecular interactions [2-4,6]:
    i) upper rim / lower rim / both rims,
    ii) *para-* / *meta-* / both (with respect to the lower rim substitution),
    iii) on the adjacent/opposite benzene rings (in polysubstituted compounds)
e) rigidity / flexibility of the molecule in solution [2-4];
f) character and reactivity of the radical intermediates, their spin state [6];
g) complexation abilities towards ions in solution.

Acknowledgements:
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References:

[1] Flídrová K, Liška A, Ludvík J, Eigner V, Lhoták P: Tetrahedron Letters *56* (2015), 1535-1538.
[2] Ludvík J, Liška A, Lhoták P: ECS Transactions *66* (2015), 26, 23-31.
[3] Liška A, Flídrová K, Lhoták P, Ludvík J: Monatshefte für Chemie-Chemical Monthly *146* (2015), 857-862.
[4] Liška A, Lhoták P, Ludvík J: Electroanalysis *28* (2016), 2861-2865.
[5] Liška A, Ludvík J: Chem Listy *104* (2010), 23-26.
[6] Liška A, Vojtíšek P, Fry AJ, Ludvík J: J. Org. Chem. *78* (2013), 10651-10656.
[7] Liška A, Rosenkranz M, Klíma J, Dunsch L, Lhoták P, Ludvík J: Electrochim Acta *140* (2014), 572-578.

OPTIMIZATION OF CONDITIONS FOR VOLTAMMETRIC DETECTION OF TUMOR BIOMARKER 5-HYDROXYINDOLE-3-ACETIC ACID USING FLOW INJECTION ANALYSIS

Mgr. Anna Makrlíková

Doc. Dr. Ing. Tomáš Navrátil

Determination of tumor biomarkers can predict some diseases and help start treatment in time or follow-up patients with these diseases. One of the tumor biomarkers is 5-hydroxyindole-3-acetic acid (5-HIAA), excreted in urine [1]. 5-HIAA is the metabolite of serotonin, neurotransmitter implicated in physiological processes and involved in sleep pattern regulation, behavioral and appetite control [2].The normal urinary concentrations of 5-HIAA are from 17.8 to 58.3 $\mu mol \cdot l^{-1}$ [3], quite different level in biological fluids indicates carcinoid tumors diagnose, hypertension, depression, migraine, and Tourette syndrome [4]. In clinical laboratories, 5-HIAA is usually determined by GC (MS) and HPLC with various types of detection [5].

Due to phenolic structure, 5-HIAA can be oxidized at carbon electrodes. In this work, determination of 5-HIAA was performed at screen-printed carbon electrodes (SPCEs) using flow injection analysis (FIA) with amperometric detection. Apparatus for FIA was composed of syringe pump, injection valve with 20 µl injection loop, flow cell (flow-cell in Teflon for screen-printed electrodes FLWCL-TEF, DropSens, Spain), and computer-controlled potentiostat PalmSens3. Used SPCEs (type DRP-110, DropSens, Spain) consist of carbon working electrode (4 mm diameter), carbon counter electrode, and silver reference electrode.

Calibration dependences were linear in the concentration range of 0.05 to 100 $\mu mol \cdot l^{-1}$ and the obtained limits of detection (*LOD*s) were 0.033 $\mu mol \cdot l^{-1}$ (calculated from peak heights) and 0.012 $\mu mol \cdot l^{-1}$ (calculated from peak areas).

References:

[1] Jong W. H. A.; Vries E. G. E.; Kema I. P. *Clin. Biochem.* **2011**, *44*, 95-103.
[2] Kema I. P.; Vries E. G. E.; Muskiet F. A. J. *J. Chromatogr. B* **2000**, *747*, 33-48.
[3] García A.; Heinänen M.; Jiménez L. M.; Barbas C. *J. Chromatogr. A* **2000**, *871*, 341-350.
[4] Yoshitake T.; Iizuka R.; Fujino K.; Inoue O.; Yamagata K.; Nohta H.; Yamaguchi M. *Anal. Sci.* **2004**, *20*, 1687-1690.
[5] Lionetto L.; Lostia A. M.; Stigliano A.; Cardelli P.; Simmaco M. *Clin. Chim. Acta* **2008**, *398*, 53-56.

Acknowledgements:
The research was financially supported by the GAUK (Project GAUK734216) and by Czech Science Foundation (GA ČR No. 17-03868S).

SIMULATION OF ABSORBTION AND EMISSION SPECTRA OF LAURDAN IN PHOSPHOLIPID LAYER SYSTEMS

Mgr. Wasif Baig Mirza

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

Fluorescent and absorption spectra of fluorescent dye LAURDAN (6-Dodecanoyl-2-Dimethylaminonaphthalene), in two phospholipid layer systems i.e. DOPC and DPPC are studied by means of excited state molecular dynamics simulations employing a quantum mechanical and molecular mechanical approach with the time-dependent density functional theory (TD-DFT QM/MM MD). The best correspondence with the experimental absorption spectra spectrum was achieved by average of different conformers of laurdan interacting with polar and nonpolar phase of the membranes. On the other, for emission spectra conformers of laurdan with specific orientation and location in the membrane gives best agreement with the experiment.

References:

[1] Parasassi, T.; Gratton E.; Levi M. J. Biophys. 1997, 72, 2413–2429.

EFFECT OF TiO_2 (ANATASE) SURFACE STRUCTURE ON SELECTIVITY OF PHOTO-ELECTROCHEMICAL WATER OXIDATION

Ing. Roman Nebel

Doc. Ing. Petr Krtil, CSc.

The photo-electrochemical water splitting research is focused on finding efficient catalysts for direct conversion of solar energy into energy storing pchemical (e.g. hydrogen or hydrocarbon). Oxygen evolution reaction is in the context of water oxidation the kinetically limiting step due to its sluggish kinetics. Achieving a fundamental understanding of photoelectrochemical anodic reactions on illuminated stable semiconductors and namely on TiO_2 polymorphs opens a way to theoretically pre-select structures that may act efficiently in the water oxidation and, consequently, be a subject of targeted synthesis.

The presentation will cover the behavior of three types of nanocrystalline TiO_2 - anatase dominated by {110}, {101} and {001} surface orientation in photo(electro) catalytical oxygen evolution reaction. Photo-electrochemical experiments were carried out in chronoamperometric mode in argon and oxygen saturated perchloric acid solution using the differential electrochemical mass spectroscopy (DEMS) technique for online quantitative determination of the reaction products.

The difference in surface structures leads to pronounced variability in selectivity of the illuminated anatase electrodes. The OER activity increases in the order: {101} < {110} < {001}. The relative amount of oxygen normalized by the passed charge varies significantly depending on the surface structure. The comparison of reactivity of anatase facets revealed that: a) {101} accommodates additional anodic reactions causing a decrease in oxygen yield, b) material with {110} faces may serve for conventional OER, c) on {001} oriented surface the OER is favored the most. The results can be extended to rationally design photocatalysts towards efficient photoelectrochemical water splitting.

References:

Minhová-Macounová, K.; et. al. The J. Phys. Chem. C. **2017**, *121(11)*, 6024-6032.

STUDY OF METABOLISM OF SYNTHETIC CANNABINOIDS. OPTIMIZATION OF METHODS FOR TOXICOLOGICAL DETECTION

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Marijuana is one of the most widely used illicit drug in the world. Due to its ilegal status the popularity of using synthetic cannabinoids is growing. These synthetic analogues mimic the psychoactive effect of cannabis and avoid positive outcome on the current screening tests for THC. The risk of these substances lie in impossibility of the detection, easily accessibility *via* the Internet without any restriction and insufficient knowledge about their potency and adverse effects. These facts lead to the necessity of developing new diagnostic method to reveal the consumption of these substances for clinical and forensis purpose [1].

The main goal of this work is the development of a reliable *in vitro* method for the rapid identification of characteristic metabolites of synthetic cannabinoids. It consist of electrochemical generation and evaluation of metabolites combined with MS methods [2], production of metabolites using human liver microsomes with advanced UPLC-MS/MS and UPLC-HRMS methods [3].

In present study I would like to introduce the first step of my study which is characteristic fragmentation of standards of synthetic cannabinoids and determination of optimal conditions for their detection using MS/MS method.

References:

[1] Gurney S. M., Scott K.S., Kacinko S. L., Presley B. C., Logan B. K.: *Pharmacology, Toxicology, and Adverse Effects of Synthetic Cannabinoid Drugs*. Forensic Sci Rev. 2014 Jan;26(1):53-78.

[2] Gul T., Bischoff R., Permentier H.P.: *Electrosynthesis methods and approaches for the preparative production of metabolites from parent drugs*. TrAC - Trends in Analytical Chemistry 2015 70 (58-66)

[3] Sobolevsky T., Prasolov I., Rodchenkov G.: *Study on the phase I metabolism of novel synthetic cannabinoids, APICA and its fluorinated analogue*. Drug Testing and Analysis 2015 7:2 (131-142)

A STUDY ON SYNTHESIS OF BIOGENIC MOLECULES FORMATION BY THE EFFECTS OF GAMMA IONISING RADIATION

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Many systems have been irradiated in the past by the gamma radiation to describe the extremely fast processes connected with radiolysis of various matters. Recently the ionizing radiation has started to be used to produce biogenic molecules from simple inorganic molecules to simulate the origin of life on early Earth. These experiments are still not very well described and are also not very numerous, particularly due to femtosecond and picosecond times where the physical and physicochemical reactions during radiolysis take place. Experiments to simulate the origin of life on Earth were mostly performed with electricity as the external energy source or laser sparks (to simulate the meteor impact energy), but now the question of importance of radioactivity as the energy source becomes to be very interesting due to obtained results.

From all the simple molecules, we focus on formamide. Formamide is the simplest amide which was present on early Earth in such amounts that allowed chemical reactions to happen. It contains all necessary biogenic elements (excluding phosphorus and trace elements) and it produces purine by simple heating to 170-200 °C readily. It was also proved formamide yields all nucleobases by heating in the presence of various catalysts. Researches like these show that formamide deserves to be explored in detail.

References:

[1] Miller, S.; Urey H., *Science*, 117, 528-529 (1953).

[2] Saladino, R.; Crestini, C.; Ciciriello, F. et al., *Chem. Biodivers.*, 4, 694−720 (2007).

[3] Ferus, M.; Nesvorný, D.; Šponer, J. et al., *PNAS*, 112, 657-662 (2014).

[4] Garzón, L.; Garzón, M. L., *Orig. Life Evol. Biosph.*, 1-2, 3-13 (2001).

EXCITED STATES OF BINUCLEAR IRIDIUM COMPLEX: EXPERIMENTAL AND DFT STUDY

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Excited states of binuclear iridium complex were investigated by time-resolved infrared (TRIR) spectroscopy in acetonitrile. This iridium complex has two possible thermal isomers - eclipsed or twisted geometry (Fig.1). The isomers have a different absorption at 470 nm (eclipsed) and 585 nm (twisted). Therefore excitation wavelengths 470 and 585 nm were selected for differentiation of isomers. The effect of polarization a light source was also tested - magic, parallel and perpendicular angle.

DFT calculations for ground and excited states were performed by Gaussian 09 program package. Calculations employed Perdew, Burke, Ernzerhof (PBE0) hybrid functional. The following basis sets were used: double-ζ 6-31g(d) basis set for H, polarized triple-ζ basis sets 6-311g(d) for C and N, and small-core quasirelativistic effective core pseudopotentials and corresponding optimized set of basis functions for Ir. Electronic transitions were calculated by time-dependent DFT (TDDFT). Vibrational analysis of ground and excited states are in good agreement with experimental TRIR data.

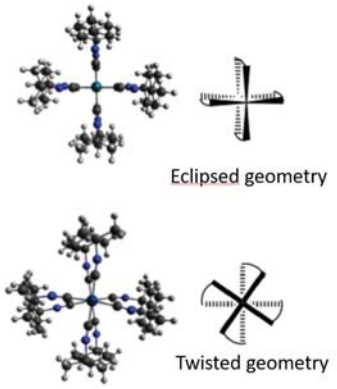

Figure 1 Thermal isomers of $[Ir_2(dimen)_4]^{2+}$

References:

Hunter, B. M.; Villahermosa, R. M.; Exstrom, C. L.; Hill, M. G.; Mann, K. R.; Gray, H. B. *Inorg Chem* **2012**, *51*, 6898-6905.
Záliš, S.; Hunter, B. M.; Gray, H. B.; Vlček, A., *Inorg Chem* **2017**, *56*, 2874-2883.

PEPTIDE ANALYTICS IN SOLUTION AND VESICLES BY LIQUID CHROMATOGRAPHY FOLLOWED BY MASS SPECTROMETRY

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Plasma membrane is responsible for various functions in living organisms. Its main components are lipids and proteins. Proper knowledge of their mutual interactions is crucial for understanding of membrane structure and function. These interactions can be readily studied in synthetic membranes composed of phospholipids and peptides. Such vesicles represent very simplified models of the plasma membrane with, as frequently stated, known composition. On the contrary, real composition of tested synthetic vesicles was only rarely analytically determined in past. Verified analytical tools for characterisation of lipid and peptide content in synthetic vesicles formed by the available techniques are missing. We employed LC/MS technique to verify the quality of peptides before and their relative content after the formation of vesicles. Our work aims to expand available tools for the characterisation of synthetic proteo-lipid vesicles often used in biophysical studies focused on membranes.

INSIGHT INTO CHEMISTRY OF STRUCTURE DIRECTING AGENTS IN RELATION TO PREPARATION OF SSZ-16 ZEOLITE

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My recent investigation was focused on development and optimization of synthesis procedure for SSZ-16 zeolite. The result of this investigation was a protocol for hydrothermal static *in-situ* synthesis of this zeolite which was optimized regarding to the SSZ-16 phase purity. Further progress is expected concerning scaling up the preparation procedure.

From the point of view of the preparation procedure, two improvements are required: (i) controllability of synthesis parameters in a relatively narrow range and (ii) further reduction of SSZ-16 crystals size. These improvements are important for zeolite application in catalytic and separation processes.

The key problem to fulfill the above requirements appears to be the stability of structure-directing species (SDA) under synthesis conditions. These species are essential for numerous zeolite syntheses. Diquaternary hexaethylpentane diammonium dibromide (Et_6-diquat-5 Br_2) was designed for the syntesis of zeolite SSZ-16. The present study is focused on chemical stability of diquaternary SDA in both nucleation and crystallization batches. It is conceived as comparative study with widely used monoquaternary tetrapropylammonium bromide (TPrABr).

Stability of the above SDAs in water solutions after heating was examined via decrease of concentrations in batch reactors. Concentrations of corresponding organic cations were measured *ex-situ* using cyclic voltammetry based on ion-transfer across interface of two immiscible liquid phases.

Water solutions of SDAs were stable in the absence of NaOH. The SDAs were stable at conditions used in nucleation batches (heating at 80 °C for 7 days) in the presence of NaOH. A considerable degree of decomposition of SDAs was, however, found for crystallization batches (heating at 140 and 160 °C for 7 days) in the presence of NaOH. The reaction kinetics of SDAs decomposition was analyzed using formal kinetic model consistent with the Hofmann elimination mechanism. In the case of $TPrA^+$ cation, the kinetics was satisfactorily described by the first order reaction. In the case of Et_6-diquat-5^{2+} cation, the first order reaction model has proved unsuitable and the question of appropriate kinetic model remains open for my further research.

ISOMORPHOUSLY SUBSTITUTED ISORETICULAR ZEOLITES WITH UTL TOPOLOGY

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The key challenges for catalytic application of extra-large pore UTL zeolite are the necessity to introduce sufficient quantity of active centers and high framework lability caused by the presence of hydrolytically unstable building units. Synthesis of aluminum-containing UTL and its post-synthesis transformation using ADOR strategy (Assembly – Disassembly – Organization - Reassembly) is a route to a series of isoreticular zeolites possessing identical structure of layers but different connectivity between them. Isomorphous substitution with aluminum results in the increase concentration of acid centers and stabilization of the frameworks. The structure, textural and acidic properties of resulted materials are dependent on the applied treatment conditions that was evidenced using XRD, SEM, FTIR and sorption techniques. Obtained materials will be used as catalysts for tetrahydropyranylation reaction as the test pore size-depending catalytic process.

References:

1. Shamzhy, M., Shvets, OV, Opanasenko, M., Yaremov, PS., Sarkisyan, LG., Chlubná, P., Zukal, A., Marthala, VR., Hartmann, M., Čejka, J, *J. Mater. Chem.*, **2012**,22, 15793-15803
2. Eliášová , P., Opanasenko, M., Wheatley, PS., Shamzhy, M., Mazur, M., Nachtigall, P., Roth, W J., Morris, R E., Čejka, J., *Chem. Soc. Rev.*, **2015**,44, 7177-7206

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