

CENTRAL EUROPEAN NMR MEETING

29th NMR VALTICE

(Theoretical NMR Predictions
for Guiding Experiments)

Valtice, Czech Republic

April 27th-30th, 2014

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29th NMR Valtice Program

SUNDAY APRIL 27, 2014

3:00-6:00 PM REGISTRATION

6:00 PM DINNER

7:15 PM OPENING REMARKS
Radek Marek

7:20 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI
SPECTROSCOPIC SOCIETY
Viktor Kanický

INTERMOLECULAR INTERACTIONS IN CRYSTALLINE THEOBROMINE
AS REFLECTED IN ELECTRON DEFORMATION DENSITY AND ¹³C NMR
CHEMICAL SHIFT TENSORS
(*J. Chem. Theory Comput.*, 2013, 9, 2629-2638)
[Martin Babinský](#)

8:15 PM SOLID-STATE NMR OF PLATONIC-SOLID GEOMETRY HIGH SYMMETRY
MOLECULES: CUBANE AND DODECAHEDRANE
[Robert Glaser](#), Wolfgang Schoefberger, Norbert Mueller

8:45 PM – 10:00 PM EURISO-TOP EVENING:
GET-TOGETHER PARTY

29th NMR Valtice Program

MONDAY APRIL 28, 2014

9:00 AM SESSION 1 – R. MAREK, Session Chair

9:00 AM PREDICTIONS OF NMR CHEMICAL SHIFTS IN HEAVY-ELEMENT COMPOUNDS: GIANT SPIN-ORBIT SHIFTS AND MORE
Martin Kaupp

9:45 AM NUCLEAR SPIN-INDUCED CIRCULAR DICHROISM IN FULLERENE COMPOUNDS
Petr Štěpánek, Juha Vaara, Sonia Coriani, Michal Straka

10:00 AM THE EFFECTS OF FAST MOLECULAR MOTIONS AND NUCLEAR DELOCALISATION ON NMR PARAMETERS
Martin Dračinský, Paul Hodgkinson

10:15 AM CONFERENCE PHOTO – IN FRONT OF VALTICE CASTLE
Radovan Fiala

10:30 AM BREAK

11:00 AM SESSION 2 – A. BAGNO, Session Chair

11:00 AM DIFFUSION IN MACROPOROUS α -ALUMINA: NMR DIFFUSOMETRY AND MONTE CARLO SIMULATIONS
Mikuláš Peksa, Martin Veselovský, Frank Stallmach, Pavel Čapek, Jan Lang

11:15 AM PROBLEMS WITH FULLERENES MODELING
Jakub Kaminský, Miloš Buděšínský, Stefan Taubert, Petr Bouř, Michal Straka

11:30 AM THE ORIGIN OF THERMODYNAMIC STABILITY OF POLYMORPH IV OF CRYSTALLINE BARBITURIC ACID: EVIDENCES FROM SOLID-STATE NMR AND ELECTRON DENSITY ANALYSES
Zahra Badri, Kateřina Bouzková, Cina Foroutan-Nejad, Radek Marek

11:45 AM DETECTING PYRAMIDAL STATE OF THE GLYCOSIDIC NITROGEN IN 8-OXO-2'-DEOXYGUANOSINE; THEORETICAL STUDY OF ¹⁵N NMR PARAMETERS
Jakub Šebera, Martin Dračinský, Radim Nencka, Lukáš Trantírek, Yoshiyuki Tanaka, Vladimír Sychrovský

12:00 LUNCH

2:00 PM SESSION 3 – M. KAUPP, Session Chair

2:00 PM PREDICTING THE NMR SPECTRA OF PARAMAGNETIC SPECIES BY DFT CALCULATIONS. FROM ORGANIC FREE RADICALS TO SPIN CROSSOVER
Alessandro Bagno

2:45 PM MODELING PARAMAGNETIC NMR SHIFTS IN COMMP-12 PROTEIN
Ladislav Benda, Jiří Mareš, Giacomo Parigi, Claudio Luchinat, Martin Kaupp, Juha Vaara

3:00 PM ssNMR CHARACTERIZATION OF PARAMAGNETIC BIS(L-VALINATO)COPPER(II) STEREOISOMERS. EFFECT OF CONFORMATIONAL DISORDER AND MOLECULAR MOBILITY ON ¹³C AND ²H VERY-FAST MAS SPECTRA
Gabor Szalontai, Jasmina Sabolović, Marijana Marković, Szabolcs Balogh

3:15 PM ¹⁹F-MRI RELAXATION AGENTS BASED ON Ni²⁺ COMPLEXES
Jan Blahut, Petr Hermann, Jan Kotek, Zdeněk Tošner

3:30 PM WHAT IS SO PUZZLING ABOUT CARBORANE RADICAL? SPIN DENSITY DISTRIBUTION IN CB₁₁(CH₃)₁₂[•] AS STUDIED BY ELECTRON PARAMAGNETIC RESONANCE
Jiří Kaleta, Ján Tarábek, Akin Akdag, Radek Pohl, Josef Michl

3:45 PM BREAK

4:15 PM SESSION 4 – SPONSORS, E. SIEVÄNEN, Session Chair

4:15 PM NEW TECHNIQUES IN STRUCTURE CHARACTERIZATION AND ELUCIDATION
Albert van Wyk, ACD

4:55 PM BRUKER NEWS
Pavel Kessler, Bruker

5:15 PM RECENT DEVELOPMENT OF HARDWARE AND SOFTWARE
Hiroaki Sasakawa, JEOL

5:35 PM WHAT'S NEW FROM AGILENT?
John Breslin, Agilent Technologies

6:00 PM REFRESHMENT

7:00-9:00 PM SCIENTIFIC INSTRUMENTS BRNO EVENING:
VISIT OF "SALON VÍN ČESKÉ REPUBLIKY"

29th NMR Valtice Program

TUESDAY APRIL 29, 2014

9:00 AM SESSION 5 – Z. TOŠNER, Session Chair

- 9:00 AM FROM GRAPE TO WINE: A NMR SPECTROSCOPY-GUIDE-TOUR
Milan Mazúr, Lucia Husáriková, Michal Kaliňák
- 9:15 AM INCREASING THE EFFICIENCY OF SPIN NOISE DETECTED NMR SPECTROSCOPY
Norbert Müller, Kousik Chandra, Maria-Theresia Pöschko, Martin Nausner, Vilko Smrecki, Gaspard Huber, Hervé Desvaux
- 9:30 AM NMR ARTIFACTS CAUSED BY DECOUPLING OF MULTIPLE-SPIN COHERENCES: APPLICATION TO SLAP EXPERIMENT
Vratislav Blechta, Jan Schraml
- 9:45 AM FITTING OF SPIN SYSTEM PARAMETERS TO NMR SPECTRA REVISITED
Stanislav Sýkora
- 10:00 AM APPLICATION OF NMR SPECTROSCOPY IN THE DEVELOPMENT OF SILICONE MATERIALS
Axel Kretschmer
- 10:15 AM NON-ROTOR-SYNCRONISED SOLID-STATE NMR
Matthias Bechmann

10:30 AM BREAK

11:00 AM SESSION 6 – R. HRABAL, Session Chair

- 11:00 AM APPLICATIONS OF NMR SPECTROSCOPY IN SUPRAMOLECULAR CHEMISTRY
Elina Sievanen, Erkki Kolehmainen, Virpi Nojonen, Jari Tamminen
- 11:15 AM SOLUTION STRUCTURE OF PSBQ FROM PHOTOSYSTEM II OF HIGHER PLANTS
Petr Rathner, Adriana Walnerova, Kousik Chandra, Christian Wohlschlager, Michaela Hornicaková, Jaroslava Kohoutová, Reinhard Wimmer, Norbert Müller

- 11:30 AM INTERACTION OF M-PMV MATRIX PROTEIN AND ITS MUTANTS WITH MEMBRANE
Tomáš Kroupa, Michal Doležal, Jan Prchal, Richard Hrabal
- 11:45 AM MOLECULAR BASIS FOR COUPLING TRANSCRIPTION TERMINATION TO NON-CODING RNA DEGRADATION
Tomasz Kabzinski, Agnieszka Tudek, Odil Porrua, Michael Lidschreiber, Karel Kubíček, Andrea Fořtová, Francois Lacroute, Štěpánka Vaňáčková, Patrick Cramer, Domenico Libri, Richard Štefl
- 12:00 INTEGRATIVE STRUCTURAL BIOLOGY APPROACH FOR UNDERSTANDING STRUCTURE AND FUNCTION OF CTD
Karel Kubíček, Olga Jasnovidová, Richard Štefl
- 12:15 LUNCH
- 1:30 PM CONFERENCE TRIP – PÁLAVA HILLS, MIKULOV
- 6:00 PM DINNER IN MIKULOV
- 9:00 PM BUS MIKULOV - VALTICE

29th NMR Valtice Program

WEDNESDAY APRIL 30, 2014

9:00 AM SESSION 7 – M. DRAČÍNSKÝ, Session Chair

- 9:00 AM HYDROSILATION INDUCED BY N→SI INTRAMOLECULAR COORDINATION. SPONTANEOUS TRANSFORMATION OF ORGANOSILANES INTO 1-AZA-SILOLE-TYPE MOLECULES IN THE ABSENCE OF A CATALYST
Miroslav Novák, Libor Dostál, Frank de Proft, Aleš Růžička, Antonín Lyčka, Roman Jambor
- 9:15 AM AXIAL-EQUATORIAL LIGATION MODE OF DINITROGENOUS LIGANDS WITH DIMERIC RHODIUM(II) SALTS: NMR AND DFT INVESTIGATIONS
Arkadiusz Leniak, Jarosław Jaźwiński, Bohdan Kamieński
- 9:30 AM CONFORMATIONAL ANALYSIS AND ENZYMATIC DECOMPOSITION OF A LOCKED NUCLEOSIDE PHOSPHORAMIDATES USING NMR SPECTROSCOPY
Eliška Procházková, Hubert Hřebabecký, Radim Nencka, Martin Dračínský
- 9:45 AM EFFECT OF pH ON CONFORMATION STABILITY OF PYRROLIDINE NUCLEOTIDE ANALOGUES
Radek Pohl, Lenka Poštová Slavětínská, Dominik Rejman
- 10:00 AM THE APPLICATION OF NEW ALIGNMENT MEDIA IN STRUCTURAL ANALYSIS OF CALIX[4]ARENE DERIVATIVES
Lukáš Vrzal, Pavel Lhoták, Hana Dvořáková
- 10:15 AM APPLICATION OF SELECTIVE 2D NMR EXPERIMENTS IN THE STRUCTURAL ANALYSIS OF A DERIVATIVE OF THE DRUG LANDIOLOL
Michal Štujber, Constantin Rabong, Igor Beseda, Martin Breza, Tibor Liptaj
- 10:30 AM BREAK** (REFRESHMENT SPONSORED BY EURISO-TOP)
- 11:00 AM SESSION 8 – M. KUZMA, Session Chair**
- 11:00 AM USING NMR SPECTROSCOPY TO FIND A 'LOST' TOXIC COMPOUND IN AN UNEXPECTED MOLECULAR COMPLEX
Lothar Brecker, Karoline Peter, Johann Schinnerl, Susanne Felsing, Yan Ma

- 11:15 AM *ESTAC*- A NOVEL TOOL FOR DETERMINATION OF BINDING CONSTANTS
Milan Bernauer, Bohumil Bernauer, Petra Cuřínová, Jan Budka
- 11:30 AM NMR TO STUDY BINDING PATTERN AND TRANSFORMATION OF UDP-GLCUA
Claudia Puchner, Thomas Eixelsberger, Lothar Brecker and Bernd Nidetzky
- 11:45 AM EFFECT OF THE ANTI-CANCER TREATMENT ON THE METABOLITE PROFILE IN CANCER CELL LINES STUDIED BY NMR
Simona Bártová, Karel Valis, Petr Novák, Julia Starková, Ivana Hermanová, Marek Kuzma
- 12:00 ¹H NMR METABOLOME CHANGES DURING THE LIFE CYCLE OF *TRICHODERMA ATROVIRIDE*
Michal Kaliňák, Ján Škorík, Peter Žemla, Martin Šimkovič, Ludovít Varečka, Daniela Hudecová
- 12:15 NMR-BASED METABONOMICS OF URINE IN THE MSG MOUSE MODEL OF OBESITY
Helena Pelantová, Jiří Anýž, Daniel Novák, Lenka Maletínská, Martin Haluzík, Marek Kuzma
- 12:30 JOSEF DADOK PRIZE**
Lothar Brecker, Radovan Fiala, Antonín Lyčka
<http://www.ncbr.muni.cz/nmrvaltice/awards>
- 12:45 CLOSING REMARKS**
- 1:00 PM LUNCH**