

CENTRAL EUROPEAN NMR MEETING

36th NMR VALTICE

Valtice, Czech Republic

April 2-5, 2023

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36th NMR Valtice Program

SUNDAY APRIL 2, 2023

**6:00-7:00 PM REGISTRATION – “CHÂTEAU VALTICE”
(GPS: 48.7393206N, 16.7496614E)**

7:00 PM GET-TOGETHER PARTY IN “CHÂTEAU VALTICE”

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MONDAY APRIL 3, 2023

- 8:30-8:55** **REGISTRATION „CENTRUM EXCELENCE“ (GPS: 48.7411942N, 16.7485308E)**
- 8:55** **OPENING – R. MAREK**
- 9:00 AM** **SESSION 1 – R. MAREK, Session Chair**
- 9:00 AM APPLICATIONS OF SOLID-STATE NMR TO THE STUDY OF CHEMICAL BONDING
David Bryce
- 9:45 AM THE HYDROGEN BOND CONTINUUM IN SOLID ISONICOTINIC ACID
Jan Blahut, Michal Šála, Martin Dračínský, Jakub Radek Štoček
- 10:00 AM OVERVIEW AND PERSPECTIVES OF NMR SPECTROSCOPY OF SOLAR CELLS AT IMC
Libor Kobera, Andrii Mahun, Sabina Abbrent, Rafal Konefal, Jiří Brus
- 10:15 AM OPTIMAL CONTROL OF EFFECTIVE HAMILTONIANS
Andrej Šmelko, Zdeněk Tošner
- 10:30 AM CONFERENCE PHOTO I
Radovan Fiala
- 10:35 AM** **BREAK**
- 11:00 AM** **SESSION 2 – D. BRYCE, Session Chair**
- 11:00 AM INTERNUCLEAR DISTANCE MEASUREMENT BETWEEN ¹H AND ¹⁴N IN RIGID SOLIDS
Yusuke Nishiyama
- 11:30 AM NMR CRYSTALLOGRAPHY OF AMINO ACIDS
Ema Chaloupecká, Martin Dračínský
- 11:45 AM SUBSTITUENT AND SOLID-STATE EFFECTS ON HYPERFINE NMR SHIFTS
Jan Novotný, Lukáš Jeremias, Patrick Nimax, Stanislav Komorovsky, Ivo Heinmaa, Radek Marek
- 12:00** **LUNCH – HOTEL KLARET (48.7413239N, 16.7505050E)**

- 2:00 PM SESSION 3 – J. BRUS, Session Chair**
- 2:00 PM PARAMAGNETIC NARROWING
Jan Blahut, Ján Tarábek
- 2:15 PM PARAMAGNETIC NMR OF OCTAHEDRAL Ru(III) COMPLEXES WITH
AXIAL PYRIDINE-BASED LIGANDS
Jan Chyba, Anna Hruzíková, Michal Knor, Petra Pikulová, Kateřina Marková,
Jan Novotný, Radek Marek
- 2:30 PM LANTHANIDE(III) COMPLEXES OF A DITOPIC MACROCYCLIC
PHOSPHINATE LIGAND
Adam Svítok, and Petr Hermann
- 2:45 PM PARAMAGNETIC HOST-GUEST COMPLEXES OF RUTHENIUM(III)
COMPOUNDS AND CYCLODEXTRINS
Jan Novotný, Jan Chyba, Anna Hruzíková, Petra Pikulová, Aliaksandra Kursit,
Michal Knor, Kateřina Marková, Jaromír Marek, Pia Jurček, Ondřej Jurček,
Radek Marek
- 3:00 PM BREAK**
- 3:30 PM SESSION 4 – R. POHL, Session Chair**
- 3:30 PM STRUCTURAL INVESTIGATION OF SUPRAMOLECULAR
PLATINUM(II) COMPLEXES
Shib S. Paul, Jan Novotný, Pia Jurček, Radek Marek
- 3:45 PM CYCLIZATION-GAINED STRUCTURAL FEATURES IN HOMOCHIRAL
BINAPHTHYLUREAS
Roman Holakovský, David Just, Martin Jakubec, Petra Cuřínová
- 4:00 PM STABILIZATION OF H-BONDED BASE PAIRS AS A FUNCTION OF
H-BONDING ALTERNATION
Zuzana Osifová, Michal Šála, Martin Dračínský
- 4:15 PM BREAK – Sandwich & Refreshment**
- 4:45 PM SESSION 5 – R. FIALA, Session Chair**
- 4:45 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI
SPECTROSCOPIC SOCIETY
Radovan Fiala
- 5:30 PM BREAK**
- 6:50 PM CONFERENCE PHOTO II (GPS: 48.7401189N, 16.7567156E)**
Radovan Fiala
- 7:00-9:00 PM BRUKER EVENING: “SALON VÍN ČESKÉ REPUBLIKY“**
(GPS: 48.7397589N, 16.7553731E)

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TUESDAY APRIL 4, 2023

9:00 AM SESSION 6 – P. CUŘÍNOVÁ, Session Chair

9:00 AM STRUCTURAL ANALYSIS USING ³¹P NMR SPECTROSCOPY
PARAMETERS
Markéta Tichotová, Aneta Ešnerová, Lucie Tučková, Lucie Bednárová, Ivana
Císařová, Ondřej Baszczyński, Ulrich Sternberg, Eliška Procházková

9:15 AM AZOPYRIMIDINE PHOTOSWITCHES WITH HIGHLY STABLE CIS
ISOMERS
Anna Hruzíková, Lucie Mužíková Čechová, Petr Knotek, Aleš Růžička, Eliška
Procházková

9:30 AM ¹H DOSY NMR SPECTROSCOPY OF BILE ACID-BASED
METALLOSUPRAMOLECULAR STRUCTURES
Subhasis Chattopadhyay, Pia Jurček, Radek Marek, Ondřej Jurček

9:45 AM ¹⁵N NMR STUDY OF AZO-HYDRAZO TAUTOMERISM IN SOME
INDUSTRIALLY PRODUCED AZO DYES
Antonín Lyčka

10:00 AM BREAK SPONSORED BY MEASUREMENT TECHNIC MORAVIA

10:30 AM SESSION 7 – M. DRAČÍNSKÝ, Session Chair

10:30 AM MD SIMULATIONS OF HOST-GUEST COMPLEXES AND NMR SHIFTS
Jakub Jakubec, Shib S. Paul, Pia Jurček, Jan Novotný, Radek Marek

10:45 AM ON RECENT 1-H NMR STUDIES OF STRUCTURAL
(ANTI)AROMATICITY
Jiří Czernek, Jiří Brus

11:00 AM NMR-CHALLENGE.COM: AN INTERACTIVE WEBSITE WITH
EXERCISES IN SOLVING STRUCTURES FROM NMR SPECTRA
Ondřej Socha, Zuzana Osifová, Martin Dračinský

11:15 AM BRUKER NEWS 2023
Philip Wurm, Pavel Kessler

12:00 AM JEOL NEWS 2023
Michal Maloň

12:30 LUNCH IN KLARET (48.7413239N, 16.7505050E)

2:00 PM FREE DISCUSSIONS

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WEDNESDAY APRIL 5, 2023

9:00 AM SESSION 8 – R. HRABAL, Session Chair

9:00 AM NMR AEROSOLOMICS STUDY OF RURAL BACKGROUND AEROSOL
PARTICLES IN THE CENTRAL EUROPE

Štěpán Horník, Petra Pokorná, Petr Vodička, Jaroslav Schwarz, Vladimír
Ždímal, Jan Sýkora

9:15 AM INVESTIGATION OF CARBONACEOUS MATERIALS POROSITY BY
LOW-FIELD NMR RELAXOMETRY

Eva Kinnertová, Václav Slovák, Tomáš Zelenka

9:30 AM TEMPLATING BEHAVIOUR IN SILICIFYING PEPTIDES

Fanny Kozak, Fabian Daus, Ludovica M. Epasto, Armin Geyer, Christian W. F.
Becker, Dennis Kurzbach

9:45 AM EXPLORING THE DIFFERENCES IN STRUCTURE AND FUNCTION OF
OUTER SURFACE PROTEINS AMONGST BORRELIA SPECIES

Libor Hejduk, Manuel Baumgartner, Martin Strnad, Filip Dyčka, Vladyslav
Lazebnyk, Jakob Schmelzer, Lukas Zajicek, Julian Widhalm, Ján Štěrba, Ryan
O. M. Rego, Norbert Müller, Adriana Rathner

10:00 AM BREAK

10:30 AM SESSION 9 – A. RATHNER, Session Chair

10:30 AM INVESTIGATING THE ACTIVATION OF A CALCIUM SENSOR PROTEIN
DIMER CONNECTED AT THE N-TERM

Manuel Baumgartner, Agrim Gupta, Adriana Rathner, Petr Rathner, Katharina
Röser, Marc Fahrner, Matthias Bechmann, Solomia Pylypchuk, Christoph
Romanin, Norbert Müller

10:45 AM STRUCTURAL CHARACTERIZATION OF FOXO4:p53 PROTEIN-
PROTEIN INTERACTION USING NMR RELAXATION EXPERIMENTS

Klára Kohoutová, Pavel Srb, Václav Veverka, Veronika Obšilová,
Tomáš Obšil

11:00 AM ‘ORDINARY’ ³¹P NMR TO STUDY THE STEREOCHEMICAL COURSE
OF AN ECAGP CATALYZED PHOSPHORYL TRANSFER

Martin Pfeiffer, Friedrich Hammerschmidt, Bernd Nidetzky, Lothar Brecker

- 11:15 AM SHORT BREAK**
- 11:30 AM JOSEF DADOK PRIZE**
Lothar Brecker & Radovan Fiala
- 11:45 AM CLOSING REMARKS**
Radek Marek
- 11:50 AM LUNCH IN KLARET (48.7413239N, 16.7505050E)**