

**CENTRAL EUROPEAN NMR DISCUSSION GROUPS**

**19<sup>th</sup> NMR Valtice**

**19.-21.4.2004**

**Valtice, Czech Republic**

# PROGRAMME

Monday April 19, 2004

Afternoon 2 p.m.

- 14:00 Opening of the Conference
- 14:10 Antonín Lyčka, Alois Koloničný, Vladimír Pejchal, Tomáš Lébl and Jaroslav Holeček  
 $^{119}\text{Sn}$ ,  $^{13}\text{C}$  and  $^1\text{H}$  NMR Spectra of Organotin(IV) Compounds Containing Two and More Tin Atoms in a Molecule.
- 14:25 Jan Chalupa, Tomáš Lébl and Antonín Lyčka  
Synthesis and Characterisation of Some Organotin Derivatives of Carbohydrates.
- 14:40 Gábor Szalontai and Gábor Besenyei  
 $^{31}\text{P}$  CP/MAS Study of Dimeric Palladium(I) Complexes. Rotation-Rate-Dependent MAS Spectra of Dipolar and Scalar Coupled Four-Spin Systems.
- 14:55 Leszek Pazderski, Iwona Łakomska, Edward Szłyk, Jerzy Sitkowski, Lech Kozerski, and Bohdan Kamiński  
 $^{15}\text{N}$  NMR Coordination Shifts in Diamagnetic Transition Metal Complexes with Heterocyclic Azines.
- 15:10 H. Štěpánková, J. English, P. Novák, J. Kohout, M. Kučera, and K. Nitsch  
Applicability of NMR to Impurities Detection in Yttrium Iron Garnet Thin Films.
- 15:25 S. M. Gerdov, Yu. K. Grishin, V. A. Roznyatovsky, N. M. Sergeyev, and N. D. Sergeyeva  
Nuclear Overhauser Effect  $^2\text{H}$  -  $\{^1\text{H}\}$ .

15:40 Break

- 16:15 Zdeněk Tošner, Jan Lang, Veronika Michlová, Jiří Vlach, Jan Budka, Ivan Stibor, and Jozef Kowalewski  
Structure and Dynamics of Calix[4]arene Complex with 2,4-Dimethylbenzoate.
- 16:30 H. Dvořáková, B. Dolenský, J. Kroulík, M. Bernátková, V. Král, J.L. Sessler, and V. Lynch

Conformational Properties of Aryl Functionalized Calix[4]pyrins.

- 16:45 Marcela Tkadlecová, Pavel Lhoták, and Petra Zlatušková  
Complexation Properties of Thiocalixarenes.
- 17:00 Veronika Deckerová, Jan Lang, and Pavel Lhoták  
Dynamics of Hydrogen Bond Array in Calix[4]arene.
- 17:15 Sejbal Jan and Zedník Jiří  
Structure and Dynamic Properties of Some Rhodium Complexes.
- 17:30 Anja Holzberger and Erich Kleinpeter  
Ag(I) and Pd(II) Complexes of Mixed O/S Crown Ethers.
- 17:45 Erich Kleinpeter and Sabrina Klod  
The  $\gamma$ - and  $\delta$ -Effects In  $^{13}\text{C}$  NMR Spectroscopy in Terms of Nuclear Chemical Shielding (NCS) Analysis.
- 18.00 Tamás Gáti, András Simon, Józef Drabowicz, Stefan Moeller, Helmut Duddeck and Gábor Tóth  
Adducts of the Chiral  $\text{Rh}_2[(R)\text{-MTPA}]_4$  Reagent with Phosphine Chalcogenides and Spirochalcogenuranes. Nature of Binding and Ligand Exchange.
- 18.15 Radek Marek, Pavlína Sečkářová, Michal Maloň, and Zdeněk Trávníček  
Proton-Transfer Processes and Metal Complexations of Purine Derivatives.

18:30 Dinner

20:00 Get-together party in wine cellar sponsored by Varian

Tuesday April 20, 2004

Morning 8.00 a.m.

- 8:00 Jiří Czernek  
Understanding Chemical Shielding Tensors in Nucleic Acids.
- 8:15 Jana Přecechtělová, Markéta L. Munzarová, and Vladimír Sklenář  
Structural Dependence of  $^{31}\text{P}$  Chemical Shielding Tensors in B-DNA: A DFT Study.
- 8:30 Lothar Brecker, Daniel Wicklein, and Arnd Petersen  
Structures of Galactan and Arabinogalactan Polysaccharides from Pollen of Timothy Grass (*Phleum Pratense* L.)

- 8:45 Jiří Brus and Alexandr Jegorov  
Through-Bonds and Through-Space Solid-State NMR Correlations at Natural Isotopic Abundance: Signal Assignment and Structural Study of Simvastatin.
- 9:00 D. Kurková, J. Kříž, P. Schmidt, J. Dybal, J. C. Rodríguez-Cabello and M. Alonso  
NMR Study of Protein Based Polymers in Aqueous Solutions.
- 9:15 Michaela Matejková, Petr Padrta, Radovan Fiala, and Vladimír Sklenář  
NMR -Distance Restraints at Low Temperatures – An Application to DNA Hairpin.
- 9:30 Petr Novák, Lukáš Židek, Petr Padrta, and Vladimír Sklenář  
Ρεφινεμεντ οφ *Τρυπανοσομα* Υ6 PNA Στεμ-Λοοπ Στρυχτυρε Υσινη Ονε- ανδ Τωο  
-Βονδ Ρεσιδυαλ Διπολαρ Χουπλινγς.
- 9:45 Jiří Vlach, Jiří Mareš, Jan Lipov, Michaela Rumlová, Tomáš Ruml, and Richard Hrabal  
Speeding up of the Assignment of Backbone Resonances of Wild-Type Matrix Protein From M-PMV.
- 10:00 Petr Sedmera, Marek Kuzma, Dietmar Haltrich, and Jindřich Volc  
Exploring the Biotransformation Potential of Pyranose Dehydrogenase from *Agaricus Meleagris* by *in situ* NMR

10:15 Break

10:45 Information about new products of our sponsors

12:00 Lunch

14:00 Informal Discussions

18:30 Dinner

20:00 Meeting of the NMR Discussion Groups - refreshment sponsored by Bruker and Scientific Instruments Brno

Wednesday April 21, 2004

Morning 8.00 a.m.

- 8:00 Radovan Fiala, Markéta L. Munzarová and Vladimír Sklenář  
Experiments for Correlating Quaternary Carbons in RNA Bases.
- 8:15 Hana Křížová, Lukáš Židek, Pavel Macek, Petr Novák, Martin J. Stone, Milos V. Novotny, and Vladimír Sklenář  
Temperature-Dependent Spectral Density Analysis and Molecular Dynamics Simulation of Major Urinary Protein-Pheromone Interactions.
- 8:30 Sándor Boros and Gábor Tóth  
Measurements of Heteronuclear Long-Range Coupling Constants on Macrolides.
- 8:45 Gyula Batta and Katalin E. Kövér  
More Line Narrowing in Trosy.
- 9:00 Zenon Starčuk, Zenon Starčuk jr., and Jaroslav Horký  
Outlasting Problems of Water Suppression in Low Field (1.5 T) *in vivo* MR Spectroscopy
- 9:15 Zenon Starčuk, Zenon Starčuk jr., and Jaroslav Horký  
About Some Magnetization Transfer Problems in *in vivo* MR Spectroscopy of the Brain.
- 9:30 Μιλαν Μαζ |ρ  
Signal Intensity Calculations from a Point-Like to an Arbitrarily Shaped Sample. A Shell Method.
- 9:45 Lenka Hanyková, Jan Labuta, and Jan Lang  
Thermotropic Phase Transition in Poly(Vinyl Methyl Ether)/Water/Ethanol Solutions as Studied by NMR Methods.
- 10:00 Gunter Wolf and Erich Kleinpeter  
<sup>1</sup>H NMR Diffusion-Ordered Spectroscopy to Study Lecithin-Based Microemulsions.
- 10:15 Catrin Tyl, Susanne Felsing, and Lothar Brecker  
*In situ* Proton NMR – Michaelis Menten Kinetics and Selectivities of Glycosidase Catalysed Reactions.
- 10:30 Jan Sýkora, Vratislav Blechta, and Jan Schraml  
HPLC coupled to NMR.
- 10:45 Miroslav Holík and Pavel Janderka  
<sup>13</sup>C Shift Increments as Substituent Constants.
- 11:00 Closing of the Conference

# **LIST OF PARTICIPANTS**

BARÁKOVÁ Lenka	CZ	
BATTA Gyula	HU	36
BÍLEK Petr	CZ	
BITTŠANSKÝ Michal	CZ	
BLECHTA Vratislav	CZ	43
BOROS SÁNDOR	HU	35
BRECKER Lothar	AT	26, 42
BRUS Jiří	CZ	27
CZERNEK Jiří	CZ	24
DECKEROVÁ Veronika	CZ	
DVOŘÁKOVÁ Hana	CZ	16
FIALA Radovan	CZ	14
GÁTI Tamás	HU	29, 33
GERDOV Sergei	RU	14
HANYKOVÁ Lenka	CZ	40
HAVLÍČEK Jaroslav	CZ	
HOLÍK Miroslav	CZ	44
HOLZBERGER Anja	DE	20
HORKÝ Jaroslav	CZ	37, 38
HORVATH Gyula	HU	
HUMPA Otakar	CZ	
CHALUPA Jan	CZ	10
CHMELÍK Josef	CZ	
CHMELIK Marek	CZ	
KESSLER Pavel	DE	
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KLEINPETER Erich	DE	20, 21, 41
KOLEHMAINEN Erkki	SF	
KOLONIČNÝ Alois	CZ	
KURKOVÁ Dana	CZ	28
KUZMA Marek	CZ	32

LANG Jan	CZ	15, 18, 40
LÉBL Tomáš	CZ	9, 10
LYČKA Antonín	CZ	9, 10
MACEK Pavel	CZ	
MALON Michal	CZ	
MANNSCHRECK Albrecht	DE	
MAREK Radek	CZ	23
MAREŠ Jiří	CZ	
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MATĚJKOVÁ Michaela	CZ	29
MAZUR Milan	SK	39
MÉHES Adam	CZ	
MIKULÍK Jiří	CZ	
NOVÁK Petr	CZ	30, 34
PADRTA Petr	CZ	29, 30
PAVELKOVÁ Anna	CZ	
PAZDERSKI Leszek	PL	12
PEJCHAL Vladimír	CZ	9
PELNÁŘ Jan	CZ	
POPA Igor	CZ	
PŮČEK Ladislav	CZ	
PŘECECHTĚLOVÁ Jana	CZ	25
PROKS Vladimír	CZ	
RIEDL František	CZ	
ŠAMAN David	CZ	
SEČKÁŘOVÁ Pavlína	CZ	23
SEDMERA Petr	CZ	32
SEJBAL Jan	CZ	19
SERGEYEV Nikolay	RU	14
SERGEYEVA Natalia	RU	14
ŠETKOVÁ Kateřina	CZ	



SCHRAML Jan	CZ	43
SIMON András	HU	22
SKLENÁŘ Vladimír	CZ	25,29,30,33,34
SRB Pavel	CZ	
STARČUK Zenon	CZ	37, 38
STARČUK, Jr. Zenon	CZ	37, 38
STAROVOJTOVA Larisa	CZ	
ŠTĚPÁNEK Josef	CZ	
ŠTĚPÁNKOVÁ Helena	CZ	13
SÝKORA Jan	CZ	43
SZALONTAI Gábor	HU	11
TKADLECOVÁ Marcela	CZ	17
TOŠNER Zdeněk	CZ	
TÓTH Gábor	HU	22, 35
TYL Catrin	AT	42
TUREČKOVÁ Milena	CZ	
VIRTANEN Elina	SF	
VLACH Jiří	CZ	15, 31
VRÁTNÍČKOVÁ Zlata	CZ	
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