

**CENTRAL EUROPEAN NMR DISCUSSION GROUPS**

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

**23.-25.4.2001**

**Valtice, Czech Republic**

# PROGRAMME

Monday April 23, 2001

Afternoon 2 p.m.

- 14:00 Opening of the Conference
- 14:10 Hana Dvořáková, Marcela Tkadlecová, Tomáš Tobrman, Dalimil Dvořák.  
Conformational and D-NMR study of chelated ( $\eta^2$ -diallylamino)carbene complexes of Cr, W and Fe.
- 14:25 Zdeněk Friedl and Svatopluk Zeman,  
Theoretical and  $^{15}\text{N}$ -NMR Study of Some High Energetic Nitramines.
- 14:40 Roman Jambor, Aleš Růžička, Jiří Brus, Jaroslav Holeček,  
Solution and CP/MAS NMR Investigation of Intramolecular Coordination Sn-N in Some Organotin(IV) C,N-Chelates.
- 14:55 V. Macháček, A. Lyčka, J. Kaválek,  
 $^{17}\text{O}$  NMR Spectra of Some Meisenheimer Adducts.
- 15:10 Radek Marek, Jiří Brus, Jaromír Toušek,  
 $\text{N}^7$ - and  $\text{N}^9$ -substituted purine analogues –  $^{15}\text{N}$  NMR study.
- 15:25 Tomáš Lébl, Jaroslav Holeček, Marek Dymák, Dirk Steinborn,  
Reactions of 2-functionalised vinylstannanes with acetyl bromide.
- 15:40 J. Pavlovský, E. Kozubek, P.Jelínek, L.Mokoš, J.Bohdálková,  
 $^{29}\text{Si}$  NMR Spectroscopy Studies of Selected Water Glass Samples for Foundry Technology.

15:55 Break

- 16:30 A. Perjéssy, W.-D. Rudolf, P. Meyer, E. Kolehmainen, D. Loos, K. Laihia, M. Nissinen, J. Koivisto, R. Kauppinen,  
Conformation and Transmission of Substituent Effects in Disubstituted Tetrahydropyridazine and Diazabicycloheptene Derivatives.
- 16:45 Andrej Petrič,  
Spectroscopic Properties vs. Molecular Geometry in a Series of Fluorescent Compounds.
- 17:00 Aleš Růžička, Libor Dostál, R.Jambor, J.Brus, J.Holeček,  
Structure of (2,6-Bis(dimethylamino)methyl)-diphenyltin(IV) derivatives.
- 17:15 Pavlna Sečkářová, Jiří Dostál, Roger Dommissé, Radek Marek,  
Structure elucidation of benzophenanthridine and protoberberine alkaloids.
- 17:30 J. Bohdalková, E. Kozubek, M. Peňáz, J. Pavlovský,  
NMR and GC-MS Analysis of Selected Coal Extracts
- 17:45 Alojz Demšar,  
NMR Study of the Solution Structures of  $\text{C}_5\text{Me}_5\text{TiF}_3$

18:30 Dinner

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

Tuesday April 24, 2001

Morning 8 a.m.

- 8:00 Robert Glaser, Dror Shiftan, and Artem Novoselsky,  
Solid-State NMR Studies of Conformationally Polymorphic Crystalline Solids  
for Stereochemical Interpretation of Fast Exchange Limit Solution-State NMR  
Spectra.
- 8:30 Jaroslav Kříž,  
NMR studies of supramolecular self-assembly: pre-micellar aggregation of  
sodium *p*-dodecylbenzenesulfonate.
- 8:45 Jiří Spěváček, Jiří Brus,  
Solid state <sup>1</sup>H CRAMPS NMR study of molecular complexes of poly(ethylene  
oxide) and benzene derivatives.
- 9:00 Radovan Fiala, Lukáš Trantírek, Erik Caha and Mikael Akke  
<sup>13</sup>C Relaxation Study of RNA Loop Dynamics.
- 9:15 Richard Hrabal, Václav Veverka,  
Simplification of NMR spectra of Mason-Pfizer monkey virus protease.

10:00 Break

- 10:30 M.Hricovini, G.Torri, M.Guerrini and B.Casu,  
NMR analysis of protein-carbohydrate interactions through evaluation of  
chemical shifts, coupling constants and transferred NOEs.
- 10:45 Hana Křížová, Lukáš Židek, Martin Stone & Vladimír Sklenář,  
NMR & Proteins Dynamics.
- 11:00 Dana Kurková, Jaroslav Kříž, Pavel Schmidt, José Carlos Rodríguez-Cabello<sup>+</sup>,  
NMR spectroscopy of an elastin-like polypeptide.
- 11:15 Václav Veverka, Helena Bauerová, Aleš Záborský, Iva Pichová., Richard  
Hrabal,  
<sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N Assignment and Secondary Structure Identification of the  
Protease from Mason-Pfizer Monkey Virus.
- 11:30 Petr Sedmera, Jindřich Volc, Ronald Mathä, Dietmar Haltrich,  
Biotransformations in NMR sample tube.
- 11:45 Daniela Suciú,  
Pulse NMR used in study of bound water in biological systems.

12:30 Lunch

14:00 Excursion to the 'Cross' wine cellar

16:30 Information about new products of our sponsors

18:30 Dinner

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

Wednesday April 25, 2001

Morning 8 a.m.

- 8:00 Christoph Seger, Wolfgang Robien,  
CSEARCH online - a free spectrum estimation tool for structure elucidation  
utilizing stereochemical information.
- 8:15 Vladimír Sychrovský, Jaroslav Vacek, Pavel Hobza, and Vladimír Sklenář,  
DFT Calculation of NMR Spin-Spin Coupling Constants in Adenine, Thymine,  
Cytosine, and Guanine.
- 8:30 Petr Padrta, Vladimír Sklenář,  
MULDER – program for extracting of torsion angles from NMR data.
- 8:45 Erich Kleinpeter and Sabrina Klod,  
Ab-Initio MO Calculation of the Anisotropy Effect of Multiple Bonds and the  
Ring Current Effect of Arenes - Application in Conformational and  
Configurational Analysis.
- 9:00 Marek Kuzma, Petr Sedmera,  
 $^4J(H,C)$  - What are they good for?
- 9:15 Milan Mazúr,  
Quantity in Magnetic Resonance Spectroscopy. - Part 4.
- 9:30 Karin Hohenthanner, P. K. Madhu, Rita Grandori and Norbert Müller,  
Cross-correlation Effects in Paramagnetic Systems.
- 9:45 Zenon Starčuk, Zenon Starčuk, Jr., Jaroslav Horký,  
Water suppression – recent developments.
- 10:00 Jan Lang, Jiří Vlach, Hana Dvořáková, Pavel Lhoták and Richard Hrabal,  
Kinetic study of thermal isomerisation of 25,26,27,28-tetrapropoxy-2,8,14,20-  
tetrathiacalix[4]arene.
- 10:15 Herwig Häusler, Arnold. E. Stütz, Peter Greimel and Hansjörg Weber,  
Mechanistic Studies on d-Xylose (d-Glucose) Isomerase (EC 5.3.1.5): NMR  
Spectrometric Investigations.
- 10:30 Hana Navrátilová,  
Enantiomeric Analysis of (3S, 4R)-4-(4-Fluorophenyl)-3-hydroxymethyl-1-  
methylpiperidine by  $^{19}F$  NMR Spectroscopy.
- 10:45 Miroslav Holík and Josef Halánek,  
Confidence Ellipses for the Quantitative Analysis from the whole NMR  
Spectrum.

11:00 Closing of the Conference