

CENTRAL EUROPEAN NMR DISCUSSION GROUPS

18th NMR Valtice

28.-30.4.2003

Valtice, Czech Republic

PROGRAMME

Monday April 28, 2003

Afternoon 2 p.m.

- 14:00 Opening of the Conference
- 14:10 M. Mazur.
Positive, Negative, and Concurrent “Lens Effect” in Magnetic Resonance Spectroscopy
- 14:25 V. Smrečki, N. Müller
Multinuclear Chemical Shielding Anisotropy Calculations in Model Peptides
- 14:40 J. Přecechtělová, M.L. Munzarová, V. Sklenář
¹³C and ¹⁵N Chemical Shifts in Deoxyribonucleosides as Studied by DFT
- 14:55 P. Sečkářová, J. Toušek, E. Kolehmainen, M. Hocek, V. Sklenář, R. Marek
Tautomerism of purine derivatives investigated by low-temperature NMR and theoretical calculations
- 15:10 L. Žídek, P. Padrta, J. Chmelík, V. Sklenář
Internal consistency of residual dipolar couplings and its effect on structure calculation
- 15:25 R. Fiala
Relaxation in Complex Spin Systems

15:40 Break

- 16:15 D. Kurková, J. Kříž, J. Dybal, P. Schmidt
How ¹H T₁ and T₂ relaxations in thermotropic materials can reveal their hydration
- 16:30 J. Kříž, J. Dybal, D. Kurková
Study of cooperative polyion-counterion interactions using SQC and DQC relaxations
- 16:45 J. Sejbal, J. Mossinger
An NMR Study of the Complexes of Porphyrins with Cyclodextrins
- 17:00 J. Lang, Z. Tošner, D. Sandström, O. Petrov, J. Kowalewski
Dynamics of Cryptophane-E Inclusion Complexes with Chloromethanes
- 17:15 M. Tkadlecová, J. Havlíček, A. Synytsya, K. Volka
NMR Study of the Metal Complexes of d-Galacturonic Acid

17:30 H. Dvořáková, J. Štursa, J. Moravcová
Conformational Study of Partly Alkylated calix[4]resorcinarenes

17:45 R. Marek, M. Lukášková, J. Toušek, J. Brus, Z. Trávníček
Protonation, Tautomerism, and Hydrogen Bonding of 6-Benzylaminopurine
Cytokinin Analogues

18:00 Dinner

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

Tuesday April 29, 2003

Morning 8.30 a.m.

8:30 M. Heydenreich, A. Koch, J. Kovács, G. Tóth, E. Kleinpeter
Electronical influence on 3J (C,H) coupling constants – their determination,
calculation and comparison of methods

8:45 E. Balentová, I. Géci, J. Imrich, K.D. Klika, J. Bernát, P. Kristian, K. Pihlaja
Structure, Protonation and Tautomerism of Acridinylthioureas and Hydrazines

9:00 T. Gátj, G. Tóth, S. Moeller, H. Duddeck
Chiral recognition of selenium compounds applying $Rh_2[(R)\text{-MTPA}]_4$ reagent

9:15 H.-J. Weber, R.F.G. Fröhlich, H. Griengl, J. Keplinger, P. Verdino
Dramatic Solvent Dependence of the Sign of Optical Rotation for (*R,R*)-1,1'-
Bis(Cyano-Hydroxymethyl)Ferrocene: An Investigation by NMR-Spectroscopy

9:30 S. Boros, G. Tóth, A. Andor, A. Kónya, É. Ilkóy, A. Tegdes
Structure Elucidation of Transformed Steroids

9:45 E. Kleinpeter, S. Klod
The anisotropic effect of the C-C single bond – the corresponding sketches in NMR
textbooks are wrong!

10:00 Break

10:30 L. Dostál, R. Jambor, A. Lyčka, A. Růžička, J. Holeček
 ^{17}O NMR spectra of some organotin (IV) O,C,O chelates

10:45 A. Lyčka, A. Klásek, K. Kořistek, M. Holčapek
Rearrangement of Some Nitrogen Containing Heterocycles Studied by 1H - ^{15}N
NMR Spectroscopy

- 11:00 B. Štíbr
Examples of NMR Methods in the Area of Boron-Cluster Chemistry
- 11:15 T. Lébl, P. Zoufalá, J. Brus, C. Bruhn
 ^1H , ^{119}Sn J-HMBC spectroscopy as a tool for the evaluation of intramolecular donor-acceptor interaction in organotin C,O-chelates
- 11:30 V. Blechta, J. Sykora, J. Schraml
 ^{29}Si - ^{13}C long range coupling constants in silylated compounds
- 11:45 J. Pavlovský
The influence of silicate module, Glucitol addition and dilution on the natriumwaterglasses by ^{29}Si NMR Spectroscopy

12:00 Lunch

14:00 Discussions

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 30, 2003

Morning 8.30 a.m.

- 8:30 L. Starovoytova, L. Hanyková, J. Spěváček, M. Ilavský
 ^1H NMR Study of Temperature-Induced Phase Transition of Poly(*N*-Isopropyl methacrylamide)/ Poly(Vinyl Methyl Ether) Mixtures in D_2O Solutions
- 8:45 Ch. Steindl, Ch. Schäffer, P. Messner, N. Müller
New NMR-results on Secondary Cell Wall Polymers
- 9:00 N. Müller, A. Obermaier
The structure elucidation of beech wood lignin with NMR
- 9:15 F. Pilichowski, T. Liptaj, M. Morel, M. Baba
NMR study of cross-linking in elastomers

- 9:30 L. Brecker, H. Janusch, D. Schwudke, U. Zähringer
Recent NMR-based Results from Structure Determination of LPS and Lipid A
- 9:45 J. Brus, J. Dybal
Hydrogen-Bond Interactions in Organically-Modified Polysiloxane Networks Studied by 1D and 2D CRAMPS and Double-Quantum ^1H MAS NMR
- 10:00 G. Pintacuda, K. Hohenthanner, G. Otting, N. Müller
Cross Correlated Curei Spin Relaxation in Proteins
- 10:15 V.Mlynárik, S. Gruber, Z. Starčuk, Z. Starčuk, Jr., J. Horký, E. Moser
High resolution multivoxel spectroscopy of human brain at 3 Tesla
- 10:30 Z. Starčuk,jr., J. Horký, Z. Starčuk, V.Mlynárik, S.Gruber, E Moser
Some Comments on Frequency Selective Excitation in Newly Proposed MRSI Sequences
- 10:45 V. Veverka, J. Lipov, J. Lang, M. Rumlová, T. Ruml, R. Hrabal.
A relationship between single point mutation of the matrix protein from Mason-Pfizer monkey virus and its three-dimensional structure.

11:00 Closing of the Conference