

Summary

The EUROMAR 2008 conference, satellite School and meeting took place in St.-Petersburg (Russia) from 3 to 10 July 2008. The conference was partially supported by the ESF Research Networking Program EMAR ("Multidisciplinary Frontiers of Magnetic Resonance"). Funding had been approved by the Program Steering Committee on its launch meeting in Tarragona. The total assigned budget was 51.000 euros.

The meeting was a scientific success and the contribution of the ESF RNP was used to help the participation of 104 students and postdoc (56 from Russia) and partially contribute to the expenses of 36 speakers.

With the help of the EMAR program, the EUROMAR kept its previous edition and gathered participants from 25 different European countries. It also consolidated the role of European Magnetic Resonance worldwide with a 18% participation of non-Europeans, coming from 18 countries of America, Australasia and Africa. EMAR received a large publicity and several non-participating countries have shown their interest in joining the network.

Description of the scientific content of the event

EUROMAR-2008

The **EUROMAR 2008 conference** took place in St.-Petersburg (Russia) from 6 to 10th of July. The conference was followed by two satellite meetings:

1 – **NMRCN School** from 3 to 5 July and

2 – **NMR and NQR studies of explosives**, from 7 to 10th of July.

The RNP “Multidisciplinary Frontiers of Magnetic Resonance” shares the same goals that inspired this series of conferences

- a) Exploring new frontiers.
- b) Bringing together the different specialties within the broad field of magnetic resonance.
- c) Integrating groups from different countries and facilitating new collaborations.
- d) Training of young researchers.

Scientific Program

Scientific program of EUROMAR-2008 was well balanced between different fields. Plenary and Key note lectures were delivered by well known scientists of the program committee from different areas of the field and included Liquid state NMR, EPR, Drug discovery, Dynamics, Biological NMR, Solid State NMR of biological and material systems, and new methods. Among the speakers were leading person in nanometer-scale magnetic resonance imaging (Prof. D.Rugar), leading person in solid state NMR of macromolecular and supramolecular systems (Prof. H.Spiess), pioneer of Xe NMR (Prof. J.Fraissard), leading person in ultrafast nD NMR (Prof. L.Frydman). Geographically speakers represent all the continents: Europe, America, Asia.

Parallel sessions were arranged thematically as follows:

Bio-Macromolecules in Liquids,

Drug discovery,

Relaxation,

Frontiers,

Molecular Dynamics and other Computational Aspects,

Applications in Catalysis,

Imaging,

Enhanced Magnetic Resonance,

Spin dynamics in solids

Biosolids,

Methods for Biosolids,

ESR methods&Paramagnetic Systems,

ESR-applications,

Solid-state physics and Polymers,

In each of the sessions a broad definition of the subject was used, so that specialists in different areas may be exposed to input their knowledge to different fields.

New methodological approaches in application to new problems also were demonstrated in each of the sessions. Thus in "Bio-macromolecules in liquids" session were suggested new signal acquisition schemes which improve NMR spectra, the latter is important for study of proteins structures as well as for mechanism of conformational transitions.

Molecular Dynamics and Computational Aspects session was devoted to investigation of protein dynamics by NMR and quantum chemical calculations. On several examples were demonstrated validation of protein dynamics obtained by NMR and molecular dynamic simulations. NMR-oriented model based on network of coupled rotators allows predict protein dynamics and thermodynamics.

Well-known EPR specialists have presented their new results in application to biological systems. Long-range constraints for the partially ordered structures that occur during folding cannot be obtained by any established technique. With site-directed spin labelling a significant fraction of such proteins is accessible to pulsed EPR experiments. However, a labelling approach implies that only a small number of constraints can be obtained whose precision appears to depend on the label size. Application of Spin-label EPR were demonstrated also by Prof. M.Drescher and Prof. G. Jeschke for protein-membrane interaction and by Prof. Yu.D.Tsvetkov for peptides.

New possibilities of modern EPR in material science were demonstrated by Prof. A.Schnegg, Prof. K.P.Dinse, Prof. E.Bagryanskaya and Prof. P.G.Baranov. Combining the high-power THz radiation in BESSY's low alpha mode with a modified FT spectrometer (operating from 100 GHz to 3 THz, which exploits THz radiation provided by a newly developed THz beamline at the Berlin synchrotron BESSY) and low noise InSb bolometers it became possible to detect the temperature dependence of spin transitions in single molecular magnets at earth magnetic fields. (A.Schnegg).

K.P. Dinse has shown that the multi-frequency approach extending to Larmor frequencies beyond 100 GHz opens the way for detailed studies of high spin systems. ESR studies of spin transitions and exchange interaction in strongly coupled spin triads were presented by E.Bagryanskaya.

High frequency (95 GHz) EPR and ENDOR experiments on ZnO nanoparticles, doped by Al unambiguously reveal the presence of shallow donors related to substitutional Al atoms located in Zn position. (P.G.Baranov).

The Imaging session included applications in humans and materials. Prof. K.P.Pruessmann has analyzed ultra-high-field MR in humans. Nowadays the number of human MR research projects involving field strengths of 7 Tesla or higher has passed the mark of 30 worldwide. Due to greater sensitivity ultra-high-field MR in humans may soon become a key modality of modern neuroscience.

Prof. T.Meersmann has demonstrated the feasibility of biological, hyperpolarized ^{83}Kr MRI with natural abundance krypton in excised rat lungs using a custom designed ventilation chamber.

Prof. P.T.Callaghan group was presented by K.W.Feindel with rheo-NMR investigations of vorticity structuring and fluctuations in shear-banded flow for a wormlike micellar solution. Their results show the existence of a fluctuating vorticity structure which is coupled to applied strain rate.

A.Jerschow has shown that intermolecular multiple-quantum coherences (iMQCs) can enhance contrast in CEST/MT/NOE experiments. These methods were demonstrated with the clinically relevant system of glycosaminoglycans (GAGs), which are important for imaging cartilage, the intervertebral disc, the cornea, and heart valves.

Advances in mobile NMR were demonstrated by its founder Prof. B. Blümich. He told about the developments of their research team in designing new magnets for mobile NMR and in applying them to new topics in materials science and chemical engineering. One class of objects that has become available to NMR analysis by depth profiling with single-sided sensors is musical instruments, in particular violins and bows, where different varnish layers and their thicknesses can be characterized.

In Solid State NMR along with the methods allowing obtain NMR parameters were demonstrated the methods allowing establishing correlation experiments between quadrupolar nuclei and dipolar nuclei, or between quadrupolar nuclei (D.Massiot). In order to reach higher and higher spinning speeds in MAS the new probe were demonstrated with the rotation frequency of 70 kHz (with 1.3 mm rotors) (D.Mueller). Ultra high field ^{91}Zr NMR investigations in 17.6 T (superconducting magnet) and in 30 T (a resistive magnet) of zirconium halides reveal empirical correlations between ^{91}Zr NMR parameters (δ , ΔCSA , CQ , ηQ) and structural parameters (coordination, bond length...). The measured isotropic chemical shift values lie between -250 and 2000 ppm, and C_Q values between 10 and 50 MHz. (O. Pauvert).

Spin Dynamics in Solids session demonstrated variable temperature solid state NMR and cryogenic investigations for study of molecular complexes, containing endohedral hydrogen molecules in fullerenes (M. Carravetta) and for dynamic disorder of sodium in two highly symmetric molecules (van Beek).

The Frontiers session included talks in NMR/medicine areas. Thus Prof.O.N. Antzutkin lecture was devoted to solid state ^{17}O , ^{13}C , and ^{15}N NMR on alzheimer's fibrils and on anti-inflammatory drug.

John Christodoulou work is allowing to describe in detail the relationship between biosynthesis and folding and also to understand how molecular chaperones that interact with the nascent chain such as the trigger factor affect protein folding. Additionally, these studies could be of importance in understanding protein misfolding disease which includes neurodegenerative diseases such Parkinson's and Alzheimer's.

The connection between NMR and EPR was further stressed.

The Catalysis application session demonstrated applications of ex- and in-situ NMR methods in heterogeneous catalysis.

In Relaxation session was demonstrated applications of the technique in different areas. Internal protein dynamics were probed by solid and liquid state NMR. Solution and in solid methyl ^{13}C relaxation is dominated by fast (~10-100 ps) methyl rotation. ^{15}N relaxation provides a different sampling of internal dynamics. In solution, nitrogen relaxation data are sensitive to the picosecond motions, whereas nanosecond (~1-100 ns) timescale dynamics contributes efficiently to the ^{15}N relaxation in solids (N.R.Skrynnikov).

The quadrupole relaxation in liquid water has been investigated by J. Schmidt both experimentally and theoretically.

In several lectures (M.Levitt, P. R.Vasos and G.Pileio) was shown the existence of singlet spin states with life-times that are much longer than T_1 . For nitrous oxide in solution approaching lifetimes was determined of half an hour.

Enhanced Magnetic Resonance included a view of the different approaches to improve NMR signals. Unique two-isocentre magnet (3.4T and 9.4T) spectrometer was constructed for NMR spectroscopy using enhanced spin polarisation generated by

dissolution dynamic nuclear polarisation (DNP).(W.Köckenberger). Hyperpolarized ^1H NMR employing low γ nucleus as a spin order storage (E.Y.Chekmenev) was demonstrated. Multiple-oscillating techniques was proposed for dipolar recoupling without dipolar truncation (N.C.Nielsen).

In Biosolids methods session Prof.L.Emsley demonstrated progress towards making the active sites in paramagnetic proteins visible to NMR studies by the use of MAS at very high speeds (>60 kHz).

P.K. Madhu has presented decoupling scheme, swept-frequency TPPM (SWf-TPPM), which performs better than the other schemes under both magic-angle spinning and static conditions of the sample. NMR-micro-probe designed for the analysis of sample volumes in the range of $V_s = 5\text{--}50$ nl for mass limited biological samples were demonstrated by Prof.T.Riemer.

Applications of NMR in biology were demonstrated in Biosolids session. Prof.S.Hediger has shown Solid state NMR study of the bacterial cell wall. Protein structure determination by MAS solid state NMR was given in Prof. H.Oschkinat lecture. A structural link between inactivation and inhibition of a K^+ channel was presented by C.Ader.

Drugs session typically restricted to liquids, included the use of solid state NMR. W. Jahnke has presented NMR-based strategies to identify novel kinase inhibitors which play critical roles in intracellular signal transduction pathways, deregulation of which can lead to a variety of pathological states and diseases such as cancer.

Quantitative online NMR spectroscopy was demonstrated in application to industrial reactions.

407 posters were presented continuously during the conference and each day two hours were allocated to individual discussions.

Satellite meetings

The specific feature of EUROMAR-2008 was the School for young participants, which was organized two days before the conference. For young participants the School was without any registration fee. Members of the Program Committee were kindly agreed and gave lectures on the School, among them: president of AMPERE (Prof.B.Meier), president of EUROMAR (Prof.G.Bodenhausen). The level of the lectures was extremely high, the same as on the conference. Each professor gave new material in the frame of conference topic. Solid state NMR was presented by the leaders in this field Prof. D.Massiot and Dr.D.Mueller. Prof.G.Bodenhausen gave a lecture about Nitrogen-14 NMR (40 years of which is noted this year). State of the art in situ Flow-MAS technique and its application in heterogeneous catalysis were represented by its founder Prof. M.Hunger. MRI – principles and applications were demonstrated by Prof. I.Koptyug and Dr.U.Eichhoff. Prof. B.Meier told how magnetic resonance force detection can be combined with NMR spectroscopy to achieve a spatial resolution of one micrometer and less.

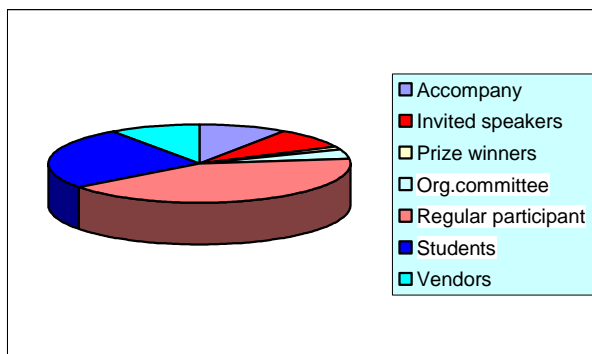
An important event of the School was the talks of Zamaraev Prize Winners (S.Arzumanov, K.Kovtunov, V.Zhivonitko). Zamaraev Prize is awarded to university or PhD students for their work in spectroscopy field. This year it was MR spectroscopy. Satellite meeting of MR for detection of explosives was directly connected to Nitrogen-14 NMR and NQR. High level specialists from USA, Australia, Germany and Russia represented their results and achievements in this field. The School and satellite meeting increased the chances of active participation for 23 speakers and attached additional participants to the main meeting.

Assessment of the results and impact of the meeting

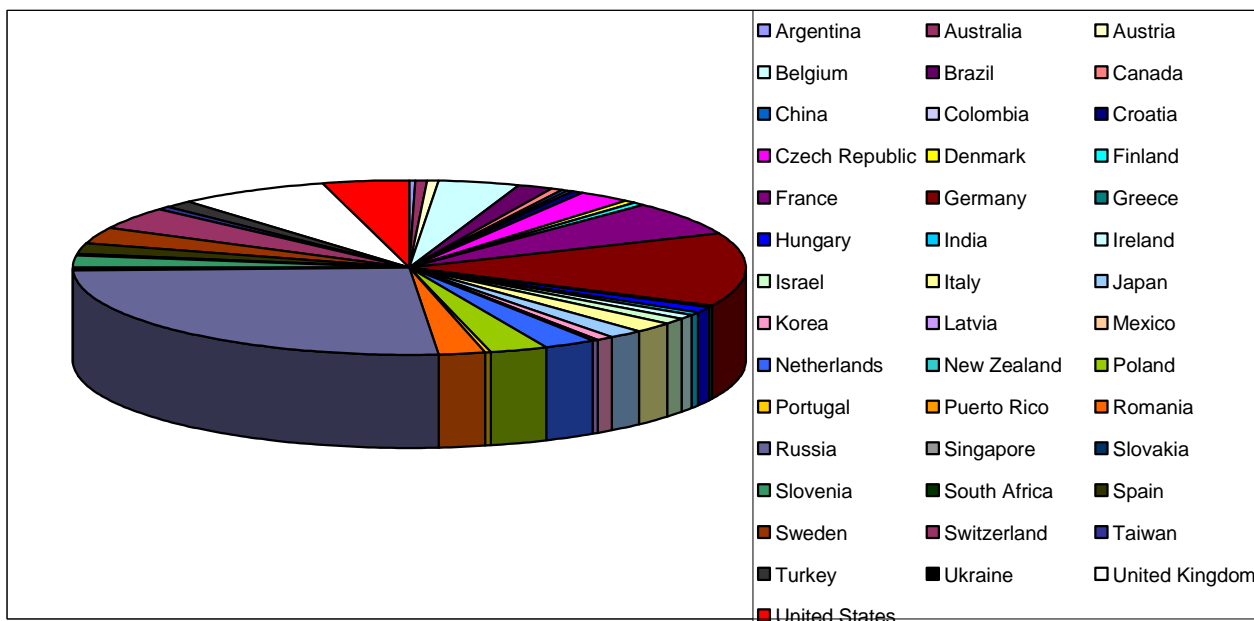
Statistics of attendance

The total number of participants was 704 (in Tarragona 673) divided in

- 9 Prize winner speakers
- 10 plenary speakers
- 14 key note speakers
- 12 speakers on the school
- 60 speakers in parallel sessions
- 284 regular participants
- 180 students
- 69 exhibitors
- 66- accompany

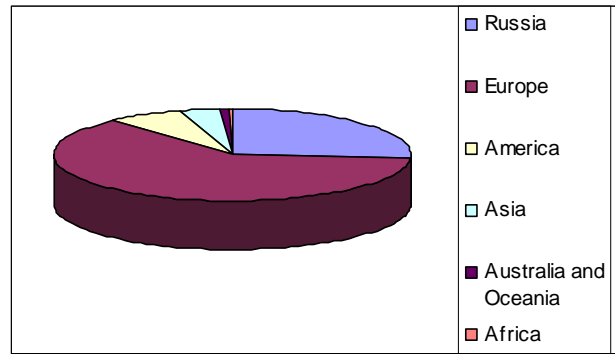


The participants came from 43 different countries (43 was in Tarragona too, but Nigeria, Tunisia, Pakistan, Iran, Bulgaria, Iceland and Guinea were replaced by Colombia, Latvia, Singapore, South Africa, Taiwan, Turkey and Ukraine).



with the following distribution per areas:

| | |
|--------------------------|-----|
| Russia | 183 |
| Europe | 439 |
| America | 48 |
| Asia | 26 |
| Australia and Oceania | 7 |
| Africa | 1 |



In comparison with Tarragona (537-Europe, 78 – Americas, 27 Australasia, 13 – Africa), it could be noted, that the number of Americas decreases (expensive trip), while the number of Russian increases. In York there were only 4 Russians, in Tarragona -8. This is very important, since only St. Petersburg open EUROMAR for Russians and I do hope that the number of Russians in the following EUROMAR conferences will never back to the York number. Certainly, it will not be 183, but it will be comparable with European countries. In St. Petersburg practically there were no African people, who are really very rare come to Russia.

Extending the network to other European countries is one of the milestone of the EMAR program. EUROMAR-2008 attracted East European countries, not only Russia, for the first time Latvia participated in EUROMAR, significantly (several times) increased participants numbering from Poland, Czech Republic and Slovenia.

The participation of students and postdocs is essential for the training objectives of the EMAR program. This year for all young participants (for 190) was organized free of charge School with extra high level lectures and fantastic social program (it is enough to tell that during 4-5 July school participants visited Tsarskoe selo, Petergohh, had nigh boat trip along the channels and the river). The EMAR has provided stipends covering part of the cost of attendance both students and their lecturers.

In summary: with the help of the ESF the 2008 EUROMAR meeting has keep and even reached its most ambitious objectives:

It has keep and even increased the participation in comparison with Tarragona

It prove to be a meeting place for the different European efforts to articulate the magnetic resonance community

It has brought together the participants from 43 different countries (including 25 European). The numbering is practically coinciding with Tarragona, however 7 new countries were attracted to EUROMAR-2008, while 7 countries – were lost. So if the next organizers will attract all these countries, the total number of the countries could be up to 50.

The scientific program of the conference and of the school was of the quality that has been rated as comparable to the most renowned magnetic conference in the world.

Summer School NMRCM -2008
St.Petersburg, Russia, 4 – 5 July 2008

Thursday 3th July, Afternoon

Hall

18:00-20:00 **Registration**

Friday 4th July, Morning

Hall

08:30-09:40 **Registration**

Lecture Hall

09.40-09.50 **Welcome by Vladimir Chizhik**
09.50-10.40 **Uwe Eichhoff**
FROM SPECTROSCOPY TO SPECTRAL IMAGING
10.40-11.00 **Break**
11.00-11.50 **Detlef Müller**
SPINS AT THE SPEED OF SOUND
11.50-12.40 **Geoffrey Bodenhausen**
NITROGEN-14 NMR
12.40-14.30 **Lunch**

Friday 4th July, Afternoon

Lecture Hall

14.30-15.20 **Igor V. Koptug**
MAGNETIC RESONANCE IMAGING – PRINCIPLES AND APPLICATIONS IN CHEMISTRY
AND RELATED FIELDS
15.20-16.10 **Michael Hunger**
STATE OF THE ART AND APPLICATIONS OF IN SITU SOLID-STATE NMR
SPECTROSCOPY IN HETEROGENEOUS CATALYSIS
16.10-16.30 **Break**
16.30-16.45 **Liudmila A. Zamaraeva**
About K.I. Zamaraev
16.45-17.10 **Sergey Arzumanov**
¹³C AND ¹H MAS NMR FOR STUDY OF CONVERSION OF HYDROCARBONS OVER
SOLID ACID CATALYSTS
17.10-17.35 **Kiril Kovtunov**
PARAHYDROGEN INDUCED POLARIZATION IN HETEROGENEOUS
HYDROGENATIONS

- 17.35-18.00 **Vladimir Zhivonitko**
AN MRI STUDY OF TRANSPORT INFLUENCE ON PROPAGATION OF A CHEMICAL REACTION FRONTS
- 18.30-23.00 **Party Tsarskoe Selo**

Saturday 5th July, Morning

Lecture Hall

- 09.00-09.50 **Beat Meier**
LOCALIZED NMR SPECTROSCOPY WITH A MAGNETIC RESONANCE FORCE MICROSCOPE: DIRECT REAL SPACE DETECTION OF NUCLEAR SPIN DIFFUSION AND OTHER APPLICATIONS
- 09.50-10.40 **Dominique Massiot**
HOW TO EFFICIENTLY OBSERVE QUADRUPOLEAR IN SOLIDS AND USE THEM IN CORRELATION EXPERIMENTS
- 10.40-11.00 **Break**
- 11.00-11.50 **Alexander Arseniev**
COMPREHENSIVE STUDY OF HELIX-HELIX INTERACTIONS IN TRANSMEMBRANE PROTEIN DIMERS
- 11.50-12.40 **Martin Billeter**
'FAST' NMR: PROTEIN CHARACTERISATION USING PROJECTION SPECTROSCOPY
- 12.40-14.30 **Lunch**

Saturday 5th July, Afternoon

Lecture Hall

- 14.00-17.00 **Excursion to Peterhoff**
- 17.00-17.30 **Break**
- 17.30-18.20 **Bekir Aktaş**
FERROMAGNETIC RESONANCE STUDIES OF MAGNETIC NANOSTRUCTURES
- 18.20-19.10 **Murat Tagirov**
A NEW ASPECT OF ENHANCED MAGNETIC RESONANCE
- 20.00 **Departure to the City**
- 24.00-03.00 **Night boat trip**

EUROMAR 2008
St.Petersburg, Russia, 6 – 11 July 2008

Sunday 6th July, Afternoon

Academy Hall

10:00-19:00 **Registration**

Manege

- 16:30-16:35 Opening of Euromar 2008 by **Olga Lapina**
- 16:35-16:50 A FEW DETAILS ABOUT MR IN RUSSIA by **Vladimir Chizhik**
- 16:50-17:00 Opening of Euromar-2008 by Ampere president **Beat Meier**
- 17:00-17:45 Opening Lecture by chair of Euromar **Geoffrey Bodenhausen**
- 17:45-17:50 Presentation of Andrew Prize by **Hans Spiess**
- 17:50-18:25 Lecture of Andrew Prize winner **Boaz Shapira**
SPATIAL ENCODING IN NMR SPECTROSCOPY
- 18:25-18:30 Presentation of Russel Varian Prize by **Vladimir Sklenář**
- 18:30-19:15 Lecture of the Russel Varian Winner **Alexander Pines**, Glenn T. Seaborg Professor of Chemistry
SOME RECOLLECTIONS OF THE EARLY DAYS OF HIGH-RESOLUTION SOLID-STATE NMR
- 19:30 **Welcome Party**

Monday 7th July, Morning

Manege

- 08:30-10:00 **Plenary Lectures**
Chaired by **Thomas Prisner** and **Beat H. Meier**
- 08:30-9:15 **Wolfgang Lubitz**
MAGNETIC RESONANCE STUDIES TO ELUCIDATE STRUCTURE AND FUNCTION OF THE WATER SPLITTING COMPLEX IN PHOTOSYNTHESIS
- 09:15-9:15 **Daniel Rugar**
NANOMETER-SCALE MAGNETIC RESONANCE IMAGING
- 10:00-10:40 **Refreshment Break**

Presidium Hall

- 10:40-12:35 Session: **Bio-Macromolecules in Liquids**
Chair: **Alexander Arseniev**
- 10:40-11:20 **Miquel Pons**
NMR AND SAXS STUDIES OF FLEXIBLE PROTEINS AND PROTEIN COMPLEXES
- 11:20-11:45 **Fred F. Damberger**
MECHANISM OF LIGAND UPTAKE AND RELEASE IN INSECT PHEROMONE BINDING PROTEINS
- 11:45-12:10 **Vladislav Orekhov**
DIVIDED EVOLUTION: A SCHEME FOR SUPPRESSION OF LINE BROADENING INDUCED BY CONFORMATIONAL EXCHANGE

12:10-12:35 **Konstantin Pervushin**
SARS CORONAVIRUS ENVELOPE PROTEIN: SOLUTION AND SOLID STATE NMR STUDIES
OF TRANSMEMBRANE OLIGOMERIC CHANNELS

University Hall

10:40-12:35 Session: **ESR methods and Paramagnetic Systems**
Chair: **Kev Salikhov**

10:40-11:20 **Thomas Prisner**
E

11:20-11:45 **Elena Bagryanskaya**
SPIN TRANSITIONS, EXCHANGE INTERACTION AND LIESST IN STRONGLY-COUPLED SPIN
TRIADS AS STUDIED BY EPR

11:45-12:10 **Alexander Schnegg**
FOURIER TRANSFORM THZ EPR ON SINGLE MOLECULAR MAGNETS

12:10-12:35 **Malte Drescher**
PROTEINE-MEMBRANE-INTERACTION MONITORED BY SPIN-LABEL-EPR

Petrovskii Hall

10:35-12:35 Session: **NMR and NQR in spotting explosives**

10:35-11:20 Plenary Lecture chaired by **Jacques Fraissard**
Allen N. Garroway*, **Joel B. Miller**
INTRODUCTION TO THE PROBLEM OF EXPLOSIVES DETECTION BY MAGNETIC
RESONANCE

11:20-12:35 Chair: **Claude Fermon**

11:20-11:45 **Janko Luznik**
POLARIZATION ENHANCED NQR DETECTION AT LOW FREQUENCIES

11:45-12:10 **Myriam Pannetier-Lecoeur**
LOW FIELD NMR WITH SUPERCONDUCTING-GMR MIXED SENSORS. Part 1

12:35-14:00 **Lunch**

Monday 7th July, Afternoon

14:00-16:00 **Poster session** in University corridor

Presidium Hall

16:00-18:45 Session: **Molecular Dynamics and other Computational Aspects**
Chair: **Alexandre Bonvin**

16:00-16:40 **Bruchweiler**
COMBINED VALIDATION AND INTERPRETATION OF PROTEIN DYNAMICS BY NMR AND
MOLECULAR DYNAMICS SIMULATIONS

16:40-17:05 **András Perczel**
THE DYNAMIC STRUCTURAL DIMENSION OF CHEMICAL SHIFTS

17:05-17:30 **François Bontems**
NMR AND SAXS STUDY OF THE RIBONUCLEASE REGB / RIBOSOMAL PROTEIN S1 SYSTEM

17:30-17:55 **Daniel Abergel**
PREDICTION OF PROTEIN DYNAMICS AND THERMODYNAMICS FROM A NETWORK OF
COUPLED ROTATORS

University Hall

16:00-18:45 Session: **Imaging**
Chair: **Igor V. Koptug**

16:00-16:40 **Alexandre Khrapitchev**
UTE VERSUS SPRITE FOR ROBUST MR IMAGING

- 16:40-17:05 **Thomas Meersmann**
HYPERPOLARIZED KRYPTON-83 MRI OF LUNGS – A FEASIBILITY STUDY
- 17:05-17:30 **Kirk W. Feindel**
NMR VELOCIMETRY INVESTIGATIONS OF SHEAR-BANDING STRUCTURE AND FLUCTUATIONS IN WORM-LIKE MICELLES
- 17:30-17:55 **Alexej Jerschow**
CEST IMAGING WITH INTERMOLECULAR MULTIPLE-QUANTUM COHERENCES

Petrovskii Hall

- 16:00-18:45 Session: **NMR and NQR in spotting explosives**
- 16:00-17:30 Chair: **Janez Seliger**
- 16:00-16:45 Plenary lecture chaired by **Daniel Canet**
Joel B. Miller
EFFICIENT EXCITATION OF NQR
- 16:45-17:10 **Alexei F. Privalov**
APPLICABILITY OF DOUBLE NMR/NQR WITH DIRECT AND INDIRECT DETECTION OF ¹⁴N NQR FOR TNT DETECTION
- 17:10-17:35 **Alan Gregorovič**
ENHANCED NQR DETECTION OF TNT

University Hall

- 18:00-18:45 **Plenary Lecture**
Chaired by **Martin Billeter**
Gunnar Jeschke
MEMBRANE PROTEIN STRUCTURE AND FOLDING - WHAT CAN EPR CONTRIBUTE?

Tuesday 8th July, Morning

Manege

- 08:30-10:00 **Plenary Lectures**
Chaired by **Igor Koptug** and **Hans Spiess**
- 08:30-9:15 **Bernhard Blümich**
ADVANCES IN MOBILE NMR: MAGNETS, VIOLINS, AND BUBBLES
- 09:15-9:15 **Gerhard Wagner**
NON-STANDARD ACQUISITION AND PROCESSING METHODS – APPLICATION TO STUDIES OF LARGE PROTEINS, PROTEIN COMPLEXES AND METABOLITE MIXTURES
- 10:00-10:40 **Refreshment Break**

Presidium Hall

- 10:40-12:35 Session: **Spin dynamics in solids**
Chair: **Zeev Luz**
- 10:40-11:20 **Marina Carravetta**
CRYOGENIC INVESTIGATION OF MOLECULAR HYDROGEN IN FULLERENES BY MEANS OF NMR, IR AND INS
- 11:20-11:45 **Jacco D. van Beek**
FAST DYNAMIC DISORDER OF SODIUM ATOMS IN THE CRYSTALLINE FORMS OF TWO HIGHLY SYMMETRIC MOLECULES
- 11:45-12:10 **Olivier Pauvert**
⁹¹Zr NMR AT VERY HIGH FIELD IN ZIRCONIUM HALIDES
- 12:10-12:35 **Oleg N. Antzutkin**
SOLID-STATE ¹⁷O, ¹³C AND ¹⁵N NMR ON ALZHEIMER'S A-BETA FIBRILS AND ON ANTI-INFLAMMATORY DRUG, INDOMETHACIN-SACCHARIN COCRYSTAL

University Hall

- 10:40-12:35 Session: **ESR-applications**
Chair: **Vadim Atsarkin**
- 10:40-11:20 **Klaus-Peter Dinse**
HIGH FREQUENCY EPR IN CHEMISTRY AND MATERIAL SCIENCES
- 11:20-11:45 **Pavel G. Baranov**
RADIO SPECTROSCOPY OF Al DOPED ZnO NANOCRYSTALS
- 11:45-12:10 **Yuri Tsvetkov**
SPIN-LABELED PEPTIDES AS STUDIED BY PULSED DOUBLE ELECTRON-ELECTRON RESONANCE(PELDOR)
- 12:10-12:35 **Sabine Van Doorslaer**
ANALYSIS OF HETEROGENEOUS CATALYSTS USING EPR TECHNIQUES

Petrovskii Hall

- 10:35-12:35 Session: **NMR and NQR in spotting explosives**
- 10:35-11:20 Plenary lecture chaired by **Karen Sauer**
Daniel Canet
FUNDAMENTALS OF PULSED NITROGEN-14 QUADRUPOLE RESONANCE : NUTATION, DATA AVERAGING, TWO-PULSE SEQUENCES, PULSE TRAINS.
- 11:20-12:35 Chair: **Hector Robert**
- 11:20-11:45 **Claude Fermon**
LOW FIELD NMR WITH SUPERCONDUCTING-GMR MIXED SENSORS. Part 2
- 11:45-12:10 **Janez Seliger**
DOUBLE RESONANCE DETECTION OF (MAINLY NITROGEN) NQR FREQUENCIES IN EXPLOSIVES AND DRUGS.
- 12:10-12:35 **George V. Mozhukhin**
THE TWO-FREQUENCY MULTIPULSE SEQUENCE IN NUCLEAR QUADRUPOLE RESONANCE OF N-14 NUCLEI.
- 12:35-14:00 **Lunch**

Tuesday 8th July, Afternoon

- 14:00-16:00 **Poster session** in University corridor

Presidium Hall

- 16:00-18:45 Session: **Applications in Catalysis**
Chair: **Michael Hunger**
- 16:00-16:40 **Clare P. Grey**
FOLLOWING THE LOCAL STRUCTURAL CHANGES BY IN-AND EX-SITU METHODS. APPLICATIONS TO BATTERIES AND ANION SEQUESTRATION
- 16:40-17:05 **Dieter Michel**
MOLECULAR MOTION OF ADSORBED MOLECULES AND GLASS TRANSITION IN CONFINED GEOMETRY
- 17:05-17:30 **Vanja Pinoie**
HRMAS NMR FOR MONITORING SUPPORTED ORGANOTIN CATALYSTS AND QUANTITATIVE DETERMINATION OF THE TIN LOADING USING THE ERETIC METHOD
- 17:30-17:55 **Anna A. Lysova**
STUDY OF THE DISTRIBUTION OF THE ACTIVE COMPONENT IN THE CATALYST PELLETS DURING THEIR PREPARATION BY NMR IMAGING TECHNIQUES

University Hall

- 16:00-18:45 Session: **Relaxation**
Chair: **Alexej Jerschow**
- 16:00-16:40 **Nikolai R. Skrynnikov**
TOWARD A CONSISTENT PICTURE OF INTERNAL PROTEIN DYNAMICS AS PROBED BY SOLID- AND SOLUTION-STATE NMR

- 16:40-17:05 **Jochen Schmidt**,
NUCLEAR QUADRUPOLE RELAXATION IN LIQUID WATER FROM QUANTUM CHEMICAL CALCULATIONS
- 17:05-17:30 **Paul Vasos**
LONG-LIVED STATES: HOW MANY SPINS CAN BE INVOLVED AND HOW?
- 17:30-17:55 **Jens Dittmer**
SUPPRESSION OF THE EFFECT OF HOMONUCLEAR J-COUPPLINGS IN RELAXATION EXPERIMENTS

Petrovskii Hall

- 15:15-18:45 Session: **NMR and NQR in spotting explosives**
- 15:15-16:00 Plenary lecture chaired by **Janko Luznik**
Karen L. Sauer
THE MANY FACES OF DOUBLE RESONANCE: FROM NUCLEAR CROSS RELAXATION TO RF MAGNETOMETRY IN EXPLOSIVES DETECTION
- 16:00-17:05 Chair: **Taras Rudakov**
- 16:00-16:40 **Hector Robert**
MODELING OF QR SENSOR PERFORMANCE FOR OPTIMIZED EXPLOSIVES DETECTION
- 16:40-17:05 **Maude Ferrari**
THE TWO PULSE SEQUENCE IN ^{14}N QUADRUPOLE RESONANCE
- 17:05-18:00 **General Discussions**

University Hall

- 18:00-18:45 **Plenary lecture**
Chaired by **Bernhard Blümich**
- 18:00-18:45 **Klaas P. Pruessmann**
ULTRA-HIGH-FIELD MAGNETIC RESONANCE IN HUMANS

Wednesday 9th July, Morning

Manege

- 08:30-10:00 **Plenary Lectures**
Chaired by **Geoffrey Bodenhausen** and **Dominique Massiot**
- 08:30-9:15 **Lucio Frydman**
PROGRESS IN SINGLE-SCAN MULTIDIMENSIONAL NMR
- 09:15-9:15 **Chris J. Pickard**
A SOLID STATE PHYSICS THEORY OF SOLID STATE NMR
- 10:00-10:40 **Refreshment Break**

Presidium Hall

- 10:40-12:35 Session: **Enhanced Magnetic Resonance**
Chair: **Christian Griesinger**
- 10:40-11:20 **Walter Köckenberger**
A DNP-NMR SPECTROMETER FOR FAST SPECTROSCOPY
- 11:20-11:45 **Eduard Y. Chekmenev**
HYPERPOLARIZED ^1H NMR EMPLOYING LOW γ - NUCLEUS AS A SPIN ORDER STORAGE
- 11:45-12:10 **Niels Chr. Nielsen**
MULTIPLE-OSCILLATING-FIELD TECHNIQUES FOR DIPOLAR RECOUPLING WITHOUT DIPOLAR TRUNCATION
- 12:10-12:35 **Mark J. Prandolini**
THE OVERHAUSER EFFECT AT HIGH MAGNETIC FIELDS

University Hall

- 10:40-12:35 Session: **Methods for Biosolids**
Chair: **Edward Fel'dman**

- 10:40-11:20 **Lyndon Emsley**
NMR CRYSTALLOGRAPHY OF PROTEINS
- 11:20-11:45 **Perunthiruthy K. Madhu**
HETERONUCLEAR AND HOMONUCLEAR DIPOLAR DECOUPLING AT HIGH MAS RATES
- 11:45-12:10 **Sabine Hediger**
SOLID-STATE NMR STUDY OF THE BACTERIAL CELL WALL
- 12:10-12:35 **Thomas Riemer**
SILICON-CYLINDER-SPIRAL

Petrovskii Hall

- 11:20-12:30 Session: **NMR and NQR in spotting explosives**
- 11:20-12:35 Chair: **Pablo Prado**
- 11:20-11:45 **Robert J. Prance**
DEVELOPMENT OF ELECTRIC FIELD NMR
- 11:45-12:30 **Taras N. Rudakov**
DETECTION OF EXPLOSIVES BY NQR METHOD: MAIN ASPECTS FOR TRANSPORT SECURITY
- 12:35-14:00 **Lunch**

Wednesday 9th July, Afternoon

- 15:00-18:00 **Excursions**
- 19:00-22:00 **Banquet**

Thursday 10th July, Morning

University Hall

- 08:30-10:00 **Plenary lectures**
Chaired by **Lyndon Emsley** and **Thomas Meersmann**
- 08:30-9:15 **Hans Wolfgang Spiess**
SOLID-STATE NMR METHODS OF FUNCTIONAL MACROMOLECULAR AND SUPRAMOLECULAR SYSTEMS
- 09:15-9:15 **Jacques Fraissard**
NMR OF PHYSISORBED ^{129}Xe USED AS A PROBE TO INVESTIGATE POROUS SOLIDS
- 10:00-10:40 **Refreshment Break**

University Hall

- 10:40-12:35 Session: **Biosolids**
Chair: **Miquel Pons**
- 10:40-11:20 **Hartmut Oschkinat**
PROTEIN STRUCTURE DETERMINATION BY MAS SOLID-STATE NMR
- 11:20-11:45 **Christian Ader**
A STRUCTURAL LINK BETWEEN INACTIVATION AND INHIBITION OF A K⁺ CHANNEL
- 11:45-12:10 **Matthias Huber**
STUDIES OF PARAMAGNETIC DIALANINATOCOPPER(II) BY SOLID-STATE NMR AND BY EPR
- 12:10-12:35 **Giuseppe Pileio**
INTERNUCLEAR COUPLINGS IN THE SOLID-STATE NMR OF MULTIPLE-SPIN SYSTEMS BY SELECTIVE SPIN ECHOES IN OFF-MAGIC-ANGLE SPINNING SAMPLES

Presidium Hall

- 10:40-12:35 Session: **Frontiers**
Chair: **Lyndon Emsley**
- 10:40-11:20 **Norbert Müller**
IMPROVING THE EFFICIENCY OF DETERMINING CROSS-CORRELATION RATES IN PARAMAGNETIC SYSTEMS
- 11:20-11:45 **Guido Pintacuda**
SUPERADIABATIC PULSES IN NMR
- 11:45-12:10 **John Christodoulou**
CO-TRANSLATIONAL PROTEIN FOLDING ON THE RIBOSOME: THE STRUCTURE AND DYNAMICS RIBOSOME-NASCENT CHAIN COMPLEXES USING NMR SPECTROSCOPY
- 12:10-12:35 **Gil Navon**
CROSS CORRELATION BETWEEN QUADRUPOLEAR INTERACTION AND PARAMAGNETIC G ANISOTROPY

Petrovskii Hall

- 10:35-12:35 Session: **NMR and NQR in spotting explosives**
Chair: **Robert Prance**
- 10:35-11:20 **Pablo J. Prado**
COMPACT, ALL-IN-ONE MR DIAGNOSTIC INSTRUMENT
- 11:20-11:45 **Jörg Mauler**
IDENTIFICATION OF LIQUIDS ENCOUNTERED IN CARRY-ON LUGGAGE BY MOBILE NMR
- 11:45-12:10 **Ramil R. Gainov**
CONTRIBUTION OF NQR-SPECTROSCOPY IN STUDIES OF SOME COMPLEX SULFIDES
- 12:35-14:00 **Lunch**

Thursday 10th July, Afternoon

- 14:00-15:00 **Poster session** in University corridor

University hall

- 15:00-16:45 Session: **Drug discovery**
Chair: **Anita Marsaioli**
- 15:00-15:40 **Wolfgang Jahnke**
NMR-BASED CHARACTERIZATION OF PROTEIN TYROSINE KINASE INHIBITOR COMPLEXES
- 15:40-16:05 **Brian Cutting**
FAST DEVELOPMENT OF PHARMACEUTICAL LEAD COMPOUNDS: HYBRIDIZING PARAMAGNETIC NMR WITH CHEMICAL SYNTHESIS
- 16:05-16:30 **Oliver Steinhof**
QUANTITATIVE ONLINE-NMR SPECTROSCOPY IN PROCESS ANALYTICS: COUPLING WITH BATCH REACTORS AND MICROREACTORS IN STUDIES OF COMPLEX INDUSTRIAL REACTION NETWORKS
- 16:30-16:55 **Julien Orts**
INPHARMA PREDICTS THE CORRECT BINDING MODE OF LIGANDS TO MACROMOLECULAR RECEPTORS

Presidium hall

- 15:00-17:45 Session: **Solid state physics and polymers**
Chair: **Jadwiga Tritt-Goc**
- 15:00-15:40 **Kay Saalwächter**
PROTON TIME-DOMAIN NMR TO STUDY INTERMEDIATE DYNAMICS IN SEMICRYSTALLINE AND MOLTEN POLYMERS
- 15:40-16:05 **Matthias J. N. Junk**
NANO-INHOMOGENEITIES IN STRUCTURE AND REACTIVITY OF THERMORESPONSIVE HYDROGELS PROBED BY EPR SPECTROSCOPY
- 16:05-16:30 **Jan Pilař**
TRACER DIFFUSION IN POLYMER HYDROGELS. ESRI, PGSTE AND QELS STUDY

16:30-16:55 **Ulrich Scheler**
SOLID-STATE NMR INVESTIGATIONS OF POLYMER NANOCOMPOSITES

University hall

17:00-17:05 *Presentation of the winner of Wiley Prize*

17:05-17:30 **Kirill V. Kovtunov**
OBSERVATION OF PARAHYDROGEN INDUCED POLARIZATION IN HETEROGENEOUS
HYDROGENATIONS CATALYZED BY SUPPORTED METAL CATALYSTS

17:30-17:35 *Presentation of the winner of Wiley Prize*

17:35-18:00 **Eugenio Daviso**
THE ORIGIN OF THE SOLID-STATE PHOTO-CIDNP EFFECT

18:00-18:05 *Presentation of the winner of Wiley Prize*

18:05-18:30 **Giuseppe Sicoli**
PULSED ELDOR METHOD FOR DETECTION OF CONFORMATIONAL CHANGES ON DNA
STRUCTURES

18:30-18:35 *Presentation of the winner of EUROMAR-2008 Prize*

18:35-19:00 **Maria Concistrè**
DOUBLE-QUANTUM NMR OF THE FIRST PHOTOINTERMEDIATE IN VISION:
BATHORHODOPSIN

19:00-19:40 **Closing of the EUROMAR-2008**

20:00-22:00 **Concert**