

BULLETIN DU GROUPEMENT

d'informations mutuelles

AMPERE



SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

September to December 2016

No. 265

Office: ETH Zürich, Laboratory of Physical Chemistry
8093 Zürich, Switzerland, www.ampere-society.org

Contents

Editorial	1
Portrait: Prof. Kurt Wüthrich	2
Presenting the Division of Hyperpolarization	4
13 th International Conference on the Applications of Magnetic Resonance in Food Science (FOODMR2016)	5
Report; AMPERE NMR SCHOOL 2016, Zakopane, Poland	7
PosterPrize Ampere NMR School 2016; P. Garbacz	11
Report on Euromar 2016	14
The Ampere Prize 2016 for Young Investigators; E. Bordignon	21
Andrew Prize 2016; F.A. Perras	24
Posterprizes Euromar 2016; S. Berkamp, J. Eills, B. Gouilleux	28
Reprint of Financial Report of the Groupement Ampere	34
Executive Officers and Honorary Members of the AMPERE Bureau	35
Future conferences and AMPERE events	40

If you would like to become a member of the AMPERE Group, you can register online under: **www.ampere-society.org**

Correspondence address:
ETH Zurich, Laboratory of Physical Chemistry, HCI F 227
Vladimir Prelog Weg 2, 8093 Zurich, Switzerland
Mail: contact@ampere-society.org

Publisher: Gunnar Jeschke, ETH Zurich, Switzerland

Editorial

Dear AMPERE colleagues,

With the conference season having (almost) come to an end for this year, it is time for Thanksgiving for the rich harvest in our field in an otherwise politically somewhat troubled year. Regarding political troubles, we should remember our motto "*Se connaître, s'entendre, s'entraider*", or "*To get acquainted with each other, to understand each other, and to help each other*". Science should bridge political divides and should not give in to those who want to divide our world. We have been there before.

Regarding the rich harvest, this issue focuses on the report on this year's truly memorable EUROMAR meeting in Aarhus and on introducing the science of the awardees of this meeting. We also have a report on the AMPERE NMR School in Zakopane and on the poster prize awarded during that school and a report on the 13th International Conference on the Applications of Magnetic Resonance in Food Science, where I would imagine that the conference dinner must also have been good (I still try to imitate the perfect tomato/vanilla combination that I encountered in Aarhus).

Our newest sub-division on Hyperpolarization is introduced on page 4. This is currently a very active field and you are invited to contribute to the life of the sub-division.

Last, but not least we continue our series of "interview portraits" of eminent scientists in the field of magnetic resonance, this time with Kurt Wüthrich (page 2). His favorite frequency is the frequency of good vibrations among human beings. In fact, this may be what unifies the field of magnetic resonance across its very large bandwidth.



Gunnar Jeschke
Secretary General of Groupement AMPERE

Portrait: Kurt Wüthrich

- Why magnetic resonance and why NMR and MRI?

In the mid-1960s, contacts with Robert Connick, Manfred Eigen, Harden McConnell and Henry Taube opened my eyes to the fact that studies of rate processes, as investigated in Eigen's laboratory with "jump methods", could be performed under equilibrium conditions when using NMR in solution. This got me hooked.

- What is your favorite frequency?

The frequency of good vibrations among human beings.

- What do you still not understand?

So many things that it keeps me going in continued attempts to satisfy my curiosity.

- Luckiest experiment you have ever done.

Observation of ring flips of phenylalanine and tyrosine inside globular proteins.

- What was the worst mistake you have made during your lab time?

Each of my contributions started with serial mistakes that led the way to unanticipated new findings.

- Most memorable conference story?

At the Biochemistry Congress in 1976, I made the first major presentation on the aforementioned "ring flips" in proteins. Max Perutz chaired the session. At the end of my talk, he delayed discussion for an exchange with a more junior protein crystallographer, Robert Huber, who had collaborated with us on analyzing the consequences of "ring flips". As Robert related to me, he was asked whether or not my lecture should be discussed or whether it was just nonsense. Thereafter the discussion was opened.

- With whom (historical person) would you like to meet?

René Descartes.

- When do you get your best ideas?

During and after strenuous physical exercise.

- If you had just one month time for travelling – where would you go to?

To a great place for fishing.

- Your idea of happiness?

Catching a big one, can be in science or out of the water.



Photo by Lukas Mäder

Positions: Cecil H. and Ida M. Green Professor of Structural Biology, The Scripps Research Institute, La Jolla, CA, USA; Professor of Biophysics, ETH Zürich, Zürich, Switzerland; Visiting Professorships at UFRJ in Rio de Janeiro, at ShanghaiTech University in Shanghai and at DGIST in Daegu, South Korea.

Education:

1957–62 University of Bern, Switzerland: Lizentiat in chemistry, physics and mathematics.
1962–64 University of Basel, Switzerland: Ph.D. in chemistry (Prof. S. Fallab); Eidgenössisches Turn- und Sportlehrerdiplom.
1964–65 University of Basel, Switzerland: Postdoctoral training (Prof. S. Fallab).
1965–67 University of California, Berkeley, CA, USA : Postdoctoral training (Prof. R.E. Connick).
1967–69 Bell Telephone Laboratories, Murray Hill, N.J., USA : Member Technical Staff, Biophysics Department (Dr. R.G. Shulman).

Awards:

Prix Louis Jeantet de Médecine, Kyoto Prize in Advanced Technology, Nobel Prize in Chemistry, a number of other awards and fifteen honorary degrees

Hyperpolarization Division of the Ampere Society

The neologism "hyperpolarization" has become the widely accepted name for a surprisingly wide range of methods that allow one to boost the polarization, and hence the much-needed sensitivity, in many branches of magnetic resonance. This burgeoning field started with optically induced hyperpolarization (now better known as SEOP, Spin-Exchange Optical Pumping) developed by Kastler (Nobel prize in physics in 1966).

A new boost to this field was due to Overhauser's, Slichter's and Solomon's immortal works, and to Abragam's and Goldman's DNP (Dynamic Nuclear Polarization). Some years later, CIDNP (chemically induced dynamic nuclear polarization) was discovered by Bargon and Fischer and explained by Kaptein and Closs. Bargon was also a pioneer of PHIP (para-hydrogen induced polarization, relying on Heisenberg's concept of spin isomers). Weitekamp provided an elegant explanation of the phenomenon. Similar physics gives rise to the Haupt effect, also called quantum-rotor induced polarization.

Very recently, new inspirations came from Griffin's MAS-DNP, Goldman's, Ardenkjaer-Larsen's, Köckenberger's, Jannin's, and Bodenhausen's Dissolution-DNP, as well as from Duckett's SABRE (Signal Amplification By Reversible Exchange) leading to many promising extensions to material science, heterogeneous catalysis, bio-solids, metabolomics, medical diagnosis, etc.

The new Hyperpolarization Division of the Ampere Society, founded in 2016, wishes to bring together both seasoned actors and beginning students of these remarkably diverse fields, by coordinating various symposia and summer schools. Another goal is to bring together the magnetic resonance community with scientists who work on applications to medicine, and who are expected to contribute to making hyperpolarization a standard analytical and diagnostic tool.

Geoffrey Bodenhausen (Paris)
Jörg Matysik (Leipzig)
Konstantin Ivanov (Novosibirsk)

13th International Conference on the Applications of Magnetic Resonance in Food Science (FOODMR2016)

Scientific Advisory Board

Søren Balling Engelsen, Francesco Capozzi, John van Duynhoven (chair), Manfred Spraul, Gisela Guthausen, Jean-Marie Bonny, Antonio Ferreira

Local Organizing Committee

Gisela Guthausen (KIT, chair), M Bunzel (KIT), T. Kuballa (CUVA, Karlsruhe), M. Rist (MRI, Karlsruhe), H. Schuchmann (KIT), B. Luy (KIT)

For the third time the International Conference on the Applications of Magnetic Resonance in Food Science (FOODMR) was organized under the auspices of the Groupement AMPERE. The conference series has built a long tradition in presenting the latest innovations in magnetic resonance and in particular new applications to understanding the functionality of foods, their processing and stability and their impact on health and sensorial perception. The 13th edition of the conference was held from 7 to 10 June 2016 in Karlsruhe (Germany) and was organized by researchers of Karlsruhe Institute of Technology (KIT), CVUA and MRI (Karlsruhe). The conference attracted 136 participants from 18 countries from Europe, Asia, Oceania, and the Americas. With this steady and broad representation of scientists the FOODMR conference has firmly established itself as an AMPERE sub-division.

The conference was preceded by tutorials on technical aspects of chemometric analysis (W. Kessler), fast data acquisition methods (B. Luy, W. Bermel) and MRI and PFG diffusometric techniques applied to food materials (D. Gross, K. Zick). The motto of the scientific part of the conference was 'Magnetic Resonance meets Food Analytics' and opened with a session on advanced method developments with inspirational presentations on future food applications. Two sessions were dedicated to applications of Low Field NMR and two to applications of MRI and Diffusion. The session 'From Method Development to Application' successfully bridged two worlds. Three sessions were dedicated to NMR applications in FoodOmics. The programme included 3 keynote speakers, 5 invited speakers and 30 oral presentations selected from submitted abstracts. The evening discussion session on Quantitative NMR was moderated by Dirk Lachenmaier and provoked lively discussions. The conference is indebted to Jan Korvink (KIT), Joseph Seymour (Montana State University), Dirk Lachenmaier (Chemisches und Veterinäruntersuchungsamt), Morten Clausen (Aarhus University), Marco Tessari (Nijmegen University), Stephano Calderelli (Aix-Marseille University), Matthew Augustine

(University of California, Davis) and Paul van der Meeren (University of Ghent) for providing excellent keynote and invited presentations. The poster session comprised 52 presentations; two poster prizes were awarded with a prize for the quality of their posters: D. Wefers and A. P. Sobolev. The poster prizes were sponsored by Wiley.

Selected oral and poster contributions will be published in the conference proceedings. These will be issued by IM Publications LLP as an electronic publication. These proceedings have gained popularity as training material for young scientists entering the field of applied magnetic resonance in food science.

At the conference dinner the founding fathers of the MRFOOD division, Peter Belton and Graham Webb, were appointed as honorary members. The MRFOOD division is indebted to them for driving the conference over more than two decades.

This conference was sponsored by ACDLabs, Antek, Bruker, Eurisotop, Lot Quantum Design, Mestrelab Research, Nanalysis, Niumag, Spinlock, Unilever, Wiley, and VWR. Without their generous support this conference would not have been able to offer such an attractive programme at low fees especially for students.

The 14th edition of this conference will be held in Brittany (France) and will be organized by Corinne Rondeau-Mouro (Chair, IRSTEA, Rennes, France). We expect to welcome (even) more participants and see many new developments in the applications of magnetic resonance in food science.



Report; AMPERE NMR SCHOOL 2016, Zakopane, Poland

Scientific Committee

B. Blümich (Aachen), Germany, V. Chizhik (Saint Petersburg) Russia, J. Dolinšek (Ljubljana), Slovenia, F. Fajarsa (Darmstadt), Germany, S. Jurga (Poznan), Poland, J. Kowalewski (Stockholm), Sweden A., D. Lurie (Aberdeen), UK MacKay (Vancouver), Canada, B. Meier (Zurich), Switzerland,

Organizing Committee

Stefan Jurga - Director

L. Szutkowska – Executive secretary, M. Walawender, J. Iżykowska, M. Dobies, Z. Fojud, M. Makrocka-Rydzik, J. Jencyk, K. Szutkowski, T. Zalewski, K. Tuśnio

The AMPERE NMR School was held between 12th–18th June 2016 in Zakopane (Poland) with over than 90 attendees, including 43 from abroad. The conference was organized by the NanoBioMedical Centre and the Department of Macromolecular Physics, Faculty of Physics of Adam Mickiewicz University in Poznań under the auspices of the Groupement AMPERE.



The meeting attracted participants from 14 countries across the world with an interest in the basic and advanced NMR techniques, recent research and interested in cooperation between the scientists. Participants represented various countries such as Germany, Bulgaria, Estonia, Israel, The Netherlands, Russian Federation, Slovenia, Czech Republic, France, UK, Canada, USA.

The programme of the School covered the following topics: NMR relaxometry, NMR diffusometry, Solid State NMR, NMR of quadrupolar nuclei, MRI and Field Cycling MRI, Novel NMR techniques and NMR in biology, medicine and material science. Programme comprised of 19 lectures, 6 trainings including online transmissions from the NanoBioMedical Centre in Poznan:

High Resolution solid state NMR
Monika Makrocka-Rydzik, Jacek Jenczyk

Diffusion studied by NMR
Kosma Szutkowski, Marek Kempka

MRI: Basic principles and application
Tomasz Zalewski

Utilization of high-resolution homonuclear and heteronuclear multidimensional NMR experiments to assignments of Backbone and side-chain resonance. Application to short cyclic cell penetrated peptide (CPP) in DPC Micelle.
Igor Żukow, Lukasz Popenda

NMR Relaxometry
Zbigniew Fojud and Maria Dobies

The lectures were given by:
Dr. Stasia Bembenek Bailey, North Carolina State University, USA
Prof. Bernhard Blümich, RWTH Aachen, Germany
Dr. Andrew B. Byrd, National Cancer Institute, USA
Prof. Vladimir Chizhik, St. Petersburg State University, Russia
Prof. Jacques Fraissard, Université Pierre et Marie Curie, France
Prof. Wiktor Koźmiński, University of Warsaw
Prof. Kanuta Kruck, University of Warmia & Maury, Poland
Prof. David Lurie, University of Aberdeen, UK
Prof. Alex MacKay, University of British Columbia, Canada
Prof. Gregor Mail, National Institute of Chemistry, Slovenia

Prof. Dieter Michel, University of Leipzig, Germany
Dr. Jürgen Schmidt, University of Kent, UK
Prof. Igor Serša, Institut Jožef Stefan, Slovenia
Dr. Jiří Spěváček, Academy of Science of the Czech Republic, CZ
Prof. Janez Stepišnik, Institut Jožef Stefan, Slovenia
Prof. Jadwiga Tritt-Goc, Polish Academy of Science, Poland
Prof. Shimon Vega, Weizmann Institute of Science, Israel
Prof. Roderic E. Wasylshen, University of Alberta, Canada
Prof. Władysław P. Węglarz, Polish Academy of Science, Poland

The participants had the opportunity to present their results during a poster session which comprised 39 presentations. The posters were evaluated by the members of "the poster committee" composed of: Prof. Alex MacKay, Prof. Jadwiga Tritt-Goc, Prof. Janez Stepišnik

The prizes were awarded to:
I. Piotr Garbacz (pl. find his abstract on page 11)

II. Egor Nasibulov, "Theoretical treatment of pulsed Overhauser DNP"
Siberian Branch of the Russian Academy of Science, Novosibirsk, Russia

III. Sebastian Vellmer, "Fast mean diffusion imaging (FAMED) to microcapillary – based phantoms"
Technical University of Dortmund, Germany

The winners were given prizes and diplomas.



All abstracts of oral presentations and posters were published as printed proceedings (book of abstracts).

The social programme included an "All together party", a dinner in a regional restaurant with folk music of the Tatra's region, a Dunajec rafting excursion, an excursion to Bielska Cave (Slovakia) and hiking in the Tatra Mountains. Participants also had the opportunity to listen to an organ recital performed by Prof. Dieter Michel. The School was a successful event, as reflected in correspondence received from the participants after the event.

The next edition of the School will be held in Zakopane (Poland) from June 25th to 1st July 2017.



PosterPrize Ampere NMR School 2016

Piotr Garbacza

CHIRALITY-SENSITIVE NUCLEAR MAGNETOELECTRIC RESONANCE

Faculty of Chemistry, University of Warsaw, ul. Pasteura 1, 02-093, Warsaw, Poland

Standard liquid-state nuclear magnetic resonance techniques cannot directly distinguish between two enantiomers of a given molecule [1]. However, it has been recently shown that an additional electric field used in the NMR experiment could induce a chirality-sensitive magnetization [2, 3]. The experiment requires a device which provides a strong electric field oscillating at the high frequency (300-700 MHz) and minimizes the unwanted time-dependent magnetic field [4].

If the electric field $\mathbf{E}(t)$ and the magnetic field $\mathbf{B}(t)$ generated by the device are, respectively, along the y -direction and in the xz -plane, then this condition can be quantitatively expressed by the dimensionless ratio between their amplitudes:

$\kappa = cB_x/E_y$, where c is the speed of light in vacuum and the static magnetic field \mathbf{B}_0 is along the z -direction [5].

The simplest compact structure that minimizes the ratio κ is the loop-gap resonator which consists of a cylinder with a slit, Fig 1 [6]. In order to obtain a sufficiently small ratio κ one has to substitute the slit with plates, reduce the cylinder to a loop, and add a second loop to obtain a highly symmetric structure as shown in Fig. 1c. [7]

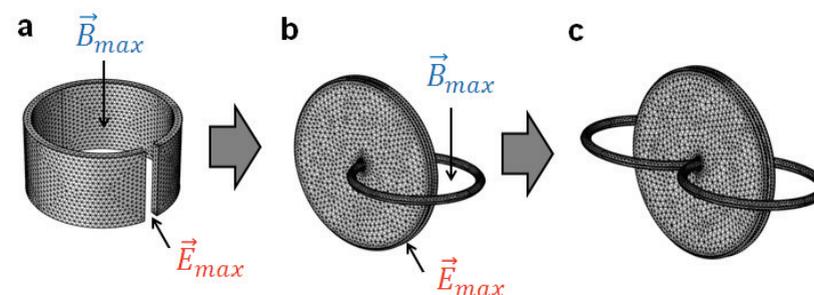


FIGURE 1. The loop-gap resonators optimised for the high amplitude of the magnetic field $\mathbf{B}(t)$ in the centre of the cylinder (a) and the high amplitude of the electric field $\mathbf{E}(t)$ between the plates (b, c).

Further minimization of the transverse time-dependent magnetic field component between plates of the resonator is obtained by increasing of the number of its loops. (Fig 2).

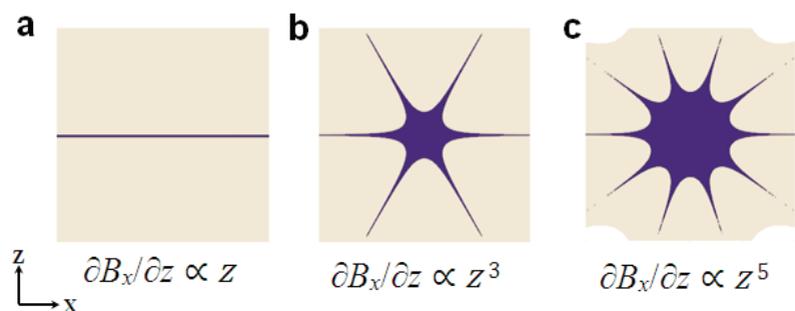


FIGURE 2. For the capacitor without any loops the area for which the ratio κ is acceptable small is a line of thickness of the order of several μm (a). For the capacitor with two (b) and four (c) loops one finds solutions for which the low- κ volume is of the order of 10-100 mm^3 .

The design of a new kind of NMR resonator based on the results of COMSOL computer program calculations, *i.e.*, numerical solutions of Maxwell's equations using finite element methods, will be discussed in detail (Fig. 3).

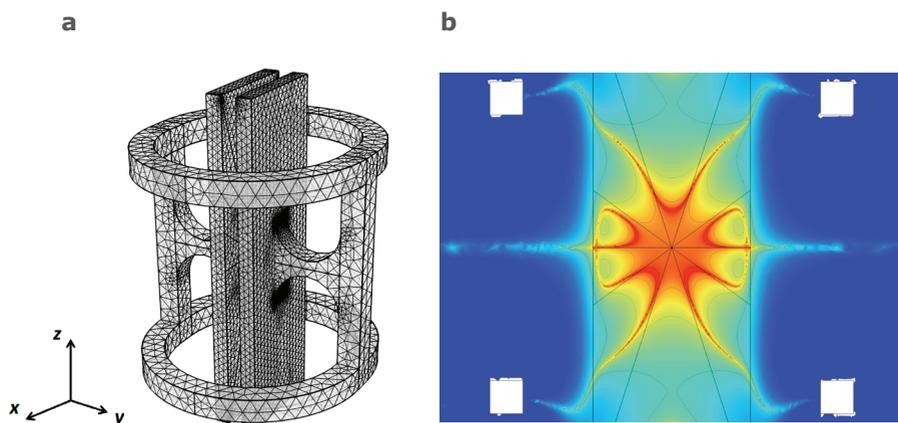


FIGURE 3. The design of the low- κ four-loop-one-gap resonator (a). The ratio between the x -component of the magnetic field and the electric field, κ , in the xz -plane between plates. The area for which $\kappa < 10^{-4}$ is marked by the red colour (b).

The chirality-sensitive NMR interaction is weak, therefore, it is necessary for the first experimental tests to find a sample for which relevant molecular properties, *i.e.*, polarisability and antisymmetry of the nuclear magnetic shielding tensor and the indirect spin-spin coupling tensor are maximized [5].

The computations performed at the coupled-cluster level indicate that for favourable samples the amplitude of the expected signal is 1-10 % of the standard NMR signal.

Acknowledgements

Support from the Max-Planck Society is gratefully acknowledged. The author thanks A.D. Buckingham, S. Krämer, P. Fischer, and G.L.J.A. Rikken for helpful discussions.

References

- [1] T. J. Wenzel and J. D. Wilcox, *Chirality* 15, 256 (2003)
- [2] A. D. Buckingham, *Chem. Phys. Lett.* 398, 1 (2004)
- [3] A. D. Buckingham and P. Fischer, *Chem. Phys.* 324, 111 (2006)
- [4] J. D. Walls and R. A. Harris, *J. Chem. Phys.* 140, 234201 (2014)
- [5] P. Garbacz, M. Jaszuński, and J. Cukras, *Phys. Chem. Chem. Phys.* 17, 22642 (2015)
- [6] G. A. Rinard and G. R. Eaton, *Biol. Magn. Reson.* 24, 19 (2005).
- [7] P. Garbacz, P. Fischer, and S. Krämer, *J. Chem. Phys.* 145, 064202 (2016)

Report on Euromar 2016

Aarhus - Denmark - July 3-7



Prof. Alexander Pines and Prof. Richard R. Ernst

International Scientific Committee

S. Aime, J. H. Ardenkjær-Larsen, M. Bennati, M. Duer, I. Felli, L. Frydman, B. Kragelund, F. Mulder, N. C. Nielsen, T. Parella, J. Skibsted, T. Vosegaard, and J. Wrachtrup.

Local Organising Committee

U. Akbey, M. Bjerring, J. Duus, H. J. Jakobsen, B. Kragelund, F. H. Larsen, A. Malmendal, F. Mulder, N. C. Nielsen, U. G. Nielsen, K. Teilum, and T. Vosegaard.

The Euromar 2016 conference

took place July 4th – July 8th in the concert hall of Aarhus, Denmark with ca 640 attendees, of which ca 150 were students. The concert hall is located in the center of Aarhus implying that most of the attendees were in hotels in walking distance from the conference site. All activities during the day took place in the concert hall, where we had access to the main lecture theater for plenary and parallel sessions and two smaller lecture theatres for the parallel sessions. The poster sessions were arranged on a balcony, a broad corridor, and a square in front of one of the lecture theaters. Exhibitor booths, registration, and coffee breaks were in the foyer in front of the main lecture theater. This setup ensured good communication between scientists and with all sponsors.



Picture from the welcome reception in the foyer of the concert hall. (photo: Mads Sloth Vinding)

Lectures

The official program started Sunday afternoon on July 4th with the major prize session. Unlike earlier, we had chosen not to have the tutorials on Sunday afternoon to allow people to travel in to Aarhus during the afternoon of Sunday.

Prize sessions

The major prize session covered three prizes. First the Raymond Andrew prize awarded to Frédéric A. Perras for his Ph.D. thesis performed at the University of Ottawa (Canada) entitled "Structural Insights from the NMR Spectroscopy of Quadrupolar Nuclei: Exploiting Electric Field Gradient and Spin-Spin Coupling Tensors" (page 24). Second, the AMPERE young investigator prize to Enrica Bordignon (Ruhr-University, Bochum, Germany) in recognition of her achievements using spin-label EPR for the characterization of large proteins, both from the methodological and application side, including orthogonal labelling approaches (page 21). Finally, Bruker has established the new Richard Ernst Prize, which was awarded for the first time in Aarhus. This prize was awarded to Prof. Alexander Pines (UC Berkely, US) in recognition of his breakthrough contributions in the fields of NMR and MRI in general, with emphasis on the invaluable input that your work has done for enabling NMR investigations on quadrupolar nuclei, as well as for your innovative approaches in hyperpolarized NMR and MRI.

The Ernst prize was presented by the chairman of the prize committee Prof. Lucia Banci, Italy and was motivated by Nobel Laureate Richard Ernst, who took the stage and made a nice and very personal introduction to the prize winner. This was truly a memorable session with both Pines and Ernst on the stage.

In the second prize session on Thursday, recipients of the MRC student travel stipends, Suraj Manrao travel stipends, and Jeol travel stipends were announced.

Scientific sessions

The scientific sessions were organised with 13 plenary lectures and 21 scientific sessions running in three parallel tracks. In each parallel session there were two invited lectures and three lectures selected from the poster abstracts, as it has been the case for the past years.

With the selection of sessions, we sought to show the breadth of magnetic resonance including MRI, EPR, DNP, methods, and applications in various areas, including low-field and high-field instruments. There was a good geographical balance reflecting approximately the number of participants from Europe, US, and Asia, as well as a good gender balance also reflecting the participant distribution.

Tutorial session

The tutorials were moved to Tuesday afternoon to ensure a high attendance at this session. We put an effort into ensuring that the lecturers addressed the newcomers of the fields in a pedagogical way. The topics covered

quadrupolar nuclei by Philip J. Grandinetti (Ohio, US), NMR of nucleic acids by Hashim Al-Hashimi (Duke, US), and product operators by Ole W. Sørensen (Denmark).

Poster sessions

There were ca 330 posters presented at the conference, divided into 22 topics. Posters were up from Sunday to Wednesday evening with poster sessions Monday, Tuesday, and Wednesday. The posters were located next to all other activities implying that many people were looking at the posters at other times than during the poster sessions.

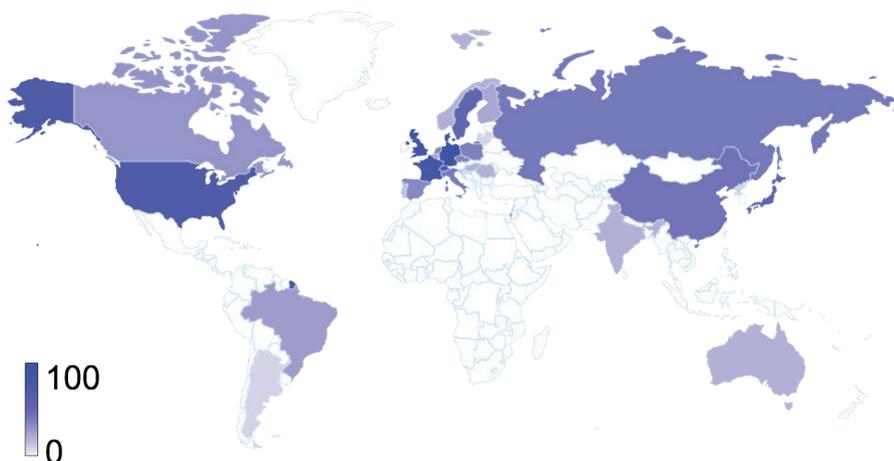
Electronic program

The conference program was printed in overview on the name badges of all people, but we chose not to make a printed version of the program with abstracts. Instead we offered a free conference app, which gave an overview of talks, floor plan, exhibitors, and the social programme. Although a few people initially expressed their concerns about not having a printed program, most of these came back later with positive feedback. In general, we had much positive feedback supporting the conference app solution, as it provides excellent possibilities to search, organise and plan the conference.



Participants from all of the World

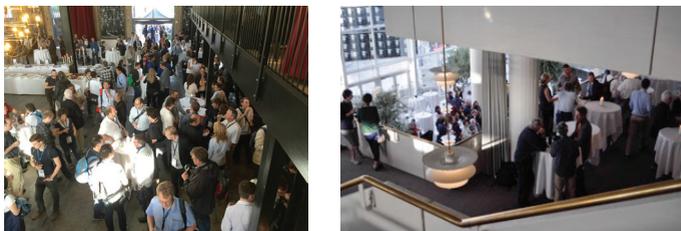
The World map below shows the distribution of participants from various Countries. The geographic diversity was good, with a quite high number of participants from both America and Asia, even Australia, New Zealand, and South America were represented.



The number of participants from different countries with most notable being 1. Germany: 125, 2. Denmark: 66, 3. United Kingdom: 65, 4. France: 64, 5. Switzerland: 48, 6. United States: 42, 7. Japan: 22, 8. Sweden: 22, 9. China: 14, 10. Russia: 13, and participants from 40 Countries.

Social events

Following the Sunday prize event there was a small welcome mixer in the foyer of the concert hall, offering food and drinks to everyone. Monday evening offered an event by Bruker, Tuesday evening was organised by Jeol, Wednesday evening was free, and Thursday evening was the conference dinner. Throughout the conference, coffee breaks and lunch breaks were accompanied by food and beverages.



Pictures from the Bruker evening (left) and Jeol reception (right). (photos: Mads Sloth Vinding)

As the concert hall is located in the center of Aarhus, we also took part in the city life. Sunday noon there was a bicycle race just outside of the concert hall. Sunday and Wednesday, people were enjoying the European championship in football on a big TV screen just outside the concert hall. Several of the conference participants took part in this. Finally, the concert hall is located next to the art museum Aros for which we provided free tickets, and according to our feedback from the concert hall, most of the

participants used this possibility.

Conference dinner

For the conference dinner, we had teamed up with a local cook and a colleague from organic chemistry, Prof. Karl Anker Jørgensen, who have developed a nice concept for molecular gastronomy. The first part of the conference dinner was a lecture by Prof. Jørgensen at the concert hall, where he talked about molecular gastronomy and about the chemistry going on during the preparation of food. Then we were transported to a large tent at the University campus where the molecular gastronomy dinner was served. Among the memorable dishes, we can mention "Chicken Maillard" in which the chicken is prepared at high temperatures to exploit the well-known Maillard reaction, "Mirror-imaged slow-roasted filet of beef" focusing on tasty chiral molecules, and "Black nitrogen ice cream" with ink-colored ice cream prepared at the table by use of liquid nitrogen. Following the dinner, people could either watch the semifinal of the European football championship in an auditorium at the Department of Chemistry at the University or enjoy a beer in the student bar that we had opened for those who wanted to stay longer.

Comments from attendees

"Thank you for a great conference. In my experience it was the best conference I have attended so far", participant from National Institute of Chemical Physics & Biophysics, Estonia.

"Thomas, this was an outstanding meeting-the caliber of Euromar talks was even higher than usual, which is a very impressive standard. I also think the idea of a „molecular gastronomy“ banquet was creative and memorable", participant from Duke University, USA.

"We attended the EUROMAR conference in Aarhus Denmark in which we were pleased to participate. We are glad to report that the science, the culture, the food and the city have made the meeting a great success", Judy Doty, Doty Scientific, USA.



Lucio Frydman and Alexander Pines after the prize ceremony (left) and Bluemich opening the conference by explaining the "Ampere tree". (photos Thomas Vosegaard and Mads Sloth Vinding)

Acknowledgements and comments

Thanks are due to all sponsors and exhibitors, the scientific and local-organising committees, the session chairmen, and my colleagues who made immense contributions to the organisation of the conference. I hope that everybody enjoyed it as much as I did.

Thomas Vosegaard
Chairman of Euromar 2016



Pictures from the conference dinner (right) and the auditorium showing the European football championship semifinal (left). (photos: Thomas Vosegaard)

The Ampere Prize 2016 for Young Investigators

Prof. Dr. Enrica Bordignon has received the AMPERE prize for Young Investigators on the 3rd of July 2016, during the EUROMAR conference in Aarhus, Denmark. The prize was given "in recognition of her achievements using spin-label EPR for the characterization of large proteins".

The Italian chemist is since April 2016 Chair of Electron Spin Resonance Spectroscopy at the Ruhr-University Bochum in Germany, where she collaborates within the Cluster of Excellence RESOLV (Ruhr Explores SOLvation). After graduation with a PhD from the University of Padova, Italy, in 2003 she moved to Germany as post-doctoral fellow in the group of Prof. Dr. Steinhoff. From 2008 to 2013, she was senior scientist at ETH Zurich, in the group of Prof. Dr. Jeschke, and in 2013 she was appointed associate professor at the Free University of Berlin.

Introducing Bordignon to her talk at EUROMAR, Prof. Dr. Meier called her "an ambassador of the EPR technique in the field of structural biology". Bordignon investigates the conformational changes of membrane proteins by means of site-directed electron spin resonance spectroscopy, in particular with dipolar spectroscopy (DEER, also known as PELDOR). She has been successfully collaborating with several groups, using EPR to investigate the structural dynamics of a series of protein complexes, e.g. the aspartate transporter (1), the muscle alpha-actinin (2), and recently she contributed to the discovery of the stoichiometry and structural organization of the Ton complex formed by a pentameric ExbB in complex with a dimeric ExbD and TonB (3). The two main focuses of her lab are: Understanding at molecular level the key interactions and conformational changes of Bcl-2 proteins at the onset of apoptosis, a form of programmed cell death (4); studying the structural dynamics of ABC transporters, which confer drug resistance to cancer cells or are involved in the immune systems (5). Within the cluster of excellence, RESOLV scientists investigate how solvents – water in particular- influence the properties of chemical and biological processes. Therefore, she will extend her EPR studies to changes in water accessibility accompanying the proteins' conformational transitions via dynamic nuclear polarization.

During her talk in Aarhus "ABC exporters: analogies and differences", Bordignon presented a comprehensive EPR study on three different ABC exporters, highlighting the species-specific response to nucleotides. ATP binding cassette (ABC) exporters are found in all phyla of life and play a key role in the transport of a variety of molecules across cell membranes. Around

half of the forty human ABC exporters are heterodimers encompassing two functionally non-equivalent ATP binding sites, which include transporters of major clinical importance such as CFTR, SUR1 and TAP1/2. Scientists in the field agree that a typical ABC exporter adopts two principal states, namely an inward-facing (IF) state with NBDs fully or partially separated and an outward-facing (OF) state with nucleotides bound at the closed NBD dimer interface, which is coupled to substrate extrusion at the transmembrane domains. Yet, the molecular events leading an open NBD dimer to a closed one having two nucleotides sandwiched at the interface (the so-called power stroke event) are still under debate.

Understanding at the molecular level how ABC exporters perform their function and what is the power stroke for substrate release is of key relevance for both fundamental and applied research – i.e. pharmaceutical applications. The heterodimeric ABC exporter TM287/288 from the thermophilic bacterium *T. maritima* is currently the only heterodimeric ABC exporter encompassing a non-canonical nucleotide binding site for which two inward-facing crystal structures are available. In contrast to ABC exporters comprising two consensus sites, the NBDs of TM287/288 remain in contact mainly via the degenerate site D-loop. In Aarhus, Bordignon showed a comprehensive site-directed spin labelling EPR study on TM287/288, and she compared the nucleotide response of this heterodimeric exporters with another heterodimeric exporter from a mesophilic organism (BmrCD) and a homodimeric ABC exporter (MsbA).

The molecular events discovered by EPR allowed to build a mechanistic model, which reconciles the data available for heterodimeric exporters and highlight species-specific differences (6).

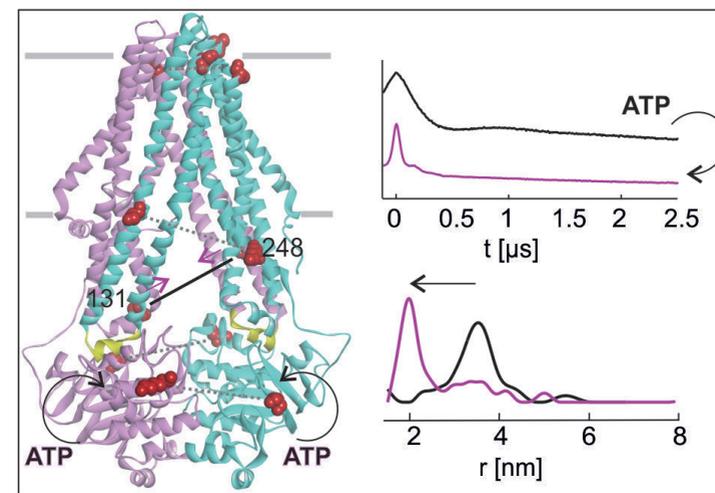


Figure 1. The side chains in the TM287/288 ABC exporter which were mutated to cysteines and then spin labeled with MTSL are highlighted in the apo crystal structure (PDB 4Q4H). Example Q-band DEER traces and obtained distance distributions are shown on the right. The conformational change from an apo inward-facing structure to an ATP-bound outward-facing structure can be easily monitored by EPR.

1. Hänel I, Wunnicke D, Bordignon E, Steinhoff H-J, & Slotboom DJ (2013) Conformational heterogeneity of the aspartate transporter GltPh. *Nat. Struct. Mol. Biol.* 20(2):210-214.
2. Ribeiro Ede A, Jr., Pinotsis N, Ghisleni A, Salmazo A, Konarev PV, Kostan J, Sjoblom B, Schreiner C, Polyansky AA, Gkoukoulia EA, Holt MR, Aachmann FL, Zagrovic B, Bordignon E, Pirker KF, Svergun DI, Gautel M, & Djinovic-Carugo K (2014) The structure and regulation of human muscle alpha-actinin. *Cell* 159(6):1447-1460.
3. Celia H, Noinaj N, Zakharov SD, Bordignon E, Botos I, Santamaria M, Barnard TJ, Cramer WA, Lloubes R & Buchanan SK (2016) Structural insight into the role of the Ton complex in energy transduction. *Nature* 538: 60–65
4. Bleicken S, Jeschke G, Stegmüller C, Salvador-Gallego R, García-Sáez Ana J, & Bordignon E (2014) Structural Model of Active Bax at the Membrane. *Mol. Cell* 56(4):496-505.
5. Herget M, Baldauf C, Scholz C, Parcej D, Wiesmüller KH, Tampe R, Abele R, & Bordignon E (2011) Conformation of peptides bound to the transporter associated with antigen processing (TAP). *Proc. Natl. Acad. Sci. U. S. A.* 108(4):1349-1354.
6. Timachi HM, Hutter C, Hohl M, Assafa T, Böhm S, Mittal A, Seeger MA, Bordignon E (2016) Exploring conformational equilibria of a heterodimeric ABC transporter. Submitted.

Andrew Prize 2016

Frédéric A. Perras

U.S. DOE Ames Laboratory, Ames, IA, USA, 50011

Structural Insights from the NMR Spectroscopy of Quadrupolar Nuclei: Exploiting Electric Field Gradient and Spin-Spin Coupling Tensors

Solid-state NMR spectroscopy (SSNMR) is one of the two main structural solution tools, along with diffraction, that are used in the characterization of materials, and the most powerful technique to study non-crystalline materials. Impressive advancements have been made, particularly in recent years, in using SSNMR to solve the crystal structures of organic materials, zeolites, and aluminophosphates. Unlike diffraction, however, the approaches used in solving solid structures by SSNMR need to be tailored to the class of materials that are studied. This fact has slowed the introduction of NMR crystallography to inorganic materials as these are generally composed of elements whose NMR-active nuclei are quadrupolar ($S > 1/2$).

Unfortunately, the extraction of structural information from the NMR spectra of quadrupolar nuclei is often far from trivial. In many cases, only the quadrupolar coupling can be measured; which is difficult to relate to structure. Contrary to this, however, with the use of PAW DFT it is relatively straightforward to predict the EFG tensor for a given crystal structure. We have then developed a least-squares method that combines accurate DFT prediction of EFG tensors and experimentally-determined ones in order to directly refine crystal structures against the NMR data in a way akin to the Rietveld approach.¹ We have shown that this approach can produce crystal structures that often rival those obtained from single crystal diffraction and are of higher quality than those produced from DFT alone. This method was applied to solve high-quality crystal structures for a near-zero thermal expansion material and a non-linear optical material, for example.²

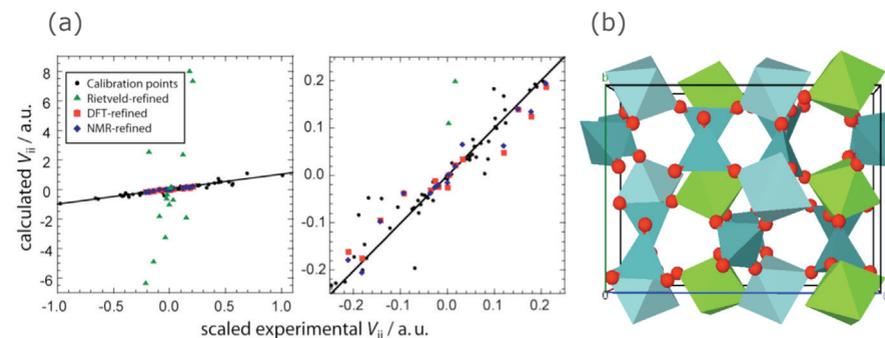


Figure 1. Results from an EFG-based crystal structure refinement of the near-zero thermal expansion material $\text{ZrMgMo}_3\text{O}_{12}$. In (a) the agreement between experimental and DFT predicted EFG tensor components are plotted for structures refined using PXRD (green triangles), DFT (red squares), or NMR (blue diamonds). The final NMR crystallographic structure is depicted in (b).

The quality of the structures obtained by such an approach of course depends on the accuracy of the EFG tensor measurements. Commonly, these parameters are obtained by fitting the spectra with the use of the high field approximation, which treats the quadrupolar interaction as a small perturbation to the Zeeman interaction. The quadrupolar interaction, however, can rival in size with the Zeeman interaction and an exact treatment of the combined Zeeman-Quadrupolar Hamiltonian is needed. We have developed a user-friendly, graphical, and fast program to simulate the NMR lineshapes of quadrupolar nuclei exactly from the complete range covering NQR to high-field NMR³. This free program, known as QUEST (QUadrupolar Exact SoftWare) has been used to analyze the NMR spectra of numerous nuclides including ^{14}N , ^{33}S , $^{35/37}\text{Cl}$, $^{79/81}\text{Br}$, ^{87}Sr , ^{91}Zr , ^{121}Sb , ^{127}I , ^{139}La , and $^{185/187}\text{Re}$.

When available, the most direct structural information that can be obtained from SSNMR corresponds to the spin-spin coupling (dipolar and J). Measuring these spin-spin coupling interactions is particularly difficult in pairs of quadrupolar nuclei due to their unfavorable spin dynamics and broad line shapes. We have shown that both dipolar and J coupling can be measured with the use of double-rotation (DOR) with which higher resolution allows for the observation of the complex multiplet structure of the resonances.^{5,6} A surprising discovery from this study is that the J coupling multiplets are still observable in pairs of magnetically equivalent nuclei if they happen to be quadrupolar. The observed multiplet structure is nevertheless unusual.

In order to simplify the measurement of spin-spin coupling between

quadrupolar nuclei we developed a series of J -resolved type experiments that enable the resolution of the J interaction with the use of broadly available MAS probes.^{7,8,9} Since only the central transition ($m = 1/2$ to $-1/2$ transition) can be accurately manipulated, the use of a double-quantum filter is necessary in these experiments in order to remove signals arising from spins that are coupling to the satellite states of another spin. Along the lines of the previous DOR work, we found that the doublet measured by these experiments is amplified when the spins are magnetically equivalent.^{10,11} This useful feature cannot only be used as a structural restraint but can also be used in order to access smaller J coupling constants. The J -resolved experiment can also be performed in static samples where it then enables the measurement of both the J and the dipolar coupling in pairs of quadrupolar nuclei possessing large quadrupolar coupling.

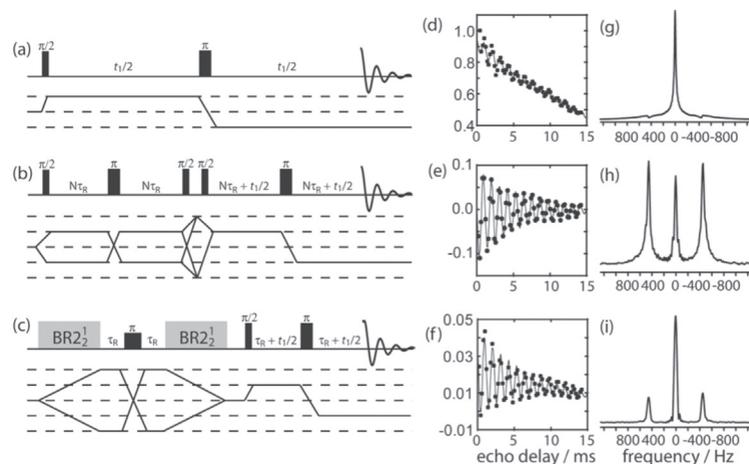


Figure 2. The pulse sequences and coherence transfer pathways for the ordinary (a), J -based double quantum filtered (b) and dipolar-based double quantum filtered J -resolved experiments are depicted. The time domain (d-f) and frequency domain (g-i) responses are also shown for dimanganese decacarbonyl demonstrating the need for the application of a central-transition selective double-quantum filter in order to observe the splitting caused by J coupling.

Lastly, applications of dynamic nuclear polarization (DNP) in order to enhance the sensitivity of difficult experiments involving quadrupolar nuclei are presented. Notably we found that the PRESTO polarization transfer technique is a good alternative to cross-polarization when performing indirect DNP experiments on quadrupoles. The improved sensitivity of PRESTO and DNP enabled the measurement of 1D and 2D ^{17}O SSNMR spectra of surface sites at natural abundance.

- ¹ Perras, F. A.; Bryce, D. L. J. Phys. Chem. C 2012, 116, 19472.
- ² Romao, C. P. Perras, F. A.; Werner-Zwanziger, U.; Lussier, J. A.; Miller, K. J.; Calahoo, C. M.; Zwanziger, J. W.; Bieringer, M.; Marinkovic, B. A.; Bryce, D. L.; White, M. A. Chem. Mater. 2015, 27, 2633.
- ³ Perras, F. A.; Bryce, D. L. Solid State Nucl. Magn. Reson., 2013, 45-46, 36.
- ⁴ Perras, F. A.; Bryce, D. L. Angew. Chem. Int. Ed., 2012, 51, 4227.
- ⁵ Perras, F. A.; Bryce, D. L. J. Magn. Reson., 2011, 213, 82.
- ⁶ Perras, F. A.; Bryce, D. L. J. Chem. Phys., 2013, 138, 174202.
- ⁷ Perras, F. A.; Bryce, D. L. J. Am. Chem. Soc., 2013, 135, 12596.
- ⁸ Perras, F. A.; Bryce, D. L. Chem. Sci., 2014, 5, 2428.
- ⁹ Perras, F. A.; Ewing, W. C.; Dellermann, T.; Böhnke, J.; Ulrich, S.; Schäfer, T.; Braunschweig, H.; Bryce, D. L. Chem. Sci. 2015, 6, 3378-3382.
- ¹⁰ Perras, F. A.; Bryce, D. L. J. Magn. Reson. 2014, 242, 23.
- ¹¹ Perras, F. A.; Bryce, D. L. eMagRes 2015, 4, 255.
- ¹² Perras, F. A.; Bryce, D. L. J. Phys. Chem. Lett. 2014, 5, 4049.

Posterprizes Euromar 2016

Sabrina Berkamp

Interaction studies of the chemokine Interleukin-8 with the G protein-coupled receptor CXCR1

Sabrina Berkamp, Sang Ho Park, Jasmina Radoicic, Ratan K. Rai, Anna A. De Angelis, Stanley J. Opella

University of California, San Diego, La Jolla, California 92093-0307, USA

G-protein coupled receptors (GPCRs) are the largest family of transmembrane receptors in eukaryotes. Although there are an increasing number of structures of GPCRs being determined, little is known about the exact conformational changes taking place in the receptor upon ligand binding. We are studying the interaction between the chemokine interleukin 8 (IL-8) and its receptor, the membrane protein CXCR1. Although a complete NMR structure of a GPCR complexed with a ligand is not available, it is known that residues of IL-8 have interactions with two sites on CXCR1: a high-affinity site on the flexible N-terminal domain and a secondary, lower affinity binding site on the extracellular loops.

wildtype CXCR1, 1TM-CXCR1 which contains only the primary binding site on the N-terminal domain as well as the first transmembrane helix, and NT-CXCR1 which is comprised of the full receptor without the N-terminal domain. Using solution NMR spectroscopy, MAS solid-state NMR and proton-detected fast MAS solid-state NMR, we observed almost complete immobilization of IL-8 on 1TM-CXCR1 as well as on wildtype CXCR1 (figure 1). When looking at the receptor, we observe the same changes in dynamics; several residues in 1TM-CXCR1 and wildtype CXCR1 become immobilized upon addition of IL-8. We have also observed chemical shift perturbation, indicating a conformational change upon complex formation. Comparison of solid-state and solution-state NMR results will provide a valuable insight into understanding the interactions of the chemokine receptor and its ligand in the early stages of GPCR activation.

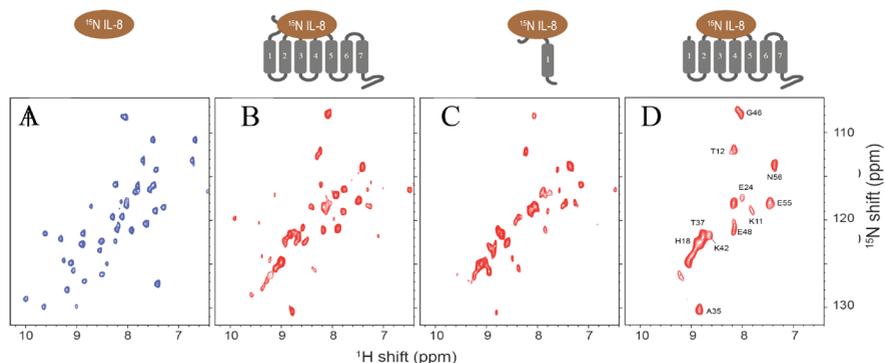


Figure 1. In A) solution NMR spectrum of IL-8. Comparison of Proton-detected HETCOR spectra of IL-8 immobilized on CXCR1 (in B), 1TM-CXCR1 (in C) and NT-CXCR1 (in D).

We published the *apo*-CXCR1 structure and are currently studying the structure and dynamics of the CXCR1 - IL-8 complex, reconstituted in phospholipid bilayers. To understand the effect the different binding sites of CXCR1 have on IL-8, we have made 3 constructs of the receptor:

James Eills Singlet Order Conversion and Parahydrogen-Induced Hyperpolarization of ^{13}C Nuclei in Near-Equivalent Spin Systems

J. Eills¹, G. Stevanato¹, C. Bengs², S. Glöggler¹, S.J. Elliott¹, J. A. Valdesueiro¹, G. Pilieo¹, M. H. Levitt¹

1. School of Chemistry and Institute for Life Sciences, University of Southampton, Southampton SO17 1BJ, United Kingdom

2. Institute of Biochemistry, Goethe University, Frankfurt am Main, Germany

Parahydrogen molecules are a repository of singlet order that can be observed if, after addition to a molecule, the protons become chemically inequivalent (PASADENA¹). Techniques to transfer this singlet order to magnetization on nearby heteronuclei have been developed to enhance the utility of PHIP.²⁻⁷

We present a novel radiofrequency pulse method to convert parahydrogen singlet order from a proton spin pair to a carbon (X) nucleus through long-range J couplings. Unlike most previous methods, this irradiation scheme works well in the near-equivalence regime of the three-spin system, which applies when the difference in the two ^1H - ^{13}C couplings is much smaller than the ^1H - ^1H coupling, and which is relevant to the sidearm hydrogenation procedure for hyperpolarising ^{13}C -labelled small molecules. This new method can give 100% transfer, and doesn't require field cycling.

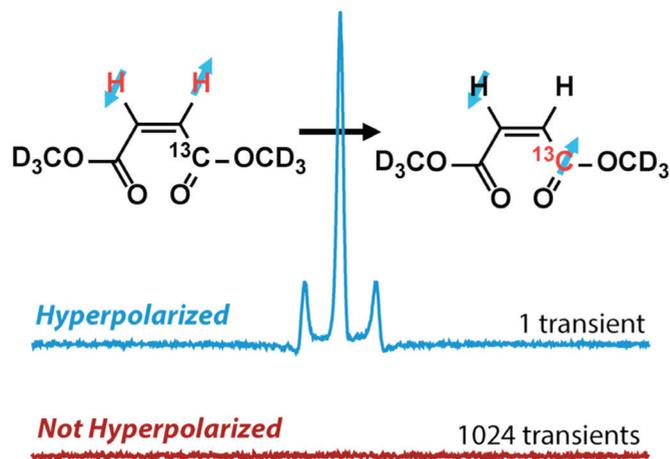


Fig. 1: We have demonstrated this pulse scheme on natural abundance dimethyl maleate- d_6 .

Initial experiments were performed on natural abundance maleic acid. We generated proton singlet order in these molecules using a standard pulse sequence⁸, and demonstrated the transfer of singlet spin order to the carbonyl carbon-13 nucleus in agreement with theory and simulations. Preliminary results are shown for parahydrogen-enhanced ^{13}C polarisation, demonstrating a NMR signal enhancement by a factor of 9000 using 50% enriched parahydrogen.

1. C. R. Bowers and D. P. Weitekamp, J. Am. Chem. Soc., 1987, 109, 5541-5542
2. S. B. Duckett, C. L. Newell and R. Eisenberg, J. Am. Chem. Soc., 1993, 115, 1156-1157
3. S. B. Duckett and R. Eisenberg, J. Am. Chem. Soc., 1993, 115, 5292-5293
4. M. Goldman, H. Jóhannesson, C. R. Physique, 2005, 6, 575-581
5. S. Kadlecěk, K. Emami, M. Ishii, R. Rizi, J. Magn. Reson., 2010, 205, 9-13
6. M. Goldman, H. Jóhannesson, O. Axelsson, M. Karlsson, J. Magn. Reson. Im., 2005, 23, 153-157
7. Field: F. Reineri, T. Boi, S. Aime, Nat. Commun., 2015, 6, 5858
8. S. J. DeVience, R. L. Walsworth, M. S. Rosen, Phys. Rev. Lett., 2011, 111, 173002

Boris Gouilleux

Ultrafast 2D NMR on a benchtop spectrometer: a promising tool for on-line monitoring and rapid screening

Boris Gouilleux,¹ Benoît Charrier,¹ Serge Akoka,¹ François-Xavier Felpin,^{1,2} Mireia Rodriguez-Zubiri,¹ and Patrick Giraudeau.^{1,2}

¹ Université de Nantes, CNRS, CEISAM UMR 6230, Nantes, France.

² Institut Universitaire de France, 1 rue Descartes, 75005, Paris, France.

The great performance reached by high-field (HF) NMR relies on strong magnetic fields, involving an expensive equipment with the need for dedicated laboratories. These economic and practical drawbacks have hampered the use of HF NMR in industrial sites and synthetic laboratories. A new generation of benchtop NMR spectrometers, more compact and cryogen-free, emerges as a relevant alternative to extend the scope of NMR in harsh environments.¹ Obviously, the use of these permanent magnets involves a reduced frequency dispersion leading to crowded spectra with numerous overlaps. 2D NMR experiments offer an appealing solution. Unfortunately their inherent long acquisition duration is incompatible with the time scale of applications such as reaction monitoring. In order to circumvent this time constraint, we developed Ultrafast (UF) NMR² on a benchtop spectrometer, yielding homonuclear 2D spectra within a single scan.³ These developments were performed on a 43 MHz Spinsolve (Magritek) including a gradient coil originally designed for diffusion experiments.

We first highlight the relevance of the UF NMR at 43 MHz through the real-time monitoring of a Heck-Matsuda coupling reaction in an on-line fashion.⁴ In the course of the reaction performed in a conventional flask, the mixture is directly analyzed through a by-pass system connected to the benchtop spectrometer, which records UF COSY spectra with well-resolved cross-peaks (Figure1).

Another potential of this approach relates to a long-standing concern: the screening of edible oils. Relevant results were recently reported using benchtop NMR for the adulteration with cheap substitutes into olive oil. Albeit promising, the accuracy of the 1D approach remains limited by the overlapped resonances from glycerides protons and those arising from the unsaturated chains. The UF COSY experiments overcome this issue by delivering well-resolved cross peaks, whose integration provides an efficient authentication tool.⁴ These first results shed light on the potential of UF NMR at 43 MHz as a promising rapid screening tool.

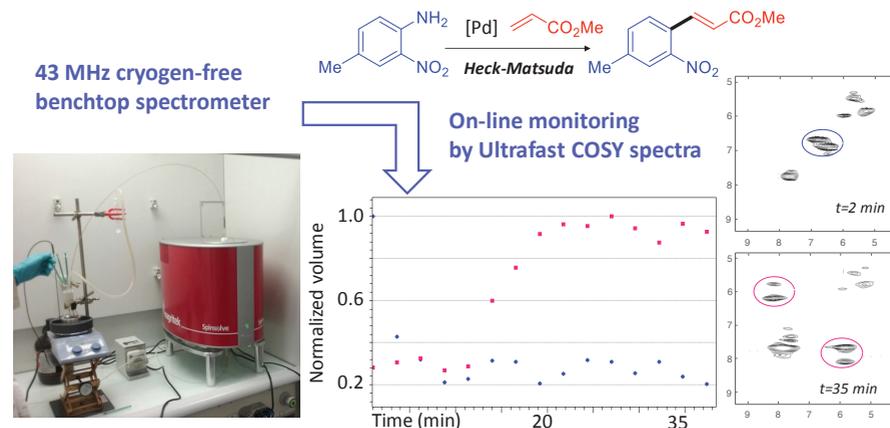


Figure 1. On-line reaction monitoring of a Pd-coupling reaction by ultrafast 2D NMR on a benchtop spectrometer.

1. E. Danieli, J. Perlo, B. Blümich and F. Casanova, *Angew. Chem. Int. Edit.*, 2010, 49, 4133-4135.
2. L. Frydman, T. Scherf and A. Lupulescu, *Prod. Natl. Acad. Sci. USA*, 2002, 99, 15858-15862.
3. B. Gouilleux, B. Charrier, E. Danieli, J.-N. Dumez, S. Akoka, F.-X. Felpin, M. Rodriguez-Zubiri and P. Giraudeau, *Analyst*, 2015, 140, 7854-7858.
4. B. Gouilleux, B. Charrier, S. Akoka, F.-X. Felpin, M. Rodriguez-Zubiri and P. Giraudeau, 2016, *Trends Anal. Chem.*, in press, doi: 10.1016/j.trac.2016.01.014

Reprint because of a typing error in bulletin 263/264

Financial Report of the Groupement Ampere

Fortune of the Society per June 21. 2016

Ampere Accounts	CHF	Euro
Savings Account	16'820.25	
Current Account	1'985.65	
Current Account Euro - <i>NEW</i>	4'502.67	4'139.73
Security Depot - <i>CLOSED</i>		
Savings Account Andrew	34'017.45	
Security Depot Andrew	83'310.69	
Total	146'636.71	
Accounts of subdivisions		
NMR school (Ampere)	2'169.11	1'994.27
MRPM	24'242.45	
Savings Account SMRM	35'424.55	
Savings Account Euromar	71'646.89	
Current Account Euromar	65'600.55	60'312.81
Hyperpolarization (past; DNP)	7'337.65	
EPR	7'418.40	
Food NMR	3'649.30	
Biol. Solidstate NMR - <i>NEW</i>	6'961.10	6'400.00
Total	224'450.00	
Grand Total	CHF 371'086.71	

Executive Officers and Honorary Members of the AMPERE Bureau

The AMPERE BUREAU includes the executive officers (which take the responsibility and the representation of the Groupement between the meeting of the committee), the honorary members of the Bureau and the organizers of forthcoming meetings.

Executive Officers 2016 - 2019

President	Bernhard Blümich
Vice Presidents	Janez Dolinšek Anja Böckmann
Secretary General	Gunnar Jeschke
Executive Secretary	Matthias Ernst
EF-EPR Representative	Graham Smith
SRMR Representative	Michael Johns
MRPM Representative	Yi-Qiao Song
MR-FOOD Representative:	John van Duynhoven
Hyperpolarisation Representative:	Geoffrey Bodenhausen
EUROMAR Representative	Lucio Frydman
EUROMAR Treasurer	Christine Redfield
Past President	Beat Meier
Honorary Member	Hans Wolfgang Spiess
Honorary Member	Stefan Jurga

Executive Officers 2016 - 2019

B. BLÜMICH

Macromolecular Chemistry, RWTH Aachen University, D-52074 Aachen, Deutschland
Tel. +49 241 802 64 20, Fax +49 241 802 21 85, e-mail: bluemich@itmc.rwth-aachen.de

J. DOLINŠEK

Institute Jozef Stefan, Department F5, Jamova 39, SI-1000 Ljubljana
Tel. +386 1 4773 740, Fax +386 1 4263 269, e-mail: jani.dolinsek@ijs.si

A. BÖCKMANN

Institute of Biology and Chemistry of Proteins, IBCP, F-69367 Lyon, France
Tel. +33 472 72 26 49, Telefax +33 472 72 36 04, e-mail: anja.bockmann@ibcp.fr

G. JESCHKE

Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 ZÜRICH, Switzerland
Tel. +41 44 632 5702, Fax +41 44 633 1448, e-mail: Gunnar.Jeschke@phys.chem.ethz.ch

M. ERNST

Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 ZÜRICH, Switzerland,
Tel. +41 44 632 4366, Fax +41 44 632 16 21, e-mail: maer@nmr.phys.chem.ethz.ch

G. SMITH

University of St. Andrews, School of Physics & Astronomy, North Haugh, ST. ANDREWS, KY16
9SS, U.K., Tel. +44 1334 462669, e-mail: gms@st-andrews.ac.uk

M. JOHNS

School of Mechanical and Chemical Engineering, The University of West Australia, CRAWLEY,
WA 6009, Australia, Tel. +61 8 6488 5664, e-mail: michael.johns@uwa.edu.au

Y.Q. SONG

Schlumberger-Doll Research, 1 Hampshire Street, Cambridge, MA 02139-1578 USA
Phone: +1 617 768 2333, Email: ysong@slb.com

J. VAN DUYNHOVEN

Unilever N.V., 100 Victoria Embankment, London EC4Y 0DY, United Kingdom, e-mail:
john-van.duynhoven@unilever.com

G. BODENHAUSEN

EPFL, Institut des sciences et ingénierie chimiques, BCH 1529 (Batochime), 1015 Lausanne,
CH, Tel. +41 21 693 94 31, e-mail: geoffrey.bodenhausen@epfl.ch

L. FRYDMAN

Weizmann Institute of Science, Department of Chemical Physics, 76100 Rehovot, Israel,
Tel: +972 8 934 4903, Fax: +972 8 934 4123, mail: lucio.frydman@weizmann.ac.il

C. REDFIELD

Department of Biochemistry, University of Oxford, South Parks Road OX1 3QU, United King-
dom, Tel. +44 (0)1865 613200, mail: christina.redfield@bioch.ox.ac.uk

B.H. MEIER

Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 ZÜRICH, Switzerland,
Tel. +41 44 632 44 01, Fax +41 44 632 16 21, e-mail: beme@nmr.phys.chem.ethz.ch

H.W. SPIESS

Max-Planck Institut für Polymerforschung, Ackermannweg 10, POB. 3148, D-55021 MAINZ,
Germany, Tel. +49 6131 379120, Fax +49 6131 379320, e-mail: spiess@mpip-mainz.mpg.de

ST. JURGA

Instytut Fizyki, Uniwersytet im. A. Mickiewicza, Zakład Fizyki Makromolekularnej, Umultowska
85, PL-61-614 POZNAN, Poland
Tel. ++48 61 829 5290, Fax ++48 61 829 5290, e-mail: stjurga@main.amu.edu.pl

AMPERE Committee

S. ASHBROOK

School of Chemistry, University of St. Andrews, North Haugh, ST. ANDREWS, KY16 9ST,
United-Kingdom

J. BANYS

Vilnius University, Department of Radiophysics, Saulėtekio 9 2040 VILNIUS, Lithuania

R. BOELENS

Bijvoet Center for Biomolecular Research, Utrecht University, Padualaan 8, NL-3584 CH
UTRECHT, The Netherlands

V. CHIZHIK

University of St. Petersburg, Quantum Magnet.Phén., Fac.of Physics, RU-198504
ST. PETERSBURG, Russia

J. DOLINŠEK

Institute Jozef Stefan, Jamova 39, SI - 1000 LJUBLJANA, Slovenia

I. FELLI

Department of Chemistry and Center for Magnetic Resonance (CERM), University of Florence
Via L. Sacconi 6 50019 SESTO FIORENTINO, (FI), Italy

P. GIRAudeau

Université de Nantes, Faculté des Sciences et Techniques, 2 rue de la Houssinière, 44322
NANTES Cedex 03, France

D. GOLDFARB

Chemical Physics Department, Weizmann Institute of Science, 76100 REHOVOT, Israel

W. KOZMINSKI

Biological and Chemical Research Center, University of Warsaw, Krakowskie Przedmieście
26/28, 00-927 WARSAW, Poland

M. PONS

Institute for Research in Biomedicine, University of Barcelona, Josep Samitier 1-5, 80828
BARCELONA, Spain

V.V. TELKKI

Department of Physics, University of Oulu, P.O. Box 3000, 90014 OULU, Finland

C. THIELE

Technische Universität Darmstadt, Alarich-Weiss-Strasse 16, 64287 DARMSTADT, Germany

J. SPEVACEK

Inst. of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 - 06
PRAGUE 6, Czechia

S. VAN DOORSLAER

SIBAC Laboratory, University of Antwerp, Universiteitsplein 1, B-2610 WILRIJK, Belgium

Emeritus members

L. KIMTYS

Department of Physics, Vilnius University, Universiteto Str. 3, VILNIUS 2734, Lithuania

F. MILIA

NRC Demokritos, Physics Department, Aghia Paraskevi Attikis, GR - 15310 ATHENS, Greece
J. HENNEL, Inst. of Nucl. Phys. Ul. Radzikowskiego 152, PL - 31342 KRAKOW 23, Poland

Honorary members

R.R. ERNST

Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 ZÜRICH, Switzerland

J. JEENER

Université Libre - Plaine, CP 223, Bld. du Triomphe, B - 1050 BRUXELLES, Belgium

P. MANSFIELD

University of Nottingham, Magnetic Resonance Centre, NOTTINGHAM NG7 2RD, U.K.

K.A. MÜLLER

IBM Zurich Research Laboratory, Säumerstrasse 4, CH - 8803 RÜSCHLIKON, Switzerland

K. WUETHRICH

Inst. f. Molekularbiologie u. Biophysik, ETH Zürich, CH-8093 ZÜRICH, Switzerland

Guest members

A. PINES

Dept. of Chemistry, University of California, BERKELEY CA 94720, USA, Delegate of ISMAR

J.A. NORRIS

Dept. of Chemistry, University of Chicago, South Ellis Ave. CHICAGO IL 6037-1403, USA
Delegate of the International EPR Society

K.A. McLAUHLAN

Physical Chemistry Laboratory, Oxford University, South Parks Road, OXFORD OX1 3QZ, UK
Delegate of the International EPR Society

D. AILION

Dept. of Physics, Univ. of UTAH, 304 J. Fletcher Building, SALT-LAKE-CITY 84112, Utah, USA

J. BJORKSTAM

Electrical Engineerin (FT-10), University of Washington, 98195 SEATTLE WA, USA

S.H. CHOH

Department of Physics, Korea University, SEOUL 136-701, Republic of Korea

D. FIAT

University of Illinois, Dept. of Physiology and Biophysics, POB 6998, CHICAGO IL 60680, USA

E. FUKUSHIMA

ABQMR, 2301 Yale Blvd., SE, Suite C2, ALBUQUERQUE, NM 87106, USA

E.L. HAHN

Physics Department, Univesity of California Berkeley, BERKELEY CA 94720, USA

O. JARDETSKY

Stanford University, Magnetic Resonance Lab., STANFORD, CA 94305-5055, USA

C.P. SLICHTER

Dept. of Physics, University of Illinois, 1110 W. Green Street, URBANA IL 61801, USA

Future conferences

Ampere Events 2016

13 International Youth School-Conference ,Magnetic resonance and its applications - Spinus-2016`	Repino (Russian Federation)	November 20-26 2016
--	-----------------------------	---------------------

Ampere Events 2017

Euromar 2017	Warsaw (Poland)	July 2-6 2017
ICMRM	Halifax (Nova Scotia)	August 13-17 2017

Other Events 2017

Spanish Biophysical Society	Sevilla (Spain)	June 6-8 2017
20 th ISMAR conference	Québec City (Canada)	July 23-28 2017
SciX2017	Reno (USA)	October 8-13 2017

Ampere Events 2018

Euromar 2018	Nantes (France)	July 1-5 2018
--------------	-----------------	---------------

Other Events 2018

SciX2018	Atlanta (USA)	October 21-26 2018
----------	---------------	--------------------

Ampere Events 2019

ISMAR / Euromar 2019	Berlin (Germany)	August 25-30 2019
----------------------	------------------	-------------------