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Groupement AMPERE

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

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Contents

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Editorial

Groupement AMPERE

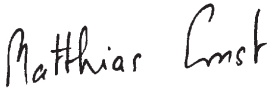
Dear Members of the Groupement AMPERE,

this year is the first year after the pandemic where conferences are fully back and it feels like there are even more of them or more concentrated than before. When the pandemic started everybody was very excited and positive about the many new online forms that came up and replaced the traditional in-person conferences that were not possible because of the many restrictions. But soon many of us realized that the online formats were good for information sharing and discussions in small groups but the important thing missing was the social component: meeting colleagues over a coffee in the break, talking to students in person at the posters, or talking about science and politics at dinner and meeting new people. There was also the hope that online formats might lower the environmental impact of conferences by reducing travel. If I look back at the conferences I attended this year, they are not different from conferences in 2019 which I find surprising after all the experiments that we did during the past three years.

I think it would be good for us as a scientific community to reflect about the role of conferences. Sharing of research results is no longer the main purpose since publishing has become very fast with preprints being available immediately. But meeting colleagues personally, networking, and getting an overview about related fields are for me the main reason to go to conferences. Personally, I think there are too many conferences, especially the big ones. Do we need EUROMAR and ENC every year and ISMAR and ICMRBS in addition every two years? What do we expect from attending a conference? Would not one main Magnetic Resonance conference be sufficient every year? Why did the hybrid formats not work? How can we reduce the travel impact of conferences?
I think these are questions that we should discuss and think about.

I wish you a good summer vacation time and if you have any thoughts on these topics, please feel free to share them.

Matthias Ernst
Secretary General, Groupement AMPERE



grapevine after unusually havy hailstorm on July 6. 2023, Cortemilia, Italy, Foto: comiotto, July 20. 2023, 08:32, work in progress

Recent experience with ‘Magnetic Resonance’, the Open Access journal of the Groupement Ampere, as seen through the eyes of a happy author.

Magnetic Resonance, the new Open Access journal of the Groupement Ampere, employs an innovative approach to peer review, inspired by various journals of the European Geosciences Union (EGU), where the entire correspondence between editors, reviewers, and authors can be read by the general public at any time.

The first two papers that were submitted in 2023 were written by Dr Deniz Sezer who is a member of Thomas Prisner’s group at Goethe University in Frankfurt:
(1) *Non-perturbative treatment of the solid effect of dynamic nuclear polarization.* It is well known that solid effect dynamic nuclear polarization can be rationalized in terms of mixing of the Zeeman energy levels. But it is less known that, even before Abragam’s explainatiojn of the phenomenon, Erb, Motchane and Uebersfeld proposed a phenomenological dynamical equation. Deniz Sezer provides a formal justification of their theory that leads to a different way of thinking about the solid effect, with novel implications for the effect in liquids. See MR, 4, 129–152, 2023;
https://mr.copernicus.org/articles/4/129/2023/.

The undersigned volunteered (somewhat foolishly?) to act as ‘handling editor’ of this first paper, but soon realized that the subject was quite challenging. Probably because the content was largely unfamiliar for many of the editors of MR, the reviewing process became rather protracted: In fact, in contrast to some other papers that I helped to edit, where almost all invited referees promptly accepted the job, no less than 5 respectable scientists declined my invitation, while 3 (perhaps wilfully?) missed the nomination deadline, before 3 others finally accepted. One of these, Malcolm Levitt, spoke of a ‘rather eccentric but interesting paper’.

One of the innovative features of MR is that the corresponding author, the handling editor, and the general public can follow in real time if proposed reviewers decline, fail to respond, or accept to serve as reviewers. This may reassure the anxious author that the review process is proceeding properly. Being able to see how the editor struggles to find reviewers may also strengthen the author’s trust.

(2) In a second paper, entitled *‘The solid effect of dynamic nuclear polarization in liquids’,* Deniz Sezer showed that the field profile in liquids (i.e., the NMR response as a function of the microwave frequency) provides rich dynamical information, in particular about the timescales of molecular diffusion, as can be determined by quantitative fits to experimental data. Some spectral features have a misleading resemblance with the signature of thermal mixing. See MR, 4, 153–174, 2023;
https://mr.copernicus.org/articles/4/153/2023/.

Again, I volunteered to act as ‘handling editor’ for Dr Sezer’s second paper. This time, only 3 colleagues politely declined my invitation to review the paper, while no less than 5 failed to respond, before 2 others finally accepted. Gunnar Jeschke wrote *‘This manuscript presents a very elegant theory on DNP under slow-tumbling conditions in liquid solution via a mechanism that is historically known as the solid effect. For a paper discussing high-level spin dynamics theory, it is astonishingly clear.’*

All of this took an inordinate amount of time, or so it seemed to me. I feared that the author might grow impatient, so, once the twin papers were finally published, I wrote to him in a private mail: *Now that the entire process has been completed, can you give me your opinion on our open review system, the handling of the files by the publisher, and the transparency (or lack of it) of the billing?*

To my delight, I received a very positive answer from Dr Sezer: *Thank you for your email and for giving me the opportunity to reflect on my experience with MR. The bottom line is that I am extremely happy that I chose to submit my research to MR. If I have to elaborate, several different factors have made my experience very positive.*

1. I really liked the fact that the manuscripts were accessible to everyone already during the review process. Although I cannot be certain, my feeling is that the visibility of my work was greatly increased in the early stage, when the paper was accessible through ‘MR Discussions’, compared to what could have been the case at a more general platform like ChemRxiv, for example.

2. I also liked the fact that I could immediately see the comments of the reviewers, as soon as they were posted, without the need to wait for the responses of all reviewers. This gave me the opportunity to reflect longer on the earlier feedback, which was very helpful when responding to all comments at the end.

3. Although I didn‘t write back to you when you first asked, I completely agree with your observation that the comments of the reviewers were well-thought and extensive. Again I cannot be certain, but I had a feeling that the open review process naturally encourages everyone (i.e., reviewers, authors and community members who comment on the manuscripts) to refrain from statements that could potentially be perceived as too aggressive.

4. I am also happy with the publisher and how they handled the publication process. (I cannot really comment on the payment side since the only thing I had to do was to specify my affiliation with Goethe University.)

While I haven't had a chance to follow the birth of MR and the subsequent (and continuing) efforts to make it the major interaction platform for the magnetic resonance community, I greatly appreciate your determination over the years toward this goal.

Coming back to my specific experience, I would also like to thank you for accepting to be the editor of my papers. Given the rather unconventional nature of my first manuscript (largely because I am somewhat of an outsider to the field), the selection of appropriate reviewers and the subsequent decision process could have been rather different. It has been truly a pleasure for me to have had the chance to interact with you scientifically, even if only in your role as an editor. I hope that there will be other similar occasions.

In a public comment that I uploaded on the website of 'Magnetic Resonance', I wrote: *'… I would like to express my appreciation for the breadth of the referees' comments and the depth of the author's response. I suspect that the mere fact that ‚Magnetic Resonance' allows the general public to have access to this correspondance ‚ad vitam aeternam' favours the quality of the exchange between referees and authors.'*

Public reviews may also serve as examples on how to write such reports. For rather sernior scientists such as myself, one can look back on the feed-back on hundreds of papers, but younger generations may not have a clue on the level of detail that is expected from referees, and may not realize how keen many authors are to respond in excruciating detail, indeed how grateful they are for constructive criticism.

Finally, I appealed to fellow editors of established journals: *'Although this would take away one of the essential competitive advantages of ‚Magnetic Resonance', I should like to express the wish that major journals such as ACIE and JACS, not to mention magazines like Nature and Science, would adopt a similar policy of open reviews. Note that this does not in any way compromise the referees' choice to remain anonymous if they wish.'*

Geoffrey Bodenhausen

Report:

Joint AMPERE and PANACEA Summer School on Biological Solid-State NMR online March-May 2023 and in Aarhus June 4-9, 2023

The AMPERE summer school on biological solid-state NMR has been a biennially recurring event since 2006, and since then it has been an important initiative for PhD students and postdocs allowing them to establish networks and gain knowledge about the state of the art within biological solid-state NMR.

During the corona pandemic, the school was extended with an online part in the spring preceding the physical meeting in Berlin in the summer of 2021. We decided to keep this setup in 2023 with an online program every Monday during the spring and a full week on-site lectures in early June.

The summer school was organized jointly between AMPERE and PANACEA, and the online part of the course was offered to both the participants of the summer school on biological solid-state NMR and participants of a PANACEA workshop on quadrupolar nuclei. There were a total of 50 participants registered for the online part, with an equal gender balance and good geographic diversity manifested by the presence of participants from 15 countries (Australia, Austria, Denmark, France, Germany, India, Italy, Mexico, Netherlands, South Africa, Spain, Sweden, Switzerland, United Arab Emirates, and United Kingdom).

The online part took place every Monday afternoon over Zoom and started in March with the legendary introduction to quantum mechanics by Beat Meier. Beat's lecture was as always thorough and with excellent historical references to the important persons in the development of quantum mechanics. Matthias Ernst followed by introducing anisotropic interactions and the concept of magic-angle spinning. Third week was devoted to exercises on the topics of the two first weeks. Third lecture was a newcomer on quadrupolar nuclei by Arno Kentgens, who demonstrated the use of NMR of quadrupolar nuclei in both materials and biological applications, and the following week was for exercises on quadrupolar nuclei. In the fourth lecture, Hartmut Oschkinat introduced product operators and how to use them for calculation of simple pulse sequences. Matthias Ernst returned and talked about linewidths and relaxation, followed by a week with exercises in these topics. In mid May, Thomas Vosegaard gave an introduction to numerical simulations and different algorithms and software packages for this, and the week after, the students tried out numerical simulations using SIMPSON and EasyNMR in the exercises. The final week of the online program was the classical

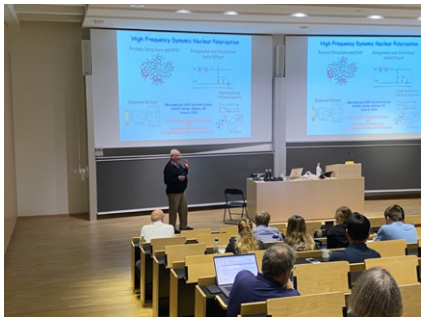
lecture by Huub de Groot on the challenges of modern structural biology.

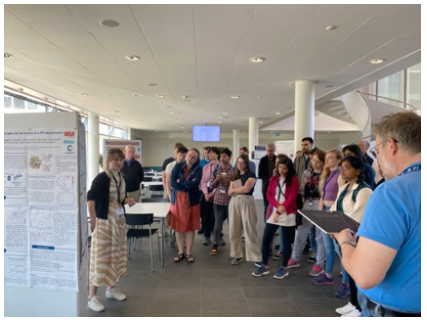
The full week in Aarhus was organized by Aarhus University and held at the Interdisciplinary Nanoscience Center at Aarhus University. 30 people were registered for the school, but there were a few absences, so we ended up having 24 participants and 12 lecturers.

	Sunday 4 June 2023	Monday 5 June 2023	Tuesday 6 June 2023	Wednesday 7 June 2023	Thursday 8 June 2023	Friday 9 June 2023
9:00-10:30		Basic concepts in NMR Meier	Setting up experiments Oschkinat	Probes (online) Engelke	Fast MAS / 1H detection Reif	
10:30-11:00		*Coffee*	*Coffee*	*Coffee*	*Coffee*	
11:00-12:30		De- and recoupling theory Ernst	New hardware Wegner / Grohe	Assignment Böckmann / Higman	Protein solid-state NMR experiments Oschkinat	
12:30-14:00		*Lunch*	*Lunch*	*Lunch*	*Lunch*	*Lunch*
14:00-15:30		De-/Recoupling experiments Nielsen	Sample preparation Böckmann	Assignment exercises Böckmann / Higman	DNP intro Griffin	In cell MAS NMR Baldus
15:30-16:00		*Coffee*	*Coffee*	*Coffee*	*Coffee*	*Closing*
16:00-17:30		SIMPSON exercises #2 Vosegaard / Nielsen	Poster pitch #1 Ernst	Poster pitch #2 Baldus	Structure calculation Higman	
17:30-18:00		Questions	Posters/beverages	Posters/beverages	Questions	
18:00-21:00	Welcome mixer				Dinner	

9:00-10:00	Dynamics Reif
10:00-10:15	*Coffee*
10:15-11:00	iNANO lecture: DNP Griffin
11:00-11:15	*Break*
11:15-12:30	Structures Oschkinat/Meier

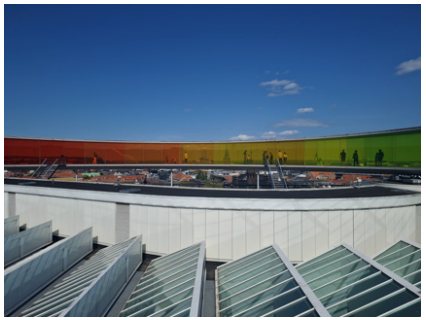
Monday through Friday was full of a good mixture of lectures and exercises by Beat Meier, Matthias Ernst, Niels Chr. Nielsen, Thomas Vosegaard, Hartmut Oschkinat, Kristof Grohe, Anja Böckmann, Frank Engelke, Vicky Higman, Marc Baldus, and Bob Griffin.





Tuesday and Wednesday afternoon was devoted to poster sessions and student presentations. There were 20 posters, and the authors presented their poster in turn in three-minute speed-presentations. The best poster was found by voting, and the poster award was given to Lea Becker from the Institute of Science and Technology Austria.

The social part of the summer school is very important to foster the best possible network between the participants. The school began Sunday evening on the 4th of June with a welcome reception with pizza and beverages.



Every evening offered new activities including playing volley ball at the beach, relaxing in the University park, visiting the AROS art museum, and playing board games in Aarhus downtown. Thanks to Armin Afrough from Aarhus University for organizing these different social activities.

Poster Prize Joint AMPERE and PANACEA Summer School on Biological Solid-State NMR

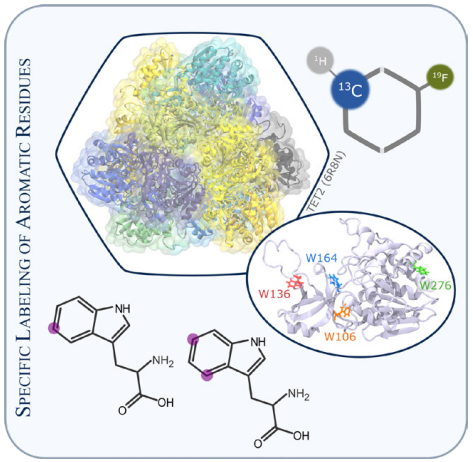
Lea Marie Becker, Institute of Science and Technology, Austria

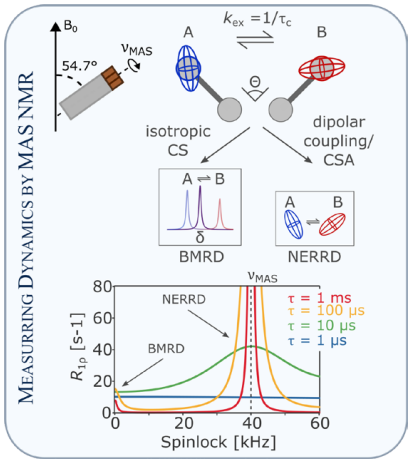
Exploring Protein Dynamics by Solid-state MAS NMR Through Specific Labeling Approaches

Lea Marie Becker, Paul Schanda
Institute of Science and Technology Austria

Aromatic residues are important reporters of protein structure and function as they are often overrepresented at functional sites, in the hydrophobic core, or at interaction interfaces. In this context, MAS NMR is uniquely suited to study their dynamics in large biological assemblies, crystalline proteins, or membrane proteins. However, measuring dynamics by MAS NMR comes with challenges and dif culties, such as broad lines, short signal lifetimes, and coherent contributions that complicate the analysis and interpretation of relaxation rates. Speci c isotope labeling in combination with deuteration yields well-separated spin systems, which signi cantly improves resolution and decreases the effects of dipolar dephasing.

On my poster, I present how we apply isotope labeling of aromatic residues with isolated ^{1}H-^{13}C spin pairs to study protein dynamics in the aminopeptidase TET2. We further aim to complement this approach with measurements on ^{19}F-labeled samples to exploit the advantages of this nucleus for sensitive and background-free dynamics measurements by MAS NMR.





Report:

AMPERE NMR School 2023 Zakopane, June 18-24, Poland

Scientific Committee:
Anja Böckmann (Lyon), France, Bernhard Blümich (Aachen), Germany, Janez Dolinšek (Ljubljana), Slovenia, Mathhias Ernst (Zurich), Switzerland, Wiktor Koźmiński (Warszawa), Poland, Danuta Kruk (Olsztyn, Poznań), Poland, David Lurie (Aberdeen), UK, Alex MacKay (Vancouver), Canada, Beat Meier (Zurich), Switzerland, Daniel Topgaard (Lund), Sweden.

Organizing Committee:
Danuta Kruk, Chair
Roksana Markiewicz, Executive Secretary
Tomasz Zalewski, Jacek Jenczyk, Jakub Jagielski, Grzegorz Nowaczyk, Nataliya Babayevska and Alicja Jorasz.

The AMPERE NMR School was held from June 18. to June 24. in Zakopane, a town in southern Poland's High Tatra Mountains. Nearly 80 researchers from research

institutions throughout the world attended the school. The conference was organized by the NanoBioMedical Centre under the auspices of the Groupement AMPERE. Like every year, young and experienced scientists from around the world attended the school to focus on basic and advanced NMR techniques. The participants had the chance to network, share knowledge about current NMR and related research, learn about new developments in the field, and form new relationships and collaborations.

The school's program covered as usual the following topics: NMR relaxometry, NMR diffusometry, Solid State NMR, NMR of quadrupolar nuclei, MRI and Field Cycling MRI, application of NMR in the area of biology, medicine, and material science, and technical aspects of NMR. In total, it consisted of 24 lectures given by:

Esteban Anoardo: Low field MRI solutions: fixed field, pre-polarized or field-cycled
Adriane Auucaise: Challenges of non-exponential NMR relaxation processes
Maria Beira: Assesing the Molecular Dynamics in paramagnetic liquid systems
Bernhard Blümich: Asymmetry in Three-Site Relaxation-Exchange NMR
Anja Böckmann: Solid-state NMR of the Multidrug ABC Transporter BmrA
Adolfo Botana: The magical world of pure shift NMR & Practical aspects of 13C qNMR
Lucia Calucci: Looking into porous materials with solid-state NMR and relaxometry
Leonid Grunin: Analysis of Strongly Dipolar Coupled Solids by Time-Domain NMR
Wiktor Koźmiński: High dimensionality and high resolution NMR experiments for biomolecules
Danuta Kruk: NMR relaxation processes in solutions of superparamagnetic nanoparticles

David Lurie: Basics of MRI & Field-Cycling Imaging
Arkadiusz Leniak: Exploring NMR Laboratory Operations in Medicinal Chemistry: Insights from Everyday Challenges at Celon Pharma SA
Olivier Lafon: NMR of quadrupolar nuclei at high magnetic fields
Beat Meier: Protein fast MAS experiments at high field
Giacomo Parigi: Field-cycling NMR relaxometry of paramagnetic-labeled proteins
Mecit Oztop: TD-NMR & MRI Applications in Food Systems
Pedro José Sebastião: Observing short-range orientational order: from liquid crystals to small molecule liquids
Claudia Schmidt: Ionic-liquid based hybrid gel polymer electrolytes as seen by NMR
Siegfried Stapf: Bicomponent fluids in porous media: what NMR can do for you
Janez Stepišnik: Chemical exchange rate studied by NMR CPMG method
Ville-Veikko Telkki: Effect of surfactant aggregation on cloud formation
David Topgaard: Translational motion and magnetic field gradients
Magdalena Wencka: ^{69}Ga and ^{71}Ga as probes of a local symmetry in diamagnetic complex metallic phases

The programme was enriched by the additional presentation of our sponsor – Jeol.
This year, five tutorials were performed, with additional online transmissions from the NMR laboratory of the NanoBioMedical Centre:
1. "Magic Angle" – Jacek Jenczyk
2. "MRI: basic principles and application" – Tomasz Zalewski and Marek Kempka
3. „NMR diffusometry" – Michał Bielejewski, Kosma Szutkowski
4. "JEOL Analytical Software Network (JASON) workshops - practical aspects" – Adolfo Botana
5. "FFC relaxometry" – Elżbieta Masiewicz

Moreover, as every year, all participants were given the opportunity to present their research in a poster session. The three equal prizes were awarded to the authors of the three best posters:

Fatima Anum from Kiel University (Germany) for the poster entitled "Synthesis of novel tracers for deuterium magnetic resonance imaging"

Krzysztof Baj from the University of Liverpool (UK), "Fast pKa determination for lead optimisation Application of Chemical Shift Imaging and Chemical Gradients into Analysis of APIs"

Marek Czarnota from the Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland for the poster entitled "Speeding up Restricted NMR Measurements for Porous Structure Determination of Biocompatible Gels"

The posters were evaluated by the Poster Committee: Prof. Pedro Jose Sebastiao, Prof. Claudia Schmidt and Prof. Marena Manley. All the winners received prizes accompanied by a certificate.

All abstracts of the oral presentations, tutorials and posters were published as printed proceedings (book of abstracts). The social programme included a welcome reception, Dinner in the Regional Restaurant “Biały Potok” with the folk music of the Tatras region, and excursion via an Alpine Path from Kalatówki to Biały Valley/ Strążyska Valley.

All the additional information about the AMPERE NMR School is presented on the website: school.web.amu.edu.pl and schools’s twitter account: @AmpereNMR.

The next edition of the school will be held in Zakopane (Poland) from June 16. to 22. 2024

Poster Prize AMPERE NMR School 2023

Fatima Anum, Kiel University, Germany

Synthesis of novel tracers for deuterium magnetic resonance imaging

Fatima Anum[a], Arne Brahms[b], Philip Saul[b], Maria Anikeeva[a], Rainer Herges[b], Jan-Bernd Hövener[a], Andrey N. Pravdivtsev[a],
[a]University Medical Center Schleswig-Holstein, Kiel University, Kiel, Germany
[b]Otto Diels Institute for Organic Chemistry, Kiel University, Kiel, Germany

Deuterium magnetic resonance imaging (DMI) is a non-invasive technique capable of generating high-resolution metabolic maps. This study explores the potential of deuterium- labeled DMI tracers for in vivo diagnostics and treatment monitoring. We present a novel deuterium based pH sensor for MRI, deuterium-labeled zymonic acid (ZA)-d4.

Protonated ZA was synthesized from sodium pyruvate (Pyr) and its pH sensitivity was evaluated. Pyr (0.1-0.2 M) was dissolved in water and maintained at a pH of 12 for two days. Acidification with HCl (pH ~1) was followed by water removal using a freeze dryer. The resulting crude ZA was diluted in acetone, filtered to eliminate NaCl, and purified using flash column chromatography with a Biotage SNAP Ultra C18 60g column and a 2-10% acetonitrile linear gradient. The purified ZA was freeze-dried, yielding a dark yellow viscous mass with an experimental yield of 50.8%.
pH-dependent changes in the chemical shifts of CH and CH_3 resonances of ZA were investigated using ^{1}H NMR analysis at varying pH values (2-3, 6-8). Two pKa values, 1.5±0.7 and 7.06±0.02, were confirmed. This chemical shift variation is planned to be utilized for pH mapping with DMI. Future steps involve synthesizing deuterated ZA and acquiring corresponding DMI pH maps.
In conclusion, deuterium-labeled zymonic acid (ZA)-d4 shows promise as a pH sensor for MRI, with its pH-dependent chemical shifts opening a new avenues for non-invasive in vivo diagnostics and treatment monitoring.

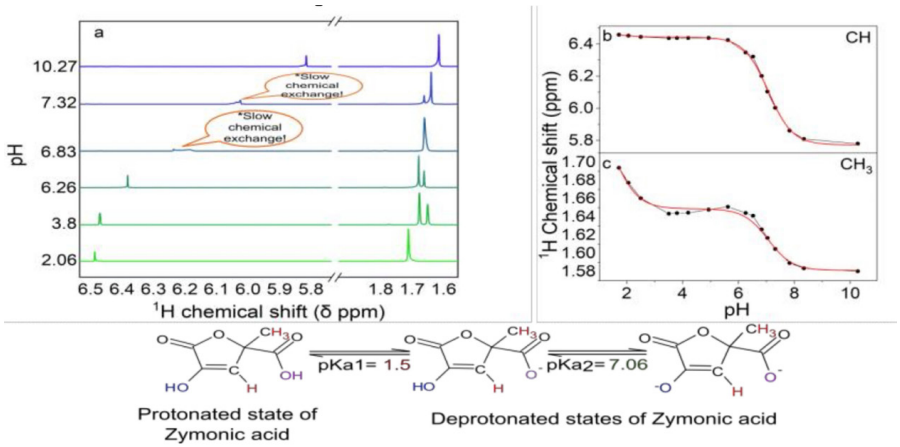


Figure 1: ^{1}H NMR spectra of ZA (a) and chemical shifts (b,c) as a function of pH. This experiment was conducted in 9.4 T at 290 K using 1:10 of H_2O:D_2O 49.64 mM ZA solution. Chemical shift variation of CH and CH_3 protons revealed to pH sensitive areas near pKa values of ~1.5 and 7.06.

Acknowledgements: We acknowledge funding from BMBF (01ZX1915C), DFG (PR 1868/3-1, HO-4604/2-2, HO-4604/3, GRK2154-2019, FOR5042, SFB1479, TRR287, HO 4604/3-1), Cluster of Excellence (EXC 2167), European Regional Development Fund (ERDF) and the Zukunftsprogramm Wirtschaft of Schleswig-Holstein (Project no. 122-09- 053) and intramural CAU funding.

Poster Prize AMPERE NMR School 2023

Krzysztof Baj, University of Liverpool, United Kingdom

Fast pKa determination for lead optimisation Application of Chemical Shift Imaging and Chemical Gradients into Analysis of APIs

K. Baj[a] A. Hindle[b] S.H. Marsden[b] J. Brammer[a] S. Demanze[c] M. Wallace[d] J.A. Iggo[a]
[a] Department of Chemistry, University of Liverpool, United Kingdom
[b] School of Chemistry, University of Leeds, United Kingdom
[c] Oncology R&D, AstraZeneca, Cambridge, United Kingdom
[d] School of Pharmacy, University of East Anglia, United Kingdom

^{1}H Chemical Shift Imaging [1] with a chemical gradient (CSI-CG) provides an efficient, one- shot method for the determination of pKa, using little analyte [2]. The technique can be readily used in DMSO-d6 [3] and has been used to analyse basicity patterns in a homologous series of bridged anilines. Density-Functional Theory (DFT) geometry optimisation and charge distribution calculations have been used to rationalise the results [4,5].

We have developed mixed solvent water-DMSO pH indicator ladders. That allows the determination of pKa in any water-DMSO ratio in a single-shot experiment and the reduction in the number of experiments required to extrapolate mixed-solvent pKa determinations to an aqueous value. As a result, we can successfully extrapolate to an aqueous pKa regardless of solvation effects on the analyte with a precision greater than that offered by computational methods.

Several pulse sequences for water suppression have been evaluated, and automation routines developed to allow the use of sample changers for high throughput of data acquisition in an industrial setting [3]. Water signals are suppressed using excitation sculpting, while pre- saturation can be used to suppress a second solvent peak if required, Figure 1.

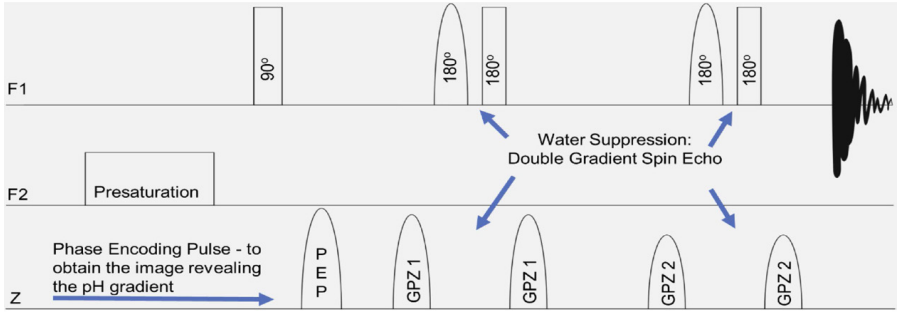


Figure 1. Pulse sequence for double solvent suppression ^{1}H Chemical Shift Imaging.

References:
[1] P. Trigo-Mourino et al., Chem. – Eur. J. 2013, 19, 7013-7019. [2] M. Wallace et al., Anal. Chem., 2018, 90, 4160-4166.
[3] G. Schenck et al., Anal. Chem., 2022, 94, 23, 8115–8119
[4] D. Bochevarov et al., Int. J. Quantum Chem., 2013, 113(18), 2110-2142.
[5] A. Hindle et al., Chem Commun., 2023, 59, 6239-6242.

Poster Prize AMPERE NMR School 2023

Marek Czarnota, Polish Academy of Science, Poland

Fast pKa determination for lead optimisation Application of Chemical Shift Imaging and Chemical Gradients into Analysis of APIs

Marek Czarnota[a], Sylwester Domański[b] and Mateusz Urbańczyk[a].
[a]Institute of Physical Chemistry,Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland
[b]Polbionica Sp. z o.o. Aleja Prymasa Tysiąclecia 79A, 01-242 Warszawa, Poland

Restricted diffusion measurements with Nuclear Magnetic Resonance spectroscopy provide us detailed information about porous structures. Restricted diffusion measurements utilize the behavior of molecules with movement limited by porous structures since the diffusion coefficient is lower than expected for free movement. The disadvantage of this measurement is it's duration, which can be shortened significantly by applying fast Time- Resolved methodology[1]. In our research, we study samples of Gelatin Methacryloyl hydrogels dissolved in water. The sample is used as a backbone structure for a 3D-printed bionic pancreas. In our work, we show the relationship between the concentration of Gelatin Methacryloyl, its degree of substitution, and its structure.

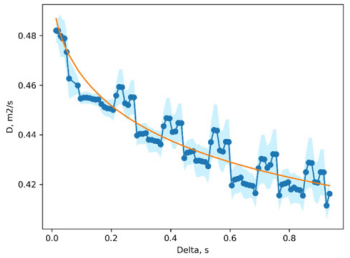


FIGURE 1. The exemplary plot of restricted diffusion of Gelatin Methacryloyl sample. Diffusion coefficient values are multiplied by the factor of 10-9. Light blue color is error of diffusion calculation.

Acknowledgements: The authors would like to thank the National Science Centre, Poland, for its support in the form of an OPUS Grant (2021/41/B/ST4/01286).

References: [1] Accelerating Restricted Diffusion NMR Studies with Time-Resolved and Ultrafast Methods, Mateusz Urbańczyk, Yashu Kharbanda, Otto Mankinen, and Ville-Veikko Telkki Analytical Chemistry 2020 92 (14), 9948-9955

Minutes of the meeting of the AMPERE Bureau

Glasgow, on July 11, 2023

Members present (13):
A. Böckmann, J. Dolinšek, P. Girardeau, M. Ernst, S. Hiller, G. Mathies, G. Jeschke, G. Bodenhausen, T. Prisner, B. Blümich, B.H. Meier, J.-N. Dumez, M. Baldus, J. Parkinson

Excused:
L. Ciobanu, Y.-Q. Song, J. van Duynhoven, G. Otting, H. Oschkinat, A. Kentgens, O. Millet, D. Kruk

Agenda:
1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Bureau meeting Online March 16, 2023
3. Report on the state of the AMPERE Society (A. Böckmann)
4. Financial Report (M. Ernst)
5. Subdivision for the AMPERE NMR School (M. Ernst/A. Böckmann)
6. More Sustainable Meetings (A. Kentgens)
7. Preparation of AMPERE Bureau elections (A. Böckmann)
8. Preparation of AMPERE Committee elections (M. Ernst/A. Böckmann)
9. Past and current meetings
   - EUROMAR Glasgow 2023 (T. Prisner)
10. Varia (M. Ernst)

At 12:50 hours, Matthias Ernst opened the meeting.

Ad 1. The agenda was approved as is.

Ad 2. The minutes of the AMPERE Bureau were approved unanimously.

Ad 3. The president A. Böckmann introduced the state and the structure of the AMPERE society. The society mourned the passing of Jean Jeener and acknowledged his contributions to NMR science, in particular the invention of 2D NMR. Sadly also, Katalin Köver, from Hungary passed way. There will be an obituary for her in the bulletin. Further notable members that had passed away in the last year include Stefan Berger and Pierre Tougne, William McFarlane, Karol Nartowski. They will be kept in the memory of the society members. A. Böckmann also mentioned the successful organization of several conferences, as well as the AMPERE Café.

Ad 4. M. Ernst presented the financial report. Finances are generally stable, with fluctuations in the normal range. Finances of the subdivisions also continue to be stable. Similarly, the EUROMAR account is stable. There will be a general assembly online later in the year to approve the finances.

Ad 5. The AMPERE NMR School in Zakopane is affiliated with the society, but not a subdivision. The school has run successfully for many years. They now are interested in becoming a subdivision of AMPERE. After some discussion in the Bureau, this proposal was strongly supported by the Bureau.

Ad 6. The Sustainability commission has met and discussed the topic of sustainability at AMPERE meetings. The committee will continue to develop possible measures. The Bureau discusses different options, including changes in conference frequencies, travel recommendations and food choices. The Sustainability commission plans to come up with more concrete suggestions at the next meeting.

Ad 7. Among the two young members of the Bureau, Q. Stern decided to step down. Consequently, there will be an upcoming re-election in the AMPERE committee for his replacement. The Prize committee had received 12 applications and unanimously selected Dariya Savchenko, from Ukraine, as the sole, highly suited candidate.

Ad 8. Four members of the AMPERE Committee, end their term wen 2023. These are all in their first term, and all four of them agreed to be re-elected: Kristaps Jaudzems LV, Predag Novak HR, Indrek Reile EE, Paul Vasos RO. The Bureau supports them for re-election by the general assembly.
Katalin Köver from Hungary passed away, and hence a new member from Hungary is needed. M. Ernst asked for suggestions.

Ad 9. The report of the EUROMAR 2023 was given by J. Parkinson. The conference is running well, with over 700 registered participants and over 370 posters. The final budget is estimated to be slightly positive. The Bureau thanked J. Parkinson for the organization. T. Prisner reported that the EUROMAR 2024 will be in Bilbao, the EUROMAR 2025 in Oulu, Finland, and the EUROMAR 2026 at Weizmann Institute, Rehovot, Israel. Both Oulu and Weizmann had convinced the selection committee with a strong proposal.

Ad 10. The general assembly will be held online on September 4 at 2 pm CEST on zoom.

The meeting closed at 14:12.
Glasgow, 11 July 23
Minutes: Sebastian Hiller

Minutes of the meeting of the AMPERE Committee

Glasgow, on July 12, 2023

Members present (28):
M. Ernst, S. Hiller, A. Kentgens, T. Prisner, J. Dolinšek, V.-V. Telkki, S. Ruthstein, B. Blümich, J. Parkinson, O. Millet, S. Ashbrook, A. Böckmann, B.H. Meier, G. Bodenhausen, J. Martins, J. Matysik, M. Baldus, G. Mathies, V. Klimavičius, L. Ciobanu, A. Lesage, D. Topgaard, P. Novak, P. Giraudeau, D. Kurzbach, P. Vasos, A. Gil, G. Parigi.

Excused: E. Bordignon, V. Chizhik, P. Crowley, I. Felli, M. Halse, K. Houben, K. Jaudzems, I. Komarov, W. Kozminski, G. Mollica, A. Pastore, M. Pons, I. Reile, F. Rise, M. Sardo, P. Schanda, G. Spyroulias, C. Thiele, L. Trantírek, J. Tritt-Goc, P. van der Wel, T. Vosegaard, Y.-Q. Song, J. van Duynhoven, G. Otting, H. Oschkinat.

Agenda:
1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Committee meeting Utrecht July 13, 2022
3. Report on the state of the AMPERE Society (A. Böckmann)
4. Financial report to be presented at the General Assembly (M. Ernst)
5. More Sustainable Meetings (A. Kentgens)
6. Subdivision for the AMPERE NMR School (M. Ernst/A. Böckmann)
7. AMPERE Bureau elections (A. Böckmann)
8. Preparation of Committee Elections at GA (M. Ernst, A. Böckmann)
9. Varia

At 12:54 hours, Matthias Ernst opened the meeting.

Ad 1. The agenda was approved as is.
Ad 2. The minutes of the previous AMPERE Bureau meeting were approved unanimously.

Ad 3. The president A. Böckmann welcomed everyone present. She gave an overview on the different branches of AMPERE. A. Böckmann then commemorated the colleagues that passed away since the last meeting and acknowledged their contributions to NMR science. The society mourns the passing of Jean Jeener, Katalin Köver, Stefan Berger, Pierre Tougne, William McFarlane, Karol Nartowski. They will be kept in the memory of the society members. G. Mathies organized an online café which was well received. Further future plans of the society are to create a searchable online directory of AMPERE members and to promote publications authored by society members.

Ad 4. M. Ernst presented the financial report of the past 2 years. Finances are generally stable. Similarly, the finances of the subdivisions including EUROMAR are stable. Generally, the society is in a financially healthy state. The budget will be voted on by the general assembly online on September 4th.

Ad 5. A. Kentgens reported on the sustainability committee. His committee will be looking into specific measures, such as nutrition, travel, remote participation. The committee briefly discussed several of these aspects.

Ad 6. The AMPERE NMR School in Zakopane so far was an associated conference but would like to become an AMPERE subdivision. There are precedencies because other schools and meetings already have a subdivision. In the Bureau meeting it had been recommended that there is a separate subdivision which could at a later stage be merged with other school subdivisions into a school division. The committee voted unanimously for the creation of the subdivision.

Ad 7. The committee discussed the prolongation and new-election of Bureau young members. The committee unanimously elected G. Mathies for a second year. The committee also voted unanimously that young members newly have terms of 2+2 years, rather than previously 1+1 years. G. Mathies gladly accepted the second year of her first term. She will be eligible for re-election for another 2-year period after the next year. Q. Stern had stepped down as the second young member. The prize committee had received 12 candidates for his succession and identified Dariya Savchenko from Ukraine as the best suitable successor and sole candidate. The committee elects D. Savchenko for a 2-year term.

Ad 8. Four members of the AMPERE Committee end their 4-year term in 2023. These were all in their first term and all four of them agreed to be re-elected: Kristaps Jaudzems LV, Predag Novak HR, Indrek Reile EE, Paul Vasos RO. The committee nominated these for re-election by the general assembly in September.
Katalin Köver from Hungary passed away, and hence a new member from Hungary is needed. The committee discussed several suggestions.
M. Ernst announced also the upcoming replacements that will be needed after 2024. These are countries UK, RU, SL, IT, FR, PL, ES.

Ad 9. The general assembly will be held online on September 4, 2 pm CEST. G. Bodenhausen says a few words about the future of Magnetic Resonance. The journal features public reviews, which is seen as a significantly positive factor for the journal. On the more negative side, Clarivate has refused to issue an impact factor, because the journal has too many special issues and invited papers. The journal will therefore stop invited papers and special issues. G. Bodenhausen appeals to the committee to publish in Magnetic Resonance. SCOPUS has listed and PubMed has agreed to list Magnetic Resonance.

The meeting closed at 14:08.
Glasgow, 12 July 2022
Minutes: Sebastian Hiller

Balance of the Accounts of the Groupement AMPERE and Subdivisions

Period from May 31. 2022 to May 31. 2023

	Balance on May 31. 2022	Membership Fees / Registration Payments	Donations/ Conference support, Copernicus	Travelgrants/ Prizes and membership fees to be pay to Ampere	Conference Sponsoring	Conference Surplus / Licence fees Copernicus & reimb. taxes	Administration, Web Bureau Meetings / domains, credit card	Bank Charges / Depot Charges/ losses on Depot	Account Closing / Account carry over	Bank Interests Account carry over, Dividends	Gains on Value Paper	**Balance on May 31. 2023**
Groupement Ampere												
Ampere (CHF)	**16'259.75**	3'310.02		58.00			972.00	37.50		2'456.21		**20'958.48**
Ampere (Euro)	**37'561.68**	19'105.25		2'512.04	7'000.00		38.52	105.22				**47'011.15**
Andrew (CHF)	**23'508.09**			2'418.51				390.15		2.25		**20'701.68**
Andrew Depot (CHF)	**94'047.78**							5'831.76				**88'253.52**
Subdivisions												
Biol. Solid State (Euro)	**13'729.72**						72.16	36.46				**13'621.10**
EPR (CHF)	**7'428.55**						20.00	2.00		0.75		**7'407.30**
Food NMR (CHF)	**615.42**					6'540.67				0.10		**7'156.19**
MRPM (CHF)	**32'614.10**				3'115.00					3.20		**29'502.30**
SMRM (CHF)	**61'894.18**						37.70			6.20		**61'862.68**
Hyp (CHF)	**4'121.00**									0.40		**4'121.40**
Publication Div. (Euro)	**281.56**					3'661.14		76.20				**3'866.50**
Euromar												
Euromar (Euro)	**98'529.22**		25'000.00	15'000.00	10'000.00			76.20				**98'453.02**

Obituary

Prof. Katalin E. Kövér PhD, a Chemist and NMR Spectroscopist and full member of the Hungarian Academy of Sciences, died on April 15, 2023.

It was with pain and shock that we learned of the news that academician Katalin E. Kövér, who was highly esteemed and loved by all of us, passed away after the Easter holidays on April 15, 2023 due to a serious illness.

Only 66 years were given to her, of which she devoted the professionally active part to NMR spectroscopy. She combined her talent with incredible work ethic and diligence, which greatly contributed to the development and international recognition of the Hungarian NMR community. With her methodological developments based on physical principles, she was able to improve the sensitivity and resolution of NMR by the introduction of novel pulse sequences, thereby expanding the application possibilities in the field of chemical and biological structure and interaction research. She was also interested in the structure discovery of biologically important proteins, oligopeptides, carbohydrates and antibiotics.

Born in Debrecen, Hungary in 1956, she obtained MSc. in chemistry at the former Lajos Kossuth University in 1979, then in 1981 she joined the NMR structural research laboratory led by Professor László Szilágyi, where an NMR spectrometer with 200 MHz superconducting magnet was put into operation for the first time in Hungary. This was a big challenge and potential for the young scientist. For a while, a Pharmaceutical Company supported her work at the Department of Organic Chemistry, then from 1999 she moved to the Department of Inorganic and Analytical Chemistry as a research associate, where she was appointed professor in 2008 at the University of Debrecen (UD). She got „candidate“ (PhD degree) in 1988, and in 2002 she became a doctor of the Hungarian Academy of Sciences (HAS). In 2013 she was a correspondent member of the HAS, then in 2019 she became a regular member, and from 2017 she was the deputy chairman of the Chemistry Section of the Hungarian Academy of Sciences.

During her career, she has received numerous awards, the most significant of which are: Bruckner Győző Award (2010), Premio Hispano-Húngaro Gamboa-Winkler Award (2010), Hajdú-Bihar County Prima Award (2014), memorial plaque of the Kajtár-Hollósi Foundation (2017), Officer‘s Cross of the Hungarian Order of Merit (2022). She took on many tasks in the organization of scientific life: from 2016 she headed the Doctoral School of UD Chemical Sciences, from 2010 she was a member of the János Bolyai Research Scholarship Expert College, editor of foreign journals and reviewer of publications. She was a PI or researcher participant of many Hungarian and international tenders. She worked as a guest researcher abroad (e.g. Tucson and Chicago, USA and Stockholm University, Sweden), had extensive international professional contacts, took on the role of organizer of conferences and often as invited speaker.

In 2019, she founded and led the „Molecular Recognition and Interaction“ Research Group in the supported research network of the HAS. During her career, she received more than 4500 citations for ca. 200 scientific publications. We remember her love of sports as her hobby: she competed for a while in the Debrecen Senior Swimming Club, but also swam Lake Balaton many times. Our condolences to his family and friends. We will preserve your memory and will continue your work.

God bless you, Kati!

Prof. Gyula Batta
President of the Hungarian NMR Discussion Group

Obituary
Stefan Berger (1946 - 2023)

Stefan Berger, born 1946 in Heidelberg, studied Chemistry in Tübingen and obtained there his PhD in Organic chemistry (1972). After a postdoc at the Caltech in Pasadena 1974, he became the head of the new NMR department at Marburg University.

While infrared spectroscopy was generally accepted as an analytical tool for structural elucidation, some chemists of the old generation rejected NMR spectroscopy. NMR was still mainly used in physics departments and physicists considered chemical shifts as a dirty chemical effect. Therefore, it was quite brave at that time to link his career to this controversial new method.

Berger then set up the first NMR service laboratory in Marburg. Since neither professors nor students had learned to interpret NMR spectra at that time, the „NMR service“ must also have been an NMR school. The possibility of once being able to calculate NMR spectra seemed utopian. So, an enormous treasure trove of data had to be gathered empirically. With Hans-Otto Kalinowski and Siegmar Braun, the book „13C NMR Spectroscopy“ (1984 in German, 1988 in English) was published. The success of this proved Berger right and the data treasure chest of NMR was immediately expanded to include numerous other non-metallic nuclei: again, with Hans-Otto Kalinowski and Siegmar Braun, four volumes of „NMR spectroscopy of the non-metallic elements“ were published (1992-1994 in German, 1997 in English).

A third book, which also canonized NMR spectroscopy for a wide audience of chemists and biochemists, gave an overview of the available NMR pulse sequences and appeared in several editions since 1996, constantly incorporating the latest pulse methods, some of which had Berger‘s signature. Once more with Hans-Otto Kalinowski and Siegmar Braun: „100 and more basic NMR experiments. The 2004 edition was called „200 and more NMR experiments“.

As a professor in Leipzig (1997-2013), he was directly involved in designing curricula in chemistry and developed two new English-language MSc programmes. In all these programmes and in further education and training courses, he taught NMR with great enthusiasm. While teaching, he developed the idea that NMR on natural substances relevant to life would certainly have to be particularly exciting for the students. Now a large series of works began in which such natural substances were investigated by molecular spectroscopy. These works were also compiled in books. Berger wrote the latest edition together with Dieter Sicker, Hans-Ullrich Siehl and Klaus-Peter Zeller: „Natural Products - Isolation, Structure Elucidation and History“ (2019).

In the last years, he started to work on nuclear hyperpolarization, in particular on the Haupt effect, which was later coined “quantum-rotor induced polarization” (QRIP). He retired in 2013. Although he suffered under Multiple sclerosis, he remained productive until his death.

Those who were lucky enough to meet Berger personally appreciated his sometimes direct honesty and his sense of humor. On April 2nd, 2023, our community lost one of our great teachers.

Jörg Matysik,
Institut für Analytische Chemie, Universität Leipzig, Germany

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.

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Jadwiga Tritt-Goc (2021-2025) Polish Academy of Sciences, Poland

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Future conferences

Ampere Event 2023

17th ICMRM	Singapore (Republic of Singapore	August 27-31
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	September 10-14
HYP23	Leipzig (Germany)	September 24-28

Ampere Event 2023

Euromar 2024	Bilbao, Spain	June 30 to July 4
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	September 10-14

Groupement
AMPERE

www.ampere-society.org