

BULLETIN DU GROUPEMENT

d'informations mutuelles



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Editorial



Dear members of the Groupement AMPERE,

In the summer and fall of 2019, on the initiative of Gottfried Otting and Geoffrey Bodenhausen, the Groupement AMPERE started the open-access journal Magnetic Resonance (www.magnetic-resonance-ampere.net) which is published by Copernicus in Germany (www.copernicus.org). This year, our journal has already 50 articles submitted in the first five month which I think is quite an achievement. I would like to thank Gottfried and Geoffrey for their hard work and continued support for this project. Of course, I also thank all the authors, editors and reviewers without whom this success would not have been possible.

One of the people who believed in the journal from the very beginning and helped shape the start by co organizing two special issues was Konstantin Ivanov from the International Tomography Center in Novosibirsk. In early March, we received the very sad and devastating news that he had passed away on March 5 at the age of 44 after falling ill of COVID. This is a big loss to the magnetic-resonance community at large, his colleagues in Novosibirsk and most of all his wife and daughter. Our thoughts are with all of them and we will remember his skills, energy, generosity and friendship he extended to many of us. Some thoughts have been collected in an obituary that we publish in this issue of the Bulletin.

I hope that many of you will be able to attend the online EUROMAR this July and to see many of you at the General Assembly of the Groupement AMPERE.

Best regards
and best wishes for a relaxing summer time,

Matthias Ernst
Secretary General, Groupement AMPERE

Preface to Portrait: Prof. Geoffrey Bodenhausen

Last 7th May, Geoffrey Bodenhausen celebrated his 70th birthday. His name has been at the forefront of NMR research for over forty years with contributions to all domains of NMR spectroscopy.

This started during his PhD thesis with Prof Ray Freeman at the University of Oxford, in the early days of 2D NMR, where he contributed to the development of correlation spectroscopy, selective excitation and relaxation, some aspects that he has been consistently exploring since.

He introduced the principles of indirect detection of less sensitive nuclei forty years ago, which has become an essential tool in modern NMR of biomolecules.

An early excursion in the domain of liquid crystals with Robert and Regitze Vold, and in solid-state NMR with Bob Griffin laid the bases for later methodological developments.

During his ETH period in the mid-80's, he contributed to the systematic and quantum mechanical description of 2D NMR: coherence transfer pathways, phase cycles, product operator formalism, and so on. This period is summarized in the celebrated book « Principles of Nuclear Magnetic Resonance in one and two dimensions » with Alexander Wokaun and Richard Ernst.

But for Bodenhausen, advancing methodology has been the possibility to explore in depth fundamental phenomena, and to use them in a spectroscopist's perspective to extract chemical information. Spin relaxation is one such domain, where in addition to earlier contributions, he developed numerous techniques based on interference effects to extend a panoply of methods to shed a brighter light onto structural and dynamical aspects of molecules.

Along the years, Bodenhausen has never stopped developing spin engineering techniques further (among which selective pulses, signal processing), whilst never overlooking more « exotic » topics (such as radiation damping or Xe-131 spectroscopy for the study of surfaces, among others). And mentioning his contribution to solid-state NMR and MRI techniques can only confirm the broad scope of his scientific interests and notable contributions to NMR.

In addition to this non-exhaustive list, Bodenhausen has also actively contributed in the past decade to the advancement of dissolution dynamic nuclear polarization techniques and applications.

Finally, beyond pure scientific achievements, Bodenhausen has been actively serving the NMR community, by taking part in the organization of international meetings (ENC, EUROMAR, in particular), and acting as editor of several NMR journals, promoting open access to scientific literature, which led to the creation of Magnetic Resonance, a journal backed by the Groupement Ampère.

Daniel Abergel, Fabien Ferrage, Konstantin Ivanov (deceased) †

Portrait: Prof. Geoffrey Bodenhausen



- Why magnetic resonance and why NMR?

Because magnetic resonance has its mysteries (is it quantum mechanical, or is it classical?) and because it is such a nice, safe and easy playground for all to try their ideas.

- What is the natural history of INEPT?

At the time, it seemed hard to think in two distinct rotating frames, one for protons and one for carbon-13, each with its own reference phase. We were baffled by the fact that heteronuclear experiments work so nicely, regardless whether two pulses are applied simultaneously or one after the other. It would only be years later that I heard about commuting propagators. I still admire Ray Freeman's unique gift for inventing acronyms, and Gareth Morris' ability to build a phase-shifter for the 80 MHz proton amplifier of our Varian CFT-20 spectrometer. Gareth was a seasoned radio amateur, while I did not even know how a transistor works (and still do not). I felt (and still feel) a bit jealous because I left the Oxford lab in November 1977, about a year before INEPT was invented in October 1978.

- What is your favourite contribution to NMR?

Carr and Purcell brilliantly described the effects of diffusion through an inhomogeneous field, and lucidly explained how multiple refocusing can fix the problem.

- What is your worst NMR experience?

Trying to read Abragam's famous book...

- What do you still not understand (and you would like to)?

Lindblad, Floquet, Landau-Zener, special and general relativity...

- How do your best ideas come to you?

By naïvely opposing simple ideas against complicated and woolly claims. And by arguing with (and against) good-willed colleagues.

- If you had the opportunity, what would you do differently?

I would do everything differently, with the exception of the labs where I had a chance to work (Oxford, UCSD, MIT, ETH, UNIL, FSU, EPFL and ENS), the people whom I met there, and the subjects that they cherished.

- Do you have any regret (NMR-wise)?

None as far as I can remember. I have a great gift for forgetting my own failures.

- Your favourite NMR anecdote?

Alex Pines, when putting their “magic sandwich” in the mailbox, purportedly said “Here goes our reputation.” John Waugh commented “But you have no reputation!”

- What is your hope or wish for future NMR generations?

Have fun! Don't be ashamed if your competitors look down on your papers, deriding them for being “elegant” and superficial rather than profound.

- Your favourite word? Attraction

- Your favourite sound? Waves crashing on pebbles.

- The work/occupation you would not have liked to have?

Being a manager and ‘making money’.

- Your favourite heroes in fiction? Ulysses

- Your favourite heroines in fiction? Penelope

- Your favourite heroes in real life?

The authors of the numerous books that have kept me company.

- Your favourite heroines in real life?

My daughters and grand-daughters.

- The natural talent you would like to be gifted with?

A talent for composing, playing and remembering music.

- What is your present state of mind?

Optimism, despite much evidence that it is naïve.

- For what fault do you have most tolerance?

Stakhanovism.

First announcement

Workshop on the Applications of Magnetic Resonance in Food Science: Multiscale Food Structures and FoodOmics

An interactive online workshop organized by the Magnetic Resonance in Food Division (MRFOOD) of the Groupement Ampere on October 28, 2021.

The workshop is aligned to the special issue ‘Multiscale Food Structures and FoodOmics’ that will be published in the journal Magnetic Resonance in Chemistry. Presenters at the workshop will be authors who have contributed to the content of the special issue.

You are therefore invited to submit manuscripts for the special issue ‘Multiscale Food Structures and FoodOmics’. A main objective of the workshop is to provide young scientist a platform for presenting and discussing their work with peers.

The scope of the special issue comprises food structure and/or food metabolites as these critically determine sensorial and nutritional attributes of foods systems and their assessment is important for designing technologies to modify biofunctionality, texture and digestion. An objective of this special issue is to emphasize the potentials of magnetic resonance (MR) techniques for the characterization of food structures on different length scales and under dynamic conditions such as temperature, shear, mass transport. Next we will wellcome foodomics studies on spatial distribution of metabolites and molecules, investigations of bioactive metabolites or constituents, the use of multidimensional NMR spectroscopy, multiple and/or advanced techniques, as well as studies focused on method development, novel data acquisition, data analysis and processing, e.g. using machine learning or other cutting-edge techniques.

First come, first serve and deadline for submission of manuscripts is October 1, 2021.

For evaluation of manuscript eligibility, please contact guest editor Prof. John Van Duynhoven, email: john.vanduynhoven@wur.nl or Prof. Hanne C. Bertram, email: hannec.bertram@food.au.dk

The interactive online workshop is organized by the Scientific advisory board of MRFOOD: [https:// www.foodmr.org](https://www.foodmr.org).

Report:

The 18th International School-Conference «Magnetic Resonance and its Applications» Spinus 2021



Since 2004 the Saint-Petersburg University holds a series of the annual International School-Conference «Magnetic Resonance and its Applications. Spinus» (an AMPERE event since 2016). The 18th Meeting “Spinus-2021” was opened on Monday, March 29, and was closed on Friday, April 02, 2021. For the first time the conference was realized in online format (via ZOOM) due to limitations of the COVID-19 Pandemic.

The goal of the School-Conference is to provide a platform to young scientists and students for the use of all aspects of magnetic resonance methods and techniques as well as computational and theoretical approaches for the solving of fundamental and applied problems in physics, chemistry, medicine and biology. The scope of the Conference included the following topics:

- Modern trends in NMR, ESR and NQR
- Magnetic resonance for fundamental science
- Magnetic resonance imaging
- Computer Modeling
- Earth’s field NMR
- Magnetic resonance in industry
- Related areas



The Meeting was attended by 113 participants from 19 countries: Australia, Cuba, England, Finland, France, Germany, Greece, India, Italy, Japan, Lithuania, Poland, Russia, Serbia, Slovenia, Sweden, Tajikistan, Turkey, USA.

The Meeting was opened by the talk of Prof. V. I. Chizhik (Saint Petersburg State University, Russia) “On history of the annual International School-Conference “Magnetic Resonance and Its Applications”.

During “Spinus 2021” there were 23 lectures, 45 oral (15-20’) and 39 poster presentations. Besides, for young scientists with poster presentations the opportunity to make oral blitz-reports (5’) was given. In particular, the lectures were given by Professors Bernhard Bluemich (Germany), Yury Bunkov (Russia), Elena Charnaya (Russia), Sergey Dvinskikh (Sweden), Jacques Fraissard (France), Prof. Jozef Kowalewski (Sweden), Olga Lapina (Russia), Malcolm Levitt (England), David Lurie (England), Thomas Meersmann (England), Georgios Papavassiliou (Greece), Yuri Pirogov (Russia), William Price (Australia), Kev Salikhov (Russia), Kazunobu Sato (Japan), Sergey Vasiliev (Finland).

The organizers published the Book of Abstracts (<http://spinus.spb.ru/>). Selected papers will be published in a special issue of the journal “Applied Magnetic Resonance”.

Barbara and Uwe Eichhoff (Germany) founded prizes of 200 and 100 Euro, respectively, for the best oral and poster reports of students and postgraduate students. Nominees were selected by an international commission. The Program Committee selected:

The best oral report

Aleksandr Koronotov (Institute of Chemistry, Saint Petersburg State University, Saint Petersburg, Russia) „2D NMR Structure Determination of 3,4-Dihydro-1,2,4-triazine Intermediate in Novel Rh(II)-catalyzed Transannulation Reaction“

Nominees:

Polina Kononova (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia) “The 1H NMR and MD study of the interaction of the antiviral agent glycyrrhizin with lipid membranes: an effect on lipid mobility and membrane fusion“

Aleksandra Kusova (Kazan Institute of Biochemistry and Biophysics, Russian Academy of Sciences, Kazan, Russia) “Protein intermolecular interactions according to the translational diffusion by PFG NMR and DLS“

Wassilios Papavassiliou (Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden) “Broadband high resolution NMR studies of topological matter“

“NMR signal enhancement in hydrogenation reactions with parahydrogen“

The best poster presentation

Aleksandra Andrzejowska (M. Smoluchowski Institute of Physics, Jagiellonian University, Cracow, Poland) „ Molecular dynamic of bound water in Antarctic lichenized fungus *Umbilicaria antarctica* Frey & I.M. observed by sorption isotherm and 1H-NMR „

Nominees:

Mark Smirnov (Institute of Physics, Mathematics and Information Technology, Immanuel Kant Baltic Federal University, Kaliningrad, Russia) “1H high-resolution NMR spectrometry and relaxometry for soybean oil research”

Julia Popova (Northern (Arctic) federal university named after M.V. Lomonosov, Arkhangelsk, Russia) “the application of nuclear magnetic resonance spectroscopy to the calculation of lignin structure formulas”

Please be already welcomed to the next meeting “Spinus-2022”:
Saint Petersburg, March 28, 2022!

Best oral report

Aleksandr Koronатов

2D NMR structure determination of 3,4-dihydro-1,2,4-triazine intermediate in novel Rh(II)-catalyzed transannulation reaction.

A. Koronатов, M. Novikov.

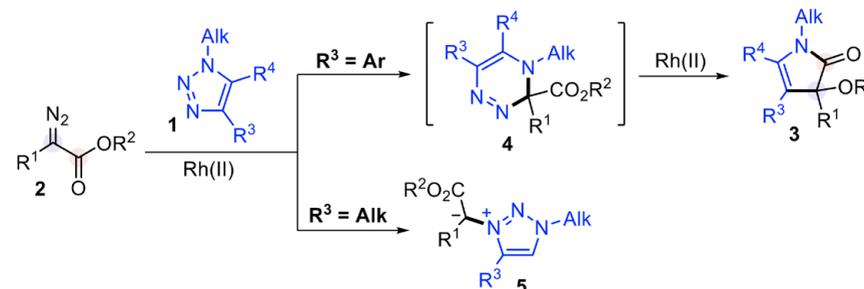
Institute of Chemistry, Saint Petersburg State University, 198504, Universitetskii prospect 26, Petergof, Saint Petersburg, Russia, E-mail: koronатов@bk.ru

Introduction

1,2,3-Triazoles are attractive compounds for various applications in different fields of chemistry. Transannulation reactions of their derivatives are usually catalyzed by transition metal complexes or light irradiation. The reactions proceed via the formation of metalcarbenes, which, when reacting with alkynes, nitriles, imines, and other unsaturated compounds, afford a wide variety of heterocyclic skeletons. Unfortunately, range of such triazoles, which could undergo aforementioned transformation, was limited to 1-sulfonyl-1,2,3-triazoles, 1-perfluoroalkyl-1,2,3-triazoles, and [1,2,3]triazolo[1,5-a]pyridines until recently.

However, in 2020 our research group discovered the first example of transannulation reaction with inactivated 1-alkyl-4-aryl-1,2,3-triazoles **1** with diazoesters **2** under rhodium(II) catalysis [1]. In fact, this approach gave the opportunity to synthesize variously substituted 3-alkoxy-4-pyrrolin-2-ones **3** (their structures were determined

by NMR and X-ray studies). The investigation of reaction mechanism showed that it proceeded through unstable 3,4-dihydro-1,2,4-triazine **4**, which could be detected and isolated if the reaction was carefully monitored. Structure of the compound **4** in one case was proved by HRMS and NMR (1H, 13C and 2D NMR). On the contrary, when the aryl substituent at C4 position of triazole ring was replaced with alkyl we did not observe the transannulation product **3**, so it was proposed that stable triazole ylide **5** was formed.



Experimental section

As was mentioned before, one of the intermediate, in particular compound **4a**, could be successfully isolated and it was shown by HRMS–ESI experiments, that it has formula $\text{C}_{14}\text{H}_{14}\text{F}_3\text{N}_3\text{O}_2$. Thus, four possible structures (A–D, figure 1) can be proposed considering the reaction mechanism.

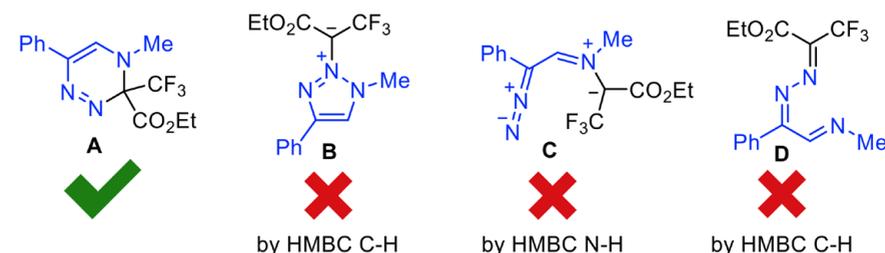


Figure 1. Suggested structures for compound **4a**.

Unfortunately, basic NMR techniques (^1H and ^{13}C NMR) did not reveal any additional information regarding the structure of **4a**. Therefore, 2D NMR of this compound was studied (figure 2). Obtained data was sufficient enough and we concluded that only one possible structural formula fitted all the criteria – 3,4-dihydro-1,2,4-triazine. To the best of our knowledge, it was the first example of this heterocyclic scaffold bearing such functionalization. Probably, it was the reason of its instability and, consequently, the reason why this unusual transannulation reaction proceeded.

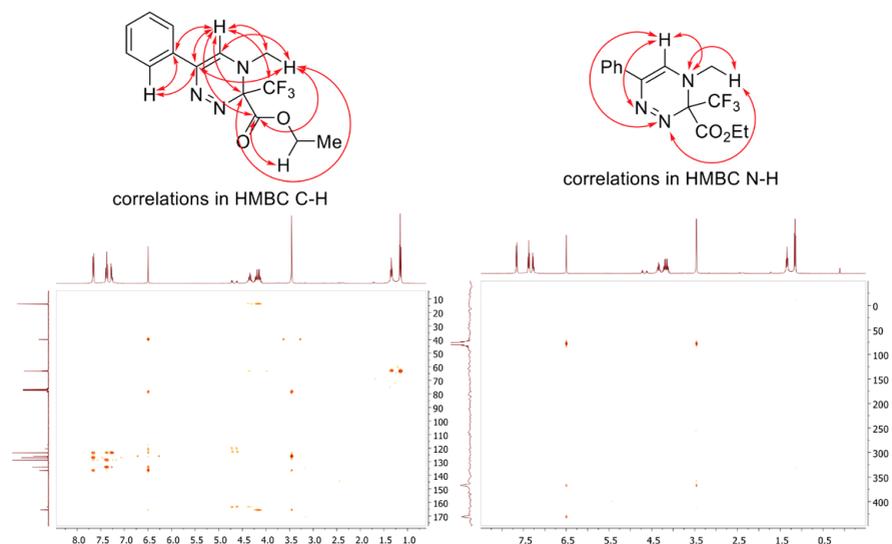


Figure 2. Correlations in HMBC C-H and HMBC N-H spectra of 4a.

In the same manner, it was impossible to verify the structures of triazolium ylides 5 by X-ray crystallography. Consequently, we proved its structural formula by analysis of ^1H , ^{13}C , 2D NMR spectra and HRMS.

Acknowledgements

We gratefully acknowledge the financial support of the Russian Science Foundation (20-13-00044). This research used resources of the Magnetic Resonance Research Centre, Chemical Analysis and Materials Research Centre, Centre for X-ray Diffraction Studies, Computing Centre, and Chemistry Educational Centre of the Research Park of St. Petersburg State University.

References

[1] Alexander N. Koronotov, Nikolai V. Rostovskii, Alexander F. Khlebnikov, Mikhail S. Novikov *Organic Letters* 2020, 22, 20, 7958–7963.

Best poster presentation

Aleksandra Andrzejowska

„Molecular dynamic of bound water in Antarctic lichenized fungus *Umbilicaria antarctica* Frey & I.M. observed by sorption isotherm and ^1H -NMR.

Aleksandra Andrzejowska¹, Karol Kubat¹, Angelica Casanova-Katny², Kazimierz Strzałka^{5,6} Maria Olech^{3,4} and Hubert Harańczyk¹

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⁴Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw, Poland,

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⁶Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, Cracow, Poland

Antarctic lichenized fungi may survive extremely low temperatures and high desiccation. This research is focused on molecular mechanisms of these abilities.

The Antarctic lichen *Umbilicaria Antarctica* collected from the sites on rocks of Isla Robert, Southern Shetlands, maritime Antarctica, on July 7th, 2018, at Chilean 54. ECA (54 Expedition Cientifica Antartica). The rate and the sequence of saturation of three bound water fractions was tested.

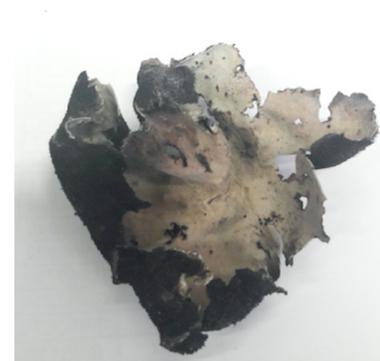


Figure 1. Thallus of *Umbilicaria antarctica*

Gaseous phase hydration and dehydration courses, sorption isotherm, ^1H -NMR spectrometry and relaxometry was used to monitor molecular dynamics of water in *U. antarctica* thalli. The hydration courses revealed bound water fractions: (i) a very tightly bound water $A_0^h = 0,01(1)$ still present after dehydration over the silica gel, (ii) a tightly bound water fraction $A_1^h = 0,08(1)$ with the hydration time $t_1^h = 2,4(3)$ h, and (iii) a loosely bound water fraction with the hydration time $t_2^h = 27(3)$ h.

For $p/p_0 \geq 88\%$ the total level of bound water significantly increases up to *ca.* 0,6 which may be interpreted as a recovery of life activity in *U. antarctica*. The dehydration kinetics is well described by a single-exponential function with the dehydration time $t^d = 10(1)$ h. The sorption isotherm showed the multilayer sorption fitted well by a sigmoidal function. We fitted two models of the sorption process, namely a classic Brunauer-Emmett-Teller (BET) model, and a newer Dent model (Guggenheim-Anderson-de Boer = GAB). The GAB fits yield the value of primary binding sites contribution equal to $\Delta m/m_0 = 0,05(1)$, as expressed in units of dry mass, m_0 . The fraction of unoccupied binding sites at $p/p_0 = 100\%$ equals $1/b_1 = 0,01\%$, which may suggest elevated hydrophilicity level of the surface of *U. antarctica* thallus.

$^1\text{H-NMR}$ spectra and relaxation times distinguish two signals of bound water: (i) a tightly bound water, and (ii) a loosely bound water fraction. $^1\text{H-NMR}$ spectrum is fitted well by superposition of Gaussian function (from partially immobilized protons of solid matrix) and one (up to $\Delta m/m_0 = 0.42$), or two Lorentzian function. The half-width of the solid Gaussian line component is equal to $\nu_G \approx 45$ kHz and does not change significantly with the increasing hydration level. The half-width of the first Lorentzian, coming from restricted in mobility tightly bound water fraction, decreases with the increased hydration level up until $\Delta m/m_0 = 0.45$ and does not change with higher hydration levels. The half-width of the second Lorentzian, coming from a loosely bound water fraction, also decreases with the increased hydration level across the entire measurement range. For tightly bound and loosely bound water the peak positions of the Lorentzian lines are different, which may be attributed to the difference in chemical shifts.

$^1\text{H-NMR}$ FID (Free Induction Decay) function is fitted well by a superposition of one Gaussian function (protons of thallus solid matrix) and one (up to $\Delta m/m_0 = 0.30$) or two exponential functions. First exponentially relaxing signal comes mainly from tightly bound water relaxes with ≈ 100 μs . Second exponential function is a signal coming from loosely bound water relaxing $T_{2L_1}^*$ g with $T_{2L_2}^* \approx 1000$ μs . *U. antarctica* thallus contains a water-soluble solid fraction. The saturation concentration of water-soluble solid fraction, $c_s = 0.55(9)$, and the dissolution effect is detected at least up to $\Delta m/m_0 = 0.7$.

Acknowledgements

This research was performed thanks to INACH (Instituto Antártico Chileno, Ministerio de Relaciones Exteriores, Chile): Sistema de Proyectos INACH, RT_27_16.

Keywords: Antarctica, extremophiles, lichens, lichenized fungi, Umbilicaria, dehydration, hydration, sorption isotherm, hydration kinetics, $^1\text{H-NMR}$, relaxometry, spectrometry

In memoriam Konstantin Lvovitch Ivanov

(10 January 1977 - 05 March 2021)

Our esteemed colleague and good friend Konstantin (“Kostya”) Lvovitch Ivanov has become one of the first victims of the pandemic in our community. He passed away in a hospital in Novosibirsk on March 5th 2021. We shall deeply miss Kostya as an exceptional human being: he was a creative yet rigorous scientist, a generous and attentive friend, a considerate and eminently civilised colleague.

Rob Kaptein wrote “[Kostya] was not only a great scientist, one of the few people who really understood magnetic resonance and spin chemistry, but also a good human being, always sincere, honest, and considerate. In addition, he was a great citizen of the scientific community; aside from his demanding job as the director of the International Tomography Center (ITC) of the Siberian Branch of the Russian Academy of Sciences, he kept his research at a high level and organized a multitude of meetings, seminars and webinars.” Kostya had built a strong relationship with Rob when they worked together in Novosibirsk, with the support of a Russian “megagrant” that Kostya had helped to secure. Kostya initiated further initiatives, so that another similar grant may soon be awarded were one of the undersigned may come to play a role, alas without Kostya’s diplomatic and scientific skills.

Rolf Boelens wrote “[Kostya’s] theoretical knowledge on NMR was phenomenal, discussing [with him was] very stimulating and never dull. (...) It was clear that Kostya was not only an outstanding scientist, but also an excellent teacher, who very well trained and stimulated his students.” Indeed, Kostya was a master of many trades, hyperpolarization, chemically induced dynamic nuclear polarization, diffusion-controlled reactions, parahydrogen induced polarization using catalysts in both low and high fields, field-dependent relaxation, long-lived states, magnetic resonance imaging, and he nurtured some challenging aspects of quantum mechanics such as avoided level-crossings with great talent.

One of his colleagues in Novosibirsk wrote “Kostya could be a humble and cheerful easy-going person, and yet be a leader with a steel hand realizing his vision of how things should be done despite numerous obstacles, never afraid of stepping up front and standing for his words. He was a lucky guy, and he passed his luck over to people whom he met. Looking back now, it is incredible how much he had



accomplished in his short but fruitful life, and how much he had started that we can continue on. It is our obligation to him to keep things that he initiated going and developing, this will be the best possible homage to Kostya.”

Kostya Ivanov studied at the Faculty of Physics of Novosibirsk State University, obtained the degrees of Bachelor of Science (1998), Master of Science (2000), and PhD (2002) under the supervision of Renad Sagdeev and Nikita Lukzen at the International Tomography Center (ITC), Novosibirsk, and of Doctor of Science in Physics and Mathematics (2008), and he was appointed Professor of the Russian Academy of Sciences.

Kostya held a Fellowship of the Alexander von Humboldt Foundation (Germany) in 2008 where he worked with Hans-Martin Vieth, and a Fellowship of the Japanese Society for Promotion of Science in 2016 that allowed him to work with Takeji Takui and Kazunobu Sato. He received the Medal of the European Academy of Science (Europea Academia Prize) in 2010, and shared the Laukien Prize with Simon Duckett and Warren Warren in 2020.

Kostya recently spent a month in Paris as professeur invité at ENS. As Fabien Ferrage wrote, “Kostya had so much strength, he was so intelligent, knowledgeable, hard-working and generous. We were of the same age, and his daughter Kseniya and my son Ravi also are of nearly the same age, which gives an even greater sense of proximity to this tragedy.”

Kostya was a key member of the of “Division of hyperpolarization” of the Groupement. Kostya was also one of the driving forces behind the creation of “Magnetic Resonance”, the Open Access journal of the Groupement Ampere. Only a few months ago, Kostya, Joerg Matysik, Rolf Boelens, Daniel Abergel and Fabien Ferrage had taken the initiative to compile two special Issues of “Magnetic Resonance” on the occasion of the 80th birthday of Rob Kaptein and the 70th of one of the undersigned. Our community will bitterly miss Kostya when these special Issues will be presented in events that Kostya would surely have wished to attend.

We shall also miss Kostya as one of the leading figures of the “Intercontinental NMR Seminar Series” (ICONS, now appropriately named after him), both in the form of regular “zoominars”, and in the form of virtual meetings extending over three consecutive days. It is clear to all of us that Kostya gave a vital impetus to such meetings, which are not merely an adequate response to the current pandemic that would be fatal to him, but may prefigure the future of many international meetings, where we shall bitterly miss Kostya’s participation as our colleague and friend.

We shall remember Kostya, not only for his remarkable achievements in many areas, but also for his energy, his ability to make things happen, his generosity, and his friendship. Please join us in extending a message of condolence to his wife Elena, his daughter Kseniya, and his colleagues at the ITC in Novosibirsk that he directed with unique skills.

Alexandra Yurkovskaya and Geoffrey Bodenhausen

Minutes of the meeting of the AMPERE Bureau in the cloud, on March 18, 2021

Members present (19):

B. Blümich, A. Böckmann, G. Bodenhausen, M. Britton, V. Chizhik, J. Dolinšek, J.-N. Dumez, J. van Duynhoven, M. Ernst, S. Hiller, S. Jurga, A. Kentgens, B.H. Meier, O. Millet, H. Oschkinat, G. Otting, J. Plavec, T. Prisner, Y.-Q. Song

Excused (2):

S. van Doorslaer, H.-W. Spiess

Agenda:

1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Bureau meeting ONLINE on September 9, 2020
3. Report on the state of the AMPERE Society (B. Blümich)
4. Financial Report (M. Ernst)
5. Report EUROMAR Division and discussion about future of EUROMAR (T. Prisner)
6. Financial report EUROMAR division (A. Kentgens)
7. Report Publication Division (Magnetic Resonance) (G. Otting)
8. Report on AMPERE and Andrew Prizes and funds to support meetings (B. H. Meier)
9. AMPERE Videos (S. Hiller, O. Millet)
10. Final reports past meetings 2020:
 - EUROMAR 2020, Bilbao (Spain), December 7-9 (O. Millet)
11. Future meetings 2021:
 - SPINUS 2021, St. Petersburg (Russia), March 29-April 2 (V. Chizhik)
 - Biological SSNMR School, Berlin (Germany), June 14-18 (H. Oschkinat)
 - AMPERE NMR School, Zakopane (Poland), June 23-29 (S. Jurga)
 - EUROMAR 2021, Portoroz (Slovenia), July 6-10 (J. Plavec)
 - 16th ICMRM, Malmö (Sweden), August 24-28 (M. Britton)
 - HYP20 Conference, Lyon (France), September 5-9 (G. Bodenhausen)
 - Alpine Conference, Chamonix (France), September 12-16 (J.-N. Dumez)
 - MRFOOD, Online, October 28 (J. v. Duynhoven)
12. Election of the AMPERE Bureau and Committee at EUROMAR 2021 (B. Blümich, M. Ernst)
13. Varia
14. Date of next meeting

At 12:00 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. B. Blümich mourned the passing of two memorably colleagues, Dieter Michel and Konstantin Ivanov. While Dieter Michel could look back at a highly successful career at the age of 80, Konstantin Ivanov tragically fell victim to COVID-19 at the young age of 44, at the height of his career. The bureau commemorates these two, as well as all colleagues that have passed away in recent years.

The pandemics lead to a cancellation of about half of the AMPERE events. The EUROMAR 2020 was held virtually and was highly successful. SPINUS conference in St. Petersburg and Modern Developments of Magnetic Resonance in Kazan took place.

For 2021, most conferences will be online, with the Euromar 2021 being hybrid or fully virtual (see below). Three conferences planned for the second half of 2021 still await a decision. Funding of events is generally impacted in a negative way, since participation fees are not at all or not in the same way available in the online formats as before, and vendors are hesitant to support meetings as opportunities for customer contacts are low. COVID-19 thus hits the society at its stem. Personal meetings have substantially declined and the society has, therefore, lost its community sense at least somewhat. As a general development, many activities move to online.

Generally, there is a sense that the society should increase its internet and social media activities. This might include twitter. A. Böckmann proposes to put up the link of new videos and events to AMPERE members via the mailing list. The age structure of the society is not favorable for new media. The bureau discusses how to best include younger and more communicative members in the society. Ideas are to take prize winners and to create a young society. A. Böckmann, B.H. Meier and Y.-Q. Song will develop a proposal for action and will present at the next meeting close to the EUROMAR.

Ad 4. M. Ernst presented the financial report. Finances are continuing to be stable. Incomes have come down because there was no EUROMAR. The financial situation of all subdivisions is stable and partially very positive.

Ad 5. Thomas Prisner reported on the EUROMAR division. EUROMAR 2020 took place online, organized by Oscar Millet. Overall perception of this online event was very positive. EUROMAR 2021 will take place in Slovenia, organized by J. Plavec and J. Dolinsek. EUROMAR 2022 is scheduled for Utrecht and 2023 in Glasgow.

Ad 6. A. Kentgens reported on the finances of the EUROMAR division. Not much has happened and finances are therefore healthy and stable, a total of around 100 kEUR is available. Two bank accounts (one in EUR and one in CHF) have been merged into one. EUROMAR 2020 did not need any financial support.

Ad 7. G. Otting and G. Bodenhausen reported on the publication division. In the first 3 months of this year, as many articles have been received as in the entire last year in Magnetic Resonance. Quality of articles is mixed. The website has been updated and the peer review system better explained.

Ad 8. B.H. Meier reported on the Andrew Prizes and the funds to support meetings. Thomas Theis received the AMPERE price at the online EUROMAR 2020 and Christian Bengs was awarded with the Andrew price. Both gave very good talks at the award ceremony. For the 2021/2022 prizes, 13 nominations for Andrew price and 5 nominations for the AMPERE price are under evaluation. The call of nominees for the latter could be better advertised in the future.

Ad 9. S. Hiller reports on the Ampere video collection. A committee has formed in December and assembled a strategy. A first video has arrived and promises for several further videos have been collected in the community. The committee hopes to have around 10 videos by summer and would then go live.

Ad 10. Final reports of past meetings:

The report of the EUROMAR 2020 was given by O. Millet. It was attempted to attract in particular young people. Overall, the conference format was very suitable with short, focused lectures. Awardees received good recognition. There were no conference fees and no organizational costs. Conference was well advertised and successfully attracted >700 attendees. The Bureau thanked O. Millet for the organization.

Ad 11. Reports of planned meetings in 2021:

- SPINUS 2021 reported by V. Chizhik. Conference will be held online, nominally in St. Petersburg. There are 108 participants from 17 countries.

- Biological SSNMR School reported by H. Oschkinat. Over 60 registered participants. The course takes currently place online and runs very well (distributed over Jan 13 – May 26). An in-person meeting is scheduled for June 14-18 in Berlin. It remains unclear at this point whether that can be realized under corona conditions. While one could hold meeting in large rooms and outdoors, a severe problem are the unpredictable quarantine rules for travelers.

- AMPERE NMR school in Zakopane reported by S. Jurga. Because a lockdown is expected, this summer school might likely be held online. 12-15 speakers are confirmed. The conference is very active on Facebook and twitter with more than 300

followers. It is expected that ~100 students will attend.

- EUROMAR 2021 in Portoroz reported by J. Plavec. The conference at this point is planned as an online event, because travelling is foreseen to become very difficult. There will be 15 plenary lectures. Sponsoring is very difficult, because companies want customer contact. A group registration price will be offered. The overall financial and organizational situation is highly challenging, also because of unpredictable pandemic rules. The Bureau notices that the registration prices are high compared to the ISMAR conference. The proposal is therefore made and agreed on that the membership fees are waived, and that AMPERE and EUROMAR make additional contributions to substantially lower the student registration fees.

- 16th ICMRM in Malmö, presented by M. Britton. The conference will be online with free registration. It will last two half days with invited speakers and the Hahn lecture by a selected young investigator.

- HYP20 reported by G. Bodenhausen. The current plan for this event is to have it in Lyon in August in a hybrid format. Uncertainties are considerable at this point and further decisions need to be made. Options are to use a smaller Hotel and run on an overall reduced budget.

- Alpine Conference, Chamonix (France) by J.-N. Dumez. Preparation is made for an in-person event as the sole option with the consequence that if that cannot be held, the meeting will be postponed. Hybrid or online versions are not an option. A decision will be made in next two weeks.

- NMR Food reported by J. van Duynhoven. The meeting has been cancelled and will hopefully be held next year. There will be a reduced online event in October, built around a special issue.

Ad 12. There are 16 members of the committee whose terms have expired in 2020 and 4 members whose terms expire in 2021. The suggestion is made that all these members are asked whether they would stand for a second term and additional members from countries with a large NMR community are added such that the termination years of all members are distributed well over the 5-year period. This suggestion is agreed on.

Regarding the price committee, B.H. Meier (president), S. v. Dorslaer and R. Kaptein step down. M. Smith is interested in staying on the committee. The next president of the price committee should be voted by the AMPERE Committee. In tradition of the society, the leaving president B. Blümich was proposed as new president of the prize committee. As additional candidates H. Oschkinat (Biosolids), E. Bordignon (EPR), A. Pastore and C. Degen are nominated.

As new president for the society, the Bureau decided on one of its last meetings that two female candidates shall be nominated. A. Böckmann is the only eligible such candidate. C. Thiele has been asked but is not available. A male alternative has been considered.

For vice president, J. Dolinšek will run. P. Girardeau is also suggested as a candidate.

(In the meantime, B. Blümich has contacted him and he has agreed to being nominated.) K. Saalwächter is also proposed for vice president by A. Böckmann, he already agreed.

Ad 13. There were no Varia.

Ad 14. The upcoming summer Bureau meeting will be held on Friday, June 25, 2021, at 12:00 and the Committee meeting on Monday, June 28, 2021, at 12:00. The envisaged date of the next spring meeting of the AMPERE Bureau: March 17, 2022, at 12:00 noon on Zoom.

The meeting closed at 15:10.

Basel / the internet, 18 March 2021

Minutes: Sebastian Hiller

Balance of the Accounts of the Groupement Ampere and the Subdivisions

Period from February 29, 2020 to February 28, 2021

	Balance on February 29, 2020	Membership Fees / Registration Payments	Donations/ Conference support	Conferences Grants / Travelgrants / Membership Fee paid to Ampere	Conference Sponsoring	Conference Surplus
Groupement Ampere						
Ampere (CHF)	14'355.01					
Ampere (Euro)	49'751.05	4'423.11		5'000.00		
Andrew (CHF)	25'518.55			544.56		
Andrew Depot (CHF)	93'515.16					
Subdivisions						
Biol. Solid State (Euro)	9'237.12	280.00	2'000.00			
EPR (CHF)	7'427.05					
Food NMR (CHF)	615.32					
MRPM (CHF)	32'607.60					
SMRM (CHF)	46'240.76					19'778.72
Hyp (CHF)	7'344.65					
Euomar						
Euomar (CHF)	71'598.89					
Euomar (Euro)	31'226.57					

Administration Bulletin print Web and Bureau Meetings / MR design	Bank Charges / Depot Charges / further Bank Charges	Account Closing / Account carry over	Bank Interests Account carry over, Dividends	Gains on Value Paper	Balance on February 28, 2021
832.65	12.00				13'510.36
24.44	44.82				49'104.90
	424.75		2.55		24'551.79
				4'260.96	97'776.12
	33.29				11'483.83
			0.75		7'427.80
			0.05		615.37
			3.25		32'610.85
41.28			5.90		65'984.10
			0.75		7'345.40
	3.00	71'595.89			0.00
	44.82		67'407.40		98'589.15

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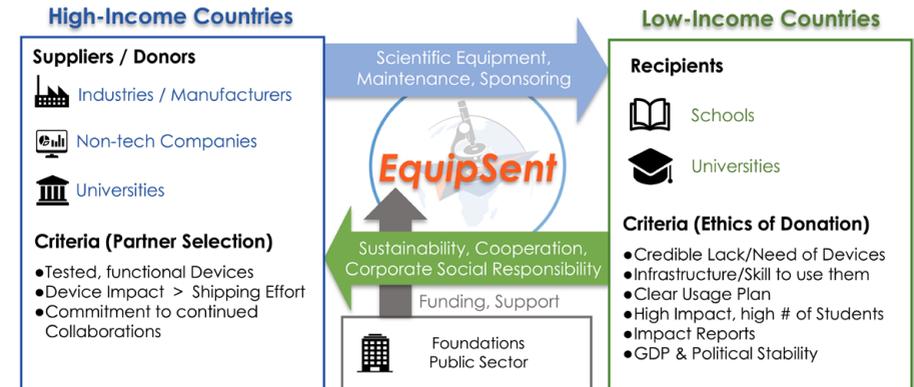
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Executive Officers and Honorary Members of the AMPERE Bureau

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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Future conferences

Ampere Event 2021

Ampere Biological Solid-State NMR School	Part 2, online	June 14-18
Ampere NMR School 2021	online	June 20-26
Euromar 2021	online	July 4-8
16 th ICMRM	online	August 1-5
HYP20	Lyon (France)	September 5-9
MR FOOD 2021	online workshop	October 28

Non Ampere Event 2021

V International School for Young Scientists, Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics	Roshchino, St. Petersburg (Russia)	Fall
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Ampere Event 2022

MR FOOD 2022	Aarhus (Denmark)	June
Euromar 2022	Utrecht (Netherlands)	July 3-7
Magnetic Resonance in Porous Media	Hangzhou (China)	August
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	September

Ampere Event 2024

HYP24	Leipzig (Germany)	September
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Groupement
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