Vol. 69, No. 1 ISSN 0432-7136

BULLETIN DU GROUPEMENT

d'informations mutuelles

Groupement
AMPERE

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

January to March 2020

No. 278

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

Contents

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

Editorial

Dear members of the Groupement AMPERE,

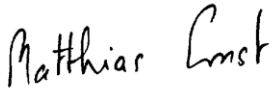
the world has changed for all of us during the past few months much more than I could have imagined possible at the start of this year. I am sure that all of you have seen changes and restrictions in your personal and professional lives. For me, closing the schools in Switzerland had the biggest impact on my personal life since I have two children that need help and support with teaching and learning at home. But also work has become much more complex with remote teaching using video conferences and labs at ETH closed for research except for emergency maintenance which means in our case filling the magnets with cryogens. Especially keeping the contact to students and advising them without personal contact is something I find demanding.

For the Groupement AMPERE, there have also been many changes in what we had planned for this year. The EUROMAR in Bilbao had to be postponed tentatively to December since it is unlikely that travel restrictions will be lifted before July. We will monitor the situation in Europe and the rest of the world carefully and make a final decision in fall. Many other conferences and schools organized by the subdivisions of AMPERE or by other organizations have also been postponed or cancelled and predictions for the future developments are very difficult. These decision carry also always a financial risk for the organizer and we hope that none of the organizers of scientific events gets hurt by a financial burden that they cannot carry. Over the years, AMPERE and the subdivisions of AMPERE have saved some money which can be used in a situation like we have now.

But especially in times like this, where many restrictions are introduced that are based on unclear assumptions, we also have to remember that we are all scientists. And scientists should ask critical questions and reflect on and think about what they are told. I think we need to ask critical questions to our colleagues that present models without explaining what assumptions have been used and on which data the models are based. We have to ask critical questions to the politicians that present us with a single solution for a complex problem. We all know that complex problems almost never have a single simple solution but require careful consideration of all possible options. We have to listen to colleagues who have dissenting view from the majority and critically think about what they tell us. We all know from our own experience that in science the majority view is not necessarily the correct one and that only critical but fair discussions lead to advancement of knowledge.

I sincerely hope, that all of you come through this pandemic unharmed and that you and the people close to you stay healthy.

Best regards, Matthias Ernst
Secretary General, Groupement AMPERE



Portrait:
Prof. Arno Kentgens

• why magnetic resonance and why NMR and MRI?
As a bachelor student I was very intrigued by quantum mechanics and was interested to get exposed to research involving QM. However, what really got me to go for an internship in NMR was the look of the solid-state NMR spectrometer home-built by our (now retired) technician Jan van Os. In this spectrometer each event was encoded binary and little lights showed each step in the pulse program when the spectrometer was running. In the evening it looked like the control room of a space ship. After laying my eye on it, I wanted to be commander of that ship! My internship, studying zeolites using 27Al NMR, convinced me to stay in this field.

• what is your favorite frequency?
I really don't have a specific favorite frequency. I have a preference for uncommon frequencies though. I like trying to get spectra from exotic nuclei.

• what do you still not understand?
There are numerous things I still don't understand. Every study also generates lots of new questions. I like this, as I love to solve complex puzzles and in science one is never done. In my thesis I had a quote from Solzhenitsyn: "You can't know everything in the world. Whatever happens you'll die a fool."

• luckiest experiment you have ever done.
A Dutch proverb says "Zonder geluk vaart niemand wel", i.e. without luck no one fares well, but in science one has to make one's own luck to a certain extend. An experiment that worked astonishingly well at the first attempt was our "Friday-afternoon" test of a microcoil; We tightly wound a coil around a single hair, connected this to a simple print board circuit and put it in the magnet. In a single shot we got a strong proton signal and the rf-field strength turned out to be of the order of 500 kHz. This certainly encouraged us to explore the use of microcoils in solid-state NMR.

• what was the worst mistake you have made during your lab time?
Parking a nitrogen vessel against the magnet. As a student I got the job to do the nitrogen fills of the (then high field 7.1T) NMR magnet during the technicians holiday. One day I put a nearly empty nitrogen vessel a little too close to the magnet, just picking the filling hose was enough to set the vessel in motion and although I tried to stop it, it got stuck to the magnet. I was able to pull it off with the help of a fellow student who held the magnet. Fortunately except for a little scratch no harm was done to the magnet, but it showed that one can't be careful enough around an NMR magnet.

• most memorable conference story?
I hold fond memories from many conferences because of hearing great presentations, funny incidents, meeting people whose papers I admired, but mostly for catching up with old friends and making new ones. A funny incident occurred at the ISMAR meeting in Morzine (1989). Paul Callaghan gave an excellent lecture illustrated with beautiful graphics which was very unique in those days. But then an elderly German professor with a very strong German accent stood up and complained that he thought the lecture might be interesting, but he was unable to follow it because of the very poor English of the speaker……
With respect to making new friends, I particularly remember a NATO-ASI summer school in Southern Italy (Maratea) in the early stages of my career. It was a beautiful place and the atmosphere was great, I met various people who were also starting out in NMR and many of us became friends for life.

• with whom (historical person) would you like to meet?
Richard Feynmann who I admire for his inquisitive mind combined with a great sense of humor. I loved reading his biographies.

• when do you get your best ideas?
Cycling home along the river dike in the evening. With my head in the wind my mind starts wandering regularly coming up with some useful ideas out of nowhere.

• if you had just one month time for travelling - where would you go to?
Travel to Norway in a campervan. I actually already did that once with my son, it took us exactly one month to drive to the North Cape and back. A fantastic journey that I would certainly love to do again.

• your idea of happiness.
Enjoying nature and being with friends and family without any obligations. There is a nice song by Joe Cocker which expresses this very clearly: "And What I've Learned Is All I Really Need Are...The Simple Things that Come Without A Price"

Position:
Professor, Magnetic Resonance Research Center, Radboud University Nijmegen

Awards:
DSM Prize of Science and Technology, 1987; Young Chemist Award, NWO, 1998; NWO-TOPO Grant, 2005; Gorter Lecturer (Casimir Research School, Leiden University) 2013

Homepage:
https://www.ru.nl/science/magneticresonance/

Education:
BSc in Chemistry and Physics, University of Nijmegen 1981; MSc University of Nijmegen 1983; PhD University of Nijmegen 1987 (Supervisors E. de Boer and W.S. Veeman)

Interests:

Science, Photography, Movies, Camping

Report: XIth Conference of the European Federation of EPR groups (EFEPR 2019)

September 1-5, 2019, Bratislava, Slovakia
https://efepr2019.conference.fchpt.stuba.sk/

International Advisory Board:
Sabine Van Doorslaer (Antwerp), David Collison (Manchester), Carole Duboc (Grenoble), Georg Gescheidt (Graz), Gunnar Jeschke (Zurich), Wolfgang Lubitz (Mülheim an der Ruhr), George Mitrikas (Athens), Thomas Prisner (Frankfurt), Anton Savitsky (Dortmund), Zbigniew Sojka (Krakow), Stefan Stoll (Seattle), Joshua Telser (Chicago)

Local Organizing Committee:
Peter Rapta, Michal Zalibera, Zuzana Barbieriková, Peter Poliak, Dana Dvoranová, Vlasta Brezová, Denisa Darvasiová, Karol Lušpai

At the beginning of September 2019, Bratislava hosted 128 participants from Austria, Belgium, Czech Republic France, Germany, Greece, Israel, Italy, Japan, Romania, Russia, Slovakia, Spain Switzerland, United Kingdom and United States at the triennial meeting of the European Federation of EPR groups (EFEPR). The conference was organized by the Slovak University of Technology (STU) and Slovak Chemical Society (SCHS) under the auspices of EFEPR, International EPR (ESR) Society (IES) and the Groupement AMPERE.

The topics discussed during the meeting covered a broad range of EPR applications from quantum technologies, through biology and in-cell EPR, to surface chemistry and catalysis, as well as the new developments in theoretical calculations of EPR parameters.
The scientific program consisted of 7 plenary lectures, 7 keynotes, 23 oral presentations and included two poster sessions with 79 contributions.

Plenary talks were given by:
Roberta Sessoli, University of Florence, Italy
Magnetic molecules for the second quantum revolution: from hybrid nanostructures to electric field control
Christiane Timmel, University of Oxford, UK
Putting a New Spin on Porphyrin Molecular Wires
Olav Schiemann, University of Bonn, Germany
Pulsed Dipolar Spectroscopy: From Model Systems to Cells
Wolfgang Lubitz, MPI CEC, Mülheim an der Ruhr, Germany
Unravelling Light-Induced Water Oxidation in Oxygenic Photosynthesis: The Contribution of EPR Spectroscopy
David Britt, University of California, Davis, USA
The FeFe Hydrogenase H-cluster: Isotope editing approaches to follow its bioassembly with EPR and other spectroscopies
Vladimir Malkin, Slovak Academy of Sciences, Bratislava, Slovakia
Calculations of the EPR and pNMR parameters in the framework of 2- and 4-component relativistic DFT approach
Mario Chiesa, University of Torino, Italy
Surface Chemistry and Catalysis by EPR: Concepts, Examples and Perspectives

The recent advances in Rapid Scan EPR were additionally presented by Patrick Carl and Sylwia Kacprzak from Bruker Biospin GmbH.

Keynote speakers gave lectures on:
Jens Anders, University of Stuttgart, Germany
EPR-on-a-chip: A new paradigm in EPR spectroscopy
Matvey Fedin, Russian Academy of Sciences, Novosibirsk, Russia
EPR of metal-organic frameworks: from defects elucidation to new functionalities
Helene Bolvin, Paul Sabatier University, Toulouse, France
First principles determination of EPR parameters in triple decker of cerocen
Marilena Di Valentin, University of Padova, Italy
Light-induced pulsed EPR dipolar spectroscopy: the triplet state probe
Maxie Roessler, Imperial College London, UK
Protein film electrochemical EPR spectroscopy as a technique to investigate redox reactions in biomolecules
Benesh Joseph, Goethe University, Frankfurt, Germany
Membrane transport explored with pulsed ESR spectroscopy
Alexey Popov, IFW Dresden, Germany
Endohedral spins in carbon cages

The Tuesday afternoon session was dedicated to the EFEPR Assembly and discussions about the future of the federation. The upcoming 8th and 9th EFEPR Schools, taking

place on November 18-25, 2019 in Brno, and in 2021 in Lille were promoted. An initiative to open the society to the younger generation was announced. This includes a more intense presence at the social media, and the Twitter account @european_epr was promplty launched by Angeliki Giannoulis and Anastasia Kultaeva.

The annual IES general assembly was also held within the conference. IES Secretary Aharon Blank and President Thomas Prisner reported on the financial status of the organization and announced calls for the nomination on IES awards. IES members also have the option to highlight their EPR - related research at IES Twitter @EPR_ESR.

Two IES poster prizes were awarded to Tomáš Hajdu (STU), for the poster on "Visible-light-responsive TiO_2-Bi_2O_3 composite photocatalyst – EPR spin trapping study" and to Kwinten Maes (Ghent University) for his contribution on "Multi-frequency electron magnetic resonance characterization of vanadium dopant sites in the metal-organic framework DUT-5(AI)". Simultaneously SCHS (Slovak Chemical Society) delivered its poster award to Ashley J. Redman (University of Oxford) for his investigations of "Triplet states of Donor-Acceptor porphyrins".

The social dimension of the event was enriched by the wine tasting, and sight-seeing trips and the positive vibrations excited there transformed into a friendly atmosphere at the Gala Dinner.
The conference manifested the enormous variety of fruitful applications of EPR in diverse fields of science, and EFEPR is looking forward to the next meeting in 2022, most likely in Leipzig, Germany.
The financial support of the Bruker BioSpin, STU, SCHS, IES and CentralChem is gratefully appreciated.

IES posterprize: Tomáš Hajdu
(EFEPR 2019)

Visible-light-responsive TiO_2-Bi_2O_3 composite photocatalyst – EPR spin trapping study

Tomáš Hajdu[1], Zuzana Barbieriková[1], Vlasta Brezová[1], Gregor Žerjav[2], Albin Pintar[2]
1) Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic
2) Department for Environmental Sciences and Engineering, National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia

One of the promising ways to improve the photocatalytic activity of semiconductor based photocatalysts and extend it towards visible light represents the combination of two semiconductors forming a suitable heterojunction. This may lead to an increased concentration of electron-hole pairs on the surface of the photocatalyst and suppressed recombination of the charge carriers. Heterojunction between two semiconductors, a visible-light-responsive (e.g. β-Bi_2O_3) and a UV-light responsive with the optimal band positions to form reactive oxygen species (ROS) (e.g. TiO_2) may lead to a promising composite with extended working region in the visible–light, while at the same time being able to decompose organic and inorganic pollutants. EPR spin trapping technique was used to study the ability of a series of TiO_2-Bi_2O_3 composites with alternating amounts of β-Bi_2O_3 (**B**) and TiO_2 (**T**) semiconductors to generate ROS upon photoexcitation. Spectra were measured *in situ* with the photocatalyst suspensions containing the spin trapping agent 5,5-dimethyl-1-pyrroline N-oxide (DMPO).

All the prepared composites (**TB**) have exhibited higher photocatalytic activity than commercially used benchmark TiO_2 (P25) when exposed to UV light (λ_{max} = 365 nm) in water suspensions (Fig. 1a).

Pure β-Bi_2O_3 has displayed inferior photocatalytic activity due to its small specific surface area and fast recombination of the photogenerated charge carriers. An apparent beneficial effect of increasing amount of β-Bi_2O_3 in the composite photocatalyst has been observed. Possible formation of the p–n heterojunction between two semiconductors may have led to an effective charge carrier separation of the photogenerated electrons and holes and to an overall improvement of the photocatalytic activity. Alongside the high UV light activity, these composite photocatalysts have shown a visible-light photocatalytic activity. When suspended in dimethylsulfoxide and irradiated by visible-light **TB** composites have shown quite a significant trend of correlation between the amounts of β-Bi_2O_3 and photocatalytic activity (Fig. 1b). Overall we observed a beneficial combination of two semiconductors obtaining a promising photocatalyst with outstanding UV light and apparent visible-light responses, which predetermines its usage in solar-light induced photocatalytic processes.

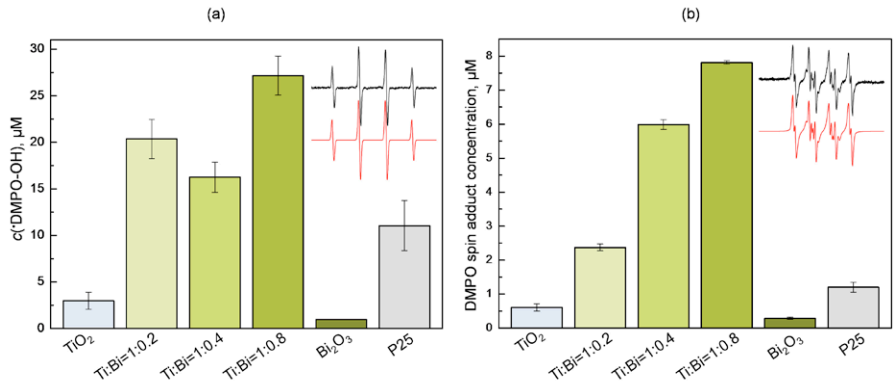


Figure 1. Concentrations of the monitored DMPO spin adducts generated either upon 180 s UVA exposure of water suspensions or upon 6 min visible-light exposure (160 klx) of DMSO suspensions of studied photocatalysts, both in the presence of DMPO spin trapping agent under air at 295 K. Insets represent experimental (–) and simulated (–) EPR spectra (magnetic field sweep width 7 mT) obtained upon either UVA photoexcitation of Ti:Bi=1:0.8 water suspension or visible-light exposure of Ti:Bi=1:0.8 DMSO suspension, both in the presence of DMPO spin trap.

Acknowledgement: This work was supported by the Scientific Grant Agency of the Slovak Republic (Project VEGA 1/0026/18) and by the Slovak Research and Development Agency under the contract No. APVV-15-0053.

IES posterprize: Kwinten Maes
(EFEPR 2019)

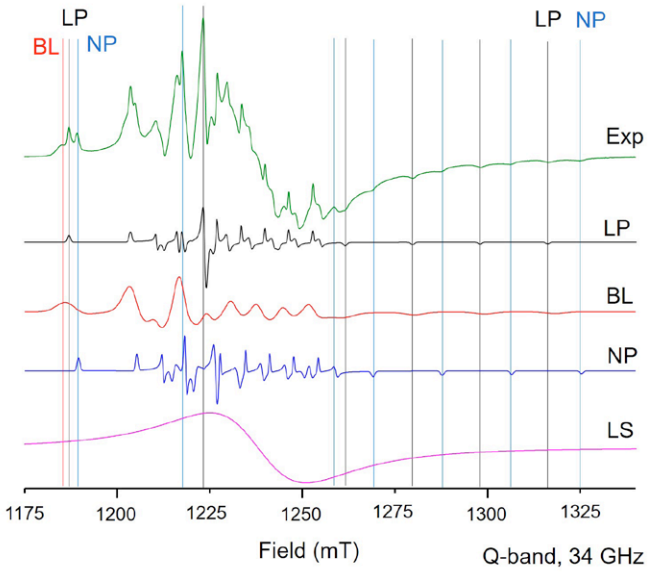
Multi-frequency electron magnetic resonance characterization of vanadium dopant sites in the metal-organic framework DUT-5(AI)

Kwinten Maes [1], Karen Leus[2], Pascal Van Der Voort[2], Etienne Goovaerts[3], Henk Vrielinck[1] and Freddy Callens[1]
1) Department of Solid State Sciences, Ghent University, Krijgslaan 281-S1, B-9000 Gent, Belgium
2) Department of Chemistry, Ghent University, Krijgslaan 281-S3, B-9000 Gent, Belgium
3) Department of Physics, University of Antwerp, Universiteitsplein 1, B-2610 Antwerp, Belgium

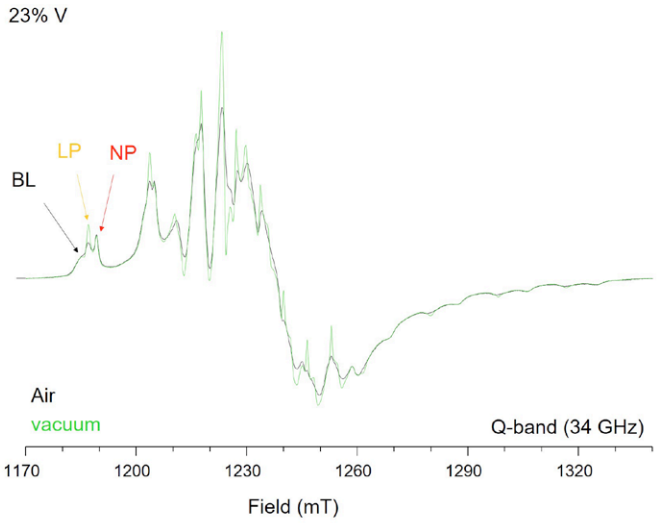
Metal-Organic Frameworks (MOFs) are ordered porous crystalline materials constructed of metal ions connected by organic linkers, for which a diverse scale of applications are being explored (e.g. catalysis, gas adsorption, separation and storage). Two characteristic types of MOFs with one-dimensional pores are DUT-5(AI) ((AI^{III}OH)BPDC, BPDC = biphenyl-4,4'-dicarboxylate)[1] and MIL-53(AI) ((AI^{III}OH) BDC, BDC: 1,4-benzenedicarboxylate).[2] The framework of the latter structure exhibits breathing: the framework can reversibly change from an open (large pore) to a closed (narrow pore) structure. Recently we have shown that EPR spectroscopy using V(IV) as a paramagnetic probe can distinguish between these two states for V-doped MIL-53(AI).[3] Whereas breathing has not been reported for DUT-5(AI), it has been observed for COMOC-2(V) ((V^{IV}=O)BPDC).[4] Measurements on V-doped DUT-5(AI) revealed an EPR spectral component that showed similar characteristics as V^{IV}=O in large pore MIL-53(AI), but also other components were found.[5]
Here we further explore the EPR spectrum of V-doped DUT-5(AI). Spin-Hamiltonian parameters are derived from X- (9.5 GHz), Q- (34 GHz) and W-band (94 GHz) spectra. At low concentrations of V two components are observed in the EPR spectrum: a large pore (LP) component and a broad-line (BL) component. Starting from 9% of V, two additional spectral components are revealed: a narrow-line (NP) component of isolated vanadyl centers that is most probably linked with a narrow pore phase of DUT-5(AI) and a broad structureless line (LS) of the V-concentrated phase (V^{IV}=O) BPDC. The relative contributions of these four components, estimated through spectrum simulations, are evaluated as a function of V-concentration. The Q-band ENDOR spectra reveal interactions with ^{1}H nuclei of the BPDC linker.

References.
1. I. Senkovska et al., Microporous and Mesoporous Materials 122 (2009) 93–98.
2. T. Loiseau, et al., Chem.-Eur. J., 2004, 10, p. 1373.
3. Nevjestic, I., et al., Phys Chem Chem Phys, 2017. 19(36): p. 24545-24554.
4. Liu, Y.-Y., et al., Inorganic Chemistry, 2013. 52(1): p. 113-120.
5. Depauw, H., et al., Journal of Materials Chemistry A, 2017. 5(47): p. 24580-24584.

Decompostion EPR spectrum DUT-5



EPR spectrum DUT-5



SCHS (Slovak Chemical Society) posterprize: Ashley J. Redman
(EFEPR 2019)

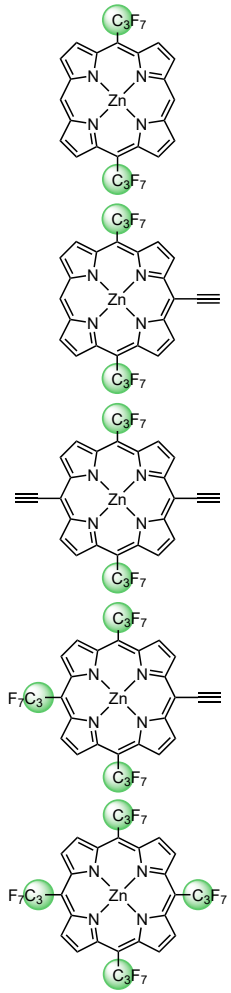
Multi-frequency electron magnetic resonance characterization of vanadium dopant sites in the metal-organic framework DUT-5(AI)

Ashley J. Redman,[1] Gabriel Moise,[1] Sabine Richert,[2] Erin Viere,[3] William K. Myers,[1] Michael J. Therien,[3] and Christiane R. Timmel,[1]
1) Center for Advanced Electron Spin Resonance (CAESR), University of Oxford, Oxford, OX1 3QR, UK
2) Institute of Physical Chemistry, University of Freiburg, 79104 Freiburg, Germany
3) Department of Chemistry, Duke University, Durham, NC 27708, United States

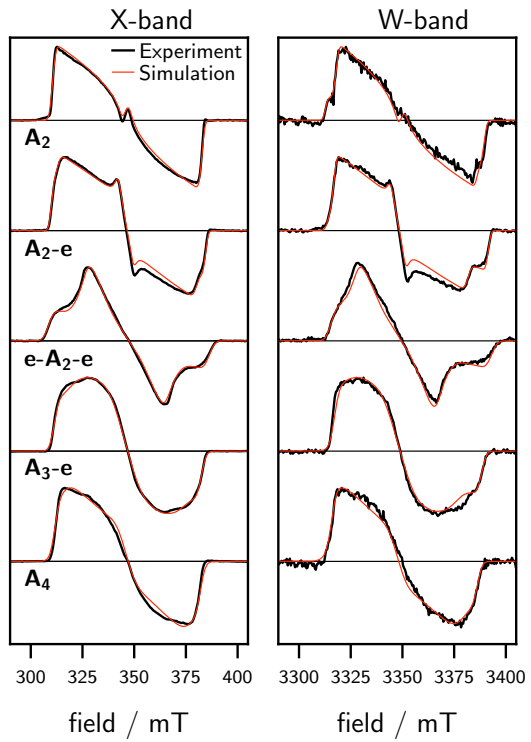
The photo-excited triplet states of π-conjugated molecules are of interest in the fields of molecular electronics and photovoltaics.[1] Porphyrin oligomers composed of meso-meso linked units have been proposed as suitable building blocks for molecular wires in nano-scale devices.[1] Controlling the electron delocalization is important for mediating the efficiency of electronic communication between subunits and there is currently no comprehensive model which relates the structure to the delocalization. Transient EPR spectroscopy in combination with pulse ENDOR has previously been employed to characterize the photo-generated triplet states of linear and cyclic zinc porphyrin oligomers.[2a] Studies have also explored the influence of the bridging linker,[2b] where varying the length or geometry of a meso-meso linker, imposes constraints on the dihedral angles between adjacent porphyrin rings. In addition, the significance of symmetry was explored by altering the distribution of side groups in porphyrin oligomers thus rendering the porphyrin units inequivalent; this work demonstrated how the symmetry of the porphyrin changes the triplet state delocalization.[2c]

Here, we extend the investigation of structure-property relations to the photogenerated triplet states of a series of linear zinc porphyrin systems with donoracceptor meso groups. Transient CW, magnetophotoselection and pulse ENDOR spectroscopies have been used to explore and gain a better understanding of the ZFS and HFC. These magnetic parameters ultimately depend on the shape and distribution of the triplet spin density. Preliminary results have so far provided information into how different combinations of donoracceptor groups can influence the triplet state wavefunction. Rationalization of the experimental trends have been performed based on a combination of DFT and CASSCF calculations.

Structures



X W TREPR simulation



References:
1.(a) Ostrowski, J. C. et al. Adv. Mater. 2003, 15, 1296. (b) Lin, V. S.-Y. et al. Science 1994, 264, 1105. (c) H. L. Anderson, Chem. Commun., 1999, (23), 2323-2330.
2.(a) Tait, C.E. et al. J. Am. Chem Soc., 2015, 137 (25), 8284-8293. (b) Richert, S. et al. J. Am. Chem. Soc., 2017, 139 (34), 12003-12008. (c) Richert S. et al. J. Am. Chem. Soc., 2017, 139 (15), 5301-5304.

Report: 8th EFEPR School 2019, Czech Republic

It was our great pleasure to welcome students and teachers across the world on the 8th European Federation of EPR groups (EFEPR) school event on Advanced EPR. The school was organised by the Czech research group MOTES (Magneto-Optical THz Spectroscopy) from CEITEC BUT (Central European Institute of Technology - Brno University of Technology) in the period from 18th to 25th November 2019.

Over 140 participants from more than twenty countries, including countries outside of Europe as Australia, Japan or USA, were brought to the Hotel Skalský dvůr on the countryside of Brno region to focus on EPR topics for seven entire days. The intensive program covered EPR theory, instrumentation, applications in bio and material sciences as well as advanced EPR techniques. In addition to the lectures given by a total of twenty professors from eleven countries, students practised their skills in three parallel tutorial sessions dedicated to EPR theory, EasySpin and DEER analysis. Two evenings were dedicated to the exhibition of 118 posters, where much vivant discussion between students and teachers took place in the poster hall ending late night. „It was nice to see so many young and enthusiastic students working in so many different areas of EPR spectroscopy. I was very much impressed by the quality of their work, presented at the Poster Sessions," adds Thomas Prisner, Presidents of the International EPR Society.

The EFEPR school was organised for the first time in a post-communist country. During the school, we introduced a bit of the history of magnetic resonance in the Czech Republic, formal Czechoslovakia, which is especially connected to the city of Brno and Josef Dadok, the pioneer of NMR spectroscopy in the Czech Republic. [1,2] Josef Dadok is well known in the EPR community dealing with Rapid Scan. His paper on correlation spectroscopy in 1973 [3] inspired Sandra and Gareth Eaton to apply this method to EPR. It took a while, but recently, in summer 2019, EPR Rapid Scan instruments were commercially released by Bruker at the Rocky Mountain Conference in Denver. The legacy of Josef Dadok in Brno is still alive. An afternoon was dedicated to visiting the CEITEC MOTES laboratories dedicated to high field EPR and the Josef Dadok National NMR Center in Brno, which was established in 2018 and 2013, respectively.

„Besides the important training aspect, EFEPR schools have had various other beneficial outcomes for the participants over the years. This type of schools has formed for many young scientists the basis of their future professional international network and have widened their view on international science. In this sense, it was crucial for EFEPR to have for the first time a school in the Czech Republic (first time in Eastern Europe). Organiser Petr Neugebauer and his team did a fantastic job and all students were enthusiastic, albeit very tired after the intense week of learning new things. The visit to the CEITEC facilities impressed everyone. „ concludes Sabine Van Doorslaer, President of the European Federation EPR Society.

In conclusion, on behalf of all organisers, I would like to acknowledge all the sponsors for their financial support, thanks to that 34 students could be financially supported. Additionally, I would like to express my acknowledgement to all teachers, who did a fantastic job and find time to participate, as well as to all students making the event more than an EPR school.

We appreciate that in the after school survey, more than 77% of students indicated that they were very satisfied with the school. Additionally, students had a chance to provide feedback to all teachers. Based on students rating the three best teachers of 8th EFEPR school are Stefan Stoll, Edgar Groenen and Gunnar Jeschke.

The program and all the lectures can be downloaded from www.eprschool.ceitec.cz.

Petr Neugebauer
On behalf of the organisers

[1] B. Král and A. Blatná, Slaboproudý obzor, 72, 4 (2016)
[2] V. Zeman, Vzpomínky na NMR v Brněnské Tesle. Stan's Library: http://www.ebyte.it/library/hist/NMR_Tesla_cs.html. ISSN 2421-1230.
[3] J. Dadok and R.F. Sprecher, Correlation NMR spectroscopy. J. Magn. Reson. 13, 243 (1974).

Group photo of participants at 8th EFEPR school, Hotel Skalský Dvůr, Brno, Czech Republic.

International committee of 8th EFEPR school:
Sabine Van Doorslaer (University of Antwerp, Belgium), Daniella Goldfarb (Weizmann Institute Of Science, Israel), Thomas Prisner (University of Frankfurt, Germany), Alexander Schnegg (HZB, Germany), Carol Duboc (Grenoble, France) Donatella Carbonera (Padova, Italy), Petr Neugebauer (CEITEC Brno, Czech Republic), Gunnar Jeschke (ETH Zürich, Swiss), Graham Smith (University of St. Andrews, UK), Zbignew Sojka (Krakow, Poland)

Local Organizers of 8th EFEPR school:
Lenka Honková, Jakub Hrubý, Oleksii Laguta, Tomáš Láznička, Andriy Marko, Jana Midlíková, Petr Neugebauer (head), Jana Prušková, Antonín Sojka, Artur Solodovnyk, Vinicius Tadeu Santana, Matúš Šedivý, Katka Vlková

Photo of poster winners at 8th EFEPR school. From left: Edgar Groenen (president of the selection committee), Fabian Hecker, Francesco Torricella, Laura Esteban Hofer, Matthias Bretschneider, Tobias Hett, Marianne Le Dantec, Petr Neugebauer (organiser of the school). All poster winners beside the certificate obtained a magnetic resonance book provided by Wiley and Springer.

Josef Dadok (28.2.1926):
Josef Dadok graduated from BUT in Brno in the early 50s. He founded The Nuclear Magnetic Resonance Department at the Institute of Scientific Instruments, Czechoslovak Academy of Sciences (ISI) in 1960 and together with his team he developed the first devices for NMR spectroscopy in the Czech Republic.

At that time, the US imposed an embargo on the Soviet Union for NMR spectrometers, which was a very unfavourable situation for research in Eastern Bloc states. The Institute of Scientific Instruments was just ten minutes away from the company TESLA Brno. TESLA had a state-sponsored monopoly on electronics production in Czechoslovakia and produced nearly all electronic products in the country until 1989. Tesla became the manufacturer of Josef Dadok's first 60MHz spectrometer, named TESLA BS477, which was put into production in 1965.

Thus, Czechoslovakia became the third country, after the USA and Japan, to succeed in the serial production of these scientific devices. This was the only production of its kind in any of the Eastern European countries, and it continued for the next 25 years. During its time, TESLA managed to produce about 500 spectrometers.
In 1967 Professor Dadok left for an internship in the USA and did not return after the Soviet occupation of Czechoslovakia in August 1968. In 1976 he became Technical Director of the Pittsburgh National Nuclear Magnetic Resonance Centre and full professor for chemical scientific instruments at the Carnegie Mellon University.

In 1977 he completed the development of the first superconducting spectrometer, with a field strength of 14.1 T and working at a frequency of 600 MHz, which remained the most powerful NMR system for high-resolution spectroscopy in the world for a full eight years.

Posterprize: Matthias Bretschneider
8th EFEPR School

Multiple quantum coherence EPR on nitroxide radicals

Matthias Bretschneider[1], Philipp E. Spindler[1], B. Endeward[1], V. Tormyshev[2], E. G. Bagryanskaya[2], Thomas F. Prisner[1]
[1]Institute of Physical and Theoretical Chemistry and Center of Biomolecular Magnetic Resonance, Goethe University Frankfurt, Frankfurt am Main, Germany
[2]Novosibirsk Institute of Organic Chemistry, Novosibirsk 630090, Russia

Multiple quantum coherence (MQC) is a method to analyze the coupling network of dipolar coupled spin label. To this purpose the measurement is performed with different quantum fiters to select one specific multiple quantum transition. The aim of the current work is to optimize pulse sequences for multiple quantum coherence (MQC) EPR.

This method can be applied to determine the oligomeric state of proteins. We could show that MQC EPR works with rectangular pulses on trityl radicals (see figure 1).

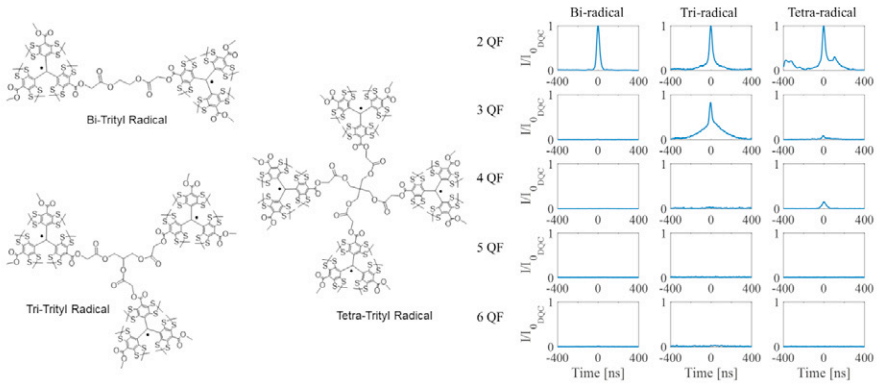


Figure 1: Left: Trityl model compounds. Right: Multi-quantum filtered echos from the bi-, tri-, and tetra-trityl radical samples. The detected echo signals for the 2, 3, and 4-trityl radicals (column 1 to 3, respectively) are shown after appropriate phase cycling to filter the n=2-6 quantum coherences (row 1 (2QF) to row 5 (6QF), respectively).

However, more common spin label used for application on proteins are nitroxides. Therefore, MQC EPR should be established on nitroxide radicals. Because of the broad bandwidth required to excite the nitroxide spectrum, broadband pulses have to be used. For this work different kind of pulses were considered. At first these pulses were tested on trityl model compounds to validate their usage for MQC measurements. Then the pulses giving a good performance were used for the measurement on nitroxide model compounds. The transversal relaxation times (T_2) of the different MQC signals were also investigated on different trityl radicals (see figure 2).

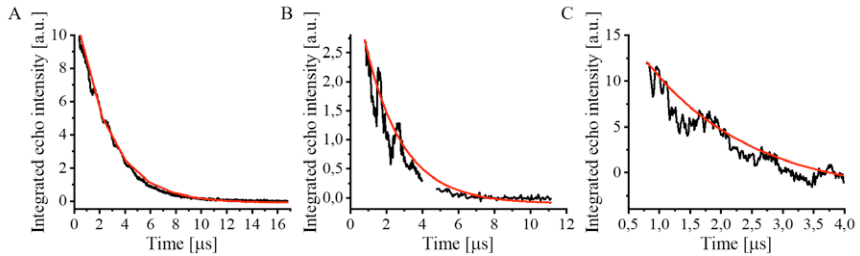


Figure 2: Determination of the single-quantum (upper left), double-quantum (upper right) and the quadruple-quantum transversal relaxation time of the tetra-trityl radical. Experimental echo signal intensity (black) is shown together with the mono-exponential fit (red).

Posterprize: Laura Esteban Hofer

8th EFEPR School

Characterization of the role of the inter-RRM linker of SRSF1 with EPR spectroscopy

Laura Esteban Hofer[1], Cristina K.-X. Nguyen[2], Antoine Cléry[2], Maxim Yulikov[1], Frédéric H.-T. Allain[2], and Gunnar Jeschke[1]

[1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland,

[2]Institute of Biochemistry, ETH Zürich, Switzerland

The RNA-binding protein SRSF1 belongs to the SR protein family of crucial regulators of gene expression.[1] SRSF1 is comprised of a canonical RNA recognition motif (RRM1) and a pseudo RRM (RRM2) connected by a flexible linker, and a C-terminal domain containing multiple arginine serine dipeptide repeats.

Isolated RRM2 contains a heptapeptide S_{133}WQDLKD_{139} that, together with Arg117 and His183, binds GGA trinucleotide motifs.[2] Although the heptapeptide SWQDLKD remains the RNA-binding surface in the pseudo-RRMs of all known SR proteins containing two RRMs, the binding affinity to the GGA motif is particularly high for the RRM2 of SRSF1. This may be related to the involvement in binding of Arg117 in the linker of SRSF1. We aim to understand the role of the flexible linker in binding to RNA in the context of RRM1 linked to RRM2.

Distance distributions obtained by DEER measurements of RRM1 linked to RRM2 in the free form and in complex with RNA can be used as restraints in RigiFlex[3] to infer the role of the flexible linker in the binding to RNA. Figure 1 depicts the preliminary ensemble models of SRSF1 in the free form and in complex with RNA (5′-UCAUUGGAU-3′) obtained using the first inter-domain distance distributions measured.

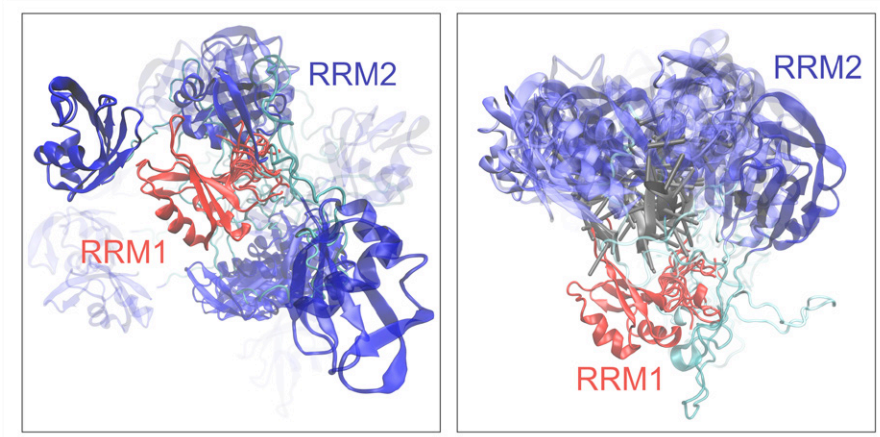


Fig. 1: Preliminary ensemble models of SRSF1 in the free form (left) and in complex with 5′-UCAUUGGAU-3′ (right). The models are superimposed on RRM1 (red) with RRM2 (blue) relative to it. The linker is displayed in cyan and the RNA in grey.

This work is supported by the Sinergia grant CRSII5_170976 from the Swiss National Science Foundation.

References:

[1] J. Long, J. Caceres, Biochem. J., 2009, 417, 15-27.

[2] A. Cléry, R. Sinha, O. Anczukow, A. Corrionero, A. Moursy, G. M. Daubner, J. Valcarcel, A. R. Krainer, F. H.-T. Allain, Proc. Natl. Acad. Sci., 2013, 110, E2802-E2811.

[3] G. Jeschke, Protein Sci., 2018, 27, 76-85.

Posterprize: Tobias Hett
8th EFEPR School

Conformational changes in a cyclic nucleotide-binding domain studied by PELDOR spectroscopy

Tobias Hett[1], Tobias Zbik[2], Reinhard Seifert[2], U. Benjamin Kaupp[2], Olav Schiemann[1]
[1]Institute of Physical and Theoretical Chemistry, University of Bonn, Germany
[2]Center of Advanced European Studies and Research, Bonn, Germany

Proteins are highly dynamic systems that can undergo large conformational changes upon ligand binding. In order to fully understand protein function, conformational changes have to be resolved in space and time. The combination of freeze-quench techniques1, site-directed spin labelling (SDSL) and pulsed dipolar spectroscopy (PDS) is ideally suited to follow such changes of the protein structure. Here, we present the application of a Microsecond Freeze-Hyperquenching (MHQ) Device[1] to the cyclic nucleotide binding domain (CNBD) of the MloK1 potassium channel from Mesorhizobium loti.2,3 The CNBD undergoes a rearrangement of α-helices upon binding of cyclic adenosine monophosphate (cAMP).[2,3]

Using MHQ, snapshots can be taken on the pathway from the ligand-free Apo state to the ligand-bound Holo state. Distance measurements via PELDOR spectroscopy reveal a change of the mean interspin distance.

References:
[1] A.V. Cherepanov, S. de Vries (2004) BBA 1656, 1-31.
[2] S. Schünke, M. Stoldt, J. Lecher, U. B. Kaupp, D. Willbold (2011) PNAS 108, 6121-6126.
[3] S. Schünke, M. Stoldt, K. Novak, U. B. Kaupp, D. Willbold (2009) EMBO Rep. 10, 729-735.

Posterprize: Marianne Le Dantec
8th EFEPR School

Electron spin resonance spectroscopy of rare-earth-ions at millikelvin temperatures

M. Le Dantec[1], M. Rančić[1], T. Chanelière[2], P. Goldner[3], S. Bertaina[4], E. Flurin[1], D. Vion[1], D. Estève[1], P. Bertet[1]
[1]Quantronics group, Service de Physique de l'Etat Condensé, CEA Saclay, France
[2]Institut Néel, Grenoble, France
[3]Institut de Recherche de Chimie Paris, France
[4]Institut Matériaux Microélectronique Nanosciences de Provence, Marseille, France

Rare-Earth-Ions are interesting physical systems because they have long lived states and record coherence times. This is due to their valence 4f electrons being very well shielded from the environment by the 5s and 5p filled shells. They are for example good candidates for quantum memories in the optical domain. Rare-Earth-Ions with an odd number of electrons in the 4f shell are paramagnetic, with an electron-spin-like transition at microwave frequency that can be studied by standard EPR spectroscopy for instance at X-band. For such transitions, coherence times in the 50-100μs range have been measured at 1-2K [1].

In this project, we explore this microwave transition using Electron Spin Resonance in a new regime of temperatures, ranging from 10mK to 1K, using a superconducting micro-resonator and a superconducting parametric amplifier [2], [3]. The sample is a crystal of scheelite (CaWO4) doped with Erbium (50ppm concentration).

During this work, we measured coherence times of the spin ensemble using Hahn echoes. For low populated hyperfine transitions of Erbium, we measured coherence times up to 1ms at 10mK. This improves considerably previous measurements of electron spin coherence times in Erbium doped crystals. This long coherence time appears to be due to the quenching of Er-Er flip-flops due to their complete polarization in the ground state at millikelvin temperatures.

References:
[1] S. Bertaina et al., Nat. Nanotech. 2, 39 (2007)
[2] P. Haikka et al., Phys. Rev. A 95, 022306 (2017)
[3] A. Bienfait et al., Nat. Nanotech. 11, 253 (2016)

Posterprize: Francesco Torricella
8th EFEPR School

PELDOR investigation on tilt angles in transmembrane β-peptides

F.Torricella[1,2], K. Halbmair[1], G.Valora[1], A. Kehl[1,3], J.Wagner[3], U.Diederichsen[3] and M.Bennati[1]
[1]Max-Planck-Institut für Biophysikalische Chemie Göttingen,
[2]University of Florence (CERM) Italy,
[3]Institut für Organische und Biomolekulare Chemi Georg-August-Universität Göttingen

Pulsed-electron double resonance (PELDOR or DEER) in combination with site-directed spin labelling has become an established experiment in structural biology for measure distances between 2 and 10 nm[1]. However, distance measurements in biological transmembrane proteins in their natural environment, pose particular spectroscopic difficulties in terms of sensitivity and reliability. To overcome this challenge suited spectroscopic setup and spin labels are required.

Here, the recently developed β-TOPP[2] was used as spin label to study the interaction of beta-peptides[3] in lipid bilayers. β-peptides are a versatile class of transmembrane peptides that can form stable secondary structures. In a model doubly β-TOPP labelled peptide, we found that the experimental interspin distances from PELDOR report on the helix pitch, both in solution and in lipid environment[4] (Fig.1). Due to their semi-rigid design, the labels deliver reliable distances with sharp - one peak - distance distributions.

We subsequently examined the tilt angle of the same peptide in an aligned lipid bilayer (Fig.2-3). Helix tilting is one of the most important hydrophobic mismatches (HMM) which can occur when the peptide hydrophobic lengths exceeds the membrane bilayer (Fig.4). Initial PELDOR distance measurements at Q-band (34GHz / 1.2T) show orientation dependence in dipolar frequencies when rotating the aligned sample in the magnetic field (Fig.5). The estimated peptide's tilt angle is consistent with the value obtained via X-ray diffraction[5].

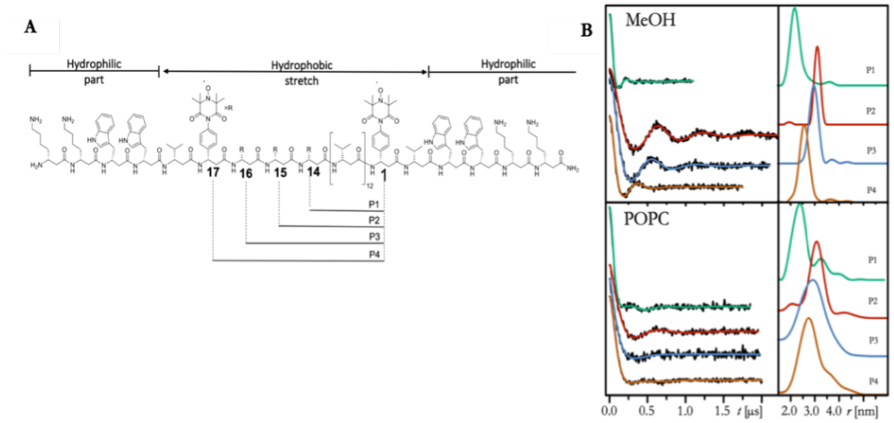


Fig. 1: β−peptides strucutres and PELDOR/DEER experiments
(A) The β−peptides structures labelled with TOPP label; label in position 1 was kept fixed while the second label was placed respectively from position 14 to position 17.
(B) "top" PELDOR/DEER experiments in MeOH solution. Background corrected time traces(black line), DeerAnalysis fit (coloured line) and resulting distance distributions (protein concentrati-on: 50 µM at 50 K)."bottom" PELDOR/DEER experiments in MLVs (Protein/lipids : 1/3000). Background corrected time traces(black line), DeerAnalysis fit (coloured line) and resulting distance distributions (protein concentration: 20 µM at 50 K).

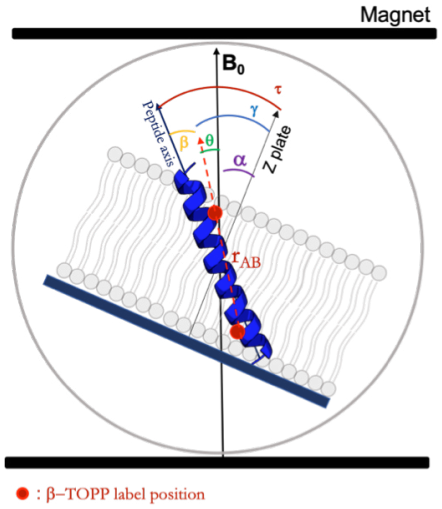


Fig. 2: Angles involved in the protein tilt angle determination using an aligned membrane sample via PELDOR/DEER spectroscopy.
Graphical representation of the top view on the EPR tube with the angles involved in the determination oft he peptide tilt angle τ. The circle line represents the EPR tube, which is rotate in 15° steps inside the resonator, as indicated by the curved arrow.

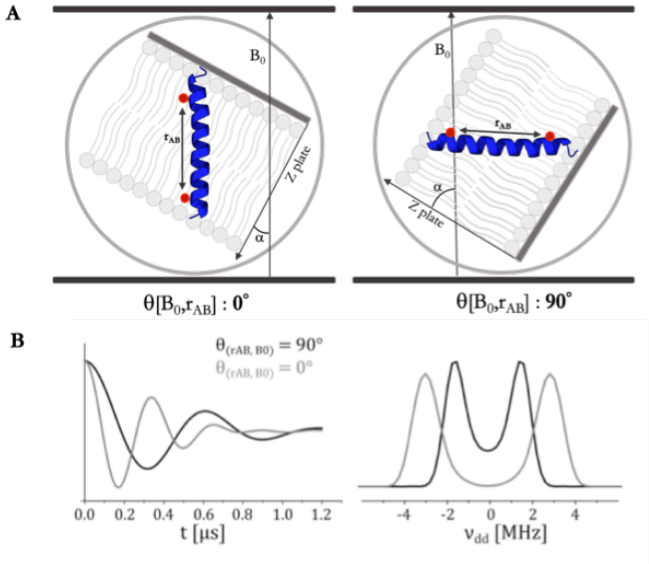


Fig. 3: Peptide tilt angle and connected dipolar frequency
Graphical top view of the EPR tube with the lipid emebedded doubly labelled sample depositated onto a quartz plate (A). (B) Theoretical PELDOR/DEER traces and relative pake pattern for the sample orientated with θ[B0, rAB]: 0° (grey line) and θ[B0, rAB]: 90° (black line).

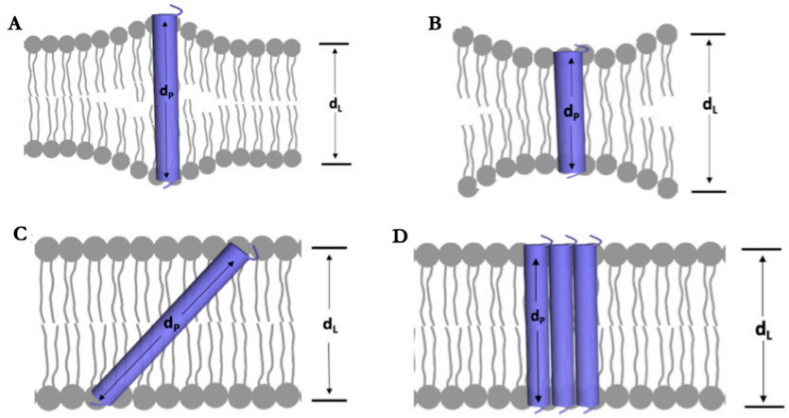


Fig. 4: Examples for hydrophobic mismatches
Schematic representation of four types of hydrophobic mismatch and possible membrane adaptations. (A) dp > dL : Under this condition, the lipids nearby the protein would get stret-ched to match the hydrophobic thickness oft he protein. (B) dp < dL : This condition leads to backbone deformation/distortion (C) helix tilting (d) oligomerization aggregation.

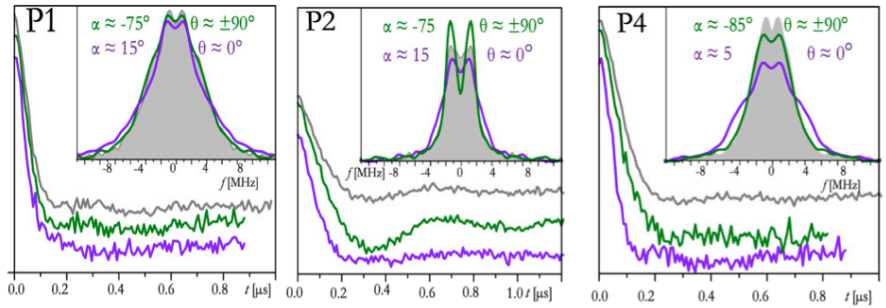


Fig. 5:Time traces at Pake pattern extrema
Comparison between the θ[B0, rAB]: 0° (purple) and θ[B0, rAB]: 90° (green) time traces. Inset: Relative pake pattern for P1, P2 and P4 samples. An orientation dependence of the dipolar frequency is visible in P2 and P4 samples. The data were plotted with the same recorded in D31-POPC MLVs vesicles (gray traces and area).

References:
[1] K. Ackermann, C. Pliotas, S. Valera, J. H. Naismith, B. E. Bode, Biophysical Journal 2017, 113, 1968-1978.
[2] S. Stoller, G. Sicoli, T. Y. Baranova, M. Bennati, U. Diederichsen, Angewandte Chemie 2011, 50, 9743–9746.
[3] K. Halbmair, J. Wegner, U. Diederichsen, M. Bennati, Biophysical Journal 2016, 111, 2345– 2348.
[4] J. Wegner, G. Valora, K. Halbmair, A. Kehl, B. Worbs, M. Bennati, U. Diederichsen, Chemistry – A European JournalChem. Eur. J. 2019, 25, 2203.
[5] U. Rost, Y. Xu, T. Salditt, U. Diederichsen, ChemPhysChem 2016, 17, 2525

First announcement HYP20

We are pleased to announce the next
Hyperpolarization Conference HYP20
from August 30 to September 3, 2020
in Lyon, FRANCE (hyp20.org).

The aim of the conference is to provide an international forum for high-level discussions on the latest developments in nuclear hyperpolarization. The meeting will focus on the state of art in theoretical, instrumental and methodological developments, in all variants of dynamic nuclear polarization (DNP), optical pumping, parahydrogen-induced polarization or quantum-rotor-induced polarization techniques, as well as on key applications in fields as diverse as clinical imaging, materials science, small molecules, structural biology, high-energy physics.

The conference has a broad scope and intends to promote interactions and synergies between the full range of hyperpolarization technologies. It will group together the best experts worldwide in the field of hyperpolarized magnetic resonance. Young scientists will be particularly encouraged to participate.

The HYP20 conference is an activity of the Hyperpolarization Subdivision of the Groupement Ampère. It will follow on, from a series of conferences on hyperpolarization organized in:
Nottingham, UK (2007), Königstein, Germany (2009), Lausanne, Switzerland (2011)Copenhagen, Denmark (2013), Egmond aan Zee, The Netherlands (2015), Southampton, UK (2018)

Plenary speakers
1. Jan Henrick Ardenkjaer Larsen (Tech. University of Denmark, Lyngby, Denmark)
2. Song i Han (University of California, Santa Barbara, USA
3. Bob Griffin (MIT, Boston, USA)
4. Matthew Rosen (Harvard Medical School, Charlestown MA, USA)
5. Carlos Meriles (City College of New York, USA)

Invited speakers
6. Lucio Frydman (Weizmann Institute of Science, Revohot, Israël)
7. Michal Leskes (Weizmann Institute of Science, Revohot, Israël)
8. Kendra Frederik (Center for Alzheimer's & Neurodegenerative Disease, Dallas, USA)

9. Danila Barskiy (University of California, Berkeley, USA)
10. Thomas Meersman (University of Nottingham, Nottingham, UK)
11. Eleonora Cavallari (University of Torino, Italy)
12. Gerd Buntkowsky (Technische Universität Darmstadt, Germany)
13. Tomas Orlando (Max Planck Institute for Biophysical Chemistry, Göttingen, Germany)

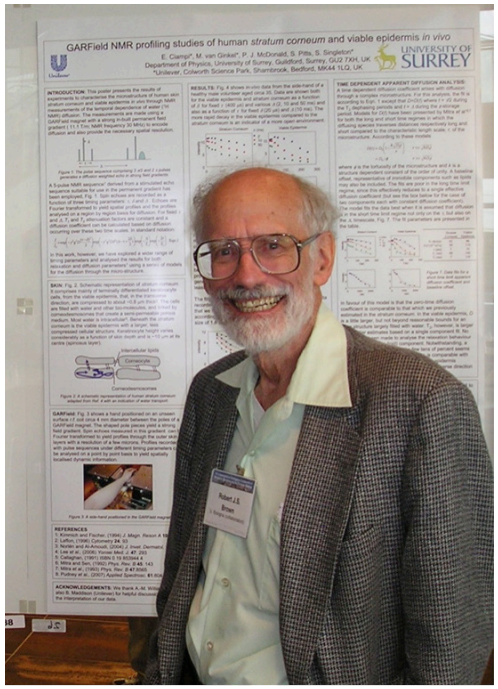
COVID-19 update:
The registrations remain open!
Note however that we have not decided yet to keep the initial dates (from August the 30th to September the 3rd) or to postpone the conference at a later period this year. Refunding registration will be possible if the conference is postponed or if travel restrictions still apply at the time of the conference.
We will follow closely the situation with the COVID-19 as well as the directives from the French government.

Regular updates will follow here: hyp20.org

Anne Lesage and Sami Jannin, co-chairs of the conference.

In memory of Dr. Robert Brown, a pioneer of magnetic resonance of porous media (MRPM)

On November 12, 2019, I received the unfortunate news from Prof. Paola Fantazzini of the passing of Dr. Robert Brown the week before. Paola informed me that Bob died peacefully at the age of 95, with his children gathered at his bedside. It is a great loss for the NMR community, and in particular for MRPM. This remembrance is largely based on the information from Paola who together with her late husband Prof. Borgia remains a close friend and long-time colleague of Bob.



Bob Brown at MRPM9, Cambridge MA, 2008

Bob was born in 1924. He started college in the fall of 1942 at California Institute of Technology and very soon had to go into the Army like many people of his time. From 1943 to 1946 he was a member of the Special Engineer Detachment at Los Alamos working under Don Hornig on the electrical engineering aspects of detonation for the plutonium bomb (https://www.atomicheritage.org/profile/robert-js-brown). After WWII, Bob graduated from Caltech with a BS degree in Physics in 1948 and finished his PhD in Physics at the University of Minnesota in 1953.

Most of his professional life, from 1953 until his retirement in 1986, was spent at Chevron Oil Field Research Co. During this period, he gave important scientific contributions to many topics related to the science and the practice for the petroleum industry, not just strictly connected to NMR. To quote a few examples, he directed a project of a downhole radar logging, including the investigation of radar attenuation in salt domes; he worked in seismology, primarily promoting three-dimensional measurement and interpretation; he studied physical properties of rocks, particularly elastic properties. Surely, his heart was always beating for MRPM, his major field of interest, a love that he continued even after his retirement, from 1988 up to the end, primarily in collaboration with the University of Bologna, Italy.

Bob was recruited by Standard Oil of California (now Chevron Oil) after getting his PhD, and his fascination for NMR began. From 1953 to 1963, Bob directed a project to develop Nuclear Magnetism Logging (NML) of oil wells. This consisted of running an instrument on up to several miles of cable to make a log of NMR properties of Earth formation outside a borehole. The project included some of the earliest work on NMR relaxation of fluid in porous media. The key feature of NML was the possibility to exploit the different relaxation times of oil and water to distinguish their signals. Much of the fascinating science and history of the NML work was reviewed by Bob in Concepts in Magnetic Resonance, 2001 vol. 13 (6) pp. 344-366.

Many of the basic features of our current knowledge of NMR relaxation in porous media were identified during this project. It was discovered that in a porous medium the relaxation rate is increased in proportion to the surface-to-volume ratio of the pore space, so water could not be distinguished from oil based on their bulk relaxation rates. Furthermore, part of the signal from water in most sandstones decays faster than the instrumental dead times, so the total porosity could not be determined. In the opening address at MRPM1 in Bologna, Bob said:

Many of the things that we found long ago looked like a disaster, but afterwards they really turned out to be something better than we had anticipated..... This was very disappointing for a while, but with a few more measurements and a little thought about what the measurements meant, we realized we perhaps could have more important objectives than we originally started out with".

Presently, relaxation and surface interaction are the key methods to study porous media for many applications.

Interdisciplinary collaboration is the characteristic of Bob's work in cooperation with the University of Bologna, Italy, doing research on Magnetic Resonance for fluids in different porous media, including rocks and biological tissues. Areas of particular interest have included the problem of getting reliable distributions of relaxation rates from multi-exponential decay data, the influence of diffusion on spin echo data in porous media, the estimation of permeability and irreducible water saturation from NMR measurements, and the NMR study of partially saturated porous media. For computing distributions of relaxation times from NMR relaxation data, the method and program UPEN (Uniform PENalty inversion) have been developed using a novel regularization method employing negative feedback to a smoothing penalty. The most recent achievement of the collaboration with the Bologna group is the extension of the algorithm UPEN to the analysis of two-dimensional data for many applications.

Bob has also contributed tremendously to the formation of the scientific community MRPM and its continuous dissemination and promotion. Many of his papers made key contributions to the field [e.g. Measurement of nuclear spin relaxation of fluids in bulk and for large surface-to volume ratios, Bulletin American Physical Society Series II, 1:216 (1956); Measurements of fractional wettability of oilfield rocks by the nuclear magnetic resonance method, Petroleum Transactions AIME, 207:262–264 (1956); Proton relaxation in crude oils, Nature, 189:387–388 (1961)]. Bob gave the opening address at the first MRPM at University of Bologna in 1990 and served on the Scientific Advisory Committee until 2016, at the age of 92. In 2008 at the 9th MRPM in Cambridge MA, Bob received the Life-Time Achievement Award with the following citation:

This award is presented to Robert James Sidford Brown for his pioneering work on ex-situ NMR instrumentation, and the magnetic resonance properties of natural fluids and granular solids. His NMR well logging apparatus was the first to make magnetic resonance measurements of earth formations from within a borehole. He has developed imaginative signal processing techniques and applied them to the problems of NMR of porous media. He was one of the founders of International Bologna Conference on Magnetic Resonance in Porous Media and has remained closely involved with the activities of the MRPM community over the years. Notably, he has continued to be an active scientific contributor many years after his formal retirement. Bob's work and career are an inspiration to all of us.

I was deeply honored to present Dr. Brown this Life-Time Achievement award together with the co-chair Dr. Martin Hurlimann. Bob's scientific work, his dedication and enthusiasm have been a long-lasting inspiration for many generations in the MRPM community both professionally and personally. We will miss his presence in the future MRPM conferences.

Yiqiao Song
Chair of MRPM, AMPERE society

Minutes of the meeting of the AMPERE Bureau
in the cloud, on March 19, 2020

Members present (17):
J. van Duynhoven, G. Otting, A. Kentgens, M. Britton, Y.-Q. Song, B. Blümich, M. Ernst, G. Bodenhausen, J. Dolinsek, J.-N. Dumez , O. Millet, B.H. Meier, S. Hiller, T. Prisner, A. Böckmann, S. Jurga, H. Oschkinat

Excused (3):
S. van Doorslaer, H.-W. Spiess, V. Chizhik,

Agenda:
1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Bureau meeting in Berlin August 26, 2019
3. Report on the state of the AMPERE Society (B. Blümich)
4. Financial Report (M. Ernst)
5. Report EUROMAR Division (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. Meier)
9. Final reports past meetings:
   - SPINUS 2019, St. Petersburg (Russia), M. Ernst
   - AMPERE NMR School 2019, Zakopane (Poland), S. Jurga
   - 15th ICMRM 2019, Paris (France), M. Britton
   - EUROISMAR 2019 Berlin (Germany), H. Oschkinat
   - XIth EFEPR Conference, Bratislava (Slovakia), S. van Doorslaer
   - 11th Alpine Conference, Chamonix (France), J.-N. Dumez
   - 8th EFEPR School, Brno (Czech Republic), S. van Doorslaer
10. Future meetings 2020:
   - SPINUS 2020, St. Petersburg (Russia), April 1-5 M. Ernst
   - NMR FOOD 2020, Aarhus (Denmark), June 2-5 J. van Duynhoven
   - AMPERE NMR School, Zakopane (Poland), June 23-29 S. Jurga
   - EUROMAR 2020, Bilbao (Spain), July 5-9 O. Millet
   - 15th MRPM, Tromso (Norway), August 24-28 Y.-Q. Song
   - HYP20 Conference, Lyon (France), August 30-September 3 G. Bodenhausen
   - Biological SSNMR School, Palma (Spain), October 4-9 H. Oschkinat
   - EUROMAR 2021, Portoroz (Slovenia), July 6-10 J. Dolinsek
11. Election of the AMPERE Bureau in Bilbao (B. Blümich, M. Ernst)
12. AMPERE Logo (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 reported that there was a number of successful conferences last year. He highlighted that the society has specific guidelines for conference organizers. These guidelines are available on the AMPERE webpage. They are meant to help organizers to consider all important points and timelines, especially to first-time organizers. The contacts to vendors and sponsors are particularly sensitive since they are a major source of income. B. Blümich urged all conference organizers to take this into account carefully.
Further key points were made: As a main concern, at least six upcoming conferences are threatened by the current coronavirus crisis; The AMPERE society has gotten a new branch of publishing, thanks to G. Otting and G. Bodenhausen; The society will have 13 committee members upcoming for re-election in 2020; Importantly, the president steps down and a successor needs to be elected at the next EUROMAR conference.
In the subsequent discussion it was pointed out, that there are two sets of guidelines, one for EUROMAR and one for other AMPERE events, and that it would be helpful to consolidate both into one with attention to the special demands of EUROMAR.

Ad 4. M. Ernst presented the financial report. Finances are very stable and substantially increased compared to previous years. The reason is that many members have paid 3-years membership fee packages. AMPERE did not have expenses for EUROMARs 2019 and 2020 yet. The financial situation of all subdivisions is stable and partially very positive. AMPERE will create an account for the publication division as soon as the first page charges come in.

Ad 5. Thomas Prisner reported on the EUROMAR division. EUROMARs will take place 2020 in Bilbao, organized by Oscar Millet, and 2021 in Slovenia, organized by Janez Plavec and Janez Dolinsek. EUROMAR 2022 will be in Utrecht and 2023 in Glasgow.

Ad 6. A. Kentgens reported on the finances of the EUROMAR division. Finances are healthy and stable, a total of around 100 kEUR is avilable. The two existing bank accounts (one in EUR and one in CHF) at Zürcher Kantonalbank shall now really be merged into one.

Ad 7. G. Otting and G. Bodenhausen reported on the new publication division. So far, two articles have been published in Magnetic Resonance. It turns out that the publisher Copernicus is perhaps slightly understaffed, leading to long response times. The open peer review system is generally perceived as attractive. There is a total of seven articles published or under discussion. The division hopes to have many more articles by the end of the year. The articles that are in the open peer review system are viewed more often than those in well-known journals. There have been minor technical issues such that reviewer invitations were considered junk by spam filters. This is now fixed by additional emails. There will be a special issue honoring Rob Kaptein. The Copernicus publishing scheme allows unique options for this, since all accepted papers are already visible while special issue is being assembled. It is noted that there exists a predatory company called Kopernikus and another one called Copernicus Publishing (compared to the original Copernicus Publication). Everyone should be aware of this.
It was discussed to alert the MR community to the issue of predatory activities to promote the new journal though mailing lists and a note in the AMPERE Bulletin.

Ad 8. B.H. Meier reported on the Andrew Prizes and the funds to support meetings. Last year's price was given to Cody Can, who gave a well-received lecture via the internet at EUROMAR Berlin, as he could not leave US due to immigration issues. The committee has received 16 nominations for the next Andrew prize and four nominations for the Ampere Young Investigator prize. B.H. Meier reported that unfortunately, the Varian young investigator prize, which was alternating in years with the Ampere prize for Young investigators, has now switched register and changed to the even years, with the result that there are now two prizes at the same year and then none in the other. All agree that AMPERE society shifts the Andrew prize to the other years, such that it will be given in Bilbao 2020, as announced, and then directly again in Slovenia 2021.

Ad 9. Final reports of past meetings:
- The SPINUS conference is an annual event with the scope to cover all kinds of NMR in chemistry, physics and related fields. It took place in St. Petersburg in 2019. Was highly successful. The report was given by M. Ernst on behalf of V. Chizhik.
- Stefan Jurga gave a report on the NMR school in Zakopane (Poland, a resort town in southern Poland, at the base of the Tatras Mountains). The conference centered around the topics of NMR relaxation, novel techniques, and solid-state NMR, around 100 attendees from over 20 countries attending. Around 20 lectures and overall very successful.
- The ICMRM in Paris was very successful in August. It was timed next to the EUROMAR ISMAR, which probably was not the best idea because presumably some potential attendants did not come therefore. Nonetheless, finances are healthy, creating a surplus of the meeting of 19 kCHF. Next meeting will be in 2022 in greater Kopenhagen area. 2024 is going to be in Singapore.

- The report of the EUROISMAR was given by H. Oschkinat. Accountants are still in the process of doing the finances. It will perhaps be ready later this week. Finances are expected to come out either at a small plus or a zero. Very likely there will have been no deficit. AMPERE society can therefore expect to get the seed money back.
- The EFEPR was very successful, a detailed report is printed in this AMPERE bulletin.
- The Alpine Conference in Chamonix in September was very successful, with over 180 participants. 130 abstracts were submitted and many great posters shown. The Vold prize was given to Melanie Rosay and the Calderelli prize to Aaron Rossini. Next conference will be held in 2021.
- EFEPR school was successful, a report is published in this bulletin.

Ad 10. Reports of planned meetings in 2020/2021:
- SPINUS 2020: M. Ernst reported on behalf of V. Chizhik. The conference has been cancelled due to coronavirus.
- NMR FOOD 2020. Local organizers are in Aarhus, while Denmark has just gone into a lockdown. The organizers want to take decision on cancellation in early April. Everyone agreed that is likely the best strategy to cancel completely as compared to shift to fall and then continue next year.
- AMPERE NMR school in Zakopane in June can likely be canceled without costs. Will likely be canceled next week.
- EUROMAR Bilbao was originally scheduled from 5-9 July. Sponsors are secured and everything was under control. But now, registrations are very low because of coronavirus. The conference has been postponed to December 6-10, the original venue is available then. The new deadline for applications will be on September 25. A minimum number of 300 registrations are needed and if this number is reached by September 25, and if the virus lockdowns are no longer in place, the conference will take place. Otherwise it will be canceled. Everyone agrees that if Bilbao December issue is cancelled, the society will re-schedule Bilbao at the next possible year, perhaps shifting some of the other planned EUROMARs by one year. EUROMAR 2021 will in any case be held in Slovenia.
- MRPM 2020 in Tromso, presented by Y.Q. Song. Attendance is very low at this point for corona reasons. Conference therefore is still at high risk. Norway is in a severe lockdown since very recently with many restrictions of movement. The local organizer is very concerned. Plan is still to move forward. Plans will be revisited in a month.
- HYP20 reported by G. Bodenhausen. There are no contingency plans yet. France is locked up since 2 days. G. Bodenhausen thinks it is likely that the meeting will be skipped and since there is an agreement with Chamonix about a bi-annual alternation, it would likely continue only in 2022.
- Biological SSNMR School in Palma. H. Oschkinat did so far not think much about a possible cancellation, because the meeting is in October. He will observe the situation closely.

- EUROMAR 2021 by Janez Dolinsek. Will be located at the Adriatic Sea, in Portoroz. The location is a particularly beautiful five-star Hotel with many lecture halls, thereof the biggest hall for 1100 participants and the second largest for 680 participants. Several smaller halls exist and plenty of space for poster session and social events. Everything is in one building with beach.

Ad 11. The elections for the new president are scheduled for the next EUROMAR, where and when-ever that is. Potential candidates were proposed by the current president Bernhard Blümich and the former president Beat Meier. In the extensive discussion it was concluded, that a list of two female candidates will be proposed by the Bureau AMPERE to the AMPERE Committee at the time of the election. If one of the nominees declines, then another candidate, preferably female, should be nominated prior to the election.

Ad 12. A new logo was presented by M. Ernst. It was generally appreciated and approved.

Ad 13. A. Kentgens brought up a suggestion to create an advanced solid-state school for materials, in alternation with the bio-solids school. He proposes to create a new subdivision for this. This was approved.

Ad 13. The envisaged date of next spring meeting of the AMPERE Bureau: March 18, 2021 in Zürich. It is proposed that the meeting may again be held via zoom only to avoid travel. It is agreed that prior to the meeting a poll is done and if less than 50% of members want to come physically to Zurich, it will be done by zoom.

The meeting closed at 14:34.

Basel / the internet, 19 March 2020
Minutes: Sebastian Hiller

Balance of the Accounts of the Groupement Ampere and the Subdivisions

Period from February 28, 2019 to February 28. 2020

	Balance on February 28. 2019	Membership Fees / Registration Payments	Donations/ Conference support	Conferences Grants / Travelgrants/ Membership Fee paid to Ampere	Conference Sponsoring	Conference Surplus	Administration Bulletin print Web and Bureau Meetings / MR design	Bank Charges / Depot Charges/ Div./Losses	Account Closing / Account carry over	Bank Interests Account carry over, Dividends	Gains on Value Paper	**Balance on February 28. 2020**
Groupement Ampere												
Ampere (CHF)	**15'311.35**	3'530.71					3'203.25	12.00	1'271.80			**14'355.01**
Ampere (Euro)	**28'520.54**	30'574.13			7'800.00		1'500.00	43.62				**49'751.05**
Andrew (CHF)	**26'009.26**			557.76				425.85		492.90		**25'518.55**
Andrew Depot (CHF)	**92'587.11**										928.05	**93'515.16**
Subdivisions												
NMR School (Euro)	**1'865.04**							7.15	1'857.89			**0.00**
Biol. Solid State (Euro)	**6'828.35**		650.00				66.00	33.12		1'857.89		**9'237.12**
EPR (CHF)	**7'425.65**									1.4		**7'427.05**
Food NMR (CHF)	**917.80**						276.63	26.00		0.15		**615.32**
MRPM (CHF)	**31'329.80**					1'271.80				6.00		**32'607.60**
SMRM (CHF)	**47'330.88**			1'096.97				2.00		8.85		**46'240.76**
Hyp (CHF)	**7'343.25**											**7'344.65**
Euromar												
Euromar (CHF)	**71'610.89**							12.00				**71'598.89**
Euromar (Euro)	**41'270.19**				10'000.00			43.62		1.40		**31'226.57**

Enable Education Everywhere…

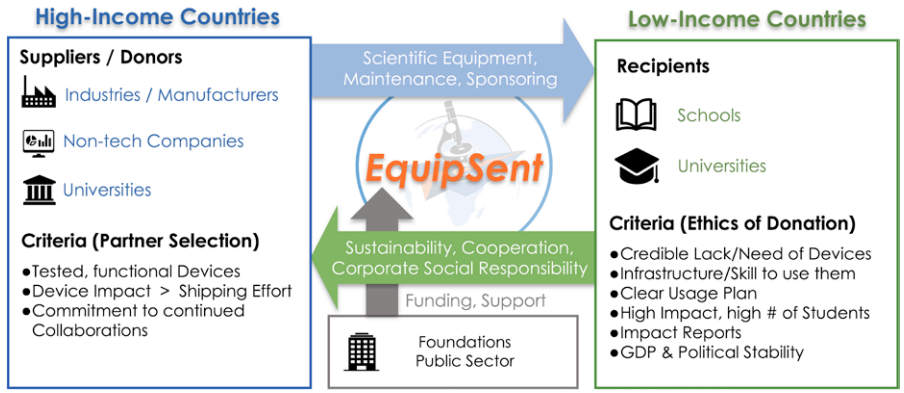
…with EquipSent!

Initial Situation
In high-income countries, scientific equipment is often stored unused after its usage time in research laboratories. Older devices are eventually discarded, even though they are still functional.
In low-income countries, schools and universities are lacking the funds to acquire even the most basic devices for adequate training of talented students. The resulting ‚brain-drain' to other countries hinders the self-development in such regions.

Our Solution
EquipSent seeks to connect these two worlds by directly matching donors of scientific equipment with those in need. As an intermediary between both parties, we reduce administrative efforts and help organizing the shipping, installation and legal contracting. Expenses are shared between the recipient and the industrial sponsors in return for CSR, new markets and advertisement.

Target Impact
• Access to Education. Students around the world will be granted access to hands-on training and education, rather than theory only.
• Collaboration and Development. The matched donor, sponsor and recipient of equipment are encouraged to collaborate on a long-term basis, which offers learning opportunities on all sides.
• Resource Efficiency & Waste Minimization. The equipment donor profits by reducing costs for space, waste and personnel, while benefitting from a positive image generated through sustainable use.

Founded by a group of ETH students, *EquipSent* is giving a second life to devices, promotes sustainable use and offers access to education and research to more people.



Do you know about no longer used, but functional scientific equipment in your research group or do you know of a university in need?

Do you want to learn more about what we do?

Check out our website *EquipSent.org* and get in touch with us!

our Partners:

CGI U COMMITMENT-MAKER 2016 AVETH Projectogether STUDENT PROJECT HOUSE

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.

Bernhard. BLÜMICH *President*
Macromolcular 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

Janez DOLINŠEK *Vice President*
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

Anja BÖCKMANN *Vice President*
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

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

Sebastian HILLER *Executive Secretary*
Biozentrum, University of Basel, Klingelbergstrasse 50/70, CH-4056 Basel, Switzerland
Tel. +41 61 207 20 82, e-mail: sebastian.hiller@unibas.ch

Sabine VAN DOORSLAER *EF-EPR Representative*
University of Antwerp, Departmet of Physics, Campus Drie Eiken, Universiteitsplein 1, 2610 Wilrjik, Belgium, e-mail: sabine.vandoorslaer@uantwerpen.be

Melanie M. BRITTON *SRMR Representative*
University of Birmingham, Birmingham, B15 2TT, UK
office: +44 121 4144391, e-mail: m.m.britton@bham.ac.uk

Yi-Qiao SONG *MRPM Representative*
Schlumberger-Doll Research, 1 Hampshire Street, Cambridge, MA 02139-1578 USA
Phone: +1 617 768 2333, e-mail: ysong@slb.com

John VAN DUYNHOVEN *MR-Food Representative*
Unilever N.V., 100 Victoria Embankment, London EC4Y 0DY, United Kingdom, e-mail: john-van.duynhoven@unilever.com

Geoffrey BODENHAUSEN *Hyperpolarisation Representative*
ENS - Département de chimie, 24, rue Lhomond, 75005 Paris, France,
e-mail: geoffrey.bodenhausen@ens.fr

Gottfried OTTING *Publication Division*
Australian National University, College of Science, Canbera ACT 2600, Australia, Tel: +61 2 612 565 07, e-mail: gottfried.otting@anu.edu.au

Thomas PRISNER *Euromar Representative*
Goethe University Frankfurt, Institute of Physical and Theoretical Chemistry, 60438 Frankfurt am Main, Germany, Tel: +49 (0) 69 798-29406, Fax: +49 (0) 69-798-29404 , e-mail: prisner@chemie.uni-frankfurt.de

Arno KENTGENS *Euromar Treasurer*
Institute of Molecules and Material, Radboud University, Heyendaalseweg 135, 6525 Aj Nijmegen, Netherland, Tel. +31 024 365 20 78, e-mail: a.kentgens@nmr.ru.nl

Beat H. MEIER *Past President*
Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zurich, Switzerland,
Tel. +41 44 632 44 01, Fax +41 44 632 16 21, e-mail: beme@nmr.phys.chem.ethz.ch

Hans Wolfgang SPIESS *Honorary Member*
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

Stefan JURGA *Honorary Member*
Instytut Fizyki, Uniwersytet im. A. Mickiewicza, Zaklad 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

Sharon Elizabeth Marie ASHBROOK (2016 - 2020)
School of Chemistry, University of St. Andrews, North Haugh, St. Andrews, KY16 9ST, United-Kingdom

Juras BANYS (2016 - 2020)
Vilnius University, Department of Radiophysics, Saulėtekio 9 2040 Vilnius, Lithuania

Rolf BOELENS (2016 - 2020)
Bijvoet Center for Biomolecular Research, Utrecht University, Padualaan 8, NL-3584 CH Utrecht, The Netherlands

Vladimir CHIZHIK (2016 - 2020)
University of St. Petersburg, Quantum Magnet.Phen.,Fac.of Physics, RU-198504 St. Petersburg, Russia

Peter CROWLEY (2018 - 2022)
Chemistry, National University of Ireland, University Road, Galway, Ireland

Janez DOLINŠEK (2016 - 2020)
Institute Jozef Stefan, Jamova 39, SI - 1000 LubljanaL, Slovenia

Isabella Caterina FELLI (2016 - 2020)
Department of Chemistry and Center for Magnetic Resonance (CERM), University of Florence Via L. Sacconi 6 50019 Sesto Fiorentino, (FI), Italy

Ana Maria Pissarra Coelho GIL (2018 - 2022)
Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aviero, Portugal

Patrick GIRAUDEAU (2016 - 2020)
Université de Nantes, Faculté des Sciences et Techniques, 2 rue de la Houssinière, 44322 NANTES Cedex 03, France

Kristaps JAUDZEMS (2019 - 2023)
Latvijas Organiskās sintēzes institūts, Aizkraukles 21, Rīga, LV-1006, Latvija

Robert KONRAT (2017 - 2021)
Max F. Perutz Laboratories, Campus Vienna Biocenter 5, 1030 Vienna, Austria

Wiktor KOZMINSKI (2016 - 2020)
Biological and Chemical Research Centre, University of Warsaw, Krakowskie Przedmiescie 26/28, 00-927 Warsaw, Poland

Birthe Brandt KRAGELUND (2018 - 2022)
Department of Biology, University of Copenhagen, Ole Maaløes Vej 5, 2200 Copenhagen, Denmark

Predag NOVAK (2019 - 2023)
Division of Analytical Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102A, HR-10 000 Zagreb, Croatia

Miquel PONS (2016 - 2020)
Institute for Research in Biomedicine, University of Barcelona, Josep Samitier 1-5, 80828 Barcelona, Spain

Indrek REILE (2019 - 2023)
National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia

Frode RISE (2018 - 2022)
Department of Chemistry, University of Oslo, PO Box 1033 Blindern, 0315 Oslo, Norway

Sharon RUTHSTEIN (2018 - 2022)
Department of Chemistry, Bar-Ilan University, Ramat-Gam, 5290002, Israel

Ferenc SIMON (2017 - 2021)
Budapest University of Technology and Economics, Műegyetem rkp. 3, 1111 Budapest, Hungary

Jiri SPEVACEK (2016 - 2020)
Inst. of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 - 06 Prague 6, Czechia

George SPYROULIAS (2017 - 2021)
Department of Pharmacy, School of Health Sciences, University of Patras, Panepistimioupoli – Rion, 26504 Patras, Greece

Ville-Veikko TELKKI (2016 - 2020)
Department of Physics, University of Oulu, P.O. Box 3000, 90014 Oulu, Finland

Christina THIELE (2016 - 2020)
Technische Universität Darmstadt, Alarich-Weiss-Strasse 16, 64287 Darmstadt, Germany

Daniel TPOGAARD (2017 - 2021)
Physical Chemistry, Lund University, Box 124, 221 00 Lund, Sweden

Sabine VAN DOORSLAER (2016 - 2020)
SIBAC Laboratory, University of Antwerp, Universiteitsplein 1, B-2610 Wilrijk, Belgium

Paul VASOS (2019 - 2023)
Extreme Light Infrastructure – Nuclear Physics (ELI-NP), Horia Hulubei Institute for Nuclear Physics (IFIN-HH), Reactorului Str. 30, Magurele Campus, Bucharest, Romania

Emeritus members

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

Richard R. ERNST
Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 ZURICH, Switzerland
Jean JEENER
Université Libre - Plaine, CP 223, Bld. du Triomphe, B - 1050 BRUXELLES, Belgium
Karl Alexander MÜLLER
IBM Zurich Research Laboratory, Säumerstrasse 4, CH - 8803 RÜSCHLIKON, Switzerland
Kurt WÜTHRICH
Inst. f. Molekularbiologie u. Biophysik, ETH Zürich, CH-8093 ZURICH, Switzerland

Guest members

Alexander PINES
Dept. of Chemistry, University of California, BERKELEY CA 94720, USA, Delegate of ISMAR
James A. NORRIS
Dept. of Chemistry, University of Chicago, South Ellis Ave. CHICAGO IL 6037-1403, USA
Delegate of the International EPR Society
Keith A. McLAUCHLAN
Physical Chemistry Laboratory, Oxford University, South Parks Road, OXFORD OX1 3QZ, UK Delegate of the International EPR Society
David AILION
Dept. of Physics, Univ. of UTAH, 304 J. Fletcher Building, SALT-LAKE-CITY 84112, Utah, USA
Sung Ho CHOH
Department of Physics, Korea University, SEOUL 136-701, Republic of Korea
Daniel FIAT
University of Illinois, Dept. of Physiology and Biophysics, POB 6998, CHICAGO IL 60680, USA
Eiichi FUKUSHIMA
ABQMR, 2301 Yale Blvd., SE, Suite C2, ALBUQUERQUE, NM 87106, USA

Future conferences

Ampere Events 2020

15th MRPM	Tromsø (Norway)	August 24-28 2020
‚HYP20' Hyperpolarized Magnetic Resonance 2020	Lyon (France)	August 30 to September 2 2020
Euromar 2020	Bilbao (Spain)	Dezember 6-10 2020

Ampere Event 2021

MR FOOD 2021 (2020)	Aarhus	June 8-12 2021
Euromar 2021	Protorož (Slovenia)	July 4-8 2021
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	12-16 September 2021

Ampere Event 2022

Euromar 2022	Utrecht (Netherlands)	3-7 July 2022

Ampere Event 2024

HYP24	Leipzig (Germany)	September 2024

Groupement
AMPERE

Correspondence address:
ETH Zurich, Laboratory of Physical Chemistry, HCI F 223
Vladimir Prelog Weg 2, 8093 Zurich, Switzerland
Mail: contact@ampere-society.org
Publisher: Matthias Ernst, ETH Zurich, Switzerland

www.ampere-society.org