

epr news letter

2012
volume 22 number 3

Nutrition Frequency



The Publication of the International
EPR (ESR) Society

Magnetic Field



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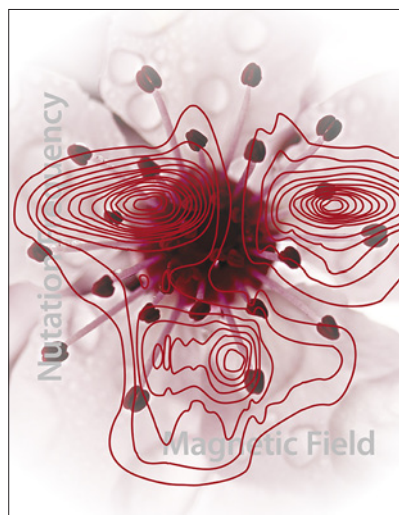
Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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The cover picture illustrates aspects of the research carried out by Seigo Yamauchi, recipient of the 2011 Zavoisky Award. It shows the time-resolved two-dimensional EPR spectrum of an excited triplet-radical pair composed of two nitroxide radicals and fullerene. EPR transitions from two excited quintet states and a ground-state doublet are separated by the nutation frequencies.

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ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

INSTRUMENT FOR ROUTINE
AND RESEARCH APPLICATIONS

CMS 8400

Bench - Top Electron Spin Resonance (ESR) Spectrometer



Affordable compact unit with accuracy of large systems and high sensitivity

Easy integration with optional equipment and accessories for X-band range



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www.epr-newsletter.ethz.ch/corporate_sponsors.html

Editorial

Dear colleagues,

To answer the unasked question in your eyes, no, you won't find an obituary for Seigo-san in this issue. In fact, Takeji Takui-san, President of the Asia-Pacific EPR Society 2012–2014, collected the relevant material and sent me most of the information but some pieces were missing. We discussed this situation and finally decided that it would be better to wait until all of the material arrived rather than split the obituaries between two issues. Thank you for your patience and understanding.

Please find the report about the IES Annual General Meeting 2012 on pp. 3–4. It gives you an insight into various aspects of the IES activities. Initiated by Sushil Misra, stories about the research performed by laureates

of the IES Awards (in the current issue by Alexander Milov, Silver Medal: Chemistry, pp. 5–6 and Laxman Mainali, Young Investigator Award, pp. 6–7) make it possible for the readers to realize what hard work, flow of creativity and flight of thought are behind their success. Glenn Millhauser (Silver Medal: Biology/Chemistry) will tell his story in the forthcoming issue *EPR newsletter* 22/4.

It is my pleasure to introduce to you our new sponsors, Adani Systems Inc., a major sponsor, and Cryogenic Ltd, a contributor. Support of our sponsors is important for the society and we look forward to the long-term collaboration with them for our mutual benefit. And if you know any other company that may be interested in collaboration with the IES, please feel free to inform CEOs about us.

Our congratulations to Richard Fessenden (p. 8) and Ohara Augusto (p. 9) and thanks for their interviews, which are of equal interest to

different generations of the EPR researchers. Also congratulations to Brian Bennett for his article that provides some guidance to users regarding sample preparation (pp. 10–12).

End of the year is a good reason to look back and to thank everybody who helped us to solve problems, shared with us our troubles and joys, laughed with us on the same jokes and understood us when we needed it. As for me, first of all I heartily thank everybody who made our newsletter possible this year and hope for the continuation of their support.

Happy New Year to all of you and your dear ones! On behalf of my colleagues from the Editorial Board of the *EPR newsletter*, Candice Klug, Hitoshi Ohta, Thomas Prisner and Sergei Akhmin, I wish you, our dear readers, the best of everything. Enjoy every moment of our life and enjoy every moment of your research!

Laila Mosina

ANNUAL GENERAL MEETING 2012

Held at the 2012 RMCAC meeting, Copper Mountain, Colorado USA on 17th July, 2012.

The meeting was opened by Sushil Misra, Secretary, IES at 5:10 pm.

The agenda of the meeting and minutes of the AGM 2011 were distributed to those present, along with the attendance sheet and membership forms. (Everyone was invited to attend the meeting even if he/she was not a member of IES).

1. Attendance and Apologies

Attendance: Alex Angerhofer, O.W.B. Benningshof, Lawrence Berliner, Aharon Blank, Christoph Boehme, Asli Cangönül, Hanjiao Chen, Alex Cruce, Tomasz Czechowski, Boris Dzikovski, Gareth Eaton, Sandra Eaton, Boris Epel, Marco Flores, Howard Halpern, Donald Hirsh, Müge Kasanmascheff, Lowell Kispert, Teruaki Koto, Periannan Kuppusamy, Adam Magyar, Dane McCamey, John McCracken, Frazer McMillan, Sushil Misra, Gavin Morley, Reef Morse, Mark Sherwin, Alex Smirnov, Tatyana Smirnova, Likai Song, Stefan Stoll, Witold Subczynski, Veronika Szalai, Susumu Takahashi, Wolfgang Trommer, Maurice van Gastel, Johan van Tol, Maxim A. Voinov.

Apologies: The President Seigo Yamauchi, Vice Presidents Klaus Möbius and Hitoshi Ohta send their apologies for not being able to attend.

2. Adoption of Agenda and 2011 Minutes

The minutes of the General Meeting held on 24 August 2011 were presented. It was moved by Lawrence Berliner, seconded by Wolfgang Trommer that they be accepted as a true record of the previous meeting. The motion was approved unanimously.

3. President's Report (read by Sushil Misra)

Dear Colleagues,

On behalf of the IES Executive Committee, I wish to welcome all participants to the 23rd General Meeting of the IES and the 54th Rocky Mountain Conference on Analytical Chemistry.

I would like to express my gratitude to the conference organizers of this meeting, especially to Rob Schurko, chair of the Conference and the Organizing Committee Members: Christoph Boehme and Gail Fanucci for allowing our General Meeting to take place during this Conference.

A major function of the IES is to honor distinguished contributors to EPR/ESR.

The awards were initiated in 1992 with the Gold Medal and extended in various specialized areas of EPR.

This year Silver Medals in Chemistry and Biology/Medicine, and the Young Investigator Award were given.

Silver Medal: Chemistry 2012

Dr. Alexander D. Milov, Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk, Russia

in recognition of his outstanding contributions to four decades of outstanding researches in EPR spectroscopy, especially PELDOR proposed in 1982.

Silver Medal: Biology/Medicine 2012

Dr. Glenn Millhauser, Department of Chemistry, University of California, Santa Cruz, CA 95064, USA in recognition of his outstanding contributions to EPR spectroscopy

Young Investigator Award 2012

Dr. Laxman Mainali (John Weil Young Investigator award), Department of Biophysics, Medical College of Wisconsin, USA

in recognition of his outstanding contributions to EPR spectroscopy

I want to thank all members of the Silver Medal and Young Investigator Award Committees for their excellent contribution.

4. Secretary Report

• IES Awards 2013

Nominations are invited for the following awards:

- Silver Medal for Physics/Materials
- Young Investigator Award (Regular)*
- Fellows of the Society

Please visit <http://ieprs.org> for full details on constitution and by-laws relating to awards.

Please send nominations to the IES President.
Closing date: 15th November 2012

• IES Activities

The Secretary is responsible for day-to-day operations of the Society, and ensures efficient functioning of the Society, e.g.

- Sending out invoices to the sponsors;

* The awards alternate between regular and John Weil awards.

– Informing members of the various items of interest to them, e.g. announcements of conferences, workshops, publication of new issue of *EPR newsletter*;

- Organization of awards given by the IES: medals, certificates and citations;
- Overlooking financial status and membership of the Society;
- Website (revamping);
- Answering any enquiries;
- Election Notices;
- Organizing AGM;
- Liaisons with the President, Treasurer, Editor of the *EPR newsletter*, and the members of the IES Executive.

• Proposed amendments to the constitution:

- (a) Raising the various membership fees:
Full member: increase to \$40 from \$30
Emeritus/retired: increase to \$15 from \$10
Post-doctoral (3 years maximum): increase to \$20 from \$10
Student: increase to \$10 from \$5
Rationale: These rates have not changed since at least 1990. Things cost a lot more now, and the IES could do with some extra money.

Discussion and voting

This item was tabled when challenged by Lawrence Berliner that increases being more than 20% required a different procedure than simply voting at the AGM as specified in the Constitution.

(b) Modify terms for Fellowship:

A fellowship shall be awarded after the normal end of a member's career, or above the age 70, whichever comes earlier. The fellows will not be eligible for nomination to silver or gold medals.

Rationale: There are some people who continue to work actively beyond the normal retirement age, but are otherwise eligible to become fellows.

Discussion and voting

An amendment to this motion was presented by Wolfgang Trommer, seconded by Alex Smirnov: "Change last year's amendment and reinstate the original version in the Constitution" – carried unanimously.

The original motion is then defeated.

I thank Jack Freed, Past President and Tatyana Smirnova (Treasurer) for their helpful collaboration on IES matters during the previous term.

- IES Web Site (www.ieprs.org): It has been recently revamped. Some representative pages follow after Treasurer's Report.



Sushil Misra (left) and Glenn Millhauser (right)



Sushil Misra (left) and Laxman Mainali (right)

5. Treasurer's Report

2011 Financial Report (\$) (self-audited)

Balance January 1, 2011	11,492.00
Deposits:	
Membership	4,845.56
Sponsors	7,175.00
Internal transfer	100.00
Total Income	12,120.56
Expenses:	
Bank & credit card fees	1,085.68
Web design / maintenance & fees	554.65
Newsletter printing	8,332.00
Newsletter Editorial	3,242.00
Awards + meetings	1,330.67
State of Illinois	24.08
Total Expences	14,569.08
Balance December 31, 2011	9,043.48

2012 (January-June) Financial Report (\$)

Balance January 1, 2012	9,043.48
Income:	
Membership	1,791.57
Sponsors	5,076.00
Total Income	6,867.57
Expenses:	
Bank & credit card fees	257.26
Newsletter	5,595.00
State of Illinois	13.00
Web support	444.93
Total Expences	6,310.19
Balance June 30, 2012	9,600.86

Comments from the Treasurer:
We were not able to balance the budget in 2011, erasing savings from 2010.

In 2012 we have gained sponsorship of KEYCOM Corporation (Japan).

We more than ever need support of the members and our sponsors.

Breakdown of memberships:
Complementary 43
Membership: paid for 2011 or 2010
Full members 195
Emeritus 21
Students 31
Postdoctoral members 27
Members represent 30 countries
Japan 19 Germany 21 Russia 28 USA 115
Some illustrative pages from the website www.ieprs.org were shown.

6. Newsletter Editor's Report (read by Sushil Misra)

Since the previous Annual Meeting of the IES in 2011 in Frankfurt-am-Main (Germany) we published four single issues, 21/2, 21/3, 21/4 and 22/1. We hope all of you had a look at these issues on the newsletter website and got copies of 21/2, 21/3 and 21/4 as well. Photos of the front pages of the above-mentioned newsletters were displayed. A tentative contents of the issue 22/2 was presented.

On behalf of the Editorial Board, I thank most heartily all contributors to the *EPR newsletter* with special thanks going to the CEOs of the IES and editors of the columns in the *EPR newsletter*: John Pilbrow, Candice Klug, Thomas Prisner, Stefan Stoll, Keith Earle and David Budil, and also to Yevhen Polyhach, our web-master, and Sergei Akhmin, our Technical Editor.

I gratefully acknowledge collaboration with Associate Editors Candice Klug, Hitoshi Ohta and Thomas Prisner.

7. Thanks

The IES thanks the following Corporate Sponsors for their contributions in 2011–2012:

- Bruker BioSpin
- JEOL Japan & USA
- Research Specialties
- Scientific Software Services
- Wilmad-LabGlass
- L&M EPR Supplies
- Molecular Specialties
- GMW
- Resonance Instruments
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All paid up members
Newsletter Editor: Laila Mosina
Technical Editor: Sergei Akhmin
Associate Editors: Thomas Prisner, Candice Klug and Hitoshi Ohta

A report of this meeting will appear in a future IES Newsletter.

The meeting adjourned at 6:10 pm.



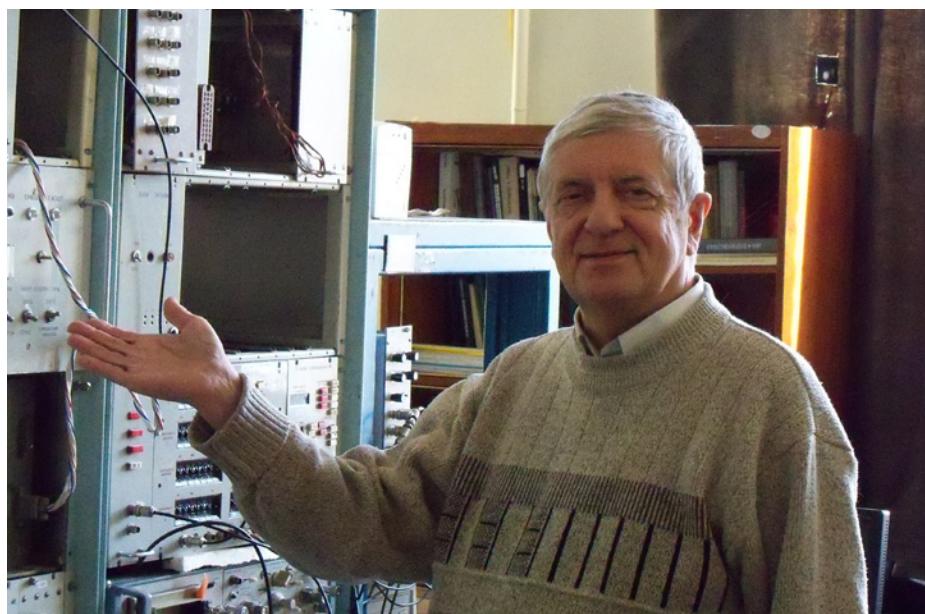
The IES Silver Medal 2012 / Chemistry

Alexander D. Milov:
PELDOR: from exotic to the
ordinarily

One of the key problems in structural chemistry is to measure interatomic distances or distances between atomic groups in molecules as well as intermolecular distances in various molecular systems. X-ray crystallography is the main classical method for these investigations. However, growth of crystals and structure determination from X-ray analysis data is still a complicated task. In addition, single crystals of biomacromolecules and their complexes may not either exhibit catalytic properties or be biologically active. Therefore, NMR and EPR spectroscopies or other spectroscopic methods of investigation of disordered samples are more useful for obtaining structural information in the liquid phase or in frozen solutions, *i.e.*, under the conditions that are more appropriate for simulation of biological systems rather than single crystals. Valuable information on the structure of nucleic acids, proteins and protein complexes can be obtained using recently developed computational methods of classical molecular dynamics (MD).

Continuous-wave (CW) EPR spectroscopy is widely used in studies of the structure and dynamics of paramagnetic species, especially, spin labels in various biomacromolecules. However, there are significant limitations on the studies of weak magnetic dipolar interactions. Nevertheless, research on just these interactions can give structural information on the systems containing nitroxyl spin labels arranged at distances of the order of 1.5 nm and longer. In this case the contribution of dipole broadening to the CW EPR line width in randomly oriented samples is much smaller than the contributions from other inhomogeneous line broadenings, *e.g.*, anisotropic hyperfine broadening or the *g*-factor anisotropy. Let us notice that electron spin echo (ESE) in solids eliminate the inhomogeneous line broadenings but the processes of phase relaxation mask the contribution of the weak dipole-dipole interaction in ESE decay.

An important step forward that offers new prospects for structural studies by EPR spectroscopy was made using the PELDOR technique. The PELDOR method is the modified



Alexander D. Milov and the first PELDOR spectrometer.

variant of ESE. In the PELDOR experiments, the spin system is subjected to the action of pulses at two different frequencies, detecting frequency and pumping frequency. The pulses at the detection frequency excite a portion of spins in the EPR spectrum (detecting spins) to generate a spin echo. Time position of detecting pulses is not changed during experiment. The pumping pulse excites another group of spins (pumping spins) and thus changes the sign of the dipole-dipole interaction between detecting and pumping spins. As a result, the amplitude of the spin echo (PELDOR signal), which depends both on the value of the dipole-dipole interaction between detecting and pumping spins and on the position and intensity of the pumping pulse, provides information on the parameters of the dipolar interaction between labels. As the position of detecting pulses does not change in PELDOR experiment the relaxation processes are excluded from PELDOR data.

The first work [1] containing the PELDOR idea was made in 1981 by a group of researchers from the Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences (Novosibirsk, Russian Federation). This work was made using an X-band PELDOR spectrometer containing a homebuilt ESE spectrometer and an additional source of pumping frequency. The authors used the simple 3-pulse PELDOR sequence consisting of two detecting pulses to form spin echo and one pumping pulse. In this work the authors measured the distances between hydrogen atom and parent ion stabilized in frozen glassy matrix after photo ion-

ization of aromatic compounds. Theoretical expressions for the case of a spin pair were obtained. In subsequent works of this group possibilities of PELDOR for studying of nitroxyl biradicals and radical clusters in solids have been shown. For the first time dipole-dipole modulation for nitroxyl biradical was observed and explained. It was shown that in the case of a radical cluster one can obtain both the spectrum of distances between the radicals in the cluster and the number of radicals per cluster.

The next step of PELDOR development was the invention of the 4-pulse PELDOR sequence consisting of three detecting pulses to form the spin echo and one pumping pulse by researchers from Max Planck Institute für Polymerforschung, Mainz, Germany in 2000 [2]. The 4-pulse PELDOR technique is characterized by zero dead time and unlike the 3-pulse sequence does not require any calibration in the course of the experiment.

In 1993 the effect of orientation selection in PELDOR was detected. In the case of nitroxyl labels, the EPR spectrum width substantially exceeds that of the mw pulses used [3]. Therefore the pulses act only on some part of the EPR spectrum from spin labels with a certain orientation relative to the magnetic field. This now gives not only information on the distance between the labels but on their mutual orientation.

In 2005 the Tikhonov regularization method was applied to obtain the distance spectra from PELDOR data assuming the absence of correlation in the orientation of nitroxyl fragments of spin labels [4].

Awards

Development and publication of the program 'DEER Analysis 2006' and subsequent versions of this program facilitate the extraction of distance spectra from PELDOR data [5].

Undoubtedly, the PELDOR technique is the simplest method of applied research and analysis of weak dipolar interactions. Researchers face difficulties only in practical implementation of the design of spectrometers with two sources of microwave radiation. Recently, these problems have been successfully solved in commercially available Bruker E580 and E680 EPR spectrometers which become more and more popular instruments.

Combined with site-directed spin labeling technique, PELDOR is used to solve differ-

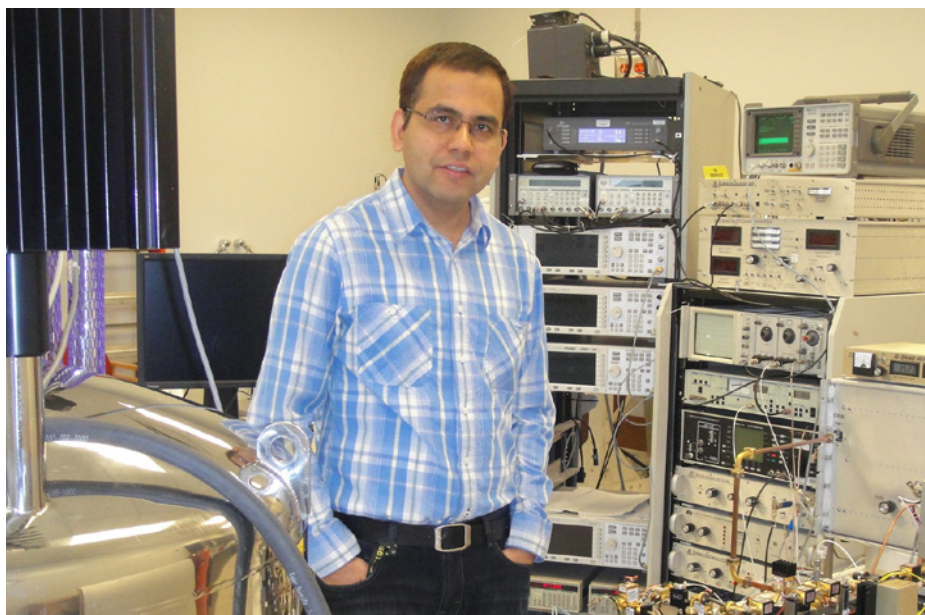
ent structural problems. The main areas of PELDOR application in solids are:

- obtaining of spectra of distances between spin labels in spin labeled biomacromolecules or polymers for distances between spin labels in the 1.5–10 nm range.
- detecting of mutual orientation of spin labels in macromolecules using the phenomenon of orientation selection in PELDOR data.
- detecting of aggregation of spin labeled macromolecules. Estimation of the number of spin labeled molecules per aggregate. Obtaining of spectra of distances between the spin labels in aggregates.
- analysis of some characteristics of disordered solids using the PELDOR data on spatial spin distribution.

Owing to the efforts of many researchers, the PELDOR method became a routine method of pulse EPR spectroscopy. Now this method is successfully employed as a "molecular ruler" used to study nanometer spin-spin distances in structural chemistry and biology.

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John Weil Young Investigator Award 2012 to Laxman Mainali

I am very honored to receive the 2012 John Weil Young Investigator Award from the International EPR (ESR) Society in recognition of my contributions to EPR spectroscopy. I would like to thank the award committee for selecting me for the award. I started my scientific career in EPR in spring 2006 when I joined Prof. Keith A. Earle's research group at the University at Albany, State University of New York, to pursue my doctorate in biomedical physics. During my studies, I was involved in four major projects: (1) development and construction of a high-field EPR spectrometer at 160 GHz; (2) development of a novel

simultaneous multifrequency fitting program based on the Bayesian inference approach for EPR parameter estimation; (3) density functional theory (DFT) calculations of EPR parameters on transition metal complexes; and (4) site-directed spin-labeling EPR studies on fibril protein construct. I am very grateful to my PhD advisor, Prof. Earle, for his intensive training in EPR in a short period of time.

Immediately after defending my thesis, I attended the ACERT workshop in 2009, Multifrequency EPR/ESR, organized by Prof. Jack H. Freed at Cornell University. During the workshop, I got a chance to attend a talk

from Prof. Witold K. Subczynski that focused on the application of EPR spin-labeling methods to study the structure and properties of the eye-lens membrane. After Prof. Subczynski's presentation, we spoke about his current research. He mentioned to me that he had just received a grant from NIH for five years of funding. He also told me that the broad objective of the proposal was to understand the function of cholesterol in the human eye lens, focusing on the cholesterol bilayer domain formed in fiber-cell plasma membranes. I was excited by the project and accepted his offer to join his research group as a postdoctoral fellow in the Department of Biophysics at the Medical College of Wisconsin. I moved to Milwaukee, Wisconsin, just after Christmas in 2009. In the first few months of my postdoctoral period, I performed experiments on model and eye lens membranes using a conventional and saturation recovery X-band EPR spectrometer. In the middle of my first year, I began conducting experiments using a W-band EPR spectrometer, which was newly constructed in the National Biomedical EPR Center, under the supervision of Prof. James S. Hyde. This spectrometer has the capability to perform saturation-recovery measurements. During my first year of postdoctoral work, I accumulated experimental results and began publishing these results the following year. During my postdoctoral research, we published nine papers. Three were published in the *Journal of Magnetic Resonance*; others were published in *Experimental Eye Research*, *Biophysical Journal*, *Biochimica et Biophysica Acta*, *European Biophysics Journal*, *Chemistry and Physics of Lipids*, and *Journal of Membrane Biology*.

In one project in which I was involved, we demonstrated the ability of conventional and saturation-recovery EPR at W-band to obtain detailed profiles of the properties of lens lipid membranes derived from a single human donor. All previous investigations were carried out at X-band using conventional and saturation-recovery EPR spectrometers with a loop-gap resonator with a sample volume of 3 μL . To complete all measurements and obtain detailed profiles, lipids were extracted from 50 to 100 eye lenses. A large amount of similar animal lenses (age is the major criterion) are not difficult to obtain. However, human lenses are more difficult to acquire in large numbers. A more serious problem is that human lenses can differ because of both age and donors' various health histories. The best solution to this problem was to perform all measurements on samples prepared from one to two eyes from a single donor. In this project, we presented results that demonstrate the feasibility of such measurements. Profiles of lens lipid-membrane properties that were obtained using spin-label EPR at X-band could also be obtained at W-band with a loop-gap resonator with a sample volume of 30 nL. Thus, the total amount of sample can be 100 times smaller at W-band than at X-band. Results obtained at W- and X-band, including profiles of membrane fluidity, the oxygen transport parameter, and data on the discrimination of coexisting membrane domains, were published in the *Journal of Magnetic Resonance* (2011, 212:86-94).

In another project, we have shown a novel method to study membrane fluidity, as deduced from saturation-recovery EPR measurements of spin-lattice relaxation times of lipid spin

labels. There were no easily obtainable EPR spectral parameters for lipid spin labels that describe profiles of membrane fluidity. The order parameter, which is most often used as a measure of membrane fluidity, describes the amplitude of wobbling motion of alkyl chains relative to the membrane normal and does not explicitly contain time or velocity. Thus, this parameter can be considered as nondynamic. The spin-lattice relaxation rate (T_1^{-1}), obtained from saturation-recovery EPR measurements of lipid spin labels in deoxygenated samples, depends primarily on the rotational correlation time of the nitroxide moiety within the lipid bilayer. Thus, T_1^{-1} can be used as a convenient quantitative measure of membrane fluidity that reflects local membrane dynamics. Profiles of T_1^{-1} obtained for phospholipid spin labels in model membranes with and without cholesterol were presented in parallel with profiles of the rotational diffusion coefficient, R_{\perp} , obtained from simulation of EPR spectra using Prof. Freed's model. These profiles were compared with profiles of the order parameter obtained directly from EPR spectra and with profiles of the order parameter obtained from simulation of EPR spectra. Profiles of T_1^{-1} and R_{\perp} that reveal changes in membrane fluidity that depend on the motional properties of the lipid alkyl chain indicated that cholesterol has a rigidifying effect only to the depth occupied by the rigid steroid ring structure and a fluidizing effect at deeper locations. These effects cannot be differentiated by profiles of the order parameter. This study was performed at X-band (9.5 GHz) and results are published in the *Journal of Magnetic Resonance* (2011, 212:418-425). As confirmed in the recent publication in the *Journal of*

Magnetic Resonance (2013, 226:35-44), these profiles can also be obtained at W-band (94 GHz) for samples of limited volume.

There are many people who helped me complete these projects at the Medical College of Wisconsin. Prof. Subczynski is very friendly and has been kind to work with on all of these projects. One of the best things about him is that he is always ready to discuss the projects at any time. While performing high-field measurements at the National Biomedical EPR Center, I have had the chance to interact with Prof. James S. Hyde. His valuable input was very crucial in completing those projects. I am grateful to Prof. William J. O'Brien in the Department of Ophthalmology and Microbiology/Molecular Genetics for his help in eye lens-membrane isolation as well as his provision of his wet lab facilities. I would like to thank Dr. Marija Raguz for her help and support during the beginning of my postdoctoral work. I would also like to thank the engineering staff at MCW, mainly Theodore G. Camenisch, Joseph J. Ratke, Jason W. Sidabras, and scientific administrator, Christopher C. Felix, for their help and support.

In April 2012, I was promoted to the rank of Research Scientist in the Department of Biophysics at MCW. My current research focuses on understanding the function of cholesterol and the cholesterol bilayer domain in the fiber-cell plasma membrane of the human eye lens across different age groups, as well as in disease. I am very excited to use the D-band EPR spectrometer, which is under construction at the National Biomedical EPR Center, to investigate these problems and hope to contribute more to the EPR field.

Laxman Mainali, PhD



Are you interested to become a member of the International EPR (ESR) Society? Please find the registration/information form for new/continuing members of the IES and non-credit-card payment instructions for individual members on this Web site: www.epr-newsletter.ethz.ch/contact.html

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Specification:

Sensitivity: $S/N \geq 10$ by $1\mu\text{M/l}$ TEMPOL at 4mW, and more at 80mW
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Magnetic field: 340mT
Sweep magnetic field: 15mT
Weight: 22kg

Application:

- Health: Exposed dosage, Superoxide, Hydroxy
- Materials: Oxidation degradation, Defect assessment dangling bonds

Richard Fessenden:

An Interview on the Occasion of His Zavoisky Award 2012

EPR newsletter: *Dear Professor Fessenden, on behalf of the readers of the EPR newsletter we congratulate you on your Zavoisky Award 2012. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

My early memories regarding a profession were always that I would take up chemistry. My father was a professor of chemistry at the University of Massachusetts and my mother a laboratory instructor also in chemistry. I was exposed to some electrochemical experiments involving plating of copper and generating hydrogen from water when I was about nine or ten. I also saw some demonstrations given by my father to the freshman chemistry class. On the other hand, several friends and I also spent much time on “experiments and projects” of all sorts, particularly involving electronics. From about age twelve we were given old radios and other electronics to try to repair. We had a shop in a friend’s attic with an extensive collection of components. Later on we built Tesla coils, audio amplifiers, and even an oscilloscope and FM tuner. At a time when tape recorders were new and expensive, we actually built both the electronics (tube type) and mechanics for one. It worked reasonably well. These experiences helped me greatly in building apparatus needed in my research.

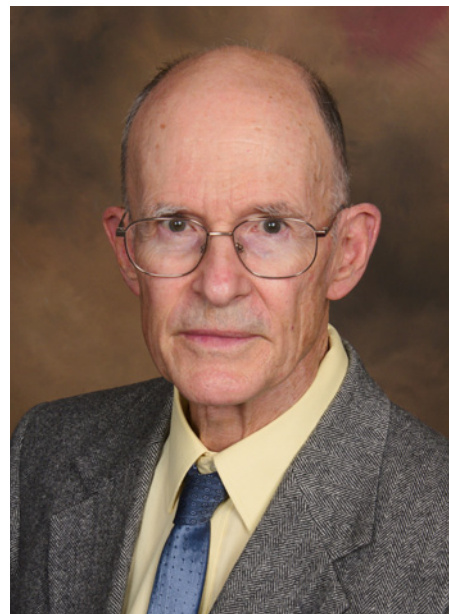
Who introduced you into magnetic resonance?

After obtaining my BS degree in chemistry at University of Massachusetts, I started my doctoral studies in NMR with John S. Waugh at MIT in January 1955. I had visited MIT and was directed to him because he was seeking another student. I had not, of course, heard of this topic. At that time, his two students were working on NMR of solids. The spectrometers were lab built and that aspect attracted me as well. I did not interview any other professors and agreed to join his group. I eventually used a 40 MHz NMR for my research. This was early in his career so I got my PhD some years before his most famous and exciting contributions to NMR. To vary my experience, I then arranged to do a postdoctoral year with Harden McConnell at Caltech and there learned ESR. It was great fortune that I was able to study

with such gifted persons. My association with radiation chemistry came about very much by chance. My girl friend (now wife) decided to further her studies in biology with a summer position at Brookhaven National Laboratory. I therefore interrupted my research to go also to Brookhaven for the summer. I worked with Robert H. Schuler in radiation chemistry but claimed I did not really understand the analysis of my results. I said to myself that I did not care to be involved with radiation chemistry again. Nevertheless, when I completed my year with McConnell I was invited to join Schuler at the Radiation Laboratory of Mellon Institute in Pittsburgh Pennsylvania. ESR had much to contribute in this field as radiation was a good way to produce radicals. In retrospect, this was very much the right choice for me.

What part of your research is most dear to your heart and why?

Although I very proud of the ESR study of irradiated liquid hydrocarbons, there are some smaller projects that I carried out by myself alone that pleased me greatly. One was the analysis of second-order splittings first seen in the spectrum of ethyl radical. Another was the explanation of a spectrum seen in the radiolysis of CF_4 and also the photolysis of CF_3OOCF_3 in NF_3 at -196°C . The similarity of the g -factor to that of FOO^\bullet (at 2.0037, much lower than for typical peroxy radicals) made me suspicious that this could be from the trioxide, $\text{CF}_3\text{OOO}^\bullet$. The parallel is that both F and CF_3O are highly electronegative. The first two oxygens were easy to show just by exposing the sample to oxygen enriched in ^{17}O and ^{18}O . Two new corresponding spectra were observed. To show the existence of a third oxygen it was necessary to synthesize CF_3OOCF_3 containing the enriched oxygen. This was done by photolysis of $\text{CF}_3\text{C}(\text{O})\text{CF}_3$ in the presence of the oxygen. No isolation was necessary. I am also very proud of my idea to use time-resolved measurement of changes in dielectric loss to determine dipole moments of excited states. I take credit for this new idea but development of the necessary issues in analysis of the data involved help from several very talented co-workers.



What is the driving force for you in your research?

Research is puzzle solving. As in looking for answers where there are only clues. That is what drives me. Because of my experience with electronics, I also enjoy designing apparatus.

What would you have done differently given the chance?

I wish I had not left as many studies unfinished. It is easy to get distracted by the current new results and I have done so a number of times. For example, the results from the radiolysis of hydrocarbons could have been even more overwhelming. For example, we had spectra of most if not all of the fluorinated ethyl radicals but they were never described by us. Also, the various inorganic radicals produced in an SF_6 matrix got only a brief communication. One spectrum we found that took quite some time to explain was eventually assigned (by others) to $^*\text{SF}_5$. The curious thing was a splitting by one fluorine that was not resolved. We had spectra from both the selenium and tellurium analogs that also showed splittings by only four fluorines! If that one splitting is small by chance cancellation of electronic effects, why does it persist in the other two radicals? This was never published.

What is your message to the younger generation of the magnetic resonance researchers?

If you like solving puzzles you should have a good chance at research. In addition, it is always important to pay attention to what might be considered side issues, that is, clues to something unexpected. Those can turn out to be important new research directions. An example is one missed opportunity of mine. It concerned small peaks in the NMR of com-

pounds with strong, single-line spectra such as acetone. These were pairs of lines separated from the main peak by a similar distance as the “spinner sidebands”, maybe ~50 Hz. These

were lines of the ^{13}C containing molecules and their study represented a considerable project for someone else to exploit. This is all the more embarrassing to me in that I had

occasionally looked at the ^{13}C NMR of some compounds at natural abundance. Of course it is important to find an area of research that can be financially supported. ●

Ohara Augusto: An Interview on the Occasion of Her Piette Lecture 2012

EPR newsletter: *Dear Professor Augusto, on behalf of the readers of the EPR newsletter we congratulate you on your Piette Lecture 2012. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

Growing up in low middle-class family, only two generations removed from illiterate immigrants, I did not consider a career in science up to the end of my undergraduate studies. During my secondary education I was motivated towards chemistry by a science teacher and finished secondary education in a technical school as a lab technician. Next, I decided to go for a BS in Chemistry at the Universidade de São Paulo but did not pay much attention to the science going on there for several reasons, including the political situation in Brazil at that time (the country was under a military dictatorship). In addition, I had to get a job and used my free time to teach chemistry to secondary students. By the end of my BS, I became friends with Francisco G Nóbrega, who was returning from his doctoral studies in the United States. I knew nothing about biochemistry, but listening to him I became fascinated by the connections between biology and chemistry, and how these basic chemical processes related to function and dysfunction of living organisms. He also lent me a copy of the recently published book by Albert Lehninger, *Principles of Biochemistry*. These facts were crucial to my decision to continue with science, and I pursued graduate studies in Biochemistry at the Universidade de São Paulo.

Who introduced you into magnetic resonance?

My PhD supervisor was an important Brazilian scientist, Giuseppe Cilento, and my PhD project was related to redox processes in biology. As soon as I read the classical work by Lawrence Piette on spin-trapping detection of hydroxyl radicals, I decided to learn EPR so as to be able to detect radicals. After I finished

my PhD, I moved to Lester Packer's laboratory at UC Berkeley to do my post-doctoral work where I gained further experience EPR working mainly with Alex Quintanilha.

What part of your research is most dear to your heart and why?

I am happy with most of the things I have done but, due to their general implications for biochemical processes, I judge my main contributions to be: (i) my work with Paul Ortiz de Montellano in finding EPR spin-trapping evidence for one-electron oxidations catalyzed by cytochrome P_{450} ; and (ii) work with Rafael Radi demonstrating by direct fast-flow EPR that the reaction of peroxyxynitrite with carbon dioxide produces the carbonate radical.

What is the driving motivation for you in your research?

I think that above all, my curiosity. Despite working in Brazil, sometimes under difficult conditions, I really attempted to contribute to the understanding of the mechanisms by which radicals and oxidants mediate biological processes ranging from physiology to pathophysiology. Redox processes are basic to life and their understanding has many implications for human knowledge and human health.

It is an interesting coincidence that exactly ten years ago you were awarded the IES Silver Medal Biology/Medicine.

What was the impact of this award on your research?

I was delighted to receive this honor. As I always have said, I am not a real magnetic resonance researcher. I was lucky to employ EPR to solve some timely biological questions. The



award brought me lots of satisfaction and recognition but it did not affect the course of my research.

What is your message to the younger generation of the magnetic resonance researchers?

They should be proud of their dedication to an extremely relevant field of science that will continue to contribute greatly to the understanding of fundamental processes and to provide important advancements to biology and medicine. On occasions, too much emphasis may be placed on translational medicine and other practical applications making it more difficult to get financial support. They should persevere, though. Progress in translational medicine and in other human endeavors will be critically dependent on the understanding of fundamental processes. ●

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Sample Preparation for Service at the National Biomedical EPR Center



Brian Bennett

National Biomedical EPR Center, Medical College of Wisconsin, Milwaukee, WI, USA

The National Biomedical EPR Center at the Medical College of Wisconsin is an NIH-funded research resource with a three decade history of technology and methodology development, technological and scientific collaboration, home-grown scientific and biomedical research, and training and service to the EPR community [1]. Service is an important mission of the Center, and service activities include rapid-freeze-quench sample preparation, multiple EPR spectroscopies, assistance with interpretation of spectra and computer simulations, assistance with resonator and spectrometer design and maintenance, and provision of novel EPR-specific chemicals such as spin traps. Potential users are encouraged to explore our service web site [2].

Resources for EPR spectroscopy are available in a number of ways, depending on the number and types of samples and the level of experience of the user. Experienced users may visit the Center and use spectrometers with little assistance from the Center staff. Inexperienced users are encouraged to apply for a training grant and visit the Center, typically for 3–5 days, to either learn how to use a technique or a spectrometer, or else to at least get an appreciation of how the EPR data are collected, processed and interpreted in the context of their research project. Users with samples that are straightforward to prepare and interrogate may simply send samples to

the Center to be analyzed by Center personnel. Whichever route is taken, it should be appreciated that the Center does not have all of the sample preparation facilities of a comprehensively equipped chemistry or biochemistry department at a research university, and users should aim to make samples as “EPR-ready” as possible at their home institution. This article is intended to provide some guidance to users with regard to sample preparation. Sample requirements vary depending on the samples, the experiment and the spectrometer characteristics, and criteria for some of the more common scenarios are described.

Frozen solutions. For frozen solutions, we offer X-band cwEPR (parallel and perpendicular B_1), cwENDOR and pulsed EPR methods including ESEEM, HYSCORE, ENDOR, ELDOR, and DEER, each over a temperature range of 4–120 K. Multifrequency options include L- and S-band cwEPR and L-band NARS [4] at $T > 77$ K, and W-band cwEPR, Q-band cwEPR and Q-band ENDOR at $T = 4$ –120 K. Q-band pulsed EPR is coming soon! Table 1 summarizes the EPR tube and filling requirements for each of the currently available systems; tubes are generally available as stock from Wilmad [5] or special order from VitroCom [6]. For very low background signals synthetic quartz tubes are recommended but clear fused quartz tubes suffice for most applications.

For X-band cwEPR/ENDOR at low temperatures (<70 K) the sample height is important. Samples much less than 3.5 cm in height may have the surface of the sample in an active part of the resonator and exhibit signals due to condensed molecular oxygen; this can often be dealt with by annealing, but is time (and helium) consuming. Samples >4 cm in height will not be completely surrounded by the cooling helium stream and will experience a temperature gradient along the sample. Samples *much* greater than 4 cm in height will partially thaw in the cryostat and are prone to breaking, presenting a hazard to the operator and potentially damaging the instrument. Samples that are frozen generally do not need to be sealed, and we recommend cutting the sample tube to 16.0 ± 0.2 cm in length (Figure 1A), to allow for annealing in the cryostat to remove O_2 signals if neces-

sary. Shorter tubes can be accommodated if the experiment requires it (e.g. rapid-freeze-quench). For tubes that must be sealed under vacuum or inert atmosphere, tubes should be sealed as close to the original top of the tube (usually 25 cm) as possible, with at least 20 cm of undistorted tube beneath the seal. For L- & S-band EPR, the same applies as for X-band, except that we do not recommend cutting the 25 cm tubes.

For X-band pulsed EPR, tubes must fit into a holder and are ideally ~10 cm in length (Figure 1B). The sample height should be greater than the resonator active length. As the entire tube is cooled, there is no rigid upper limit on sample height. Sealed sample tubes must be sealed very carefully because the seal itself should not protrude outside the walls of the cylinder projected by the EPR tube, otherwise the sample may not fit into the holding rod. The “4 mm” pulsed resonator is designed for 3.8 mm tubes, but samples in 4 mm tubes can be loaded manually through the bottom of the resonator and held in place with a PTFE tape harness (Figure 1C). The tubes will be cut to ~7 cm in length and users should be generous with the sample height because the sample moves during the coupling procedure and precise sample location is not assured (Table 1).

Two common questions relate to **sample concentration** and the use of **cryoprotectants**. For X-band DEER of spin labels, a concentration of 0.2 mM is generally recommended. Though spectra have been obtained on as low as 70 μ M, an eight-fold longer acquisition time is needed to collect data of the same nominal quality as from 200 μ M and eventually environmental factors negate the advantages of very long scans (numbers of days). For transition ions, the necessary concentrations are highly dependent on the experiment and the metal ion. For cwEPR, a very rough guide would be >100 μ M for $S = 1/2$ ions, octahedral Mn(II), rhombic $S = 5/2$ Fe(III) and high-spin heme; >200 μ M for $S = 3/2$ Cr(III); and >500 μ M for $S = 3/2$ Co(II) or integer-spin systems. ESEEM and ELDOR-NMR have slightly lower sensitivity whereas ENDOR (cw and pulsed) may have *much* lower sensitivity. Cryoprotectants are commonly used to maintain the structural integrity of biological macromolecules that would otherwise be susceptible to conformational change or damage from ice crystal formation, and to prevent solute concentration at grain boundaries during freezing that can lead to intermolecular spin-spin interactions. Cryoprotectants are deemed necessary for DEER, which is sensitive to long range

Resonator or cryostat	Experiment	Tube dimensions	Sample height (approx. volume)	Suggested supplier (part number)
Oxford Instr. ESR900 cryostat	X-band cwEPR, cwENDOR	~4 mm O.D.	3.5–4.0 cm (250–300 μ l)	Wilmad (707-SQ-250M)
Bruker EN4118X-MD-4W 4 mm dielectric	X-band pulsed (incl. ENDOR)	3.8 mm O.D. <i>or</i> 4.0 mm O.D.	>1.3 cm (100 μ l) <i>or</i> >2.0 cm	Wilmad (706-PQ-9.50) <i>or</i> (706-SQ-250M)
Bruker ER4118X-MS-2 2 mm dielectric	X-band pulsed (not ENDOR)	<2 mm O.D.	>1.3 cm (10 μ l)	VitroCom
MCW EPR Ctr. 4 mm loop-gap	L- & S-band	~4 mm O.D.	>1 cm (100 μ l)	Wilmad (707-SQ-250M)
Bruker ER5106-QTE cavity	Q-band cwEPR/ENDOR (4–70 K & 295 K)	1.6 mm O.D. (Figure 1D)	>1.4 cm (10 μ l)	Bruker, VitroCom <i>or</i> Wilmad (WG-221T-RB)
Varian Q-band cavity	Q-band cw-EPR (>77 K)	2 mm O.D.	>1.3 cm (10 μ l)	VitroCom

interactions, but are not generally necessary otherwise (some line-narrowing sometimes results from a lowering of strains in g and A , and/or in the zero-field splitting).

Rapid freeze quench. Rapid freeze quench (RFQ) sample preparation for EPR (and other techniques) involves the rapid mixing of two or more solutions and freezing the mixture as a spray in a cold, immiscible

solvent contained in a cooled EPR tube assembly. Typically, reactants (*e.g.* enzyme and substrate) are mixed at 2–40 °C and frozen in 2-methylbutane (isopentane) at –110 °C. Reaction times of 10 ms and beyond are accessible with the Center's equipment. EPR, ENDOR, DEER *etc.* reveals changes in metal ion geometry and coordination, or in protein folding or conformation using spin labels. The species of interest will be diluted by a factor

of either 3 or 4 in the final sample (1.5 or 2-fold dilution with *e.g.* substrate, and a further 2-fold “dilution” due to aqueous spheres packing in the isopentane matrix) depending on how the experiment is carried out. Therefore, concentrations of starting material for *e.g.* EPR, ESEEM, ENDOR need to be increased accordingly. For DEER, the final concentration *in the aqueous phase* should not exceed 0.2 mM, so the stock solution should be 0.3 or 0.4 mM. Generally, *cryoprotectants cannot be used with RFQ*; fortunately, the freezing is so rapid that they are not necessary, even for DEER. RFQ can be expensive in material, and users should plan on having at least 0.5 ml of sample for a single RFQ time-point, though some

of this material is recoverable. A 1 ml sample may allow for up to four time-points.

Aqueous samples. Aqueous samples absorb the microwave electric field (E_1) non-resonantly and require that either the sample is precisely positioned in a cavity along an axis of lowest E_1 , or else a resonant structure is used that concentrates E_1 outside the active (high B_1) region of the resonator such as the loop-gap resonator developed at the Center [7]. Both options are available and both are well-suited to the use of very small capillaries (*e.g.* 1 mm O.D.; Figure 1E) with sample volumes as low as 5 μ l. Borosilicate capillaries (micropipettes) are cheap and work well for reasonably concentrated samples, and are available at the Center. For more challenging applications, clear fused quartz capillaries are available from VitroCom. For weak signals, a flat cell can be used in conjunction with a rectangular cavity, though the loop-gap resonator has largely superseded this approach. Capillaries are sealed at one or both ends with sealing compound (*e.g.* Cha-Seal; Figure 1F). For gas exchange experiments, TPX capillaries are available from Bruker [8].

Solid samples. The Center has historically had very few requests for single crystal studies on minerals or other materials science studies and we recommend that any potential users contact us directly. On the other hand, we have had many samples of powders for study. ►

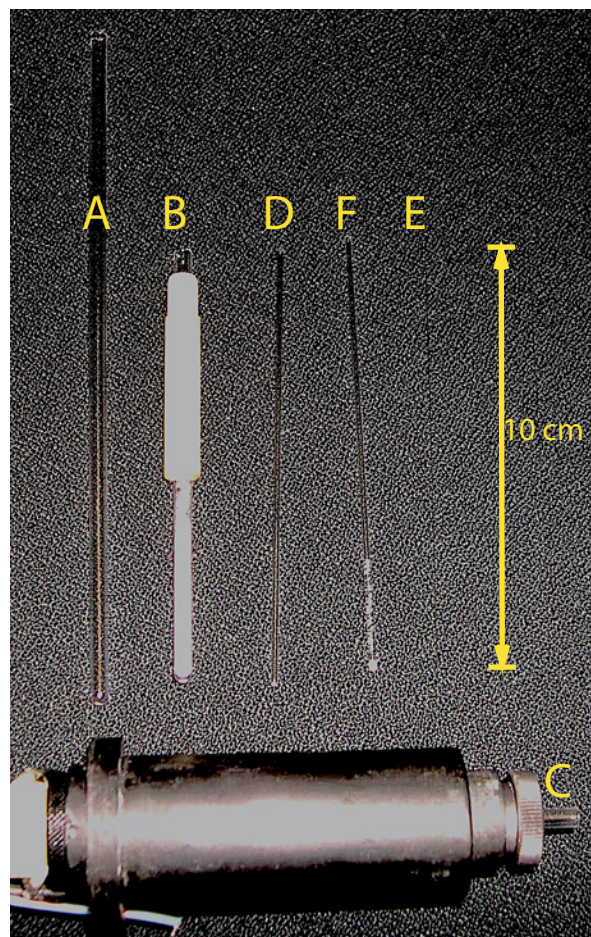


Figure 1. Sample tubes for EPR. (A) 160 × 4 mm O.D. X-band EPR tube for cwEPR/ENDOR. (B) 100 × 3.8 mm O.D. tube for pulsed X-band EPR, mounted in sample holder. (C) 70 × 4 mm O.D. X-band EPR tube bottom-mounted in pulsed EPR resonator. (D) 100 × 1.6 mm O.D. Q-band EPR/ENDOR tube. (E) 10 × 0.32 mm O.D. capillary for aqueous solution EPR at X- or Q-band. (F) 100 × 1.6 mm O.D. capillary for aqueous EPR at X-band, sealed at the bottom with ChaSeal and containing ~2.5 cm of aqueous sample.

Tips & techniques

At room temperature, a powder sample in an EPR tube is straightforward, though we urge the user to be careful to ensure that the outside of the tube is clean. At cryogenic temperatures, heat transfer is very poor from the sample to the cryostat, and if the powder can be suspended in an inert matrix, such as paraffin oil or glycerol, then heat transfer will be much improved and temperatures reliable. Powders of undiluted paramagnetic complexes may absorb very strongly, and it is recommended that the sample be ground very finely with an inert material, e.g. 1% sample in boron nitride. Polycrystalline material will exhibit incompletely averaged powder spec-

tra; again, fine grinding helps alleviate this. Finally, undiluted paramagnetic complexes may exhibit quite strong intermolecular spin-spin interaction and paramagnetic doping, where possible, will remove this problem (e.g. 1:99 Co(II):Zn(II)).


Safety. It is imperative that the Center is made aware of *any* safety issues regarding samples *at the time of the initial application*. Potentially hazardous samples include human material, pathogens, toxins, poisons, oxidants and corrosive compounds, pyrophoric and explosive compounds, and environmental hazards. Sealed samples should be tested thoroughly for leaks

that could admit gas at low temperature that can explosively expand upon warming the tube.

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notices of Meetings



EUROMAR 2013
30th June - 5th July
Hersonissos, Crete, Greece

NCSR
"Demokritos"

Colloque Ampere on Advances in Solid State Broadband Magnetic Resonance

cost European Network on Spin Hyperpolarisation
Physics and Methodology in NMR and MRI 28th & 29th June 2013

EUROMAR is the main annual meeting of the European magnetic resonance community covering all aspects of magnetic resonance including NMR, EPR and MRI.

EUROMAR 2013 will be held in Hersonissos, situated in the beautiful island of Crete, Greece. The aim of the conference is to provide an educational and stimulating forum where participants can exchange ideas on the latest scientific breakthroughs in a unique Mediterranean location.

On behalf of the organizing committee and the EUROMAR board, it is my pleasure to cordially invite you to join us in making EUROMAR 2013 a memorable scientific and personal experience.

Georgios Papavassiliou

Chairman EUROMAR 2013

Key Dates

Conference Registration Opens 01/12/2012
Early Registration Closes 01/04/2013
Deadline for Oral Submission 01/05/2013

55th Annual Rocky Mountain Conference on Magnetic Resonance: 36th EPR Symposium

Denver, Colorado, USA, July 28 – August 1, 2013

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It is our pleasure to invite your participation in this year's Rocky Mountain EPR Symposium, July 28 – August 1, 2013. In addition to several vibrant and exciting sessions, we will be located at the Crowne Plaza Hotel in Denver, Colorado.

Our change from the customary mountain locale to Denver this year is intended to accommodate those that have expressed a desire for a lower elevation urban locale. Please check back here for updates as our program

materializes. We look forward to having you join us in Denver.

Gail Fanucci (Chair) and Mark Sherwin (Co-Chair) 2013 EPR Symposium

Program:

Sunday, July 28 – Bruker EPR Meeting, Monday, July 29 – Oral presentations, Posters & Conference Reception, Tuesday, July 30 – Oral presentations, Posters & EPR Reception, Wednesday, July 31 – Oral presentations & Posters, Thursday, August 1 – Oral presentations & Posters (ends at noon).

Deadline for Poster Submission 31/05/2013 Program Committee

Claude Berthier, Ivano Bertini †, Bernhard Blumich, Geoffrey Bodenhausen, Muriel Delapierre, Janez Dolinsek, Sabine Van Doorslaer, Lucio Frydman, Ioannis Gerathanassis, Malcolm Levitt, Beat Meier, Gil Navon, Georgios Papavassiliou, Thomas Prisner.

Local Organizing Committee

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Contact Us

Conference e-mail: info@euromar2013.org
Conference Chair: Georgios Papavassiliou,
Phone: +30 210 6503307,
Fax: +30 210 6503323,
e-mail: gpapav@ims.demokritos.gr

Piette Lecture: TBA

Topics & Invited Speakers:

Materials: Dane McCamey (University of Sydney) – Chair

Methods: Christoph Boehme (University of Utah) – Chair

EPR for Spin Devices: John Morton (Oxford University) – Chair

Biological Macromolecules: Kurt Warncke (Emory University) – Chair, R. David Britt (University of California Davis), Victoria DeRose (University of Oregon), Brian M. Hoffman (Northwestern University).

Radicals: Frederick Villamena (Ohio State University) – Chair, Valery Khramtsov (Ohio

State University), Ronald Mason (NIEHS), Andrzej Rajca (University of Nebraska).

Frontier in Spin Labeling: Fraser MacMillan (University of East Anglia) – Chair, Daniella Godfarb (Weitzmann Institute), Gunnar Jeschke (ETH Zurich).

In vivo: Howard J. Halpern / Boris Epel (University of Chicago) – Chair.

Scientific Committee:

Gail Fanucci (University of Florida) – Chair, Mark Sherwin (University of California, Santa Barbara) – Co-Chair 2013, Chair 2014; Kurt Warncke (Emory University) – Co-Chair 2014, Chair 2015; Christoph Boehme (University

of Utah), Howard J. Halpern (University of Chicago), Fraser MacMillan (University of East Anglia), Dane McCamey (University of Sydney), John Morton (Oxford University), Frederick Villamena (Ohio State University).

4th International DNP Symposium
Konvention Conference Centre and Hotel
August 28, 2013 – August 31, 2013

www.dnpsymposium.org/index.php/DNP/4thDNP

The 4th International Meeting on Dynamic Nuclear Polarization will be held August 2013,

in Copenhagen, Denmark, following the highly successful meetings in Nottingham (2007), Koenigstein (2009) and Lausanne (2011).

An array of key players of this emerging field will assess the present state of the art while participants will be encouraged to reveal and discuss the current issues and new trends in DNP, including the developments in Overhauser effect, dissolution DNP, gyrotrons, magic angle spinning, low temperature DNP, radical chemistry, and hyperpolarized imaging.

Registration will open January 2013 and closes June 1st, 2013.



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**54th Annual Rocky Mountain Conference on Analytical Chemistry:
35th EPR Symposium**
Copper Mountain, Colorado, USA, July 15–19, 2012

Rocky Mountain EPR Symposium sees highest attendance in eight years.

The 35th International EPR Symposium of the 54th Rocky Mountain Conference on Analytical Chemistry took place in the Colorado Ski Resort Town of Copper Mountain from July 15 to 19, 2012. The Symposium did not only reach new heights in terms of its location (2960–3740 m above sea level) but also in terms of size, as the 133 registered participants marked the largest attendance in almost a decade.

In contrast to the past three years when the meeting was held in Aspen/Snowmass, this year's meeting did not only cover its traditional emphasis on chemistry and biology related EPR but with equal emphasis also new sessions focused on physics and materials science. For the first time, the meeting featured a session on "Spin Devices" which covered EPR related aspects of quantum information and spintronics research. The symposium also featured an independent "Methods" session for the first time in years – a good move as this turned out to be the most demanded and oversubscribed session. These changes to the EPR Symposium reflect the current renaissance of EPR as an important area of contemporary materials science and condensed matter physics.

The symposium's various presentations of new and alternative EPR detection techniques involving solid state spin probes such as nitrogen vacancy centers in diamond or phosphorus donors in silicon were indicative of a fundamentally new range of EPR applications that has evolved in recent years. Some of these new methods allow for EPR spectroscopy at the single spin level and are currently explored intensively for application ranges like magnetometry, spintronics, spin-quantum information, spin memory and semiconductor defect spectroscopy.

The range of covered topics also showed that the rapid development of electrical-, optical-, force- and microresonator-detected EPR methods takes place along with a possibly equally rapid development of new spin excitation schemes and sequences. One of the frequently heard terms at the EPR Symposium was "arbitrary wave form generator, AWG" which represents a new generation of digital pulse formers that have become available to EPR users. These radiation sources allow for the generation of radiation trains with arbitrary and continuously changing frequencies, intensities and phases - a new technology with the potential to introduce radically new ways to conduct EPR spectroscopy using adiabatic or highly concatenated pulse sequences which previously have not been seen at all or only for NMR applications.

The EPR Symposium featured 68 oral presentations, including 19 invited presentations, the Piette lecture and the award presentations of the International EPR Society (IES) whose annual general meeting was hosted by the Rocky Mountain Conference this year. The IES awarded the John Weil Young Investigator Award to Laxman Mainali from the Medical College of Wisconsin for his outstanding EPR studies of membrane fluidity profiles in small volume samples. The 2012 IES Silver Medal for Biology/Chemistry was awarded to Glenn Millhauser for his seminal EPR studies on prions, metal ions and neurodegenerative processes. The 2012 Piette Lecture was given by Ohara Augusto from the University of Sao Paulo, who presented a review of connections between superoxide dismutase, carbonate radical, protein oxidation, protein aggregation and neurodegeneration.

The excellent scope of speakers seen at the EPR Symposium was accompanied by a diverse range of equally outstanding poster contributions. Two poster sessions took place, covering 48 presentations. As all posters were exhibited throughout the entire conference, plenty of opportunity was given for discussions and an exchange between the symposium attendees. In addition to the scientific presentations, the Rocky Mountain Conference also hosted an exhibit by EPR related vendors, the traditional, and this year extraordinarily well attended Sunday night presentation by Bruker about latest technological developments as well as social events such the conference and a symposium receptions.

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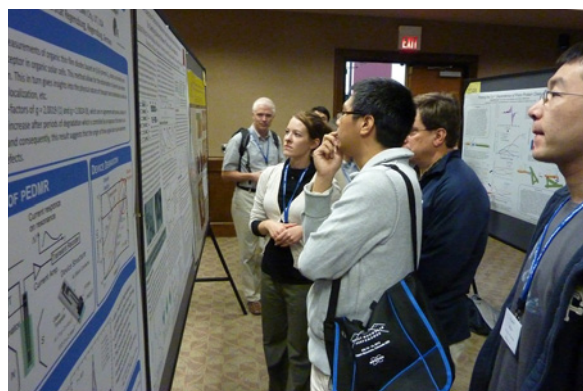
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A midsummer morning view from the Conference venue to the nearby Copper Mountain Ski slopes.



The oral sessions of the Rocky Mountain EPR Symposium featured a new range of topics including a new session of "EPR for Spin Devices".



Many excellent posters and plenty of poster space allowed for lively discussions and a productive

The 2012 EPR Symposium ended with the announcement of future Rocky Mountain Conferences. Following the tradition that the EPR Symposium is alternately chaired by researchers from the physics/materials community and the biology/chemistry community, the 2012 Chair (Christoph Boehme from the University of Utah) stepped down while the 2011 and 2012 co-chair Gail Fanucci (University of Florida) assumed the chairpersonship for 2013. As the rapid developments within the EPR community and the general magnetic resonance communities continue, the Rocky Mountain Conference will continue

to evolve as well. After 53 years, the “Rocky Mountain Conference on Analytical Chemistry” will finally change its name into “Rocky Mountain Conference on Magnetic Resonance”. Similar as in 2011, it will feature only the EPR Symposium in 2013. The meeting will take place from 07/28 to 08/02 in Denver, Colorado returning one

more time to its original location after more than eight years. In 2014 it will move back to Copper Mountain when both Symposia, EPR and Solid State NMR, will take place again.

Christoph Boehme

VIII Voevodsky Conference “Physics and Chemistry of Elementary Chemical Processes” (VVV-2012) & Satellite School “Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics” Novosibirsk (Akademgorodok), Russia, July 15–21, 2012

The VIII Voevodsky Conference “Physics and Chemistry of Elementary Chemical Processes” (VVV-2012) was held in Akademgorodok of Novosibirsk (Russia) on July 15–19, 2012. The conference was organized by the Institute of Chemical Kinetics and Combustion (ICKC) of the Siberian Branch of the Russian Academy of Sciences (SB RAS) and by International Tomography Center (ITC), both located in Novosibirsk. All conference events took place in Akademgorodok. The unique atmosphere of the “town of science in the forest” is created in Akademgorodok by over 30 research institutes located in pristine natural surroundings.

The first Voevodsky Conference took place in 1977, in honour of Academician V. V. Voevodsky’s contribution to various areas of chemical kinetics and his role in the development of physical methods in chemistry. This conference has become a tradition and is held every five years. Since V. V. Voevodsky was the founder of the scientific school of chemical radiospectroscopy in Akademgorodok, EPR was one of the main topics of this strongly interdisciplinary conference (the other topics are NMR, chemical dynamics, photo- and

biochemistry). Totally about 200 scientists participated in the conference. EPR was represented by pioneering scientists as invited speakers, viz. E. G. Bagryanskaya (Novosibirsk, Russia), V. L. Berdinsky (Orenburg, Russia), M. K. Bowman (Tuscaloosa, USA), E. Goovaerts (Antwerp, Belgium), G. Grampp (Graz, Austria), V. V. Khrantsov (Columbus, USA), G. I. Likhtenshtein (Beer-Sheva, Israel), O. G. Poluektov (Argonne, USA), A. Savitsky (Mülheim an der Ruhr, Germany), A. Schnegg (Berlin, Germany), V. F. Tarasov (Moscow, Russia), L. M. Weiner (Rehovot, Israel), A. M. Ziatdinov (Vladivostok, Russia), to name a few.

The conference started on the evening of July, 15 with a welcome party at a lovely lawn of ITC where participants mixed together for informal discussions. Each morning on July 16–19 plenary sessions were held in the House of Scientists of SB RAS. The official

program began with welcome addresses of the President of SB RAS A. L. Aseev and of the VVV-2012 co-chairmen R. Z. Sagdeev and S. A. Dzuba. Then the Voevodsky Prize was



R. Kaptein is presenting his Voedodsky Prize lecture.



M. Bowman (right) is handing IES Silver Medal to A. D. Milov (left).



Group photo of VVV-2012 in front of the House of Scientists, Akademgorodok of Novosibirsk.

Conference reports

awarded to R. Kaptein (Utrecht, The Netherlands / Novosibirsk, Russia) “for outstanding contribution to the theory and practice of chemically induced nuclear spin polarization and the development of novel applications of nuclear magnetic resonance in structural biology”. He delivered an intriguing lecture on structure, dynamics, and allosteric interactions of lac repressor – a “classical” protein for NMR structure studies.

After lunch parallel sessions were held simultaneously at ICKC and ITC. Also ITC hosted two poster sessions with 50 posters presented at each of those. These sessions were accompanied by snacks and beer, which added energy to already vivid discussions. The very busy program of the second conference day was finished by the “Evening of Memoirs about V. V. Voevodsky” – an informal event inspired by A. I. Burshtein (Rehovot, Israel) and chaired by Marianna Voevodskaya, the daughter of V. V. Voevodsky. During this homely evening in ICKC M. Voevodskaya and the followers of Voevodsky (Yu. N. Molin, Yu.

D. Tzvetkov, V. I. Azatyan, A. I. Burstein, L. M. Weiner) shared their impressions of the unique personality of V. V. Voevodsky. They also talked about different obstacles which Voevodsky had to pass on his way in science in Soviet time. Many of impressive details of Voevodsky’s biography were mentioned. A video recording of this event and its English translation (all the discussions were in Russian) will be posted at ICKC site www.kinetics.nsc.ru.

The plenary session of July, 17th started with the ceremony of IES Silver Medal awarding to A. D. Milov (ICKC SB RAS) for numerous pioneering works in the field of electron spin echo spectroscopy and for development of PELDOR. Then, a lecture on Russian-Dutch collaboration in EPR and PELDOR study of spin-labeled peptides was presented by J. Raap (Leiden, The Netherlands), a long-term collaborator of A. D. Milov.

Between lectures there were several excursions to museums of Akademgorodok, including Museum of History and Culture of Sibe-

ria and Far East, where the famous mummy of the “Princess of Altay” was displayed. On the evening of July, 18th we had conference dinner in the House of Scientists where we enjoyed live music and exciting singing of R. Z. Sagdeev. After the official closing of the conference there was an informal “after-party” with volleyball and tennis playing and dancing at ICKC lawn.

The School for young scientists “Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics” was held as a satellite meeting of VVV-2012 (July 16–21, 2012). The lectures on basics and advanced methods of magnetic resonance were presented on July 20 and 21 by Yu. D. Tzvetkov, G. I. Likhtenshtein, S. A. Dzuba and other eminent scientists.

The participants of VVV-2012 witnessed an extremely hot week (both climatically and scientifically) in Siberia. The next Voevodsky conference will be held in 2017, again in Novosibirsk.

Leonid Kulik, ICKC SB RAS

The 2nd International Symposium on Electron Spin Science (ISESS2012) Matsushima, Japan, July 23–25, 2012

The 2nd International Symposium on Electron Spin Science (ISESS2012) took place at Hotel Taikanso in Matsushima, one of the three most scenic spots in Japan. There were 103 participants including accompanying persons from seven countries (Germany, USA, UK, Russia, Israel, Taiwan, and Japan). This was the second symposium in a series

that started in Shizuoka, Japan (2007) sponsored by the Society of Electron Spin Science and Technology (SEST). This symposium was postponed from November 2011 to July 2012 due to the terrible earthquake and the related accidents which occurred on March 11, 2011. The tsunami along 500 km of coast line caused serious problems in northeastern

Japan. But fortunately the Matsushima area was almost protected by the numerous islands. The aim of the symposium was to stimulate in-depth discussions in all aspects of electron spin science; photoreceptor proteins, photosynthesis, organic solar cells, quantum computing, ESR imaging, distance measurements, high field ESR, etc.

The symposium started with a welcome address by Seigo Yamauchi (Japan) who was the chairperson of the symposium and



President of the IES. He really enjoyed the symposium, but unexpectedly, he has passed away on September 26, 2012, due to a sudden illness. The scientific program was opened with an invited talk by Klaus Möbius (Free University Berlin/ Max Planck Institute for Bioinorganic Chemistry) "News and Views of High-Field Dipolar EPR Spectroscopy: Probing Conformational Changes in Photosynthetic Protein Complexes". Further invited talks were delivered by Daniella Goldfarb (Weizmann Institute of Science) "High Field and High Spin – A Different Approach for Long Range Distance Measurements by EPR Spectroscopy", Michael R. Wasielewski (Northwestern University) "Fast Photo-driven Electron Spin Coherence Transfer: A Quantum Gate Based on a Spin Exchange J-Jump", Christiane Timmel (University of Oxford) "A New Net Won't Catch an Old Bird – But Will New Techniques Catch an Old cryptochrome?", Mark Sherwin (University of California) "Free-Electron Laser-Powered Pulsed EPR Spectroscopy", Olav Schiemann (University of Bonn/ University of St. Andrews) "Unravelling Conformational States of Materials and Proteins with PELDOR, DQC and New Labels", Jian-Ren Shen (Okayama University) "Atomic Structure of Photosystem II and the Mn_4CaO_5 -Cluster that Enables Photosynthetic

Water-splitting", Wolfgang Lubitz (Max Planck Institute for Bioinorganic Chemistry) "Unravelling Structure and Function of the Water Oxidizing Complex in Photosynthesis by High Field EPR, ENDOR and ELDOR-Detected NMR", Harold M. Swartz (The Geisel Medical School at Dartmouth) "Clinical EPR: Challenges and Progress", Osamu Sato (Kyushu University) "Control of Magnetic Properties in Molecule-Based Magnets", Elena G. Bagryanskaya (International Tomography Center/ Novosibirsk Institute of Organic Chemistry SB RAS) "Thermal and Optical Switching of the Exchange Interactions in Nitroxide-Copper(II)-Nitroxide Clusters", and Gerd Kothe (University of Freiburg) "Quantum Oscillations and Spin Entanglement in Photoexcited Triplet States". There were presented 38 oral and invited talks, and 38 posters. The Best Poster Awards were selected by an award committee from the posters that were presented by students, which were given to



Kohdai Fujimoto (Kobe University), Mizue Asada (Nagoya University), and Lauren E. Jarocho (University of North Carolina). The final event on the programme was a post-conference tour, in which participants visited Higashimatsushima city, which was hit by the earthquake and tsunami in order to understand the latest situations of the disaster-stricken areas. Finally, we are grateful to all sponsors, speakers and participants of the symposium, and to every person who contributed to its organization.

Hideto Matsuoka

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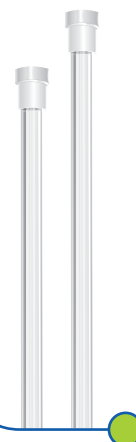
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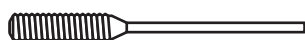
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Alistair Fielding became a Bruker Applications Scientist/Senior Lecturer in the Department of Chemistry at the University of Manchester, United Kingdom, in May 2012. He obtained a BSc in Chemistry at the University of Sussex and a MSc with Distinction from University College London. He achieved his PhD under the supervision of Prof. Brian Roberts, studying the free radical chemistry of thiol polarity – reversal catalysts. During this time he became interested in EPR spectroscopy and went on to learn pulse EPR in the Eaton Laboratory, Denver, USA. This was followed by stays in CEA-Saclay and MPI-Göttingen, where his work became more biologically orientated. Recently, he has focused on studying the catalytic properties of

peroxidase and P450 enzymes. His current position is sponsored by Bruker and based at the EPSRC National EPR Research Facility & Service which provides access to state-of-the-art experimental techniques for multi-frequency continuous wave and pulsed EPR spectroscopy, and associated methods. His work aims at driving new applications and techniques in advanced EPR spectroscopy in the study of biomacromolecules. Currently, he is setting up laser photo excitation experiments and contributing to the development of an optical detected magnetic resonance (ODMR) instrument. He is keen to use his position to advance the use of EPR spectroscopy in research across the United Kingdom and globally.

Readers corner

Dear IES members,

I recently opened my home page with the title of “Spin Chemistry & Solution Flow in the MCM-41 Nanochannel” and uploaded a few articles including two accounts on our own works: 1) Reaction control by spin manipulation on the photochemical reactions and 2) Solution dynamics in the nano-channel of MCM-41 as studied by the radical-pair probe and spin probe techniques. Please visit my home page and read those.

We published many papers on these two subjects but I could not find time to write review articles on these with covering all the progress made until now, though a part of theme 1) has been reviewed in “Dynamic Spin Chemistry” as chapter 8 (Kodansha & John-Wiley, 1998). Since I retired from the research job in AIST (National Institute of Advanced Industrial Science and Technology) Japan, I cannot publish an article in a journal from AIST. Under the circumstances, I wrote accounts of these works and uploaded on my

home page. Critical comments are welcome, which may be written in the blog page.

Home Page:

<http://sky.geocities.jp/xhcwt890>

Blog:

<http://sky.geocities.yahoo.co.jp/gl/xhcwt890>

Sincerely,

Dr. Masaharu Okazaki,
National Institute of Advanced Industrial
Science and Technology, Chubu-branch,
Shimo-shidami, Moriyama-ku, Nagoya,
463-8560, Japan.

Market place

POSITIONS

**Associate Director
Electron Paramagnetic Resonance Center
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Location: Hanover, New Hampshire.

Position Description: We are seeking an Associate Director for our highly successful EPR Center. This individual will work closely with the director, Harold Swartz, to continue and expand the activities of the Center. He/she will be expected to play an active role in the development of the clinical and preclinical

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Qualifications: The ideal candidate must have a Ph.D. and direct and extensive experience with in vivo EPR and active funded research that can be transferred to the Geisel School of Medicine. Extensive experience in the administration of complex high quality research programs is strongly desired.

Compensation, etc.: This will be a tenure track position with a competitive salary.

The individual will receive an appropriate academic appointment as a member of the faculty of the Geisel School of Medicine.

Application Process: Qualified applicants should send their contact information, CV

with research interests and current funding, letter describing their qualifications, and the names and addresses of five references to:

E-mail: Traci.Rosenbaum@Dartmouth.edu

Mail: Traci Rosenbaum, Administrative Director, EPR Center, Geisel School of Medicine at Dartmouth College, Vail Building 705, Hanover, NH 03755

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The EPR community has available to it a list server. The address is epr-list@xenon.che.ilstu.edu. To subscribe to the list, send the words SUBSCRIBE epr-list to majordomo@xenon.che.ilstu.edu. That sends a message to Reef Morse who will then manually place you on the list. This honors only legitimate requests to join the list. Reef also moderates the list which keeps it spam-free.

POSITIONS



Research Positions – Advanced EPR of Biochemical and Chemical Systems

Several research positions (doctoral and postdoc level) are presently available in the Biophysical Chemistry Department of the Max Planck Institute for Chemical Energy Conversion in Mülheim/Ruhr, Germany. We are looking for highly motivated young scientists in the field of Electron Paramagnetic Resonance who are interested in studying biochemical and chemical systems related to the topic of the institute.

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- Hydrogenase enzymes and related model systems;
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- EPR instrumental developments dedicated to EPR studies of (single) protein micro crystals;
- Advanced EPR investigation of highly reactive chemical intermediates and their weakly bound intermolecular complexes.

Our lab is equipped with 10 modern EPR spectrometers covering the frequency range from 2 to 244 GHz capable of the complete repertoire of CW EPR and pulse techniques (ENDOR/TRIPLE, ELDOR, ESEEM) in combination with laser excitation and freeze quench techniques. More details can be found on our website: www.cec.mpg.de.

Candidates should have project relevant knowledge and be trained in Magnetic Resonance Spectroscopy, preferably in EPR. Candidates with an interest in EPR instrumental development and microwave engineering are specifically encouraged to apply.

Please send your application including CV and the scope of scientific interests to:

Prof. Wolfgang Lubitz

Max Planck Institute for Chemical Energy Conversion, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany

e-mail: wolfgang.lubitz@cec.mpg.de

Faculty position wanted

As an experienced theoretical and experimental physicist, I desire to take my career to the next level through a faculty position. I'd like to focus my research on EPR method development. The marvels of digital revolution, fast arbitrary waveform generators and digitizers,

together with novel data processing methods are about to reshape EPR spectroscopy and imaging. I've been working on a number of projects with the common goal to enhance sensitivity and functionality of CW, rapid scan and pulse EPR. Some of these methods are being implemented into standard commercial instruments and software. I look forward to starting a lab where students from a variety of disciplines: electrical and mechanical engineering, math, biology and chemistry, can contribute to new developments in the methodology and applications of EPR.

Mark Tseytlin (Tseitlin in publications), Research Scientist at the University of Denver. Portfolio: <http://portfolio.du.edu/mtseytli>; e-mail: mark.tseytlin@du.edu

Post doctoral/Ph.D positions available

Two post doctoral (or Ph.D) positions are available in the laboratory of Prof. Daniella Goldfarb at the department of Chemical Physics, Weizmann Institute, Rehovot, Israel.

The research focus is development of pulse EPR methodology, including distance measurements using standard and new spin labels, and applications of pulse EPR to biological systems.

The positions require background in Magnetic Resonance, and/or Biochemistry/Structural Biology.

Information about the groups and the Weizmann Institute can be found at www.weizmann.ac.il/chemphys/EPR_group and www.weizmann.ac.il.

Interested candidates should contact Daniella Goldfarb (daniella.goldfarb@weizmann.ac.il) for further information.

For serious suitable candidates the possibility of a funded visit to the lab will be offered prior to final decisions.

Bruker BioSpin Corp

Bruker BioSpin Corp is looking for a highly motivated individual to join our EPR Service team to install and support high technology EPR Spectrometer Systems in customer research labs. This individual will install and service our EPR Spectrometer Systems and train customers for basic operation of the equipment. A BS in electrical engineering, electronics or related fields or equivalent experience is required. Experience diagnosing and repairing electronic, electromechanical and/or mechanical equipment is required. General understanding of analog electronics, digital electronics, high voltage circuitry/circuits, microwave technology, vacuum tech-

nology, cryogenics; strong technical skills on analytical instrumentation required.

Please send resume, cover letter and salary requirements to bruker.jobseprfse0620@bruker-biospin.com

EQUIPMENT

Design and construction of EPR electronics

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 kHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field-control units to voltage-controlled scan operation. A 6-digit 1-ppm frequency counter is available in X-, C-, S-, L-band, or MHz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the University of Denver. **Please contact:** Richard W. Quine, e-mail: rquine@du.edu, phone: 1-303-871-2419

For sale: Varian and ESR equipment

Resonance Instruments has available: (1) Replacement klystrons for Varian EPR bridges and some Bruker bridges (at reduced prices) and other klystrons; (2) Resonance Instrument's Model 8320A is a general purpose Hall-effect based magnetic field controller that provides direct control and precise regulation of the magnetic field between the pole pieces of an electromagnet. Its high resolution permits precise adjustment of the magnet's field either through the front panel keyboard or through an RS232 serial interface with your PC.

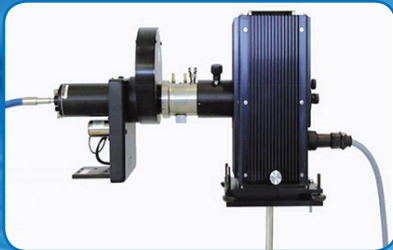
Please contact: Clarence Arnow, President, e-mail: 8400sales@resonanceinstruments.com, phone: 1-847-583-1000, fax: 1-847-583-1021.

Available: Used Varian EPR equipment

(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (3) Varian TM cavity with flat cell holders and flat cells. (4) Varian E-257 variable temperature controller with heater sensor and insert holder. (5) Varian E-272B field/frequency lock accessory.

Please contact: James Anderson, Research Specialties, 1030 S. Main St., Cedar Grove, WI 53013, USA. phone/fax: 1-920-668-9905, e-mail: janderson36@wi.rr.com

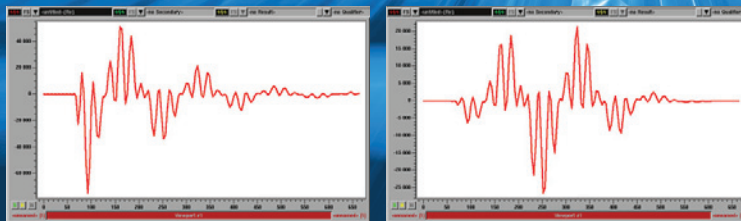
The Xepr API



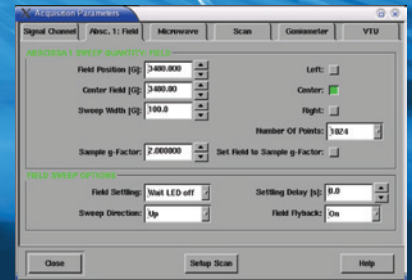
Device Monitoring



Device Control



Data Manipulation



Full Xepr Access

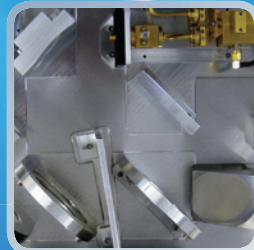
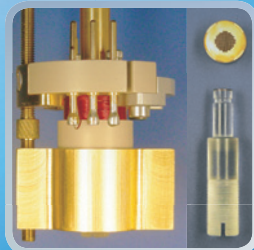
Xepr via Python scripting

- Direct access to Xepr for data acquisition and manipulation
- Does not block Xepr GUI during scripts
- Interactive Python scripting
- Python scripting for experiment settings and data processing
- Interface to devices via USB, GPIB, and Ethernet

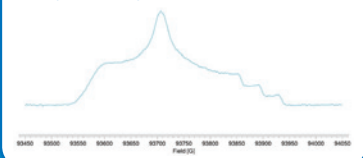
Discover our powerful EPR software: www.bruker.com/epr

mm-wave EPR

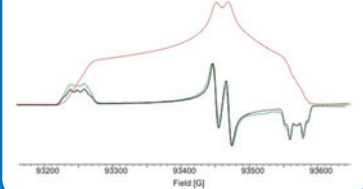
E780 quasi-optical spectrometer



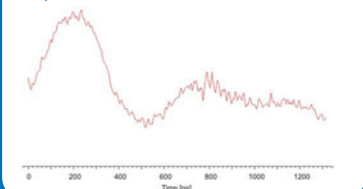
WSS Probehead
100 μ M Tempol at 50K



TE₀₁₁ Probehead 580 μ M
RNR-Y122 at 10K



TE₀₁₁ Probehead DEER of
50 μ M RNA at 30K



Data courtesy:
Marina Bennati, MPI Göttingen

- 263 GHz, $g=2@9.4T$
- 12 T cryogen free superconductive magnet (main and sweep coil)
- Quasi-optical front-end
- Single mode VT TE₀₁₁

- Non resonant wide sample space VT probe (WSS)
- ELEXYS based single door console
- Bruker IF concept
- Operation modes: CW and Pulse/ENDOR/ELDOR

Find out more about our cutting-edge EPR technology:
www.bruker.com/epr