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The Publication of the International
EPR (ESR) Society

IES Anniversary issue

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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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ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Editorial

Dear colleagues,

I think it was a good idea to prepare a special issue of the *EPR newsletter* devoted to the 20th anniversary of the International EPR Society. Frankly speaking, it was crucial to remember that 2009 marks this important event. You understand that everyday life is full of urgent things to do: grant submissions, grant reports, conference presentations, writing papers, etc. However, I feel it is just great to have an excuse to have a celebration!

As a youngster of twenty, the IES is not completely mature yet it is already grown-up with the fascinating past, the glorious present and looking to the breathtaking future. This statement is nicely illustrated by the articles in the '*EPR newsletter* Anecdotes' column (thanks to Jack Freed, past IES CEOs and Hitoshi Ohta who contributed to this column) and the 'Reader's column' (thanks to Sushil Misra).

I presume the IES members have their own way to the Society and supposedly they get the feedback they need. As for me, if I remember right, it was in 1990 that I saw an announcement at our Zavoisky Physical-Technical Institute that the IES was organized and EPR spectroscopists all over the world were invited to join it. I do not remember exactly what the driving force was for me to join the IES, but I can say that my IES membership added a new dimension to my life as an EPR experimenter. I started receiving Linn Belford's *EPR newsletter* and every new issue, with its comprehensive EPR-related news, was a source of invaluable information I could get nowhere else.

I am pleased that when the editorial office of the *EPR newsletter* moved to Kazan we could continue the high standards set up by Linn Belford and also add some new columns to humanize science. Between-you-and-me-and-do-not-tell-anybody, in this issue my name is mentioned many times and in such a complimentary manner that it makes me blush. In fact, the true story is that during this move one of the crucial aspects was that Bruker BioSpin agreed to cover the extra cost of the hard cover in color. It was like a touch of a magic wand transforming a pumpkin into a nicely decorated carriage in this fairy tale we all read as kids. Another big help is that we have a terrific team of Associate Editors: Thomas Prisner, Candice Klug, Hitoshi Ohta (also in the past Takeji Takui and Graham Timmins), and Technical Editor, Sergei Akhmin, preparing a high-quality layout. Editors of the *EPR newsletter* columns include John Pilbrow (*EPR newsletter* Anecdotes), Thomas Prisner (Pro&Contra), Candice Klug (IES Young Investigator Award Revisited, New EPR Faculty and EPR Faculty on the Move), Stefan Stoll (Software), and Keith Earle and David Budil (Tips and Techniques). And last but not least, we had to find a new printer and you can imagine how happy I was to get an email message from Sandy Formichella (Bruker, Billerica) telling me about LaPlume and Sons Printing, Inc. Since then we have enjoyed our collaboration and Scott Morton and his team are extremely efficient.

I cannot rob you of the delight to have the adventure of reading this issue and to discover what we prepared for you. Join us in congratulating John Weil on his 80th birthday (p. 23), and Yuri Molin and Aleksander Milov on their 75th and 65th birthdays, respectively (see also 14, pp. 11–12). And enjoy George Feher's interview in the 'Five Years After' column (p. 25; see also 14, p. 10). Dear George, let you live till your120th birthday (this is a must) and then as much as you wish!

Special congratulations go to the ESR group of the Royal Society of Chemistry, the elder brother of the IES, on its 40th anniversary and special thanks go to Shirley Fairhurst for her continuing support of the *EPR newsletter*. We greatly appreciate the help of our web-masters from ETH, Fabienne Ruffieux, Besnik Kasumaj and Yevhen Polynach.

Welcome, dear reader, to this special issue of the *EPR newsletter*! And who knows, maybe after you finish reading it, you will agree that it was a good idea to prepare it ...

Laila Mosina

Twentieth Anniversary of the IES

Jack H. Freed
President of the IES

It is a great pleasure for me to introduce this special issue of the *EPR newsletter* commemorating the 20th anniversary of the IES. I am very pleased that, in response to my invitation to the past IES Presidents, Executives, and IES Medalists to contribute their thoughts on the IES and its role in promoting EPR/ESR, we have received many thoughtful and entertaining responses. In this spirit, I would like to present an introductory overview to these recollections in a celebratory fashion.

We must credit Hal Swartz as the Founding Father of the IES. In his recollections he details the circuitous path and his major efforts in bringing our Society about. The guiding principles and structure of the IES remain today very close to those Hal established 20 years ago. This even included the establishment of the *EPR newsletter* as the public voice of the IES, and the one in which we are able to disseminate the thoughts and contributions for this special issue.

Let me give another example of Hal's prescience and wisdom of 20 years ago that seems so appropriate today. It was Hal who named the society: International EPR/ESR Society. I must say that over the many years over which I have contributed to the field, I have preferred to call our field ESR. After all, most work is done with systems wherein the g value is very close to the free electron *g*-value of 2.00232, possibly deviating in the third decimal place. Thus it is predominantly a spin phenomenon. On the other hand, as we know, many transition metal ions can have *g*-values deviating greatly from this, due to orbital contributions, so EPR becomes more appropriate in those cases. However, my prejudices in favor of ESR transcended these considerations.

We all feel that ours is a unique field, so we deserve a unique name. but as many of you are aware, EPR also stands for the Einstein, Podolsky, Rosen paradox in quantum mechanics, and a Google search even today shows this clearly. Not only that, of growing importance with respect to worldwide issues of energy is the European Pressurized Reactor, a.k.a. the EPR Nuclear Reactor, which is a current version and very popular on Google. Hence my past preference for ESR. Unfortunately, I recently took the trouble to Google ESR only to find: Erythrocyte Sedimentation Rate (ESR), Equivalent Series Resistance (ESR) Meter, European Society of Rheology, European Society of Radiology, and so on. However, when I Googled EPR/ESR, our Society, as well as some of our regional societies, predominated. How did Hal get that so right 20 years ago, long before Google?

The seat of the Presidency moved to Oxford, Britain when Keith McLauchlan became the second President. Keith's indefatigable skills and good natured friendliness served the IES well. As he describes, and as is typical for the second president, he had to face up to a number of practical issues such as the funding of IES functions, as well as the improvement of the methods of making awards of the Society, including instituting the Fellowships of the IES. I am personally indebted to Keith, because whenever it was my honor to receive an EPR/ESR award, he was ready, willing, and able to deliver it to me. In 1990, he handed me the Bruker Prize as head of the ESR Group of the RSC, and in 1994 he handed me the IES Gold Medal in his role as President. So not only do all of us in the IES today owe Keith thanks for his important contributions, I must give him my own personal thanks.

When Jim Norris became the third President, the U.S. again became the center of IES activity. Jim was an able and dedicated President under whose direction the IES continued to prosper. It was always a pleasure for me to see Jim as he represented the IES at many international EPR/ESR meetings and at his home base in Chicago. Jim has in recent years developed a strong interest in fishing. I wish him continued success in all his endeavors. Perhaps, he will be willing to teach me how to fish when I finish my tenure as President of the IES.

Our fourth President, John Pilbrow brought the focus of the IES to a new continent, Australia. While some of those who do not know John might think that is a bit out of the way for our field, John is an inveterate traveler. He can (and does) pick up any day of the week to travel 24 hours to practically any point on the globe. We got to know each other during a common 12 hour layover in Frankfurt, Germany, where we could compare travel tricks and experiences, matters we continue to expand upon over the years. John, as President, took advantage of his propensity for travel and was able to represent the IES at countless EPR/ESR meetings around the world. He truly helped to make the IES a closer knitted world-wide community, as his recollections make clear.

With Yuri Tsvetkov's appointment as the fifth President, the great contributions of Russian scientists to EPR/ESR, including those of Yuri and his group in Novosibirsk, Siberia were recognized. It also brought the center of IES activity to a new continent, Asia. As Yuri points out in his recollections, this is a double anniversary given that 65 years ago EPR/ESR was first observed by Zavoisky in the Soviet Union. Yuri continued to foster the international spirit of the IES, and he brought the editorial office of the *EPR newsletter* to Kazan, where it is today in the hands of the Editor-in-

My recollections of the establishment of The International EPR (ESR) Society

First, I would like to clearly state that this is a decidedly subjective, non-referenced, idiosyncratic discussion on the topic, uncontaminated by reference to historical documents! But perhaps, by highlighting those aspects that are most vivid in my memory about the process, this may provide insights into some of the issues and critical decisions that led to the founding of the Society and its operation during the early years. The article is composed under section heads, to provide the reader with guidance as to what I am trying to say.

Early discussions about whether such a society should be established

I believe that I must shoulder much of the blame and perhaps a little credit for the initial formation of the Society. There always had been concerns expressed among EPR people about our lack of recognition as a separate discipline, but generally people were resigned to this state as being inevitable. I felt that we could ameliorate this by forming a society of our own and took the initiative to stimulate discussions about the topic. The initial responses were decidedly mixed, with some enthusiastic about the idea, a few adamantly opposed, and most indifferent. But those who saw the potential value of the society persisted and gradually the discussions, over 2-3 years, began to take on reality, as more and more people perceived the potential benefits. From this point the development was the product of many people and many ideas and my role, quite properly, became more limited and principally involved trying to organize these thoughts, suggestions, and support into a cohesive proposal that could be distributed to the larger community of EPR spectroscopists in a credible manner.

The impetus for forming an EPR Society came especially from our experiences in participating in joint magnetic resonance conferences and societies with our NMR colleagues. It seemed that EPR always was the poor sister, with the planning and the decision-making dominated by people who were primarily involved in NMR. The NMR people always tried to make us feel welcome, but the reality was (and still is) that EPR was a minor perturbation on the NMR program. While this was in some ways quite reasonable because of the larger numbers of NMR people involved, the result was a loss of identity of the EPR people.

A second factor was the recognition that although there were a lot of EPR scientists in the world, they were involved in so many different disciplines that in meetings organized for other purposes, there was little overlap and therefore few opportunities to share those aspects of common interest.

The third factor was a feeling of optimism about the prospects for further development of EPR, which had for a while seemed to be a lagging field. If the exciting new instrumental developments, concepts, and applications

Chief, Laila Mosina who continues to be outstanding in this role. I myself have had many associations with Yuri and his group, including my various service roles for the IES. I might mention that Yuri was one of the first distinguished visitors to our Cornell National ESR Center, ACERT, shortly after it was formed.

The sixth President, and my immediate predecessor, Wolfgang Lubitz describes the twenty years of the IES in the context of how his own career developed over this period. His tenure as President has been from a united Germany. He relates how the year 1989 is also when the separation of Germany ended followed shortly by its reunification. Thus a celebration of the 20th anniversary of the IES also brings to mind the inception of closer relations between colleagues in the East and West as the barriers came down. Clearly our Society has benefited greatly, and this has added to its international character. Under Lubitz' direction this East/West interaction continued to prosper. I am particularly grateful to Wolfgang for his special efforts in helping me get started as the current President of the IES, and his ongoing willingness to help and advise me. This is a continuation of what is now a long line of cooperation between successive IES Presidents.

Other distinguished members of the IES have also contributed to this special issue. Klaus Moebius provides his recollections from Berlin. He fills us in on how difficult it was for scientists to communicate when East and West Berlin were separated by the wall, and on the exciting political events of 1989 concurrent with the inception of the IES. Klaus, as we all know, has contributed greatly to international cooperation in our field. Kev Salikhov tells about developments in Russia during that period. Kev, aside from his many distinctions, was a pioneer in establishing the International Zavoisky Award and the international journal of Applied Magnetic Resonance, of which he is the editor from his base in Kazan, Russia. Haim Levanon, writing from Jerusalem, Israel, reminisces on his postdoctoral years with the great EPR/ESR pioneer Sam Weissman in St. Louis. Back then one could argue (if one was disposed to such things) whether science was stronger in Russia or the U.S. For Sam's answer to the eminent Russian scientist Voevodsky, see Haim's recollections.

Takeji Takui and Hitoshi Ohta, writing from Osaka and Kobe respectively, provide insight into how the IES has helped to foster interactions of the EPR/ESR community in Japan with those elsewhere. They make particular mention of the formation of the Japanese Society of Electron Spin Science (SEST) which helped to bring together EPR/ESR scientists in Japan working in the diverse fields of physics, chemistry, biology, and medicine. In fact, Takeji is the Founder

that were becoming evident 20 years ago were to be fully realized and appreciated, it seemed to many of us that we needed to have a better forum for sharing and disseminating these developments.

Composition of the initial board of trustees and the initial set of officers

We deliberately established the initial board of trustees with two complimentary goals in mind: (1) to have the board consist of individuals who would achieve instant recognition of their scientific excellence and (2) to include people who would be likely to be of significant help in establishing and governing the society. The members of the board also were chosen to provide adequate representation reflecting the diversity of both geographic involvement and areas of application. In retrospect I think we did accomplish these goals. We recognized that all of the criteria would not apply to everyone on the board, but felt that the name recognition of the members of the board was extremely important for establishing immediate credibility.

We tried to follow the same principles in choosing the first set of officers, but here we needed to make a compromise choosing individuals, especially for the President, more on the basis of organizing capabilities rather than the most prestigious people in the field. We did better with the other officers, combining both characteristics.

Naming the society

This topic warrants a separate section because of the insights that it provides on the nature of the EPR (ESR) community and some of the early thinking about what the society should represent. Initially I had the naive concept that the use of the two different terms was strictly an historical circumstance, signifying nothing of importance and, accordingly, an easy topic on which to achieve consensus. The impetus for trying to settle on a single name for the discipline arose from the conversations that many of us had had with colleagues from other fields when, after a long discussion about our particular research, we were brought up short by the question: is that at all related to ESR (or EPR as the case may be). This, of course, shattered the illusion that the colleague understood what we were talking about, as well as illustrating how our small field was being further sub-divided by the name that we chose to use.

My own reasoning for naming the discipline arose early when I found that while ESR seemed to be the common usage, Varian Associates inevitably used EPR. My reaction to this was that we should not give in to this crass commercial entity (which was essentially our only source of commercial equipment) and so I used ESR in my papers. When we began to develop the Society the topic of the name came up and in another naïve moment, I assumed that we could have a discussion and then a vote (the venue was the Rocky Mountain meeting) and go with whatever the majority preferred, and thus issue would be settled. It turned out that the assemblage of scientists at that particular meeting preferred EPR and the matter was settled – or so I thought. Of course, the result was quite different. Soon afterwards there were vigorous discussions in person, by mail, email, and phone with very passionate explanations why only one or the other was the proper term. Some suggested, in the vein of compromise, that we choose a neutral name, EMR, for which there was some logic. At this point I gave up, because probably the last thing in the world we wanted to do was to try to establish a third name and thereby divide up knowledge of what we were doing into three portions instead of two. I suggested (and the convention was rapidly adopted that exists to this day) of calling ourselves the International EPR (ESR) Society. Simultaneously, I began and still strongly advocate that in every paper one should consistently use one of the two terms and in the first instance where the technique is named, to note that it is completely equivalent to the other. Historically this evolution has led to my being associated with the founding of both EPR or ESR centers, with the initial one at Milwaukee still using ESR and the subsequent ones at Illinois and Dartmouth being EPR Centers. And I am sure that the world couldn't care less!

Establishment of awards

This was an aspect where I probably pushed my own agenda harder than for most other aspects. I was convinced (and remain so) that one of the most useful things that we could do to advance the field and the people in it was to establish a broad but appropriate set of awards to recognize their achievements in the field. Because of our previous limitations to being part of the magnetic resonance community, which was so numerically dominated by the NMR community, there had been a paucity of opportunities for recognition of the achievements of the EPR community. I certainly received a lot of criticisms and concerns about having too many such awards, but I believe that that these awards have made a significant difference to the field and to the individuals who received them. Perhaps with the exception of the first silver medal in Biology & Medicine, all of the recipients, even in hindsight, richly deserved these awards. Later it was decided by others to curtail the number of awards and while I understood the rationale, I did not and still do not agree with that change. A well deserved recognition by an established scientific society has considerable credibility and usefulness with one's institution and among one's peers.

Annual meetings

The *sine qua non* of most societies is the annual meeting, where the members have an opportunity to interact professionally and socially, find positions, see the latest offerings from vendors, etc. But it quickly became apparent that there were too many disparate interests, loyalties, and habits in the EPR community for it to be feasible, at least initially, to have our own meeting. Some felt that the existing joint magnetic resonance meetings still served their particular needs and others had local or regional EPR societies. I rapidly made the decision that if I were going to be able to herd these cats into a society; I would need to drop the possibility of establishing still another meeting. This prob-

President of SEST. Takeji and Hitoshi emphasize the close association of SEST with the APES symposia and the importance of the participation of IES presidents in these symposia.

Finally, Gareth and Sandy Eaton note that, whereas the formal creation of the IES dates from 1989, the "real genesis" might well have been in 1987 during the annual International EPR Symposium that Gareth and Sandy organized in Denver, Colorado for so many years, and which continues to this day. The first annual meetings of the IES took place at that venue, and in the 20th year of the IES it again returns to this venue, or rather nearby in Snowmass Colorado in the beautiful Rocky Mountains.

lem was perhaps made more acute by the fact that the initial organizational discussions about forming the society took place at the Rocky Mountain conference, and any new meeting would be a potential rival to this well established meeting. At the same time, it was clear that we could not make this regional USA conference the annual meeting of the EPR society. The perception was that it is principally a USA meeting, and thus there would be no opportunities for it to be held elsewhere, while the goals of the society were to be a world-wide. Perhaps more fundamentally, the field of EPR was (and is) so diverse that it might be very difficult to encompass the full interest of the members in a single meeting and achieve critical masses for each of the subfields.

Instead we adopted the principle, which is still operational, of having the EPR Society co-sponsor other meetings. This appears to be working reasonably well, although my prejudice remains that we should have our own annual meeting, perhaps rotating it in conjunction with other meetings.

In the early years of the Society I did make several attempts to establish a main meeting of the EPR Society in association with established magnetic resonance society meetings. These initiatives went fairly far along until floundering on the rock of the NMR domination of all of the joint societies and their unwillingness to delegate the responsibilities for the EPR part of the meetings to the EPR Society. That was a disappointment to me, because I think that we could have significantly augmented one of the joint magnet resonance meetings by having a larger and more vigorous participation of EPR scientists.

Relationships with existing societies, both EPR and magnetic resonance

This was an especially challenging aspect, which I believe has been satisfactorily solved only after many years through the work of many people. The EPR community was quite fractured with aggregates of people involved in societies that were formed at multiple levels of geography and disciplines. It became clear, even in the initial discussions about forming the society, that each society and grouping was very concerned about the impact of an international EPR society on their organization. This was not surprising in view of the already fractured nature of the EPR community (e.g. one country had three different and competing EPR societies, each of which felt that they were the dominant one!).

In the early days, in spite of considerable effort and sensitivity to the problem, we had to battle the impression that the EPR Society was an organization that was primarily American. We finally resolved the concerns only when we had non-USA Presidents, (and later added regional vice-presidents as well), but I suspect that even 20 years later that there are those who still think of this society as being a USA organization, even though the membership is widely distributed world-wide.

There was a long series of discussions with some of the magnetic resonance societies about the possibility of incorporating the society entirely into their structure and having the EPR Society assume responsibility for the EPR portion of the meetings. While there were some positive responses and in some cases prolonged discussions with several groups, eventually all of these initiatives did not work out—probably to the ultimate benefit of our Society.

Evolution of the working model

The EPR Society has been dynamic and constantly changing over the years, as we have found out what works and does not work and what is feasible. Very early the basic structure and function of the society was established, and subsequent changes have been evolutionary. We quickly adapted to the concept that the Society would not have its own meetings. Initially we overcame this potential handicap, which prevented the members from meeting as a group, by informally using the Rocky Mountain meetings as the venue for formal meetings. Sandy and Gareth Eaton were most accommodating in this respect, and that venue still is used frequently. The down side of this arrangement was the somewhat limited geographic and disciplinary representation at this meeting and also, the perpetuation of the impression that the Society was an American one. Therefore, periodically the "annual meetings" of the Society have been held in conjunction with other EPR oriented meetings, especially the European Federation of EPR Societies that gradually emerged. But this aspect has never been fully implemented, because each of the existing meetings only serves a small portion of the international EPR community. Consequently, the Newsletter and the awards have been the glue that has given the society an identity and a value.

The finances of the society have always been both problematic and sufficient, due to a combination of planning and good luck. The biggest expense, the Newsletter and the support for it, initially was subsidized by the EPR Center at Illinois, but there also were very significant contributions from the various sponsors and the members via their dues. We always have been constrained by the fact that many of the Society members resided in countries where there was little access to hard currency. Because of this a system evolved whereby dues in such countries were able to be paid in the local currency and at rates that were consistent with the availability of funds of the scientists. This allowed everyone to make a proportionate contribution of dues according to their salaries, but resulted in little flow of cash from these countries to support the infrastructure of the Society. As far as I can recall, we never had to curtail any of the essential activities of the society because of limited finances; we only were constrained from doing some of the additional accomplishment that we would have liked to achieved, such as travel support for young investigators.

The role of the newsletter

The newsletter has been an extremely important and valuable part of the Society from the very beginning. And over time it has gotten even better and better. For many years it was based at the University of Illinois where we were able to take advantage of the

personnel of the EPR Center to carry out the considerable amount of work involved in assembling and distributing the Newsletter. Also from the start, Bruker has provided very significant support in the distribution of the Newsletter. The transition of the newsletter to Kazan has been especially fortuitous, where Laila has been unstinting in her advocacy and energy in improving and enhancing the newsletter, and Kev has been a vigorous supporter of it, enabling Laila to devote the very considerable amount of time needed to do such an excellent job. Other key developments that have facilitated the development of the newsletter building on the achievements of the previous editor to maintain the status of the Newsletter as a state-of-the art quality publication that presents a very positive impression of the Society include the support of Bruker to cover the cost of the color hard cover; the involvement of Sergei as the Technical Editor who prepares a professional high-quality layout of the newsletter; and the collaboration with LaPlume and Sons Printing, Inc. (Lawrence, MA) for the printing.

Over time it has provided an excellent source of scientific and technical material that would not readily be available through conventional means. And especially through the energy and insights of Laila, the personal dimension of the science and the scientists has had splendid exposition.

The magical transformative power of reality

After all of the initial angst and doubts about the need and viability of the Society, as soon as we established its existence, it generated a very positive effect on the members and the outside scientific world. The doubters often became strong advocates of the role of the Society and other organizations, and scientific and governmental agencies almost immediately acted as if this were a real, important, and appropriate scientific society.

Letting go and reflections after 20 years

I remained very much involved in running the Society for many years and responded to the absolutely essential and desirable change of leadership with very mixed emotions. It seemed impossible that the Society could continue unabated without my constant attention (for many years I did put in 20–30 hours per week on the Society and my administrative assistants did most of the organizational tasks) and it was unlikely that however well motivated and capable, my successors could not keep up all of the required effort. The reality, of course, was quite the opposite. The Society did not miss a beat after the new set of officers was elected, and eventually I found that they functioned quite well without my advice and help! In the intervening years the Society has continued to grow and become more useful and more important. And I rapidly found other activities to fully fill the void in my activities when I no longer needed to carry out the work of the Society.

Now I look back with considerable pride at the EPR Society, which has been so ably continued and expanded, still nursing the conviction that perhaps I did make some real contribution to its origin and thereby a contribution to the field. In fact, the existence and the success of the International EPR (ESR) Society is something in which I take great pride and satisfaction, and I will be eternally grateful to all of you who allowed me to participate in this wonderful enterprise and to continue to be involved. We all have done a great job – and the best is yet to come!

Hal Swartz
Founder President of the IES

Impact of IES

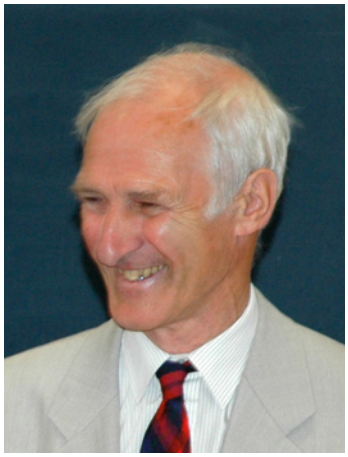
Although the International EPR (ESR) Society was formally created at the 12th International EPR Symposium in 1989, the real genesis might be traced to the1987 Workshop on the Future of EPR, which was held in conjunction with the 10th International EPR Symposium. Looking back two decades, through the filter of all that has transpired since then, we perceive that the 1987 Workshop was a community-building event. Although the EPR Symposium had brought people together to share excitement about new developments in EPR for a decade already, it was in the 1987 Workshop that people came together to think collectively about the future of EPR, what the potential applications were, what the impediments to progress were, and what the enabling technologies might be. Importantly, people from Bruker, Wilmad, Oxford Instruments, and other companies joined with academic, industrial, and government lab scientists from many countries to solve problems together. After that Workshop, people began to perceive that we really were a society of researchers, and maybe we should formally create a society. It took the enthusiasm and skills of Hal Swartz to stimulate many people to put a lot of effort into creating the formal structure of IES. Hal agreed to be the first President of the Society and asked us to contribute as secretary and treasurer. To avoid having the female automatically be the secretary, Gareth became secretary and Sandy became treasurer. Immediately, the question of a journal was raised. By that time, Kev Salikhov was hard at work founding Applied Magnetic Resonance, which, together with Journal of Magnetic Resonance and Organic Magnetic Resonance, met the needs we perceived, so we argued against creating a new journal, just as we had argued against those who wanted us to publish volumes based on papers at the EPR Symposium. However, a newsletter seemed to be needed. The benefit of a newsletter for EPR had already been demonstrated by the EPR Centers Newsletter, which was edited by Linn Belford, who agreed to convert it to the IES Newsletter and continue as editor.

Over the years, this has grown to the present very valuable Newsletter, with international contributors. For many years, the International EPR Symposium in Denver allocated time in the program for an annual meeting of the Society.

From the beginning Hal and we worried that our involvement as officers, and having annual meetings at the Symposium in Denver would cause others to think of the Society as a US society, although we all wanted it to be the society for people in all countries. Hal and subsequent presidents put a lot of effort into creating or linking to Associated Societies in other countries or regions of the world. There were many currency problems inhibiting international membership in the early years of the Society, so one of the roles of the Associated Societies and regional officers was to coordinate membership, collect dues, and distribute the Newsletter in those regions.

Many corporate and other donors, and much volunteer effort, keep the Newsletter and the Society strong. For example, Bruker has financed the distribution of the Newsletter to the benefit of all members of the Society.

Gareth and Sandra Eaton
IES Secretary and Treasurer 1989–1992



The Second Presidency

Following Zavoisky's discovery of EPR, Brebis Bleaney quite independently did the equivalent experiment in Oxford and EPR became quickly established in the physics community in the U.K. Chemists here realized its potential and soon Alec Waters, Dick Norman, Martyn Symons, David Whiffen and Alan Carrington became involved, all establishing research groups so that the community expanded rapidly. In the early 1960 period the desirability for forming a society became evident and the Electron Spin Resonance Discussion Group (ESRDG) was founded, and quite soon was assimilated into the Chemical Society (now the Royal Society of Chemistry). This for some years formed the focus for ESR research in Europe but a strong Italian group soon emerged besides rather smaller ones in other European countries. All retained, and retain, their independence but it became apparent that a European Confederation was desirable, and this resulted from a meeting arranged by Marina Brustolon in Padova, with Klaus Möbius and others strongly involved. At this time no EPR society existed in the United States although many of the major advances in technique, theory and application originated there. This, and the desire for a world-wide organization, was one reason that provided Hal Swartz with his motive to establish the IES. Another was that there was little formal recognition of EPR scientists in the world scientific community.

When Hal, who I had not met before, arrived at my office in Oxford one morning I was just finishing a period as Chairman of the ESRDG and was also involved in the European initiative. Being the persuasive person he still remains he talked me into accepting the Presidency of the IES, which he saw as a means of globalizing the Society. I did so with considerable misgivings especially as the new Society was largely resented in Europe as a U.S. upstart which appeared to be usurping the position of the pre-existing ones. Indeed, for some years it was very difficult to persuade members of the U.K. group to join the IES.

This, however, was not my main difficulty. I inherited from Hal what was apparently a carefully worked out constitution and code of practice under which the Society was run. It was very detailed but, as I rapidly realized, utopian in its ambitions. Right from the start he realized there would be expenses involved and some support for the new Society was written into the grants awarded to his Institute in Illinois. This was crucial to the embryonic IES for inter alia it gave us some of the time of Lynn Belford and Becky Gallivan, whose significant contributions were very properly recognized with awards some years later. Becky, one of the nicest people I ever met, worked for us much more than her contract demanded and I depended on her completely. However whilst some funding was assured it failed to meet the running costs of the Society, especially in the employment of a second secretary at the time and in funding the expenses of the Chairmen of several sub-divisions created by Hal to whom members could apply for grants to attend Meetings. The problem was that no budget had been established for them and when I collated all the information I discovered that the IES was heavily in debt. This was overcome by removing this funding (although it was always hoped to re-establish it) and unfortunately by getting rid of the second secretary. Hal and I also continued to expand backing from our sponsors and we were greatly helped by Bruker accepting the circulation costs of the Newsletter. Most of those who supported us then still do, for which the IES must be eternally grateful.

Soon after its inception the IES established prizes in the various branches of EPR application and, eventually its top award, the Gold Prize. Independently the Bruker Prize was established in the U.K. and the Zavoisky Prize in Russia. But although these satisfied the desire for public recognition of our community this came after a period when no awards had been made and the world was full of very distinguished, but slightly elderly, ESR scientists who would naturally have received most of them. Our solution was to create the Fellowships of the Society to recognize these whilst allowing us to award to younger people. A further move was to recognize Hal's seminal contribution by creating the honorary position of "Founder President".

By the time my two years of office came to its end the financial problem had been solved and the membership was growing rapidly. I received a lot of credit at the time but the secret was that I had Arthur Schweiger as the Secretary of the Society during my reign. Arthur was the source of many of the new ideas, especially those that were concerned with the help to, and recognition of, young scientists. His was the human face of the Society, although his modesty prevented this from being widely known, and it was a sheer joy to work with him. For a man who was personally so brilliant to put so much time and commitment into the welfare of others was a lesson to us all.

But I must end on a final note about Hal. The IES is the only society I know which grew from the imagination and foresight of one man and, although I did not appreciate it too strongly at the time, I was lucky that he came to my office that morning!

Keith A. McLauchlan
IES President 1993–1996

EPR (ESR) Society's 20th Anniversary: 1989 – Recollections and Second Thoughts

It was in August 1988, at the 11th International EPR Symposium in Denver organized by Gareth and Sandra Eaton, when the only announced scientist from the Soviet Union, Gertz Likhtenshtein from the Academy of Sciences in Chernogolovka, ultimately arrived, eagerly awaited for his invited lecture. He came with enthusiasm about what he wanted to see, but without any dollars from the Soviet authorities. To obtain an exit visa was apparently the utmost to be feasible at that time of still intact Cold-War barriers. In early June 1990, Gertz contacted me from East Berlin where he was staying at an agricultural institute of the Academy of Sciences in Berlin-Wartenberg as a guest scientist. He asked me for an invitation letter to apply for a short-term visa at the Soviet Embassy in East Berlin to visit the Free University in West Berlin. Since he had only three more days left to stay in East Berlin, we quickly figured out that there is no chance to get this visa in time. Instead, we managed to come within sight of each other at the opposite sides of a hole in the still standing Berlin Wall that I knew to have been punched recently by the new species of "wallpeckers". And, when the patrolling East German border soldier turned his back to the hole, Gertz quickly wormed his way into West Berlin. After half a day of exciting excursions and discussions, he returned happily to East Berlin (through the same hole as far as I remember). Still, a very unusual way for scientific exchange!

This was almost a year after the International EPR Society was founded, in July 1989, by the attendees of the 12th International EPR Symposium in Denver, following an initiative of Harold Swartz from Urbana-Champaign together with a group of dedicated supporters (see *EPR newsletter* vol. 2, #1, 1989). In what kind of historical environment did this launching of a new international society happen?

Really, several breath-taking historical events had happened in 1989 that I remember vividly since they dramatically affected the notoriously bad East-West relations – and thereby my daily living in a divided city and a divided country. In this regard, the year started with good news: At the Paris Chemical Weapons Conference, January 7–11, 1989, 149 nations solemnly affirmed their commitments not to use chemical weapons, and stressed the necessity of the prohibition of the development, production, stockpiling, transfer, and use of all chemical weapons, and the necessity of their destruction. Unfortunately, the bad news on the nuclear arms race continued to come out: During the whole year of 1989 about 30 nuclear weapon tests were still performed by the US, France, USSR and Great Britain (in this order of prevalence). Moreover, we had to learn that, on June 4th, the students' protest at Beijing's Tiananmen Square had ended in a horrible massacre of hundreds of students by Chinese soldiers.

In the second half of the year, fortunately the good news prevailed: Thanks to wise statesmen in the East, the Iron Curtain started to become full of holes, and in September/October thousands of East Germans fled to the West, often via embassies and summer resorts in more tolerant neighboring countries. In my memory, as a Berliner, the final opening of the Berlin Wall on November 9th and its subsequent demolishing was the best news of the year! This opened new horizons not only in global politics, for instance terminating the hard-line party governments in Eastern Europe, but also changing completely our life by allowing to meet friends and family members separated for so many years. And to meet EPR colleagues from East Berlin and East Germany as well as friends from Eastern EPR laboratories, specifically from Poznan, Moscow, Kazan and Novosibirsk, whom to see had previously been possible only under rather unusual circumstances (see above).

As a charter member of the freshly formed International EPR Society I was very much in favor of its published aims (see *EPR newsletter* vol. 2, #1, 1989): to stimulate the scientific development of EPR spectroscopy; to communicate information and news about EPR ...; to encourage appropriate and useful application of EPR in a wide variety of fields ...; to provide a central voice for the EPR community by promoting support for research and development ...; to stimulate educational programs on EPR and related spectroscopies .... But, to be honest, I missed an explicit mentioning of the aim to foster scientific and human exchange between the EPR scientists from both sides of the Iron Curtain, whose ultimate lifting nobody could foresee in July 1989.

The abstinence in formulating such a political aim was different from what I knew from other scientific societies, for example the Groupement AMPERE, a European association of scientists active in the fields of magnetic resonances. It was founded in Paris already in 1952 under the motto "*mutual knowledge, understanding and cooperation*" with the precise purpose of supporting links between different European laboratories, explicitly including as an aim to help scientists in difficult economic and political conditions. And to keep an efficient scientific and human exchange between Eastern and Western European countries. As certainly many of the older magnetic-resonance scientists will remember, this objective of the Groupement AMPERE was realized most successfully, even during the coldest periods of East-West politics. And I want to add that it was in this spirit that a substantial driving force for the activities of the European Federation of EPR Groups, founded in 1991/92, has been the fall of the Berlin Wall, opening new chances for cooperation between EPR colleagues throughout Western and Eastern Europe.

It is tempting to speculate about the reasons for this apparent difference in formulating explicitly the aims of these international magnetic-resonance associations. Could it be that this difference simply reflects the different awareness in 1989 of the consequences of the East-West shism for scientists in Europe and the US? I don't think that it was abstention in political issues as a matter of principle that motivated the founding scientists of the International EPR Society not to mention the Iron-Curtain issue (in particular when reading their names as members of the Organizing Committee and Members-at-Large). I rather believe that they were convinced that in the new Society "*Actions speak louder than words*".

To my admiration, right from the beginning until now, the International EPR Society followed exactly this claim. The Society was extremely successful in promoting EPR world-wide, particularly by bridging gulfs between political, economic and cultural systems of its members, by fostering personal contacts and exchanges of scientists from vastly different corners of the globe, by

encouraging, via a variety of specific Awards, young and senior scientists to enhance the significance of EPR spectroscopy in all its facets, such as instrumental and theoretical developments and relevant applications. This success, reaching far beyond the written aims of the Society, could only be achieved by highly dedicated members and officers of the Society, in particular the Presidents, their Vice Presidents, Secretaries and Treasurers. And, last but certainly not least, by the Editors of the *EPR newsletter* with its steadily growing scientific and cultural attraction.

By the way: It was not a coincidence that in the same issue of the *EPR newsletter* (vol. 2, #1, 1989), in which the foundation of the International EPR Society was reported, a new international scientific journal was announced: *Applied Magnetic Resonance* (AMR), edited by Kev Salikhov from the Zavoisky Institute of the Academy of Sciences of the USSR. The first issue of AMR appeared in early 1990. Surprisingly, this was the first journal on magnetic resonance at all that was published in the country where the phenomenon of EPR was discovered (by E. K. Zavoisky in Kazan, in 1944). Even more surprising is the fact that the USSR authorities permitted that in AMR all articles must be written in English; a novelty at that time in the USSR! And in the Introduction to the first issue the Editor consistently claimed "that this journal will bridge the gap between scientists from East and West".

So, when leaning back and giving the 20th anniversary of the International EPR Society and the historical events in 1989 a second thought, there remain no doubts that the Society has played – and is still playing – a pivotal role in the renaissance of EPR spectroscopy in a time of political and scientific paradigm changes. EPR is distinguished by its on-going growth in significance as a spectroscopic tool in a wide variety of fields including physical, chemical, biological and medical applications. This success story is based on world-wide cooperations among EPR scientists, often with very different background in terms of political, cultural and economic systems, but united by common goals of intellectual curiosity, scientific honesty and mutual understanding. I want to wish the International EPR Society continuing success while working for the benefit of all of us.

Klaus Möbius
IES Vice-President 1997–1999

Some recollections as President and Secretary of the Society

When I was approached by Hal Swartz (or was it Linn Belford?) in 1990 to be a Charter Board Member of the new International EPR Society, I was pleased to know this would be a society devoted to EPR that would not be overshadowed by the much larger NMR community. I had attended enough meetings to realize that the NMR community was always going to be many times larger than the EPR community. I was therefore, very happy to have my name associated with this new Society.

Here in Australia in the early '90's, I undertook to be Regional Treasurer and we established a local IES Bank Account. After some years Graeme Hanson took over. Now with credit card arrangements in place, there is probably less reason for having a Regional Treasurer here these days.

Early in September 1997 I received an email from Keith McLauchlan, former IES President, asking if I would consider becoming Secretary as Arthur Schweiger wanted to step down. After pondering his email for a while I realized that Keith was visiting my alma mater, the University of Canterbury in Christchurch, New Zealand! So in my reply I said something like "*I'm delighted that you are visiting my home town*". Keith responded immediately with, "*If this is your home town, why ever did you leave?*" Part of that story has been told a few times in *EPR newsletters*. After a day or so I replied to Keith saying that I would be pleased to become Secretary to the Society. I had had some hesitation as I was already Vice-President of the Australian Institute of Physics and was to be President during 1999 and 2000.

A month later I was able to talk with Keith about the Society during the Spin Chemistry meeting in Jerusalem, organized by Haim Levanon. My return journey took me to Urbana, where I met with my old friend, Linn Belford, and also Becky Gallivan, who really did the administration. From there I visited Milwaukee to meet with Balaraman Kalyanaraman and Chris Felix to discuss the parlous state of the finances and the poor rate of dues payments and what we might do about that. I was unable to meet face-to-face with the then President, Jim Norris, as he was on a sabbatical in Japan at that time.

Then, in December 1997, I attended the ANZMAG meeting on Fraser Island, off the coast of Queensland where Arthur Schweiger was the keynote EPR speaker. Over dinner one evening, he handed me a folder containing a small number of documents with the words, "*It won't take much of your time!*" I have heard that kind of thing a lot during my career and have often been foolish enough to believe it, though always knowing deep down that it is never true!

The following April [1998], on my way home from the UK ESR Group Meeting in Manchester, I stopped off in Chicago for an Executive Meeting. Those present were Jim Norris [in the Chair], Linn Belford [as Editor of the *EPR newsletter*], Chris Felix [Treasurer] and I. Becky Gallivan and Martha Moore, both of whom were involved in IES administration, record keeping and in preparing the *EPR newsletter*, were also in attendance. Another Executive Meeting took place during the joint AMPERE/ISMAR Meeting in Berlin the following August. Jim Norris [in the chair], Klaus Mobius [Vice-President] and I were the only Office Bearers present. We invited Arthur Schweiger as former Secretary to attend.

On my way to the meeting, Tengize Sanadze from Tsibilisi accosted me and asked how he and his Georgian colleagues might become IES Members. He explained that they could not afford to pay the regular subscription but he asked if there was something they could do for the Society. Without thinking I remarked, "*The Society awards Medals but there are no medals!*" to which he replied, "*We could make medals*". So I reported this conversation to the meeting with the upshot that we decided to set up a competition for the design of a Society Logo.

Further, I reported that we were not operating according to the Constitution. So with Jim's encouragement I set about revising the Constitution so that it reflected what we actually did. My experience in this regard was previously limited to rewriting the Constitution of the University of Canterbury Athletics Club back in 1959; though at the time [1998] the Executive of the Australian Institute of Physics was starting to think about revising its Constitution. The revised document was circulated amongst past and present Office Bearers and a number of others including Wolfgang Lubitz. After some minor changes, the new Constitution was circulated to the Membership in time for a vote at the Annual Meeting of the Society in Denver during August 1999, when it was adopted. New features in the Constitution included the appointment of three Regional Vice-Presidents to represent, respectively, Europe, the Americas and the Asia-Pacific. This has ensured that all major regions of the world have a voice on the Executive irrespective of where the other Office Bearers are from.

As I was an Australian delegate to the International Union of Pure and Applied Physics Congress to be held in Atlanta during March 1999, I arranged to spend two days in Chicago on the way so that we could hold an Executive Meeting. Jim and Carol Norris kindly invited me to stay with them. At that meeting, we considered the several logos submitted for our consideration and in the end we accepted that submitted by Tengiz Sanadze which is what we see on the *EPR newsletter* today. Tengiz also submitted a sample medal about the size of a US silver dollar with the logo on one face. We all liked the idea but felt that the medal should be bigger. By the time of the Denver meeting in August of that year, Tengiz had produced medals not only for the 1999 medal winners but also for all past winners – some 30 in all! In addition to the presentations made to 1999 winners during the EPR Symposium in Denver, a great many past winners also received theirs during the Symposium Dinner. The remaining 15 or so medals were mailed to those unable to receive them in person.

A word about award presentations. One of the practices I instituted was to have prepared citations of about 2 minute's duration which are read at the time of the presentations. In this way we have been able to ensure that all winners receive a considered prepared statement about their work and the reasons for the award. Actually they receive two certificates – a formal one and the other containing the citation. It has ensured that presentations keep to time, very important for our Society which does not organize its own conferences, when piggy-backing on other conferences. We are indebted to other organizations such as AMPERE, ISMAR and the annual Denver Symposium for making it possible for our presentations to take place.

In my remaining time as President, I invested a good deal of effort in chasing up members to pay their subscriptions. This involved a lot of emailing but it worked. By the time I handed over to Yuri Tsvetkov in 2002, the Society had a bank balance of more than $US15,000. Interestingly, I found it necessary to adopt the same policy as President of the Australian Institute of Physics. It is amazing what a message from the President of a society can achieve!

My last important and very satisfying duty concerned the Editorship of the *EPR newsletter*. It was obvious that the team in Urbana could not continue for ever and Becky Gallivan was under pressure to back off from helping with IES administration. During the Voevodsky Conference in Novosibirsk in July 2002, I invited Laila Mosina to consider taking on the editorship of the Newsletter. She was at first reluctant, wondering if she'd be up to the task. A week or two later she emailed to say she would do it. We would all agree that she and her team have done an outstanding job. What more can I say?

I have counted it a great privilege to serve the Society as its Secretary and President. I thank all those who worked with me to make my period in those roles as enjoyable as it was challenging.

IES has fulfilled the hopes of the founders in giving the EPR community its own voice.

John Pilbrow
IES President 1999–2002,
Secretary 1997–1999

IES forever!

Sometime in the beginning of the 1990s, of the recent but already past century, I received a letter from Prof. Hal Swartz. He proposed to organize the International EPR Society. I remember enthusiastically supporting his idea. It was a very interesting period in my life. Not long before that, "perestroika" started in my country. In the institutes of the Academy of Sciences of the USSR the scientific collectives were electing their directors. I was elected director of the Kazan Physical-Technical Institute, named after E. K. Zavoisky, the pioneer of EPR. At that time, I proposed establishing the International Zavoisky Award and developed the idea to publish the international journal of Applied Magnetic Resonance. Imagine that at the same time Hal's proposal reached me! Of course, I supported the idea because it synchronized with my own desire to enhance the prestige of EPR as an experimental method with great prospects and vast potentials. The creation of the International EPR Society was a very important milestone on the way to achieve this aim. We gratefully acknowledge Prof. Hal Swartz's role in this for the international EPR community and the whole scientific community.

I think that the creation of the IES stimulated the creation of the regional professional associations of the EPR spectroscopists including: the Russian EPR Society, the Asia-Pacific EPR Society (APES) and the European Federation of EPR Groups. I would also emphasize the activities of APES on promoting the EPR research performed in their enormous region.

Talking about the IES, we should certainly mention the *EPR newsletter*. This publication plays an important role in the integration of the community of EPR spectroscopists worldwide.

I wish all colleagues good health and success.

Kev Salikhov
IES Vice-President 1999–2002

Sam Weissman and the *EPR newsletter*

It is my pleasure to accept the invitation to commemorate the 20th anniversary of the International EPR (ESR) Society. The excellent review article by Prof. Jack Freed (see *EPR newsletter*, 18/4, p. 3) demonstrates the contribution of the IES not only to the EPR field, but to the scientific community at large. My contribution will be presented by two anecdotes, which are related to someone I deeply admire.

For me, EPR spectroscopy goes jointly with Sam Weissman, who was honored by the IES gold medal, just a few years before passing away in 2007. Sam was a mentor to many students, postdocs and colleagues who walked by his office, always open. In this short communication I would like to show another side and less known aspect of his activities, where I consider Sam, not only as a scientific pivot, but also an expert in telling jokes.

I was lucky and fortunate to be a postdoc of Sam Weissman at Washington University (1969–1971). His office consisted of a working desk, a blackboard and a few books, lying on some shelves. All of our scientific interactions were carried out on the blackboard and napkins. It was difficult for me to follow his derivation, written on these two "important" items. I remember asking Sam "please do not erase the blackboard and keep the scientific napkins for me." The combination of optical and EPR spectroscopies was rather a new field, requiring advanced state-of-the-art electronics related to time-resolved EPR. I remember coming in the evenings and on weekends, repeating the experiments and the electronic setup. Sam designed the experiment; the electronic shop built the right circuits. The keychain in Sam's pocket was an integral part of the experiment. At this stage, I came to Sam asking him to recommend a book or a review article that will assist me. Sam's answer was typical: "Haim, I can not help you, I was born with it." Indeed, during our acquaintance, I learned that his response was absolutely correct.

In addition to being a brilliant scientist, Sam was gifted with a fantastic sense of humor. As a member of the American National Academy of Science, he hosted at Washington University a colleague from the Russian Academy, Professor Voevodsky. After dinner and some drinks, the scientific conversation became less formal. "Dear Professor Weissman, don't you think that Russian science is more dynamic than that of the American one." "You may be right" answers Sam, "but we know how to employ Fourier Transformation in our research".

These two examples are typical to Sam, a scientist and a "mench".

Haim Levanon
IES Secretary 1999–2002

On the 20th Anniversary of the IES

At the end of 2002, after long reflection, I decided to accept the proposal by John Pilbrow, then the President of the IES, to become the next President of the IES. I would like to emphasize, at once, that both John and Shirley Fairhurst (Secretary of the IES) have helped me immeasurably in my IES activities during my tenure, the period of 2002–2005.

Now, four years later, the role and influence that the IES plays in the life of the EPR community has become clearer to me – the international cooperation, the personal contacts of the IES members, the creation and support of an atmosphere of respect and benevolent criticism both at personal meetings and conferences, the acknowledgement of achievements by peers, and the joint search of the ways to further develop the method and its applications. I tried, as did all Presidents of the IES, to support this atmosphere in our community.

The major activity of the IES is the annual selection for the IES medals of the best works in various areas of EPR. The competition at this top-level of works is intense and the evaluation by our relevant committees, though complicated, is fairly weighed. I am most appreciative of the activities of Jack Freed, Brian Hoffman, S. Subramanian, Ron Mason, and Peter Dinse, Chairmen of the relevant committees, during my presidency.

Undoubtedly, one of my major decisions coordinated with vice-presidents was to transfer the editorial office of our publication, *EPR newsletter*, from Urbana to Kazan in 2002. I am proud that we made the right choice with the Editor-in-Chief. Laila Mosina demonstrates the best qualities of a highly qualified scientific editor combined with a deep and abiding interest in the future of EPR spectroscopy. Because of the high caliber of activity of Laila and her team of Associate Editors, Candice Klug , Hitoshi Ohta and Thomas Prisner (in former years also Graham Timmins and Takeji Takui), and the Technical Editor Sergei Akhmin, we have a quality publication which presents the activities of the IES and the EPR community on the whole.

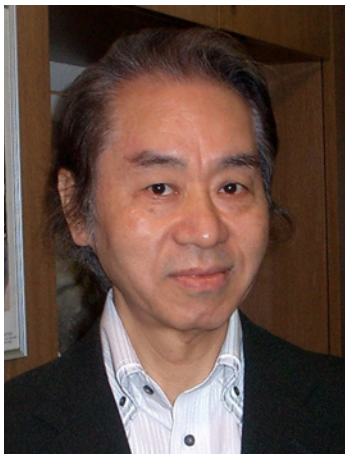
Three years ago I have transferred the powers of President to Wolfgang Lubitz who did an excellent job. Now, Jack Freed assumed the presidency from him and I congratulate Jack. I have known him for many years as an outstanding scientist and an organizer and I am absolutely certain that he will do much to strengthen the IES and its authority and influence in the international scientific community.

This year we celebrate a double anniversary: 65 years ago EPR was first observed by E. K. Zavoisky. Twenty years ago the IES was organized on the initiative of Harold Swartz. Through these years, EPR developed from single laboratory experiments

to a powerful method studying the structure and properties of matter and materials, kinetics and mechanisms of chemical and biological processes. EPR applications are surprisingly wide and diverse, including wide areas of human activity, from geology and materials science to history and medicine.

In view of the anniversary year I wish all IES members the best successes in science and strong Siberian health.

Yu. D. Tsvetkov
IES President 2002–2005



In Celebration of the 20th Anniversary of IES, from the Japanese ESR/EPR Community

I, as Founder President of The Society of Electron Spin Science and Technology (SEST), would like to celebrate the 20th anniversary of the International EPR (ESR) Society. The last two decades, through the successive presidents and officers of IES, IES has won a worldwide reputation as the most active and influential group in the field of electron magnetic resonance. Particularly, among its accomplishments, the Society has stimulated scientific and technological progress in ESR (EPR) worldwide. I have imagined how hard the charter members and founder organizers of IES worked for IES to have become so influential that it now enjoys the present worldwide reputation. I did have an opportunity to work with Professor John Pilbrow, Former President of IES. John was really a global frequent flyer, willing to help scientists and researchers of the ESR community. I learned a lot from him under his unfailing guidance.

Especially, I came to see that the ESR community in Japan needed to take a more global view of our interaction with ESR communities outside of Japan. In terms of new waves of global standards in science in Japan, even among people in our ESR community, there had been many discussions which contained some seemingly controversial ideas. Professor Noboru Hirota, an IES Fellow, led us in many crucial ways through these discussions. Nearly three years and elaborate continuous talks among our ESR community resulted in the formation of SEST in 2002 with some explicitly stated missions.

SEST members represented all areas relevant to electron spin science and technology in pure and applied natural sciences. Our ESR community in Japan then began formal interactions with IES on many levels and our young scientists and graduate students began to enjoy easy and frequent meetings with distinguished scientists of the worldwide ESR community. The situation reminded me of the kind of impact that I felt when I first "saw, met or talked with" Klaus Moebius, Jack Freed, the Late Daniel Kivelson, Peter Atkins, Charles P. Scholes and many MRI people in Banff in 1976, when I was young and all of them were young as well. During this first international conference that I participated in, I learned of their eagerness and passion for science at extraordinary levels. I believe that it is this in particular that is the most important for young Japanese students – to build up their own international benchmarks to accomplish their scientific activities. Their involvement, while they are young, with this international scientific community and its personal connections can have a significant impact.

I trust that IES will continue to serve as such, as an international center for the young scientists and students, to advance all aspects of electron magnetic resonance spectroscopic technology and to foresee future progress in electron spin science and technology.

Finally, in closing, I must express the appreciation of the Japanese ESR community for all of the effort and conscientiousness of Laila Mosina and the founder/charter editors of The *EPR newsletter*.

Takeji Takui
IES Vice-President 2002–2005

Are you interested in becoming 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

20th Anniversary of the International EPR(ESR) Society: A personal perspective

This year the International EPR/ESR Society is celebrating its 20th anniversary. It was founded in 1989 in Denver at the Annual EPR Symposium of the Rocky Mountain Conference on Analytical Chemistry stimulated by a proposal of Hal Swartz, who also became its first president. After Keith McLauchlan, Jim Norris, John Pilbrow, Yuri Tsvetkov, Wolfgang Lubitz our current president is Jack Freed, and after 20 years it is time to look back on the IES and the development of EPR. Since these 20 years exactly parallel my own career as an EPR spectroscopist I will try to do this flashback from a very personal perspective.

It was exactly 20 years ago that I left my home town and Alma Mater, the Free University Berlin, where I had worked during my PhD and Habilitation with Harry Kurreck and Klaus Möbius and, after my postdoctoral time with George Feher, also as a young assistant professor. From there I accepted my first permanent position as a professor in the Physics Department of the University of Stuttgart. This institute was headed at this time by Michael Mehring, who developed and applied both NMR and EPR in his laboratory. This was an exciting time in a physics department, with excellent workshops and facilities and many ideas floating around in the NMR group – where pulsed and FT methods were already the standard – stimulating new developments also in EPR spectroscopy. Peter Höfer had just finished his PhD with Mehring, pulse ENDOR was used extensively and HYSCORE was developed during this time. In my group we were still doing mostly cw EPR and ENDOR with applications to photosynthetic systems.

The year 1989 also marked dramatic political changes in Germany with the silent revolution in the East, the opening of the wall and soon after the peaceful reunification of Germany. This had a profound impact on the German universities and research institutes in the East and West. Only two years later I moved from Stuttgart back to Berlin – the old and new capital – and started to build up our EPR laboratory at the Technical University Berlin with the help of Friedhelm Lendzian, Robert Bittl and several other coworkers from Stuttgart who went with me to Berlin. It was during this time that commercial pulsed EPR equipment became mature, and we acquired a Bruker pulse EPR/ENDOR X-band machine. Later on we obtained the first Bruker W-band instrument sponsored by a large equipment grant from the DFG. The development of high-field EPR had a profound effect worldwide, which is seen from the steep rise of publications in this field after 1990.

I vividly remember when my colleague Dieter Ziessow at the TU Berlin asked me to chair the joint ISMAR-Ampere Conference together with him at the TU Berlin. We went together to the 1995 ISMAR Conference in Sydney to present the concept and were successful. The joint conference took place in summer 1998 in Berlin and was a great success with close to 900 participants from both NMR and EPR. A large number of prominent scientists from around the world attended this conference. Berlin as a gateway to the East attracted many scientists from East Europe, in particular the former Soviet Union. This country had – and still has – a large EPR community with a tradition going back to the first experiments performed 65 years ago by E. K. Zavoisky in Kazan. It was also in Kazan where in 1989 a new journal, *Applied Magnetic Resonance*, was announced by the chief editor Kev Salikhov; the first issue appeared in January 1990. This was the first journal published in Russia entirely in English. Thus, we are also celebrating the 20th birthday of *Applied Magnetic Resonance* this year.

Ten years ago I decided to leave Berlin and soon after started to work at the Max Planck Institute for Radiation Chemistry (later renamed Max Planck Institute for Bioinorganic Chemistry) in Mülheim/Ruhr. The resources of the Max Planck Society allowed us to develop better equipment together with the permanent staff scientists, technicians and excellent workshops. We succeeded to set up a large multifrequency EPR laboratory in Mülheim, as the central part of the biospectroscopy facility. This opened the possibility to tackle more complex systems, e. g. metalloenzymes like wateroxidase and hydrogenase and related biomimetic systems.

A very important development parallel to EPR spectroscopy took place at this time in the field of quantum chemical theory, where DFT methods were increasingly used to not only calculate energy minimized structures but also spectroscopic parameters, e.g. by the group of Frank Neese in our institute. The concerted use of advanced experimental and theoretical methods allowed us to determine reliable structures of reaction intermediates, e.g. in enzymatic processes. This forms the basis for the elucidation of the underlying reaction mechanisms. The high time resolution of transient or pulsed EPR makes it possible to follow the dynamics of species in fast reactions on a nanosecond time scale, e.g. in photoinduced processes. The combination with NMR – in form of ENDOR spectroscopy – opens the possibility to resolve the nuclear hyperfine and quadrupolar structure, even of large and complex species living only a few microseconds. Thus information about the local characteristics of the electronic wavefunctions of such transient systems is obtained. The dynamical range that can be studied by these techniques covers many orders of magnitude including the interesting range where most chemical reactions occur. In molecules with more than one paramagnetic center distances and orientations of these spin-carrying domains can be determined by PELDOR/DEER spectroscopy. The technique of spin labeling – e.g. using nitroxide radicals or paramagnetic ions – opened new vistas of EPR by allowing also the investigation of diamagnetic systems. The sensitivity of these methods allows distance measurements up to 80 Å in favorable cases. All these applications make EPR a powerful and in some respect unique technique to gain insight into the spatial and electronic structure of paramagnetic systems and their dynamical behavior.

Many scientists in their various fields now start to realize the power of EPR and related methods; thus the number of applications is constantly rising. Clearly, the foundation of the IES 20 years ago has been a very important milestone in this development of EPR in all its facets. The presidents and other members of the IES Executive have enormously helped to advance the field by providing a central voice for the EPR community, and by stimulating new developments and applications. Not less important are the educational programs on EPR stimulated by IES members and officers thereby fostering personal contacts between students and scientists

around the globe. The IES bestows medals and fellowships upon EPR scientists who have contributed substantially to the progress of EPR. This award program enhances the visibility of EPR in the general magnetic-resonance community. It is also very stimulating for young researchers and senior scientists alike. In recent years the IES has become even more interdisciplinary encouraging applications in such diverse fields as spin physics and chemistry, material science, enzymatic reaction mechanisms, structure determination of macromolecules and medical imaging, just to name a few. A very important part in the development of EPR spectroscopy has also been played in this respect by the *EPR newsletter*. This periodical was founded by Linn Belford right from the beginning of the IES. Since 2003 it is being edited by Laila Mosina and her crew and published in a new format. Laila has to be congratulated for her impetus and efforts to steadily improve the quality of this IES publication.

EPR is clearly the most versatile method to study paramagnetic systems, both stable and transient, on the molecular and nanoscopic levels and time scales of pico- to milliseconds. Therefore, it is frequently used in many areas of physics, chemistry, geology, biology and medicine. A particular advantage is the possibility to study liquid and solid samples, single crystals and whole cells. Even entire biological objects can be studied through EPR imaging and spatially resolved spectroscopy, an area of increasing importance in the medical sciences. I am therefore convinced that modern EPR has a great future. Last but not least it is a great subject to study for the young generation. Students will frequently work in an interdisciplinary environment, get to know a modern spectroscopic technique with all its facets, learn data analysis and interpretation, which often includes modern quantum mechanical calculations and molecular modeling. To me this is an ideal field to work in that will provide a broad education at the interface of several scientific disciplines.

I would like to congratulate the IES on the occasion of its 20th anniversary for the great work done during the past 20 years and I sincerely hope that this success story will continue.

Wolfgang Lubitz
IES President 2005–2008

My impressions of IES

My first contact with IES was during the 2nd Asia-Pacific EPR/ESR Symposium 1999 in Hangzhou, China, which started from the establishment of the Asia Pacific EPR/ESR Society (APES) in 1997 by the Founder President Prof. Rudowicz. Prof. Pilbrow, President of IES at that time, provided some introductory comments about IES during his speech at the reception. I received a membership form from him at the end of the reception and joined IES after the symposium.

To confess, I did not know about IES at all before 1999. One of the reasons for this is that EPR/ESR scientists in the field of physics in Japan had almost no contact with EPR/ESR scientists in the field of chemistry in Japan, who had more contact with IES. However, the situation started to change after the 3rd Asia-Pacific EPR/ESR Symposium, October 2001, Kobe, Japan. I helped Prof. Kawamori, the chairperson, to organize the symposium as a secretary general, and this symposium was almost the first occasion where the EPR/ESR scientists from Japan in the fields of physics, chemistry, biology and medicine joined together. This symposium provided the impetus for the establishment of the Society of Electron Spin Science and Technology (SEST, Japanese EPR society), and the attendance of IES President, Prof. Pilbrow, promoted this closer affinity to IES in APES scientists. The custom continued at the 4th (2004, Bangalore, India) and 5th (2006, Novosibirsk, Russia) APES symposia with the presence of IES Presidents Prof. Tsvetkov and Prof. Lubitz. At this same time, APES became an affiliated society of IES due to the efforts of Founder President of APES Prof. Rudowicz. Moreover, IES silver medalists from the Asia-Pacific area, including myself, feel honored and our efforts recognized. And, our recognition by IES was a source of encouragement, especially for young APES scientists.

From my experience as President of APES (2004–2008), I feel that strengthening the link between IES and APES or the EPR Society of each country, for instance SEST or the Indian EPR Society, will stimulate increased activities of the EPR/ESR society. In that sense, I think the idea of Prof. Lubitz, Immediate Past President of IES, to hold the IES Annual Meeting not only in North America and Europe but also in the Asia-Pacific area is a good move. The 2008 IES Annual Meeting was held during the 6th Asia-Pacific EPR/ESR Symposium, July 2008, Cairns, Australia, and the new IES Executives were announced. I hope such a move will continue with the new IES Executives, and it will open a brighter future for IES world-wide.

Hitoshi Ohta
Kobe University

On behalf of the Asia-Pacific EPR/ESR Society (APES), I would like to congratulate the International EPR/ESR Society on its 20th anniversary.

APES was created in 1997 with the aim to promote EPR studies in the countries of the Asia-Pacific region. At present, Japan, Russia, China, India, and Australia are its active members. The most important activity of APES is the organization of biannual conferences. APES positions itself as a part of international EPR community, therefore these conferences are attended by many scientists from Europe and USA.

We wish your society success and are looking forward to the further strengthening of the productive cooperation between EPR spectroscopists of different countries.

Sergei Dzuba
President of Asia-Pacific EPR/ESR Society,
Institute of Chemical Kinetics and Combustion,
Russian Academy of Sciences, Novosibirsk, Russia

Groupement AMPERE

On the occasion of the 20th anniversary of the International EPR (ESR) Society I wish to extend my heartfelt congratulations on behalf of Groupement AMPERE.

As a European organization dedicated to the whole of Magnetic Resonance, Groupement AMPERE has always included EPR spectroscopy as a vital part of its activities, as is apparent from several Specialized Colloquiums on this subject. Many members of the International EPR (ESR) Society are also members of Groupement AMPERE. We feel that both our organizations could profit from further coordination of their efforts.

For your endeavor of supporting communication among EPR spectroscopists and shaping the future of this interesting field of research we wish you much success.

Gunnar Jeschke
Secretary General, Groupement AMPERE,
Laboratory of Physical Chemistry, ETH Zürich

The International EPR/ESR Society celebrates its 20th anniversary. Initiated at the Rocky Mountain Conference in 1989 by Hal Swartz, who also became its first president, the society today is as lively as ever. The activities

range, amongst others, from editing the *EPR newsletter* to selecting honourable prize winners. For an outside observer the *EPR newsletter* is certainly the most visible activity. It became a communication platform which is recognized worldwide and is the figurehead of the IES.

The Society's 20 years have closely matched Bruker's development and popularization of commercial pulse EPR. The IES community has inspired us and initiated many new developments. We have utilized the *EPR newsletter* to inform the readers and our customers about our latest developments, such as W-Band, DEER, pulse Q-Band, EPR Imaging and now 263 GHz spectrometers.

The whole EPR community is using the *EPR newsletter* as a platform to advertise positions,

sell used equipment and report on conferences. Credit has to be given to all those who write scientific and tutorial articles giving insight into sometimes controversially discussed topics. Bruker has been proud to underwrite the distribution costs for the Society.

The enormous efforts by Laila Mosina to put together an attractive issue each time has to be acknowledged greatly. We hope that the IES and the Newsletter stay as active as now for many more years and congratulate to the first successful 20 years.

Art Heiss
Peter Höfer
Dieter Schmalbein

EFEPR

Dear *EPR newsletter*,

It is a great moment to congratulate you on the 20th anniversary of the day that Linn Belford has brought you into life to strengthen the worldwide community of researchers using EPR spectroscopy. Indeed, the news and information that you brought to all of us over the years has been an important ingredient for the healthy development of this community, showing how others were applying the EPR methods, keeping us aware of the important events such as conferences and schools, and publicizing the activities of the International EPR (ESR) Society, in particular the medals, awards and fellowships. The latter was coming with a very precious human touch, as those involved were offered a forum for their ideas and personal interests. It is no wonder that the thriving forces that have been fostering your success, Prof. R. Linn Belford and Mrs. Rebecca J. Gullivan, have been honoured with Special Gold Medals for Distinguished Service at the Denver meeting in 2002.

It is obvious that as a teenager you have lived an amazing transformation, turning into a quite sexy appearance (I hope you can forgive me this expression). Indeed, in full colours and with a lay-out throwing into the shadows most of the other journals we (have to) read, you were made ready for at least another fifteen years of success. While growing up in Urbana, IL, USA, you decided to go international, taking Kazan – where EPR was discovered – for your residence, having a website in ETHZ, Switzerland, and rolling out of printing offices back in the USA, …, quite remarkable! You give us also more than before a sense of perspective in the evolution of EPR methods, and in the experiences of younger and more experienced EPR spectroscopists with the new items, Another passion, Anecdotes, YIA revisited, …, while keeping high the standards for the news and professional information. Your total makeover did not happen accidently, you owe it indeed to the very international editorial team under guidance of Laila Mosina, her assistant editors, nowadays Candice S. Klug, Hitoshi Otha, Thomas Prisner (also previously: Graham Timmins and Takeji Takui), and last-but-not-least the Technical Editor: Sergei M. Akhmin. There is no doubt that this team deserves our admiration and gratitude for their continuing service to the IES and its members.

At this point let me, in the name of the European EPR community gathered in EFEPR, wish you a splendid future as the newsletter of the international community of EPR spectroscopists, with many more years to come in which you can continue to foster the relationships between scientists over the whole world. Sincerely,

Etienne Goovaerts
President of the
European Federation of EPR Groups
www.physics.ua.ac.be/EFEPR

ISMAR

On behalf of the International Society of Magnetic Resonance (ISMAR), I would like to send my greetings to the International EPR (ESR) Society on the occasion of its 20th birthday.

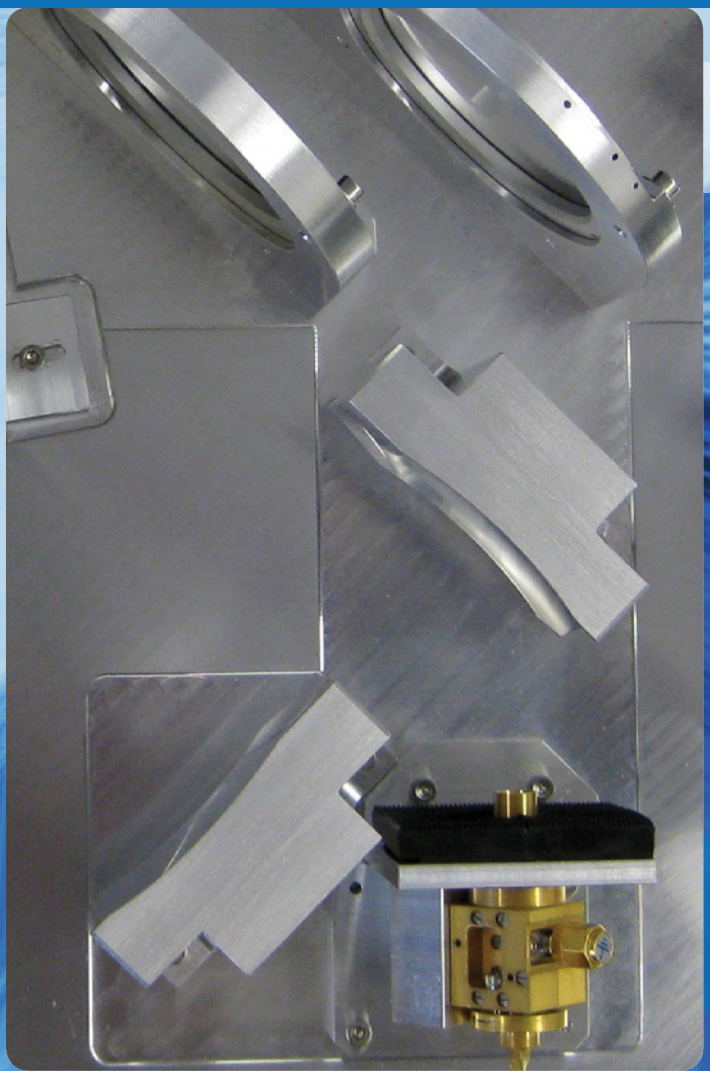
As you know, ISMAR has always embraced EPR/ESR as a vital part of worldwide magnetic resonance, acknowledging the proud history of EPR and its origins in Kazan before the first NMR experiments were performed in condensed matter.

We are proud to count among our Members and Fellows some of the leading experts in EPR world-wide.

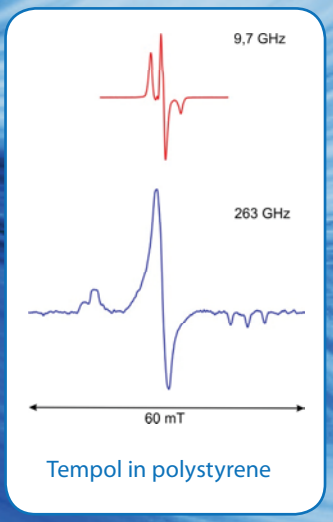
We wish your society a prosperous and active future in this exciting field of scientific endeavour.

Paul Callaghan, President, ISMAR
School of Chemical and Physical Sciences
Victoria University of Wellington, New Zealand

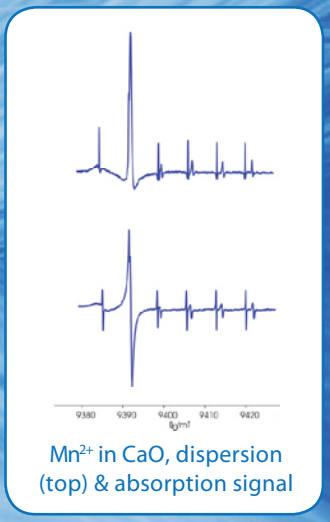
Bruker **BioSpin**



Routine mm-wave EPR!



Tempol in polystyrene



Mn^{2+} in CaO, dispersion (top) & absorption signal

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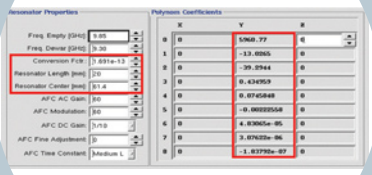

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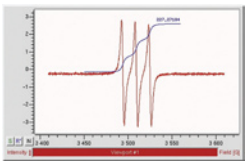
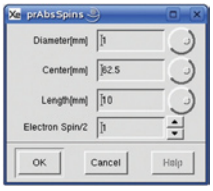


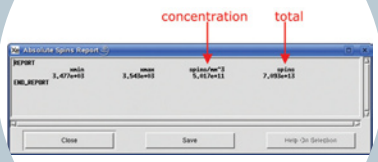
New tool for high precision double integration

User Input



Minimum user interaction

Software Reporting



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think forward

EPR Solutions

2009 IES Silver Medal for Chemistry to Takeji Takui

Takeji Takui (Specially Affiliated Professor, Emeritus Professor, Osaka City University) obtained his BEng, MEng and DEng (1973) degrees from Osaka University. He has applied modern EPR spectroscopy to molecular chemistry and materials science to study organic molecule-based magnetism. Prof. Takui is one of the world leaders in electron-spin science, not only in the application, but also in the development of new methodology and spin technology in EPR spectroscopy. Especially significant to note is Prof. Takui's contribution to the establishment of the high-spin chemistry underlying organic molecular magnetism by his pioneering research on EPR/ENDOR spectroscopy of electronic structures of high-spin molecules and their clusters. These studies are also important for the emerging spin technology of quantum computers and quantum-information processing.

In recognition of his many contributions to high-spin chemistry studies in EPR, Professor Takeji Takui eminently deserves the 2009 Silver Medal for Chemistry of the International EPR (ESR) Society.

2009 IES Silver Medal for Biology and Medicine to Garry Buettner

Garry R. Buettner (Professor, Radiology Oncology, College of Medicine, The University of Iowa) has advanced EPR spectroscopy in Biology and Medicine by his fundamental contributions. He was the first to spin-trap superoxide produced by xanthine oxidase. This experiment is undoubtedly the most repeated experiment in all of EPR spectroscopy. To be successful he recognized and overcame several key issues with respect to the chemistry of DMPO and the superoxide spin adduct; especially important in this work, he discovered that low levels of adventitious catalytic metals, e.g. iron, could change the course of oxygen radical chemistry. His 1987 compilation of spin-adduct parameters in Free Radical Biology and Medicine and the subsequent Database have been invaluable for all EPR spectroscopists doing spin trapping. He introduced the concept that ascorbate is the terminal small-molecule antioxidant and that the EPR detection of the ascorbate radical can be used as a real-time indicator of oxidative flux in biological systems; he provided the thermodynamic and kinetic foundation for these fundamental advancements.

In recognition of his many contributions to advanced EPR spectroscopy, Professor Buettner eminently deserves the 2009 Silver Medal for Biology and Medicine of the International EPR (ESR) Society.

2009 IES Young Investigator Medal to Stefan Stoll

Dr. Stefan Stoll (Department of Chemistry, University of California at Davis, California) is certainly one of the most versatile and influential EPR spectroscopists of his generation. His contributions include new pulse sequences, new insights into spin dynamics in ESEEM experiments involving multiple nuclear spins and into the influence of nuclear spin relaxation on pulsed ENDOR experiments, application of advanced EPR techniques to transition metal complexes, spectrometer control software, and most importantly- the freely available software package EasySpin for simulation of EPR, ENDOR, and HYSCORE spectra in liquids and solids. EasySpin has by now become the standard program for spectrum simulation in many of the leading EPR groups worldwide. Currently the paper introducing this software gathers more than 50 citations per year. Last but not least, Dr. Stoll is an active and good teacher at EPR Summer Schools and workshops and an interesting and knowledgeable partner in scientific discussions.

In recognition of his many contributions to EPR spectroscopy, Dr. Stefan Stoll eminently deserves the 2009 Young Investigator Medal of the International EPR (ESR) Society.

Segre Prize

On behalf of the Ulderico Segre Family, GIRSE announces that the first SEGRE PRIZE has been awarded ex-aequo to

Dr. Reinout Declerck
of the University of Gent (Belgium) for his Doctoral Thesis "Development and implementation of theoretical methods for the calculation of EPR parameters in periodic simulations"

and to

Dr. Mirco Zerbetto
of the University of Padova (Italy) for his Doctoral Thesis "Advanced computational tools for the interpretation of magnetic resonance spectroscopies"

The winners will receive the prize during the VII EFEPR Meeting that will be held on September 6–11, 2009 in Antwerp (Belgium).

The Segre Prize Committee wishes to congratulate all the applicants for the outstanding quality of the works they submitted.

The Segre Prize was jointly established last year by the Segre family and GIRSE to honor the memory of Prof. Ulderico Segre (1946–2008) who passed away in early 2008.

Ulderico Segre was an Italian scientist whose research activity greatly contributed to the advancement of theoretical and computational modeling applied to magnetic spectroscopies.

The Prize, of the amount of 4000 Euro, is awarded on a two-year basis to an outstanding doctoral thesis in the field of theoretical and computational modeling and advanced methodologies for magnetic resonance spectroscopies.

Further details on the Segre Prize can be found at
www.chimica.unipd.it/~girse/girse.html

Prof. Gian Franco Pedulli
President of GIRSE

The Zavoisky Award 2009

Daniella Goldfarb

Weizmann Institute of Science, Rehovot, Israel

in recognition of her outstanding work in EPR, in particular her pioneering contributions to pulsed high-field electron double resonance methodology and applications in metalloproteins and zeolites

ISMAR International Society of Magnetic Resonance

Fellow of the International Society of Magnetic Resonance

Klaus Möbius

Free University Berlin, Berlin, Germany

in recognition of distinction in contributing to the field of magnetic resonance

Fellow of the International Society of Magnetic Resonance

Brian M. Hoffman

Northwestern University, Evanston, Il, USA

in recognition of distinction in contributing to the field of magnetic resonance

President

Secretary General

ISMAR is a society devoted to the advancement of magnetic resonance and its applications

IES Young Investigator Award Revisited

This column features former recipients of the IES Young Investigator Award.

In Resonance: From EPR to MRI

When Dr. Laila Mosina asked me to write a brief article for the IES Young Investigator Award revisited column I was a little hesitant at first. I missed the first deadline which we had agreed upon, but she insisted that I write a small column. She specifically asked me to write about my thoughts on my research, the IES award and my very simple life in science before and after this award. Our current IES's President stated that 'Laila Mosina has been a very dedicated Chief Editor since 2003', and I felt it would be my duty as a member of the EPR society to fulfill her simple request.

My previous research has focused on investigating the electronic and molecular structure of small molecules using optical and magnetic resonance spectroscopic methods, namely EPR, pulsed EPR and ENDOR. I have also extended my experience and interests into the structure-function relationships of biological macromolecules, particularly those of metal-requiring enzyme systems. Our work on enzyme substrate complexes, using chemical syntheses, cryoenzymology, spectroscopy, and state-of-the-art molecular graphics, provided the first direct structural characterization of a true, kinetically competent enzyme reaction intermediate in solution. I have also been involved in studies on the structural basis of insulin mimetic effects of vanadyl chelates of organic ligands with Marvin Makinen at the University of Chicago. Our research on the structure and activity of insulin mimetic compounds such as vanadyl chelates has led me to consider the use of analogous compounds for detection of metabolic activity in cancers.

It was really a true honor and privilege to receive the first Young Investigator Award from the EPR Society in 1994 (awarded in 1995). Since graduate school I have been trained in EPR, pulsed EPR and ENDOR spectroscopy (Dave Doetschman, Ph.D. advisor). I have learned so much not only from the renowned experts in the field, but also from my peers. The EPR society is more like an extended family; the annual meeting in Denver is like a big get-together, where people gather to discuss good science for a week. I have truly benefited from those discussions, and I've also met many outstanding scientists in the field of magnetic resonance spectroscopy. Two outstanding scientists in the EPR Society who have especially inspired me are the late Professor Clyde A. Hutchison Jr. of the University of Chicago and Professor Harden M. McConnell of Stanford University. When I was struggling with a fundamental question about the point-dipole approximation, even when the unpaired electron spin is not located in an s-orbital or an f-orbital, they were able to explain the concept to me in laymen's terms. This is just an example; I could bring up many similar valuable experiences such as this one. I feel very fortunate to be associated with the EPR Society.

I am now primarily involved in research towards developing cancer-specific contrast agents for magnetic resonance imaging (MRI). This research builds upon my previous experience as an EPR spectroscopist and biophysical chemist with expertise in structural biology, while taking my research in a new direction by focusing on biomedical applications.

Although I have had an ongoing interest in MRI for many years, my involvement in the development of MRI contrast agents has greatly increased over the past few years. Recently, I have been collaborating with Professor Gregory Karczmar at the University of Chicago. We took on a pilot project on the anti-angiogenic effects of green tea, wherein we used functional and anatomical MRI methods to evaluate the effects of green tea on angiogenesis in rodent prostate tumors. These studies led me to think about using vanadyl complexes for selectively detecting cancer and monitoring metabolic activity. I became motivated to change the focus of my research, because I saw the possibility of developing targeted MRI contrast agents that could have a direct impact on patient care. I felt that doing more translational and applied research would be an exciting way to use my background in physical biochemistry. I also felt that the combination of my previous experience with my new training in MRI physics and cancer biology would allow me to make significant contributions to clinical care.

I am now involved in three main avenues of MR imaging of cancers. First, as mentioned above, I'm investigating the development of improved vanadyl based MRI contrast agents that would enter into cancer cells with high glycolytic activity and could provide high-resolution functional images of tumor boundaries and internal structure, which cannot be achieved by conventional contrast agents. Second, I'm researching the development of improved MRI methods that would detect colitis (colonic inflammation) and monitor the progression of colitis to colorectal cancer in a clinically relevant murine model. Non-invasive MRI studies of colitis and early colorectal tumors in mice will improve understanding of this disease, guide development of new therapy, and produce new MRI markers to improve diagnosis. Third, I have been developing an improved method for making agar phantoms for MRI that mimic human tissue in terms of their relaxation pathways, including T_1, T_2, and T_2^*, and other magnetic interactions. Agar phantoms have potential advantages because they can be designed to mimic human tissues. However, air bubbles in agar present an important challenge to the development of agar-based phantoms. Air bubbles produce large susceptibility gradients, leading to distortions in the images that would render these phantoms un-usable. Homogeneous and heterogeneous agar phantoms, free of air bubbles, will assist in the standardization of scanner performance and assist in quantitative measurements of contrast media concentration as a function of time after injection.

And now I'd like to end my column by expressing how delighted I am to contribute to the IES's newsletter. I wish the best for this great society of ours and for my fellow members. Cheers!

Devkumar Mustafi
The University of Chicago
dmustafi@uchicago.edu

80th Birthday of John Weil

It is an honor and pleasure for me to write about my friend John Weil, who will be celebrating his 80th birthday in March 2009.

Professor John Weil is certainly well known in the EPR/ESR community, and has many friends around the world. His research and personal interests are eclectic. Hopefully the discourse below will illustrate his broad range of interests.

John A. Weil (born 1929, Germany) took his Ph.D. in Chemical Physics at the University of Chicago (1955), under the tutelage of Professor C. A. Hutchison Jr. His doctoral thesis dealt with then-unknown triplet states in aromatic molecules, and with spin concentration analysis in free radicals.

Dr. Weil then spent two years as a Corning Post-doctoral Fellow in the Department of Chemistry, Princeton University. He set up electron paramagnetic resonance (EPR) spectroscopic equipment and worked with gas adsorption on charcoals as studied by EPR spectroscopy. He stayed on for two years as Instructor in Chemistry in the Chemistry Faculty, was involved with a number of Physical Chemistry Courses, and created his own research program. He spent summers at the Mellon Institute as Visiting Fellow, sponsored by the Pittsburgh Plate Glass Co. His research interests in silicate systems originated during this period.

In 1959, Dr. Weil accepted a staff position at Argonne National Laboratory, and became a Group Leader soon thereafter. He set up an EPR/ENDOR laboratory, and initiated studies of magnetic defects in irradiated covalent solids. Dr. Weil spent one year away from ANL as a Fulbright Scholar at the Department of Physics, University of Canterbury in New Zealand (1967–68). Besides teaching several courses there, he began a (10-year) theoretical study of the effects of crystal symmetry on magnetic resonance spectra, and was involved as well in several experimental projects. After 12 years at Argonne, during which he progressed to the Senior Scientist rank, Dr. Weil moved to the University of Saskatchewan (1971) in Saskatoon, Sask., Canada to take up a tenured Professorship in Chemistry.

Since coming to Saskatoon, until his retirement, Prof. Weil was heavily involved with teaching, and of course research. Several generations of graduate students were trained in Prof. Weil's laboratories. His research efforts centered on the defect structure of crystalline quartz (a very important industrial material), plus sophisticated theoretical and free-radical studies.

Prof. Weil has collaborated actively with various other research groups, in France, Germany, in Japan and Korea, in New Zealand, and in the USA, and continues to do so. His group's quartz work, including frontier techniques, such as pulsed microwave and optical detection as well as large-scale Hartree-Fock cluster modeling, has gained international recognition, particularly also in view of the applied importance of this material. It is Prof. Weil's intention to continue this program as his primary one, ongoing and expanding, and he visualizes decades of exciting developments in it. Certainly the progress and success of his research constitutes his highest priority. As a result, approximately 150 publications have appeared, so far.

Prof. Weil, as the senior author, has completed an introductory text to the field of "Electron Paramagnetic Resonance", first published in February of 1994 by John Wiley & Sons, as a totally revised 2nd edition of the 1972 book co-authored by J. E. Wertz and J. R. Bolton. Since demand materialized, there now is a new much-updated edition, under the authorship of J. A. Weil and J. R. Bolton, which appeared in early 2007.

A major computer program, EPR-NMR, developed by Prof. Weil's group to do advanced analyses of magnetic resonance spectra, is now being used internationally by 200+ research groups. Relevant to this, a review article "The Simulation of EPR Spectra" by him appeared in 1999.

In 1983, Prof. Weil was elected Thorvaldson Professor of Chemistry (five-year term) at the University of Saskatchewan. A D.Sc. degree was awarded to him by the same institution, in 1985.

Prof. Weil also is involved in various extra-scientific activities. One notable one is his interest in the cultural aspects of crystalline quartz, ranging from anthropological/archaeological aspects to visual aesthetic ones. A bibliography (2500+ references) has been copyrighted, and various articles and books on these topics are planned. A venture in Northern New Mexico has led to discovery and characterization of a buried shamanic kit, containing a quartz-crystal fetish of the Largo-Gallina culture.

Prof. Weil was selected to be the 1996 Distinguished-Researcher Awardee at the University of Saskatchewan, in the spring of that year. As of July 1, 1996, he formally retired and began his career as Professor Emeritus there. In 1999, he was elected to be a Fellow of the International EPR Society. In 2000, he was awarded the Gerhard Herzberg Award by the Spectroscopy Society of Canada.

Prof. Weil at this time has only minor support funds from Canadaís research agency, but continues seeking to improve this situation. Happily, other support has materialized at times.

More details of all recent publications can be found on Prof. Weil's Websites:
http://chm15127.usask.ca/ &
www.usask.ca/chemistry/weil.html.

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40th Anniversary of the ESR Group of the Royal Society of Chemistry

E. K. Zavoisky first observed an EPR signal in January 1944 but it was some years before EPR spectroscopy became important to Chemists and Physicists. In Britain, the first formal meeting on magnetic resonance seems to have been in Oxford in 1956 (see *EPR newsletter* 16, 13–14 (2006) attended by about 50 people, covering both nuclear and electron magnetic resonance in half a day! After this time, the two disciplines followed their separate ways but with ESR spectroscopy often forming part of early meetings and was mainly concerned with free radical Chemistry. NMR spectroscopists formed the NMR Discussion Group in 1964 – affiliating to the Royal Society of Chemistry (RSC) in 1970. The ESR Group became a subject group of the RSC in 1969, following a meeting in Southampton. Since 1969 the group has hosted forty-one international ESR conferences: generally held annually, in the spring, at a UK University. The meetings last for several days and cover theory and applications of EPR and related subjects usually centred around a few themes. A major strength of these conferences is that they are sufficiently small to enable scientists with very different interests and passions to meet, to talk and to exchange views and ideas.

Since 1986 the Conference is the occasion to annually award and host the presentation of the Bruker Lecture, sponsored by Bruker Biospin.

Bruker Prize Lecturers 1986–2009: Martyn C. R. Symons, Klaus Möbius, Hans Fischer, James S. Hyde, Jack H. Freed, Neil M. Atherton, Arthur Schweiger, Harden M. McConnell, Brian M. Hoffman, Keith A. McLauchlan, John R. Pilbrow, Jan Schmidt, Dante Gatteschi, Jürgen Hüttermann, Sandra and Gareth Eaton, Wolfgang Lubitz, Wayne L. Hubbell, Klaus-Peter Dinse, Yuri D. Tsvetkov, Daniella Goldfarb, Edgar Groenen, Gunnar Jeshke.

In 2007 the 40th meeting was marked by having as many of the previous Bruker Lecturers as possible attend and contribute.

With an eye to securing the future development of ESR, young postgraduate students and postdoctorate workers are en-

TAKEN BY SHIRLEY FAIRHURST

Bruker Prize Lecturers, Oxford 2007: Neil Atherton (1993), Jack Freed (1990), Gareth Eaton, Sandra Eaton (2002), Jan Schmidt (1999), Dante Gatteschi (2000), Daniella Goldfarb (2007), Keith McLauchlan (1997), John Pilbrow (1998), Yuri Tsvetkov (2006), Jürgen Hütterman (2001), Klaus Möbius (1987), Klaus-Peter Dinse (2005), Wolfgang Lubitz (2003)

couraged to present their work during the meeting. JEOL UK sponsor student lectures with the JEOL medal being awarded for the best oral presentation. The competition is between three students selected from those offering oral presentations and is restricted to 2nd and 3rd year Ph.D. students and postdoctoral workers in the 1st year of their research. Posters are always an integral part of the conference with the prize of a bottle of whisky for the best poster. The conference has a lively Social Program with several receptions, a sightseeing excursion, and a Conference Banquet.

This year the 42nd International Conference was hosted by the University of East Anglia (UEA) and took place on April 19–23 at the Ramada Hotel, Norwich. The 2009 Bruker lecture 'Measuring the nano-world' was presented by Gunnar Jeschke (ETH Zürich, Switzerland). Keynote lectures were presented by: Wayne Hubbell (UCLA, USA) 'Functional protein dynamics from site-directed spin labelling', Martin Kaupp (Universität Würzburg, Germany) 'Quantum chemical calculations of EPR parameters as a tool to study metalloenzyme sites', Richard Cammack (Kings College London, UK) 'Biochemical targets for advanced EPR weaponry' and Fraser MacMillan (UEA Norwich, UK) 'Correlating the structure and function of proteins using EPR'.

More information on the group and a full listing of conferences is available:

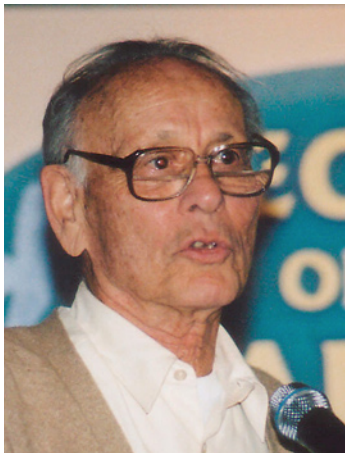
www.esr-group.org.uk

Shirley Fairhurst

Anniversaries

Five Years After

George Feher: An Interview to the *EPR newsletter*



EPR newsletter: *Dear Professor Feher, on behalf of the readers of the EPR newsletter we congratulate you on your 85th birthday. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science and why was it EPR?*

I was always wondering how things worked and was tinkering with electrical and mechanical gadgets since I was a small boy. Experimental science is just that - only on a more sophisticated level.

Where do you see EPR going?

I never considered EPR as a discipline by itself. It is a tool, among many others, to help solve problems. With the development of more sophisticated EPR techniques it is becoming a more useful and valuable tool. But it is the choice of the problem and not the tool that is of prime importance.

What do you think about the young generation of the EPR researches and what is your message to them?

My message to the young generation of EPR researchers is the same as to any other young researchers. Don't listen to us 'old fogies', go your own way and do things that the old generation says cannot be done.

In what way do you think your research ever influenced anybody in the EPR community?

That you really have to ask the members of the EPR community, preferably those who use ENDOR.

What would you have done if given a different opportunity?

It depends on the opportunity. But by and large, I prefer to pick rather than be given an opportunity.

Concerning the role of the IES in the life of the EPR community, I consider the most important part the Newsletter.

Software

Analysis of DEER signals with DEFit

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Motivation

Dipolar modulation data obtained from biological samples are often characterized by medium-to-high noise levels which render reliable analysis difficult. It is critical to determine the uniqueness of a best-fit solution and the associated parameter uncertainties. Statistical analysis is crucial when the background subtraction is imperfect, intramolecular distances are long (above about 3.5 nm), or the distance distribution is wide. Within the time domain, the sensitivity to long distances and broad distributions is low and the resolution can be obscured by experimental noise. This is a quite common situation in biological systems where low sample concentrations are common and molecules usually display large disorder to backbone dynamics or structural heterogeneity. In these cases it is of paramount importance to know the uniqueness (parsimony) of a determined best-fit solution, the associated errors and potential correlations between parameters describing the distance distribution.

Approach

We have attempted to address the above problems in a program DEFit for analysis of DEER signals (Sen, Logan, and Fajer 2007). The implemented approach uses Gaussian shaped distance subpopulations to describe the total distribution of distances between two spin labels. Although this is a model-dependent approach, it can approximate non-Gaussian distributions by overlapping Gaussian curves, analogous to the expansion of a complex shape in terms of Gaussian basis functions. DEFit tries several random parameter sets as starting conditions and finds the best solution by minimizing the sum-of-squares deviation using the Simplex algorithm. This combined Monte Carlo/Simplex approach is very robust and efficient and has been successfully used in fitting EPR spectra (Fajer, Bennett et al. 1990; Fajer, Fajer et al. 1990; Fajer 1994; Li and Fajer 1994; Sale, Sar et al. 2002; Sen, Sienkiewicz et al. 2006). The comparison to Levenberg-Marquardt (LM) optimization, NLS2NO, or "trust region" LM in its efficiency and accuracy was described in (Khairy, Budil and Fajer, JMR 2006). The current version of DEFit is available as a Matlab source code and is routinely used in our lab on Windows XP and Linux systems. The programs and a quick start guide are available at http://kadirilkersen.googlepages.com or http://fajerpc.magnet.fsu.edu.

F-Statistics

The objective in developing DEFit was to provide statistical analysis of data; hence it might be worthwhile to explain how the program evaluates the fits. The most important aspect is the evaluation of the number of Gaussians adequate to describe the solution. The program automatically tests distance distribution models with n = 1, 2, 3 and 4 Gaussians. After a series of random (Monte Carlo) trials for n Gaussians are completed, the program compares the results to the results obtained for $n-1$ Gaussians by calculating the F and P values. F is defined as the ratio of χ^2 values of the more complicated models to the less complicated model (2 Gaussians to 1, etc.). We use a normalized χ^2, defined as:

$$\chi^2 = \frac{1}{\nu}\sum\left(\frac{y_{data} - y_{fit}}{\sigma}\right)^2,$$

where ν, the degrees of freedom, corresponds to the number of data points minus the number of parameters in the fitting function. F itself is not used to assess the improvement of fit versus the cost of introducing additional parameters for more complex distributions, but it is used to calculate a probability (the P value) of the *null* hypothesis: "if the simpler model is really correct, what is the chance that you would randomly obtain data (for instance with a repetition experiment) that fits the more complex model better?" If the P value is greater than the accepted threshold of 5% (Hoel, Port et al. 1971), DEFit decides that the simpler solution ($n-1$ Gaussians) is correct. For P values lower than the threshold, DEFit concludes that the more complicated model is statistically better and increases the number of Gaussian in the next trial. This is analogous to using an L-shape curve with the number of Gaussians along the x axis and χ^2 along the y axis and letting the statistics decide whether the change in the slope of the curve warrants an increase in the number of components.

χ^2 Surface

Once the best number of Gaussians and the corresponding best parameter set are determined, the user needs to initiate the error surface calculations. Here DEFit generates a large family of solutions in a user-defined neighborhood of the best solution, and calculates χ^2 for each of them. The resulting χ^2 surface is then used to estimate the plausible solutions within the desired confidence limit (default is 68%), and hence the error value. Because the χ^2 calculation is normalized to degrees of freedom, the 68% confidence limit corresponds to the solutions in the interval between χ^2_{min} and $\chi^2_{min} + 1$.

Example

Figure 1 shows a comparison of analyses of two real data sets. The surface in Fig. 1C consists of the χ^2 values corresponding to the mean distance (r_0) and width (Δr) of the Gaussian curve it represents (Fig. 1B). The colored areas in the χ^2 surface plots

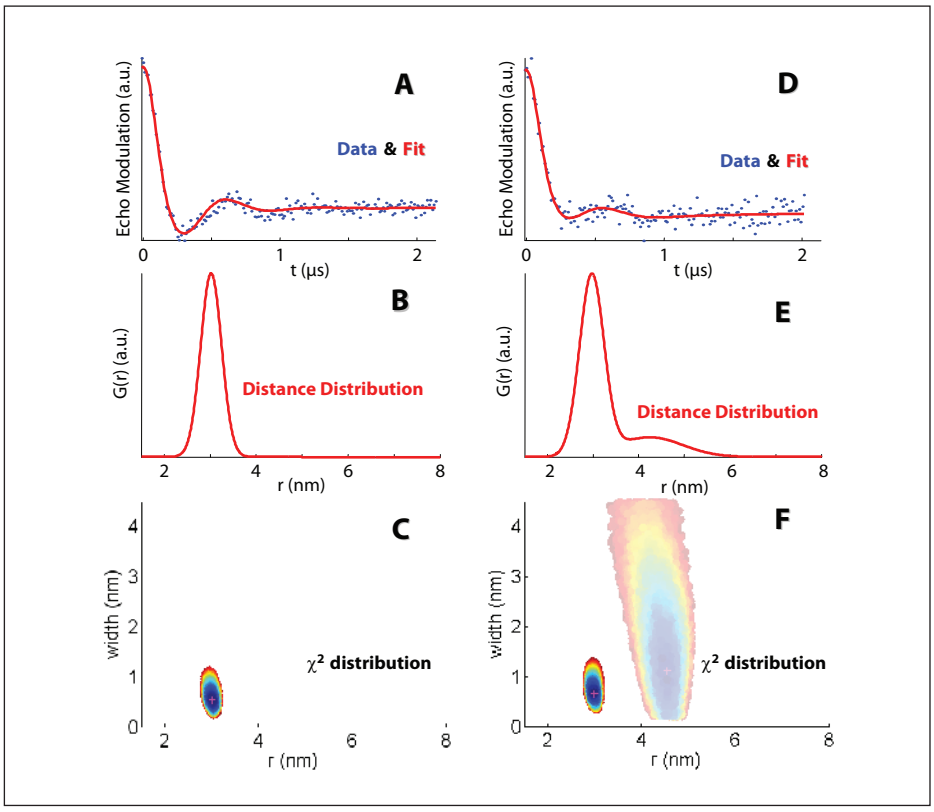

Figure 1: DEER time domain data (A-blue), least-squares fit (A-red), the corresponding distance distribution (B), and the χ^2 error surface of the fit (C) of two example data sets. The magenta cross in C denotes the location of the best solution (lowest χ^2). Dark blue points correspond to lower χ^2 values and red to higher ones. The color saturation reflects the relative fractions of population, with paler colors indicating lower fractional population.

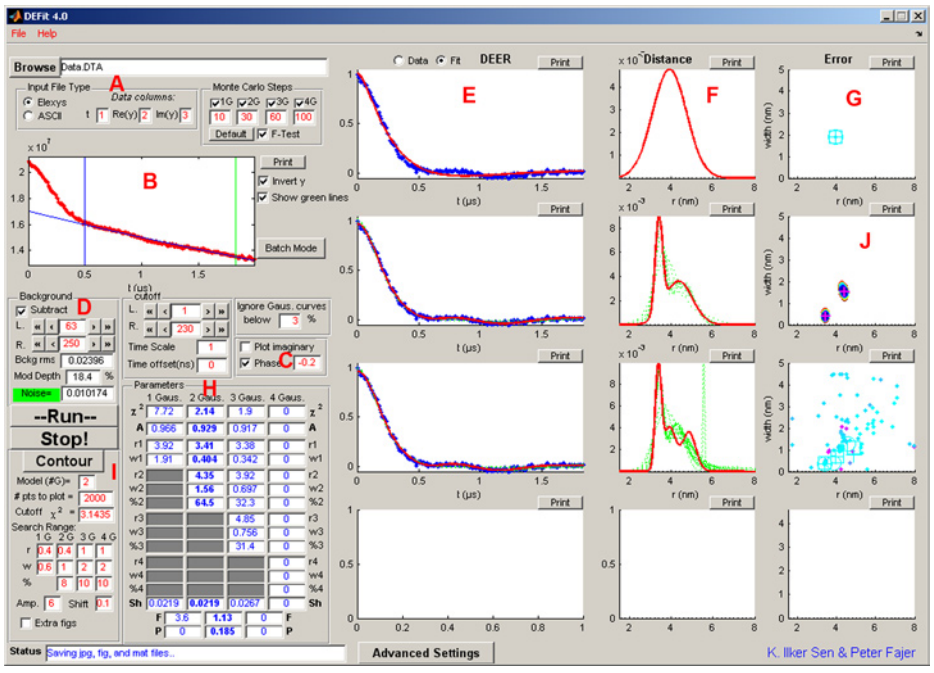

Figure 2: The graphical user interface of DEFit showing input file selection (A), input data (B), phase correction (C), background subtraction (D), background subtracted and normalized data (E, blue points), best fit to data -assuming 1 Gaussian shaped distance distribution - (E, red line), distance distribution (F), error plot showing overlapping circle, cross, and square, hence indicating a unique solution (G), parameters which yielded the best fit (H, selected number of Gaussians by F-test, 2 in this case, is set in bold), settings for χ^2 surface (contour) calculation (I), χ^2 surface of 2 Gaussian fit (J) showing narrow surfaces, which indicated well-defined solutions.

correspond to solutions within 68% confidence limit. The χ^2 surface on the left has one minimum – the distance distribution is described by a single Gaussian curve. The widths along r and Δr of the minima region represent the uniqueness of this solution. The χ^2 surface in Fig. 1F has two minima because the solution has two Gaussian populations as shown in Fig. 1E. The population with the shorter mean distance (≈3 nm) has a narrow χ^2 distribution, and hence it represents a well defined solution. On the other hand, the second Gaussian is not as well defined; the contours in the r axis are narrow imply a well defined average distance but the contours along the Δr dimension are broad, indicating large uncertainty in the estimate of the distribution width. The tilt of the distribution (not observed in Fig. 1) is indicative of parameter covariance.

Program Features

- System requirements: 500 Mb free memory, 2 Gb disk space, tested on Windows XP and Linux (Ubuntu); Matlab 7.0.4 and higher. A compiled version with runtime library can be provided on request.
- Input formats: Bruker Elexsys (DSC, DTA), ASCII (2 or 3 columns).
- Outputs: Matlab .fig and .mat files, screenshot (JPEG format), Excel file of results.
- Automatic or manual choice of number of Gaussian components (maximum: 4).
- Batch operation on all files in a given folder.
- 3D homogenous background subtraction.
- Phase correction.
- Adjustable data range analysis.
- User defined parameter space.

Usage Tips

The quick start guide which comes with the DEFit package is a reference on how to start using the program, and includes several useful tips. The CPU time increases significantly as the number of parameters increase (especially for models including 3 or 4 Gaussian), hence the users may want to fine tune the parameter space in the Advanced Settings. Depending on the data set, the default number of Monte Carlo Steps may have to be increased until there are multiple hits on the same solution. This is easily seen when the cross, square, and circle markers overlap in the Error plot. χ^2 distribution calculation also takes a significant amount of computa-

Tips & Techniques

Fitting Slow-Motional EPR/ESR Spectra: Practical Guidance and Guidelines

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Words of warning and encouragement

Fitting slow-motional spin label spectra can be an extremely useful technique for refining models of dynamic motion, which can in turn provide insight into function or mechanism. The widespread availability of least-squares slow-motional EPR programs on personal computers has significantly aided the quantitative interpretation of spin-label dynamics in many systems. At the same time, the ready accessibility of these programs has opened the door to a variety of misapplications. Here we offer some advice for avoiding common pitfalls in the application of least-squares analysis, and determining reliable fit parameters for some of the diffusion models that are commonly used.

Perhaps the most important point we can make is that fitting is not a substitute for physical understanding. Uncritical use of fitting programs will (almost) always give you an answer, but the first question to ask is, "Is it reasonable?". We encourage everyone who uses fitting programs to spend a fair amount of time constructing a model to test, including estimates of the relevant parameters. If the fit results are close to the predictions of the model, great! Or, maybe great. If you restart the fitting procedure from a different set of initial parameters does it converge to the same set of parameters or a different set? If different, how different? Do you understand all aspects of the output of the fitting program? For example, are there strong correlations among the fit parameters? Can you reparameterize your fit to reduce correlations? It can seem as if the list of questions to ask is dauntingly long.

We assume that most readers have access to a lineshape fitting program, such as NLSL [1] or EasySpin [2]. For the purposes of this note, though, it is more important to understand the theoretical notation commonly used in the field. Our recent review article may be of assistance to newcomers to the field [3].

Prepare

It's always wise to set yourself up properly before attempting a fit. Don't make the common mistake of forgetting to specify appropriate diffusion axes. You can control the transformation from magnetic axes to molecular axes by setting the diffusion tilt angles. If you keep the diffusion tilt angle β_D at its default value ($\beta_D = 0$) you're assuming that the fastest axis of rotation is along the magnetic *z*-axis, which only works for fatty acid probes. Most spin labels with a tether

DEFit Software DEFit Software DEFit Software DEFit

tional time. We recommend starting with 100–200 points to plot (and maybe a higher χ^2 cutoff) to get and idea about the range of parameters, then setting these in the Search Range and rerun with a higher number of points. Unchecking the Extra Figs and Autosave options in the Advanced Setting dialog will also increase the performance.

The companion of DEFit is CWdipFit, which analyzes the dipolar broadening in a cw spectrum. CWdipFit uses identical fitting algorithm and is also available on the website. We thank Dr. Likai Song for helpful discussions in developing of this program.

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have the principal diffusion axis closer to the N–O bind direction, which is typically the magnetic *x* direction! When in doubt, one common solution that often works for the popular MTSL spin probe is to set β_D to about 36° to represent the composite motion of the probe around the last two bonds of the tether [4].

If you want to explore the effect of more complicated diffusion tilts involving α_D or γ_D as well as β_D, remember that this comes with a price. Keeping the α_D and γ_D parameters at their default values of zero will reduce the size of the basis set required for the calculation, and your computations will run faster. So save α_D and γ_D for those occasions when you know or strongly suspect that β_D alone is insufficient.

As you refine your spectral fit, consider using the MOMD (microscopic order, macroscopic disorder) model. Most spin-labeled systems do exhibit local ordering of the spin probe. We suggest that an iterative approach is useful here. That is, it's often easiest to start with a simple diffusion model. In certain favorable cases, such a model may be all that's required, particularly if the motion is very fast or the ordering is very weak. In order to use the MOMD model, you must specify not only an ordering potential, the part that models the microscopic ordering, but also the number of domain orientations, the part that models the macroscopic disorder. If you forget to increase the number of domain orientations you will only calculate the spectrum of a single domain that is ordered relative to the applied field direction ($\psi = 0$).

Because spin-labeled spectra often do show local ordering effects, it is often worthwhile to explore the MOMD model, even if you achieve apparently satisfactory results with a simple model of diffusion. It must be admitted that the MOMD model does increase the computational burden, as it will multiply the number of spectra you have to calculate for each iteration of your fitting procedure by the number of orientations. On the other hand, if the more complex model is a more faithful representation of the underlying physics, your fitting results will be more reliable.

There are a couple of important things to keep in mind if you use an ordering potential. First, the ordering axis is assumed to coincide with the principal diffusion axis (*z*), so the c20 parameter will line the labels up along that axis. This generally works for tethered labels, but it may also happen that ordering occurs along another axis in the presence of steric effects, so don't be surprised if, say c22 ends up bigger than c20. Finally, if you do use an ordering potential, remember to increase the limit on the M basis set quantum number. The default for this index is two times the nuclear spin, and the common mistake of failing to change it will lead to unreliable results.

Don't use too many parameters

With all the fitting parameters at your disposal, it's tempting to over-fit your data. Remember that there's only so much information available from an EPR spectrum, so choose your variable parameters wisely and hold all the others fixed. There's almost never a good reason to vary magnetic parameters to fit a slow-motional spectrum. Always fix these by fitting a rigid limit spectrum of the system if you can.

Increase the number of fit parameters by small increments. It's best to work by making successive approximations to your spectrum, starting with the highest symmetry and adding symmetry breaking terms as necessary. For example, start out by fitting the spectrum with isotropic motion, then add axial anisotropy to improve the fit and rhombic anisotropy only if you have to. With care and caution, you can develop a parsimonious parameter set that will lead to efficient spectral simulation. Of course, if you know from modeling or prior experience on similar systems that a fully anisotropic rotational diffusion tensor is called for, by all means use one. The important point is that you shouldn't use low symmetry parameter sets without cause. The same thing holds true for potential coefficients: if you've got the geometry right, the lowest-order ($L = 2$) coefficients may be all you need.

Ockham's Hatchet

Where possible, look for ways to eliminate parameters (or components) from your fit. You can use the information available to you from the fit to guide your choices. It's very important to keep a careful eye on the covariance or correlation matrix of your fitting parameters. If you don't, you can fool yourself into thinking you know more than you do. If two fitting parameters (including scaling factors for individual components in a multicomponent spectrum) have a correlation greater than 0.85, it's time to consider folding them together into a single parameter. If your fitting program doesn't return a covariance matrix, get a fitting program that does. Your data deserves no less.

Know the limitations of model

If you've tried every imaginable combination of diffusion geometries, anisotropies, and components (which can be very time intensive, given the number of fit parameters that are available) and you're still not satisfied with the results, it may be time to reconsider whether the model you're using is really right for your data. Is there a possibility of some sort of composite motion in your system, which a simple diffusional model simply can't fit? If this is the case, you might want to consider a more complex diffusion model, such as the Slowly Relaxing Local Structure (SRLS) model. The Earle/Budil article provides some guidance on choosing parameters for the SRLS model [3]. If you think SRLS is relevant for your application, we encourage you to explore the relevant literature, much of which can be found at the ACERT website [1]. Software for using the SRLS model is also available at the ACERT website. For those whose experience with spectral fitting is limited, we urge caution before employing the SRLS model (see the section on Ockham's hatchet). However, if you know from modeling or prior experience on similar systems that SRLS is likely to be needed, we encourage you to explore the refinements that SRLS affords.

Check your results

After you've gone through the careful procedure we advocate to extract model parameters from your spectral fitting, you may find that you have a set of parameters that generates a calculated line that is barely distinguishable from your data, except for a modest amount of perfectly normally distributed noise. You may think that you're done. However, there are some important checks that you need to make. Never trust a minimum by itself. The smart thing to do is to get a feel for the likelihood of your parameters given the data, and that can take a lot of computation. One way that is not prohibitively expensive, is to restart your fit a couple hundred times (a fitting program that can be run from a shell script is a big help here) starting from parameters chosen at random within a reasonable range). They won't all come back to the same set of parameters, and the resulting scatter in the solutions will tell you lots about the uncertainties and correlations in your fitting parameters. You might even find a new minimum you didn't know existed.

This method of restarting the fit multiple times is sometimes called 'poor man's Monte Carlo'. An alternative method, which imple-

ments the recently developed 'nested sampling algorithm' [5], suitable for EPR/ESR spectral fitting, is an active area of research [6, 7].

More Than Two Roads Diverged

If you find that two models work equally well to explain data obtained at one frequency, you have encountered the spectral ambiguity gremlin. One way forward is to consider a multi-frequency approach. Spectra at different EPR/ESR frequencies are sensitive to different parameters and can act as powerful constraints on candidate models. The price is more computer time, but the payoff is typically more reliable fit parameters.

Parting thoughts

We hope that we've been able to make some useful suggestions for fitting EPR/ESR spectra of spin-labeled systems. We encourage you to try different models in order to sharpen your insights, but we also admonish you to think about what you're doing. We take our motto from the words of Hamming, "The purpose of computation is insight, not numbers." [8].

Endnotes

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Notices of Meetings

Molecular Imaging 2009: Routes to 3-Dimentional Imaging of Single Molecules
Kavli Institute, Cornell University, Ithaca, New York, USA, August 9–13, 2009
www.research.cornell.edu/KIC/events/mr-fm2009/

The 11th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena
Brock University, St. Catharines, Ontario, Canada, August 9–14, 2009
www.brocku.ca/scm09

The 10th International Conference on Magnetic Resonance Microscopy (ICMRM 10)
West Yellowstone, Montana, USA
August 30 – September 3, 2009
www.icmrm10.montana.edu

2nd International Symposium on Dynamic Nuclear Polarization: Theory - Hardware - Applications - Radical
Goethe Universität, Frankfurt AM Main, Königstein, Germany, September 2–4, 2009
www.bio-dnp.uni-frankfurt.de/dnpsymp/

7th European Federation of EPR Groups Meeting and Closing Meeting of COST P15
Antwerp, Belgium, September 6–11, 2009
www.efepr2009.ua.ac.be

School on Dynamic Nuclear Polarization (DNP)
Weizmann Institute, Safed, Israel,
October 11–16, 2009
www.weizmann.ac.il/conferences/DNP/

38th Southeastern Magnetic Resonance Conference
Vanderbilt University, Nashville TN (USA),
November 6–8, 2009
structbio.vanderbilt.edu/nmr/SEMRC_09
e-mail: semrc2009@vanderbilt.edu

International Workshop Electron Magnetic Resonance of Strongly Correlated Spin Systems (EMRSCS2009)
Kobe, Japan, November 8–9, 2009
extreme.phys.sci.kobe-u.ac.jp/EMRSCS2009

Molecular Photoscience Research Center, Kobe University will be organizing an international workshop "Electron Magnetic Resonance of Strongly Correlated Spin Systems" on November 8 and 9, 2009, prior to the 48th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2009) in Kobe. This international workshop will cover the recent advances of high frequency and high field EMR and its applications to the study of strongly correlated spin systems. Invited speakers from overseas include O. Cepas (France), S. Demishev (Russia), O. Portugall (France), G. Smith (UK), J. van Tol (USA), S. Zvyagin (Germany). The deadline for the submission of the abstract is August 10, 2009. For further information, please see the web site or contact:

Hitoshi Ohta (Chairperson), Eiji Ohmichi (Secretary), Organizing Committee, e-mail: emrscs@ruby.kobe-u.ac.jp

The 48th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2009)
Kobe, Japan, November 10–12, 2009
extreme.phys.sci.kobe-u.ac.jp/sest2009

SEST2009 will be held at the Centennial Hall of Kobe University during November 10-12. This is the 48th Annual Meeting of the Society of Electron Spin Science and Technology. The conference site, where the APES2001 was held previously, gives a splendid view of the sea, and the annual meeting will cover the wide range of EPR/ESR applications in physics, chemistry, biology and medicine. Following the tradition of the annual meeting of SEST, several distinguished scientists from overseas, including G. Smith (UK), will give plenary lectures at the meeting. Participants from all over the world are welcome. For further information, please see the web site or contact:

Hitoshi Ohta (Chairperson), Susumu Okubo (Secretary), Organizing Committee, e-mail: sest@kobe-u.ac.jp

Workshop on Structure and Dynamics by Multifrequency ESR/EPR
ACERT, Cornell University, Ithaca, New York, USA, November 15–17, 2009
www.acert.cornell.edu

COST P15 Spin Echo Workshop
Karlsruhe, March 10–13, 2009

A COST P15-sponsored seminar series, entitled "Spin Echo Workshop", was held at Bruker BioSpin in Rheinstetten on March 2009. The workshop was convened in response to the fact that there is a strong need especially of a new starter, but also of those who would like to improve/recover their basic knowledge, for an intensive overview on the state-of-art in the field of EPR. For this purpose, not only some basic EPR lecture series presenting briefly the theoretical background, but also a number of hands-on practical sessions which cover a diverse set of c.w. and advanced pulse EPR experiments were scheduled. In order for these components to meet each other, Bruker BioSpin, being the pioneer in this field, is really the particular place for realizing and experiencing the above-mentioned goals.

The workshop consisted of two main parts: (1) A series of general lectures: In-depth introduction to the spectrometer design as well as to the methodology of advanced EPR experiments covering a wide scope of applications.

The first two days consisted of lectures which started from a basic level and gradually advanced to more sophisticated aspects of EPR instrumentation and experiments. They concentrated on the principles of EPR, how these are implemented in the software/hardware of the spectrometers and how the scientist can obtain optimum results. The latter consists of understanding what we want to measure and how to perform the most appropriate experiment with maximum efficiency. These lectures though quite intense, were lively and allowed direct interaction between the speakers and the students. The theoretical part was on the whole well equilibrated and put through in 'simple words' by our two lecturers Dr. Peter Hoefer and Dr. Patrick Carl, whose presentations were clear and concise. (2) The workshop continued with two-day practical courses. The participants were divided into small groups of 5 people to attend the practical sessions. Each group attended 4 sessions in a 'clockwise' rotating manner. The topics covered were: ESEEM, Pulse ENDOR, ELDOR and Molecular Sophe. Dr. Fraser MacMillan gave an introduction to ESEEM and HYSCORE techniques. Experiments were carried out using both pulseSPEL as well as the software incorporated 'easy experiments'. The pulsed ENDOR technique was elaborated by Dr. Jeffrey Harmer in a W-Band spectrometer. We were given the opportunity to familiarise with the 'high-frequency' experiments, to setup a number of Mims and Davies ENDOR sequences. The demonstration of the advantages and limitations of each ENDOR technique, as well as the 'setting up' of TRIPLE ENDOR were very educational. Dr. Patrick Carl gave a very thorough introduction into the ELDOR techniques and their potency in measuring hyperfine couplings and distances. All these experiments were organised in a quite well manner, i.e. not only the parameter optimization "tricks" were presented, but also suggestions were given for possible troubles likely to be faced with for our own samples (usually different from model systems). In this sense all of the instructors were quite helpful, and they made sure that even a fresh-starter got the essential points. Thus, after these sessions, even if you face for the first time a certain experiment, you feel like you will be able to perform them yourself back at your EPR spectrometer. Finally, the last session consisted of an interactive demonstration of the 'under development' program molecular Sophe by Dr. Peter Höfer. It was shown to be efficient for c.w. and pulsed EPR experiments, though some limitations in the more advanced pulsed techniques like HYSCORE are still present.

The key output of the workshop was a dynamic and interactive introduction to the EPR techniques by combining a better understanding of the spectrometer design as well as of the theoretical basics supporting the hardware/software implementations. The important message is that even though the spectrometer configuration is nowadays more user friendly and more straightforward, the input of the user is still what defines a successful experiment. Nevertheless it is fair to say that Bruker Biospin has developed things in such a manner, where EPR measurements are favourably predetermined to be successful. Thus, the workshop being organized "on-place", was quite informative and educational for all attendees though having a wide range of backgrounds.

Maria-Eirini Pandelia and
Özlen Ferruh Erdem
Max Planck Institute for Bioinorganic Chemistry, Mülheim an der Ruhr, Germany

Reader's Corner

Electron Paramagnetic Resonance (EPR): Cutting-edge topics and future

Sushil K. Misra

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EPR has recently gone through a renaissance and the future appears to be very bright. However, in order to outline the cutting-edge topics, it is first important to review current EPR spectroscopic techniques, as well as future perspectives and desirable advancements in EPR instrumentation. Historically, applications have driven instrumentation development and, to some degree, also vice versa. Forecasting of applications that are driven by instrumental developments is feasible. However, forecasting of applications that are not driven by instrumentation progress must be based on existing knowledge that lies outside the field of EPR. The following description is not only based on the author's opinion, but relies equally on input from prominent researchers in the field (as listed below in acknowledgments).

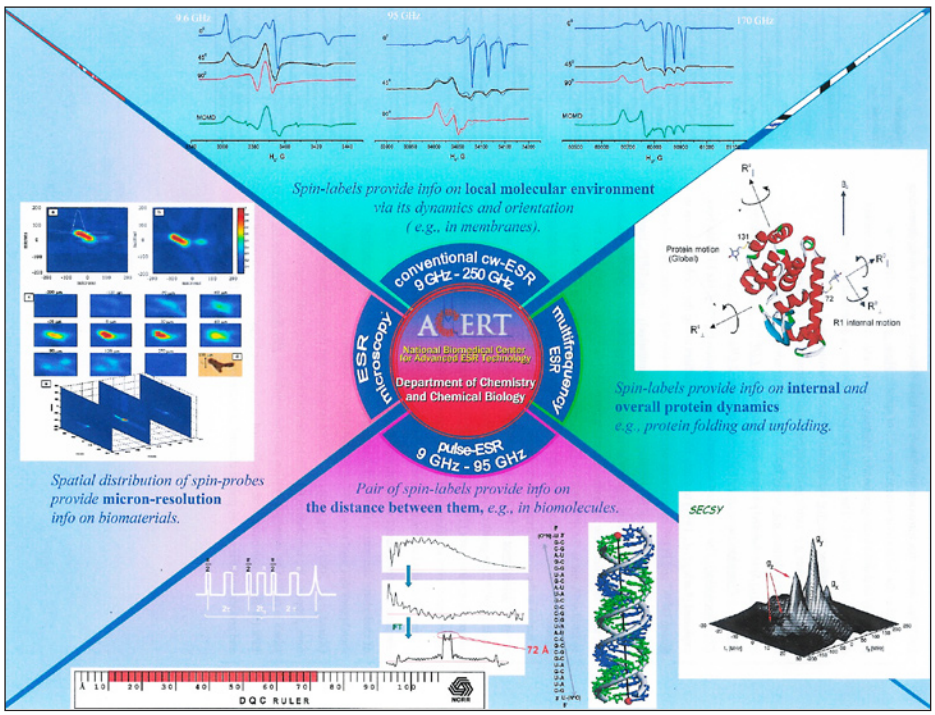
Spectroscopic techniques currently available in EPR. They are: multifrequency continuous-wave (CW) and pulse EPR, augmented by time-resolved (TR) and rapid-scan capabilities, EPR operating at high magnetic fields and high microwave frequencies (HFHF EPR) up to the submillimeter region. These are extended by multi-resonance and multi-pulse capabilities such as electron-nuclear double resonance (ENDOR), electron spin echo envelope modulation (ESEEM), hyperfine sublevel correlation spectroscopy (HYSCORE), double quantum coherence (DQC), pulsed electron double resonance (PELDOR) – also known as double electron-electron resonance (DEER), which play important roles, and will continue to do so. At the high-frequency end, for commercially available spectrometers, Bruker now has a W-band (95 GHz) spectrometer available and a 263 GHz machine will be on the market shortly. Further improvement of new pulse schemes, such as those developed by the late Arthur Schweiger and his group, is very important, and is still in progress, for example, modified versions of HYSCORE, originally introduced by Höfer and Mehring, for measuring small couplings of metal nuclei and heteronuclei in organic systems. Development of dedicated multi-frequency/multiple-resonance EPR instrumentation has enabled several outstanding applications of state-of-the-art EPR spectroscopy. It is anticipated that the advancement of EPR will depend largely on the development of novel and sophisticated instrumentation involving the latest inventions in microwave and magnet technologies. The trend to higher and higher magnetic fields will continue. In NMR, the "magic" 1 GHz limit has already been passed and in EPR, although the terahertz domain has been reached, it has not yet exceeded the *g*-strain limit of the Zeeman field for many systems, beyond which no more resolution improvement will be gained. In fact, increased resolution at increased field is very species-dependent. For some species the trade-off between hyperfine, Zeeman, and *g*-strain favors lower frequencies. The choice depends on information sought. The following examples of recent instrumental developments demonstrate how modern EPR and NMR complement each other to the benefit of future magnetic resonance spectroscopy: (i) Dynamic nuclear polarization (DNP) at high magnetic fields, as well as photochemically induced DNP in magic-angle-spinning NMR. DNP is a very 'hot topic' that brings HFHF EPR and NMR together; (ii) Pulsed terahertz EPR with synchrotron radiation and magnetic fields; (iii) Fourier-transform high-field EPR with broadband stochastic microwave excitation.

Future perspectives in EPR instrumentation. Based on natural evolution steps in improved computers and digital devices the following appears feasible. (i) Exploitation of software to accomplish the processes of phase shifting, mixing, quadrature detection, and filtering, or narrow banding such as that achieved with time-constant selection in CW EPR. Analogue-to-digital (A/D) converters are now used in a routine manner for direct digitization at 3 GHz, with 10 GHz not far away. (ii) As for resonators, digital design and automated fabrication will be the rule rather than the exception. (See the chapter on resonators by J. Hyde in the forthcoming book: *Multifrequency EPR: Theory and applications*, mentioned below.) There will be increased use of resonators, specifically optimized for a particular experiment. (iii) With respect to sample excitation, hard pulses will generally remain beyond reach; however, hybrid methods, such as those initially used in NMR under the rubric of correlation spectroscopy, will be used. There will be increased use of very fast field sweeps, very fast microwave frequency sweeps, and the use of multiple irradiation arms, with each arm under its own temporal control. The distinction between pulse and CW methods will blur. In addition, improved computers will enable advanced solutions of Bloch equations, spin Hamiltonians, and Liouville equation, required to interpret EPR data. (iv) There will be continued interest in multifrequency EPR, including zero-field EPR, especially because the high-field approximation is no longer a limitation with modern simulation programs. (v) In view of (i) and (ii) above, the cost of EPR spectrometers will be sharply reduced. The long-sought goal of a really cheap EPR spectrometer that can be used in mass routine applications may be within reach. EPR-based assays may become routine. (vi) Digital design will vastly improve stability of

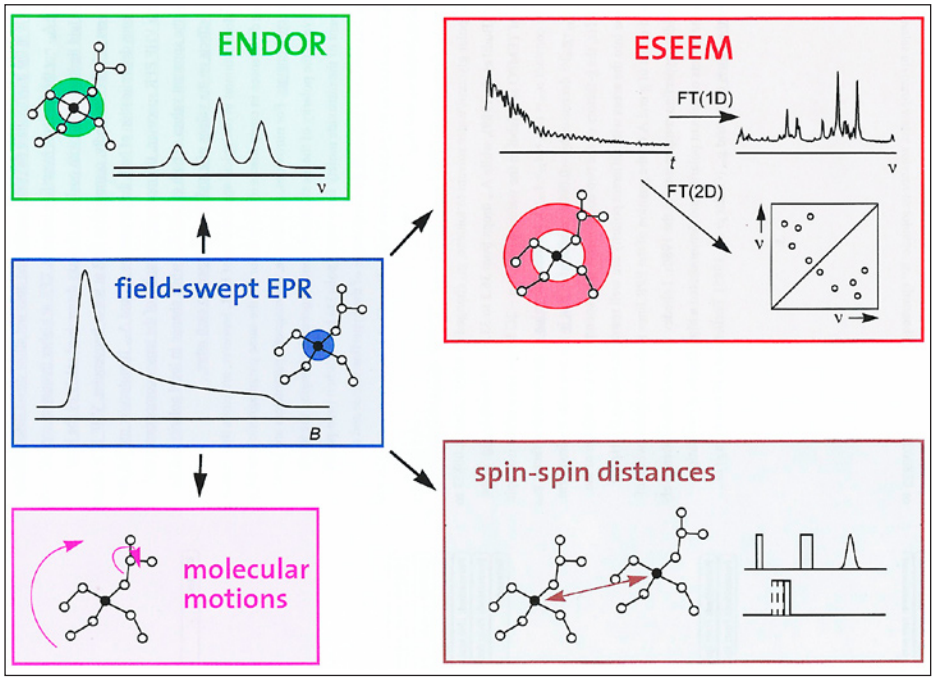
EPR spectrometers. This will 'open the door' to much improved sensitivity by being able to scan over a long period of time, as in NMR. This increased sensitivity will become the principal driver of new applications. There will be further developments in sensitivity and resolution with induction detection and also with new methods, such as MRFM, NV centers, and Hall probes.

Desirable advancements in EPR instrumentation. (i) The combination of optical (laser) excitation with pulsed EPR has a much larger application field than is currently realized. This technique should be developed to a point where it is no longer the specialty of a few groups but can be applied with relative ease as a routine technique. (ii) Exploitation of high-field pulse EPR with ultra-short pulses and ultra-short dead times is already underway to increase sensitivity and time resolution significantly. It would allow for new Fourier-transform EPR experiments and broader application of many of Jack Freed's techniques that were almost exclusively confined to his own group in the past. Although financial constraints on both the users and the manufacturers direct us toward multi-purpose spectrometers, for cutting-edge research single-purpose instruments can be designed to yield better signal-to-noise (S/N) and more nearly optimized information. Throughout the history of EPR, improvements in instrumentation, and primarily improvements in S/N, have made possible entirely new areas of research. Thus, the main advances that will facilitate new applications of HFHF EPR are improvements in low-noise sources, low-noise amplifiers, and detectors.

Cutting-edge topics, involving applications of HFHF EPR and its multiple-resonance extensions, which represent near-future challenges in EPR, are now described. They are exploited to investigate challenging problems in studies of structure and dynamics, notwithstanding the fact that, currently, sensitivity issues exclude application to several interesting classes of (biological) samples. The following examples are noteworthy. (i) **Resolution of small *g*-anisotropies**. (a) For cofactor radicals the canonical *g*-tensor orientations in their powder spectra can be resolved, even in disordered samples. Thereby, orientation-selective spin interactions within the molecule and with its micro-environment can be detected. (b) **Study of transient intermediates of several radical species with overlapping EPR spectra**, often generated in chemical reactions, are distinguished by clearly detecting small differences in their *g*-factors and hyperfine interactions using high Zeeman fields in HFHF EPR. (ii) (a) **Study of high-purity biological samples**. They are often produced only in minute quantities. Very high detection sensitivity of HFHF spectrometers is quite suitable in this context. However, many HFHF spectrometers are not designed to facilitate control of the environment of the biological sample, such as exclusion of oxygen, keeping the sample cold or in the dark at all times. (b) **Study of mixed biological samples**. The high spectral range allows discerning, e.g., different carbon-based radical nitrone adducts that could never be resolved at lower frequency. (iii) **Determination of the absolute sign of the zero-field splitting (ZFS) parameter**. ZFS characterizes, e.g. a two-spin system, such as a biradical or triplet state, or a single spin with $S \geq 1$. Considerable Boltzmann thermal spin polarization to accomplish this can be easily achieved well above liquid-helium temperature at high fields. As for the absolute signs of hyperfine couplings, simulations yield the relative signs of the principal values, and initial steps have been made in determining absolute signs, but a robust method for reliably measuring absolute signs is needed. (iv) **Study of dynamic processes**. HFHF CW EPR generally provides shorter time windows down into the picosecond range for determining correlation times and fluctuating local fields over a wide temperature range. (v) **Real-time access to specific molecular slow motions in the nanosecond time-scale**. This is achieved by pulsed HFHF EPR in the form of two-dimensional field-swept electron spin echo (ESE) spectroscopy. Here, even motional anisotropy, generated by anisotropic interactions, e.g., hydrogen bonding, can be traced. (vi) **Orientation selection of molecular sub-ensembles in powder or frozen-solution samples**. It is achieved by ENDOR at high magnetic fields, so that even in the case of small *g*-anisotropies, ENDOR can provide single-crystal-like information about hyperfine interactions, including, e.g. anisotropic hydrogen bonding to the protein. (vii) **Differentiation of strongly and weakly hyperfine-coupled nuclei in protein systems**. This can be accomplished by properly adjusting the Zeeman field in multifrequency pulse EPR experiments to record ENDOR and ESEEM spectra, e.g. those of remote and coordinated nitrogens in histidines of metallo-proteins. (viii) **Revealing subtle changes in polarity and proticity profiles along segments of proteins or their micro-environment of the plasma or membrane**. This is well accomplished by combination of CW and pulse high-field EPR spectroscopy with site-directed spin labelling (SDSL) tech-

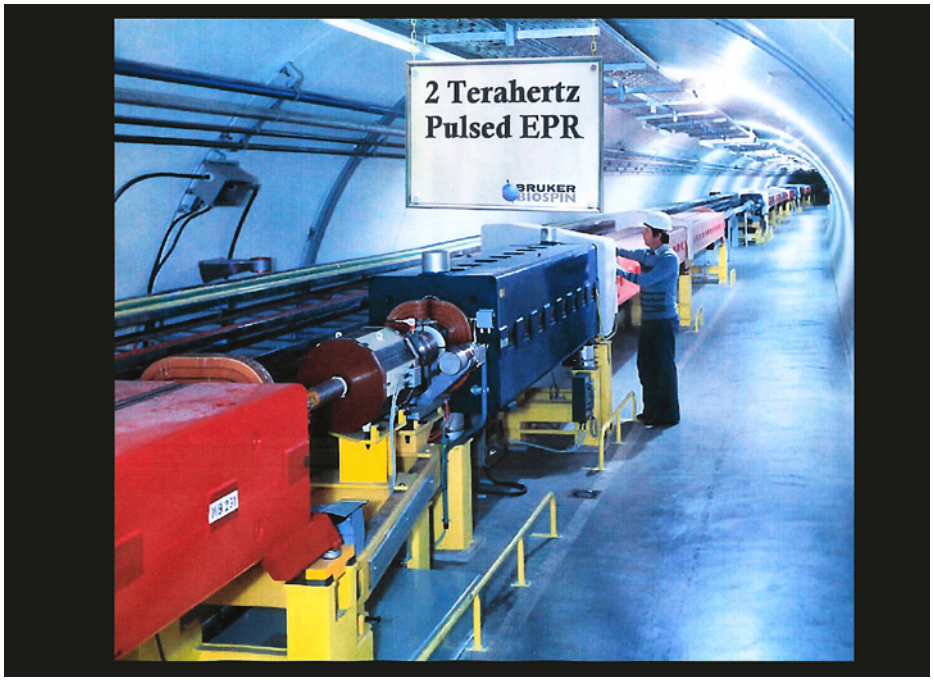


Some cutting-edge research projects being carried out at ACERT, Cornell University, USA (from Jack Freed's lecture, given at the EUROMAR conference, Eindhoven, The Netherlands, 2005)



Some cutting-edge research projects being carried out at ETH, Zurich, Switzerland (from the late Arthur Schweiger's lecture, given at the APES 04 conference, Bangalore, India, 2004)

niques employing nitroxide radicals. This information can be obtained from the g_{xx} and A_{zz} (hyperfine) components of the nitroxide spin label, but also from the quadrupole-tensor component P_{yy} of the ^{14}N nucleus, measured by high-field ESEEM, which can be exploited for probing subtle matrix effects. (ix) **Characterization of the environment of the probe in more detail**. This can be achieved by advanced instrumentation in conjunction with SDSL. The complex motional information so acquired may lead to new insights on biomolecular dynamics. As for choices of SDSL, it is desirable to go beyond nitroxides. (x) **Other studies of proteins using spin labels**, e.g. multifrequency EPR of nitroxide spin labels for increased resolution in analysis of protein rotational dynamics; bifunctional spin labels attached to two Cys residues, used to detect global protein orientation and microsecond rotational dynamics (using saturation transfer (ST) EPR); unnatural nitroxide-bearing amino acids such as TOAC that could be rigidly inserted into the protein backbone to report on the rotational dynamics and interspin distances; Pulsed EPR used to resolve multiple structural states of motor proteins; (xi) **Redox imaging**. Use of EPR in conjunction with magnetic resonance imaging (MRI) to study blood flow and metabolism; (xii) **High-field EPR applications to inorganic materials, containing various transition-metal ions**. This has not yet reached its full potential. The main unresolved issue here is improving the sensitivity of EPR spectrometers operating at very high magnetic fields/frequencies as these currently lack suitable resonator cavities. (xiii) **Determination of three-dimensional structure (distance and relative orientation) of stable or transient radical-pair systems with large inter-spin distances (up to about 8 nm), even in frozen solutions**. The possibility to measure not only distances up to about 10 nm, but also to obtain orientational information (at high field) using DQC, PELDOR (DEER) would provide much needed data for biophysicists. Such data would be complementary to solid-state NMR for short distance NOE constraints, and are envisaged to become extremely important for structure determination of large proteins and/or protein complexes. Here the development of new spin labels, in addition to nitroxides, and labeling techniques is desirable to increase the sensitivity and the distance range. (xiv) **Study of molecular magnets and other high-spin systems**. For this, multifrequency HFHF high-spin EPR is very well suited. (xv) **Study of disordered systems**. This can be achieved with the use of currently available EPR techniques, without requiring single-crystal preparations, e.g. that of a protein, to obtain detailed structural information with atomic resolution. As well, structure and dynamics of transient states of proteins in action on biologically relevant time scales are readily characterized. The combination with labeling techniques opens the possibility to access diamagnetic compounds that are otherwise EPR-silent. Here an important research objective is to understand, on the basis of structural and dynamics data, the dominant factors that control the specificity and efficiency of electron- and ion-transfer processes in proteins. Parallel to high-resolution X-ray crystallography, theory-assisted EPR spectroscopy in all its facets is being used currently in this endeavour. Structure and dynamics of biomacromolecules and biomacromolecular complexes, in particular membrane proteins and their complexes, are fields where EPR can potentially yield unique insights. (xvi) **Study of transient paramagnetic states**. When detected immediately after (photo) initiation of the reaction, characteristic electron spin-polarization (CIDEP – chemically induced dynamic electron polarization) effects are exhibited. They can be exploited for signal enhancement in EPR and ENDOR experiments to provide valuable information on structure, dynamics and reaction pathways of short-lived intermediates. (xvii) **Study of catalysis**. (xviii) **Study of organic systems**. Here important developments are emerging due to enhanced sensitivity and time resolution. For example, triplet states, characterized by a few microseconds life time, are not only easily detected by TR EPR, but also by pulse ENDOR, e.g. at Q-band. As a consequence, spin-density distribution in this $S = 1$ state can be investigated via the resolved hyperfine structure. Other examples of interesting applications to organic radicals are: amino acid radicals that occur in many reactions, e.g. in the water-splitting complex of photosystem II and in ribonucleotide reductase of "radical enzymes". Flavine radicals and triplet states have seen a renaissance, e.g. in the study of cryptochromes. (xix) **Study of transition metals in bioinorganic chemistry**. EPR and related methods are particularly useful to study transition metals in chemical and biological systems. Together with methods to trap intermediates, EPR has been instrumental to set-up reaction mechanisms for many enzymes, and to study the action of other proteins, e.g. nitrogenase, hydrogenase and water oxidase – a topic related to solving future energy problems; (xx) **measurements using the**



A dream for EPR in the future (from the late Arthur Schweiger's lecture, given at the APES 04 conference, Bangalore, India, 2004)

torque method with cantilever; (xxi) **organic molecular magnetism, with applications to molecular spin quantum computing and quantum information processing**; (xxii) **electron-spin quantum information processing** using the techniques of high-field pulse EPR, ENDOR, and EDMR; (xxiii) **HFHF EPR using accelerator-based terahertz light sources**; (xxiv) **single-spin detection**; (xxv) **EPR microscopy and nanoscopy**; (xxvi) **application of EPR to quantum-information processing**; (xxvii) **in-vivo EPR** (300 MHz – 9 GHz); (xxviii) **low-temperature tissue EPR**, e.g. that of myocardial tissue.

Topics related to theoretical interpretation of EPR data. The objective here is deduction of structure and dynamics from EPR parameters. (i) **Spin-Hamiltonian parameters**. The following parameters are not yet well predicted: ZFS, hyperfine couplings of transition metal ions, as opposed to the ones of ligand nuclei, which are reasonably well predictable, and exchange couplings. However, quantum chemistry is on the verge to change that. (ii) **Ab-initio methods to calculate EPR parameters** with a focus for future research on systems with non-dynamic correlation untreatable with single-determinant methods (Hartree-Fock, Kohn-Sham, density-functional theory (DFT)) (iii) **Dynamics of spin-labeled macromolecules**. Despite much research in the past four decades, detailed, precise information cannot yet be extracted from CW EPR spectra of nitroxides. Jack Freed's new rotamer approach to the problem bridges the gap between more abstract, fast simulations and more detailed, slow MD simulations that are fraught with problems of full sampling of the conformational space. (iv) **Interpretation of distance measurements**. EPR is currently the most precise method for measuring distance distributions in the range from 1.8 to 5 nm, in favorable cases to 8 nm, in disordered systems. This allows for insights in macromolecular conformation that no other method can obtain. The relation between statistical mechanics descriptions of macromolecule conformation and the measured data needs to be further investigated to make full use of this potential. (v) **Pulse EPR theory**. Most pulse sequences with good application potential are well understood for systems consisting of a single electron spin $S = 1/2$ and a single nuclear spin $I = 1/2$. They are reasonably well understood for a single electron spin and a single nuclear spin $I > 1/2$. The response of systems with more than one electron spin, with electron group spins $S > 1/2$, and with multiple nuclear spins is generally not very well understood, and needs further development for its application to detailed data analysis of many systems of interest. Multifrequency EPR is crucial to understanding electron-spin relaxation mechanisms. One advantage of high-frequency EPR is that for the same resonator Q the dead time due to ring down following a pulse is shorter, allowing shorter relaxation times to be measured.

Desirable applications of EPR. Systematic strategies that apply a whole arsenal of EPR techniques and well-defined measurement protocols need to be developed. Current molecular modeling approaches are not very well suited to the information EPR can provide and to combining information from diverse techniques. EPR-restraint modeling of structures and structural transitions needs to be developed. Analogous techniques and approaches are well suited for materials based on supramolecular assemblies. This field is almost unexplored, due partly to non-health related funding being scarce in the US.

Future of EPR. It appears very promising, particularly in anticipation of cheaper spectrometers becoming available in the coming years (see above), and continuous progress being made in experimental and theoretical research. There are many EPR centers and specialized research laboratories in existence at present around the world, in particular, in Australia, France, Germany, Israel, Italy, Japan, Russia, UK, and USA. In view of its applications to science and industry as described above, particularly in biology and medicine, quantum computing, photosystems, and magnetism, and the effective role played in understanding the environment of a paramagnetic ion, EPR offers excellent opportunities to attract strategic funding and commercial development.

Better organized details with references of these topics can be found in the forthcoming book: *Multifrequency EPR: Theory and applications*, edited by S. K. Misra (Wiley-VCH, Fall 2009). This book will also include detailed descriptions of many of the topics by prominent researchers mentioned in this article.

Acknowledgments

I am grateful, in particular, to Aharon Blank, Larry Berliner, Peter Dinse, Gareth R. Eaton, Sandra S. Eaton, Daniella Goldfarb, Steve Hill, Brian Hoffman, Jim Hyde, Gunnar Jeschke, Wolfgang Lubitz, Klaus Möbius, Thomas Prisner, Alex Smirnov, and Hans van Tol for detailed specific input on the topics covered here. In addition, I thank the following for their input – Chris Chang, Jack Freed, Balaraman Kalyanaraman, Gavin Morley, Hitoshi Ohta, Hal Swartz, David Thomas, and Dmitry Tipikin. I apologize to anyone whose name may have been inadvertently omitted.

Market Place

POSITIONS

Research Positions - Advanced EPR of Bioinorganic Systems

Several research positions (Ph.D. and Postdoc level) are presently available in the EPR department of the Max Planck Institute of Bioinorganic Chemistry in Mülheim/Ruhr, Germany.

We are looking for highly motivated young scientists in the field of Electron Paramagnetic Resonance who are interested in studying metallo-enzymes and related model systems. The main focus is on the investigation of photosynthetic systems (reaction centers, water oxidation), hydrogenase (biohydrogen production), radical enzymes and protein maquettes.

Our EPR lab is equipped with the full range of modern Bruker EPR spectrometers including E500 CW X-band, E580 CW/pulse X-band, E700 CW/pulse Q-band, and E680 CW/pulse W-band. In addition a high field CW/pulse spectrometer operating at 122 and 244 GHz (fields up to 12 T) is available next to several other CW EPR systems at S-, C-, X- and Q-band. We are using the complete repertoire of pulse and CW EPR techniques (ENDOR/TRIPLE, ELDOR, ESEEM) in combination with laser excitation and freeze quench techniques. More details can be found on our website: www.mpibac.mpg.de/lubitz.html.

The selected persons should have relevant training in Magnetic Resonance Spectroscopy, preferably in EPR. Candidates with an interest in EPR instrumental development and microwave engineering are specifically encouraged to respond.

Please send your application to Prof. Dr. Wolfgang Lubitz, Max Planck-Institute for Bioinorganic Chemistry, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany

E-mail: lubitz@mpi-muelheim.mpg.de

Postdoctoral position at Physics Department, National Dong Hwa University, Taiwan

A postdoctoral position is available in the laboratory of Prof. Shyue-Chu Ke at the Physics Department, National Dong Hwa University, Taiwan. The research will involve the application of EPR and pulsed EPR spectroscopy to understand the fundamental questions related to adenosylcobalamin-dependent enzymatic reactions. Additional information about the laboratory is available at: www.phys.ndhu.edu.tw/teachers/ke/ke.htm. Applicants should have experience in analytical techniques and continuous or pulsed EPR methods and data analysis. Experimental physical chemists with experience in cell culture or synthesis would be beneficial, but is not essential. The position is available this summer and appointments are for up to 3 years. If interested, please send a CV and summary of previous research experience to ke@mail.ndhu.edu.tw.

EQUIPMENT

Design and construction of ESR modules

The Magnetic Resonance laboratory at the Israel Institute of Technology has developed a variety of electronic modules, systems and probes for ESR and NMR. We are open to disseminate these projects and share our designs and modules either in a collaborative or in a service mode of action. Major recent instrumentation projects include: (1) 6–18 GHz pulsed ESR microwave bridge; (2) 33–36 GHz pulsed ESR microwave bridge; (3) 6–18 GHz CW ESR microwave bridge; (4) Pulsed gradient drivers for ESR and NMR (for imaging and/or field jump experiments); (5) Retrofitted Lakeshore Magnetic Field controller with improved resolution; (6) Retrofitted Walker electro-magnet power supply with improved stability.

Contact details: Aharon Blank, ab359@tx.technion.ac.il

Web address: www2.technion.ac.il/~ab359

Available: EPR accessories and supplies

We have some excess EPR accessories and supplies that might be of use to other labs. For example, we have a lot of chart paper, pens and ink for older recorders, and some spare parts and accessories such as VT Dewars for older spectrometers. If you need something for an older-style Varian or Bruker spectrometer, ask us – we might be able to help. Most items are available for shipping costs.

Gareth R. Eaton geaton@du.edu

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 electromatnet. Its high resolution permits precise adjustment of the magnet's field either though the front panel keyboard or though 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

Reader's Corner

EPRBioMed.org: User Groups for the EPR Community

Over the past five years, the Internet has grown, not only in its available content but also in the sense of community between its users. Virtual communities have sprung up on a variety of subjects, driven by the free exchange of ideas, opinions, and collaborations between users all over the world. EPRBioMed.org was commissioned to serve the EPR community specifically by the creation of community driven user groups to allow for the exchange of ideas on subjects related to EPR.

Two main features inspired by other community Web sites drive EPRBioMed's user groups: the bulletin board and the wiki. A bulletin board allows users to interact with each other similarly to e-mail, but unlike e-mail the whole community can join in the discussion and provide insight on the specific problem. Once a problem is solved or the discussion has ended, it remains in a searchable archive for users to learn about and expand on at a later date. The wiki allows for a collective collaboration on building information for a specific subject. At EPRBioMed.org we invite anyone to create and manage a user group. This is made possible with straight forward administration tools.

Management of the domain is done in a hierarchical manner. The internet dissemination coordinator (IDC) is in charge of the main Web site content and the delegation of management positions to each user group. Initial software and updates will be provided by the IDC, along with general user group help. A user group is administrated by a manager who has full responsibility for the content and for upkeep of that particular Web space. Content guidelines and software-help guides will be provided to new managers. Each user group is contained in its own subdomain, allowing for isolation from other projects and the ability to be directly linked. Promotion of individual user groups is made easier by having short, but descriptive, subdomain names.

EPRBioMed's first user group, the finite-element modeling group, focuses on creating a community to increase the knowledge-base of finite-element modeling programs. This group's main goal is to improve sensitivity in EPR spectroscopy, but over the past year, has grown to include an assortment of general-help question and answer discussions about finite-element programs. Additionally, the finite-element modeling Group has a wiki to collect the general knowledge of the community and create a user-driven manual to help ease the learning curve associated with commercial software programs. Another user group that has been formed is the spectral simulation group. This group focuses on providing support for anyone with questions about EPR spectra and how to properly simulate them.

The current user groups set an example of the type of communities that can be built at EPRBioMed, but there is room to grow. We invite you to inquire about forming your own user group and expanding the EPR community using 21st century tools.

Jason Sidabras and James Hyde

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