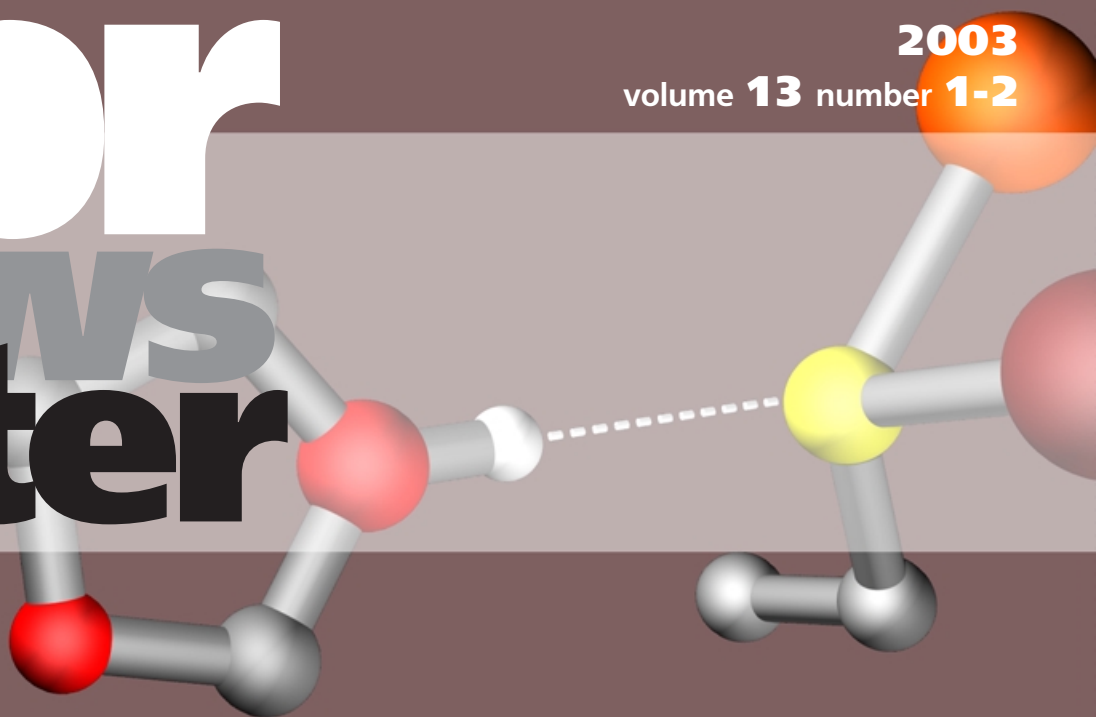


# epr news letter

2003  
volume 13 number 1-2



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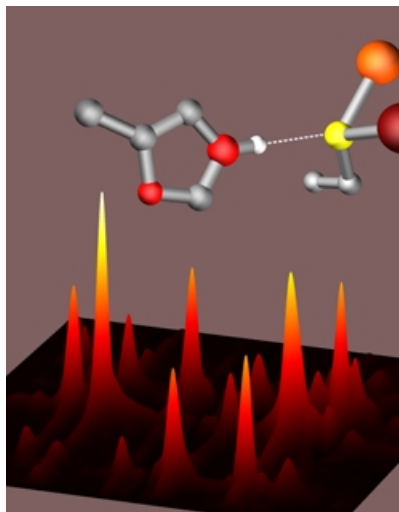
Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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The cover picture illustrates the research carried out in the group of Wolfgang Lubitz, the Zavoisky Awardee 2002 and Bruker prize 2003 winner. It shows a 'surface plot' of a 2-dimensional DONUT-HYSCORE (5-Pulse ESEEM) spectrum at X-band obtained from a [NiFe] hydrogenase in its oxidized "ready" state ( $S = 1/2$ ) containing a  $\text{Ni}^{\text{III}}\text{Fe}^{\text{II}}$  center. Investigated was a hydrogenase single crystal from the sulfate reducing bacterium *Desulfovibrio vulgaris* Miyazaki F. The large g anisotropy allowed selection of one crystallographic site of a specific paramagnetic species termed Ni-B. As an inset, a conserved histidine residue of the protein is shown that forms a hydrogen bond to a cysteine sulfur bridging the Ni and Fe in the active site of the enzyme. The HYSCORE data yield the nuclear quadrupole and hyperfine couplings of the proximal  $^{14}\text{N}$  nucleus of the attached histidine and thus information about the interaction between the metal center and surrounding amino acids that affect the functional properties of the enzyme. (M. Brecht and W. Lubitz, unpublished data.)

The cover picture has been prepared by Carlos Calle and Cinzia Finazzo, ETH Zurich.

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<http://www.epr-newsletter.ethz.ch/contact.html>

# Editorial

Little Lailechka  
takes the ball and  
runs with it...



Dear colleagues,

This is my first editorial and it is inevitable that I am a bit nervous. When John Pilbrow asked me if I could consider the possibility of becoming the Editor of the *EPR newsletter*, my first uncontrollable reaction was to say: oh, this is a great honor and a great responsibility, I am flattered and happy that you thought of my candidature, but I doubt I would be able to manage this. However, the good thing about first uncontrollable reactions is that they do not last long, and then second thoughts come into play. And my second thought was that if the editorial office has to be moved from Urbana, it is Kazan where the *EPR newsletter* belongs to rightfully. Kazan, the Motherland of electron paramagnetic resonance, the 998-year old city on the banks of the Volga river where East and West meet. Thus, I have accepted this proposal and Yuri Tsvetkov, President of the IES, nominated me as the Editor of the *EPR newsletter*.

Being a member of the IES, I received the newsletter during all these years and read it from the beginning to the end and I always found something interesting or instructive. In our everyday life we have plenty of sources of information. The local newspapers give us the feeling of belonging to the community of our neighbors. All-country newspapers make us feel that we are citizens of a country and the news worldwide gives us the feeling that we belong to humanity. We live in different countries and use different EPR techniques to study a wide variety of problems and we attend different conferences on magnetic resonance but we are all members of one and the same International EPR (ESR) Society. We (hopefully) regularly pay our dues but this is not what gives us the feeling that we belong to the same community. It is the *EPR newsletter* that unites us and gives us the feeling that we are of the same blood, if I may say so.

This is how I understand the place and role of this newsletter in the life of the EPR community. Maybe my being from a country which recently had lived through dramatic changes makes me less of a revolutionary concerning the changes to be made in the newsletter by the new team. The Belford team did a brilliant job with this newsletter and over the years the lists of contents cover various aspects of EPR. What I would like to add is a human touch to science. To this end, we introduce a new column "Another Passion". I have to confess it is my personal curiosity. Talented people are usually talented in many things. This column is about people who achieved success in EPR but also have a passion for something absolutely different. By realizing this passion they have achieved success as well. I am happy to start this column with a contribution from George Feher. We have several firm commitments for this column and I hope the curiosity about people to be featured there will keep you in a good waiting-for-the-next-issue mode. In the column "For Your Perusal" Arthur Schweiger kindly serves as your personal guide in the abundance of EPR and EPR-related literature starting from the year of 2000. 2002 marked the 95th anniversary of E. K. Zavoisky, the man who made this fascinating discovery of EPR. In this issue you will find an interview with his daughter, Nataliya Evgen'evna Zavoiskaya, who tells us some personal details about her father. And, finally, to have a feedback from our readership, we introduce the column "The Reader's Corner". You are welcome to give your input to anything which is related to EPR or you have the feeling EPR spectroscopists could be interested in. Please note the new Web site of the newsletter: [www.epr-newsletter.ethz.ch](http://www.epr-newsletter.ethz.ch)

You should certainly not miss the article by Richard Ernst about Kurt Wüthrich's 2002 Nobel Prize in Chemistry. A Nobel Prize Winner telling about another Nobel Prize Winner gives it a special flavor. Interestingly, some of the first publications of Kurt Wüthrich were on EPR.

It is my pleasure to express my gratitude to Graham Timmins, Takeji Takui and Thomas Prisner who agreed to serve as Associate Editors for Americas, Asia-Pacific and Europe, respectively. I owe special thanks to John Pilbrow. Meeting him in Novosibirsk in July 2002 and abundant e-mail correspondence contributed a lot to my understanding of aims and goals of the newsletter. He also kindly agreed to edit a column about the pioneers of EPR and in this issue you find his story about Oxford in the early 1960's. I really enjoyed my e-mail correspondence with George Feher, Arthur Schweiger and Joan van der Waals who gave me a wider and deeper outlook on my task on editing this newsletter. Linn Belford and Becky Gallivan willingly and kindly helped me to get acquainted with the inner life of the *EPR newsletter* and provided me with guidelines to ensure its functioning. The input from Shirley Fairhurst and Chris Felix could hardly be overestimated. I am glad that my colleague from *Applied Magnetic Resonance*, Sergei Akhmin, serves as technical Editor of the newsletter.

To make a long story short: it is you who produce the news, we just present it in the *EPR newsletter*.

Laila Mosina



# Fellowship of the IES to Daniel Kivelson<sup>†</sup>

The International EPR/ESR Society is delighted to announce that Professor **Daniel Kivelson** (University of California at Los Angeles) is awarded a Fellowship of the Society for his outstanding contribution to the development of theories and experiments on electron spin relaxation and line shapes in liquids.



Professor Kivelson's name will always be associated with the early development of ESR theory of line shapes in solution. His interests over his long and distinguished career have included: microwave spectroscopy; electron spin resonance spectroscopy; nuclear magnetic resonance; low-energy electron-

molecule scattering; dynamic light scattering; relaxation phenomena in liquids and viscoelastic fluids; supercooled liquids and glasses (attempted to develop an overall theory of supercooled liquids and glasses); polyamorphism (multiple apparently amorphous solid metastable phases).

During his distinguished career Professor Kivelson has been honoured with many awards: Including a Guggenheim Fellowship, 1959; American Chemical Society California Section Award, 1967; American Physical Society: Fellow, 1976, Langmuir Award in Chemical Physics 1999. UCLA: Harvey L. Eby "Art of Teaching" Award, 1970, and College of Letters and Science Faculty Award, 1987.

The title of Fellow of the Society is conferred on those who have made truly outstanding contributions in EPR theory and/or practice. It is intended for particularly distinguished scientists who are either retired or are close to retirement.

It is fitting that Professor Kivelson should be honoured with Fellowship of the International EPR (ESR) Society.

Yu. D. Tsvetkov, President IES  
S. A. Fairhurst, Secretary IES

<sup>†</sup> Professor Kivelson died shortly afterwards and an Obituary is included in this issue

## IES General Meeting 2003

The General Meeting of the International EPR (ESR) Society was held during the 26th International EPR Symposium in Denver from July 27–31 2003. All IES members

and Symposium attendees were cordially invited to attend. Further details on this meeting will be given in a future issue of the *EPR newsletter*.



## IES Awards 2003

### Silver Medal for Chemistry

**Michael K. Bowman**

William R. Wiley Environmental  
Molecular Science Laboratory  
Pacific Northwest National Laboratory  
USA

### Silver Medal for Physics/Materials Science

**Edgar J. J. Groenen**

Huygens Laboratory  
Leiden University  
The Netherlands

### Silver Medal for Biology/Medicine

**Michael Davies**

The Heart Research Institute  
University of Sydney  
Australia

### Young Investigator Award

**Stephan Zech**

Department of Chemistry  
Columbia University  
USA

Full citations for all of the award winners will be given in a future issue of the *EPR newsletter*.



# The New Team of the *EPR newsletter*

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**Laila V. Mosina**

(see vol. 12, no. 4 for the details on Dr. Mosina)

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### AMERICAS



**Graham Timmins**

(see vol. 12, no. 2 for the details on Dr. Timmins)

### ASIA-PACIFIC



**Takeji Takui**

(see vol. 12, no. 3 for the details on Prof. Takui)

## EUROPE



**Thomas Prisner**

Thomas Prisner studied physics at the University of Heidelberg and graduated in 1984 with the diploma thesis "ESE on Photo-excited Benzophenone Molecular Crystals" prepared in the group of Karl H. Hauser at the Max-Planck Institute for medical research. He obtained his Ph.D. in 1988 from the University of Dortmund under the direction of Klaus P. Dinse, studying stochastic and coherent excitations in electronic spin systems. Then he was a postdoctoral fellow in the group of Robert G. Griffin, Chemistry Department at the Massachusetts Institute of Technology, Cambridge, USA, working in high-field EPR and DNP at 140 GHz and 5 T. In the period 1991–1996 he worked on his habilitation thesis "Pulsed High-Frequency/High-Field EPR" at the Department of Physics, Free University Berlin, in the group of Klaus Möbius. Starting in 1997, Thomas Prisner is Full Professor at the Institute for Physical Chemistry at the Goethe-University in Frankfurt am Main. In 2001, he became Director of the Institute for Physical and Theoretical Chemistry.

His research interests are focused on the following: EPR spectroscopy, method developments (pulse EPR and multifrequency EPR), kinetics and reaction dynamics of electron-transfer reactions, photo- and electron-transfer reactions in proteins, conformational dynamics of macromolecules, reaction dynamics and structure of catalytical metal centers, protein-ligand interactions, determination of the structure of paramagnetic centers in proteins, and DNP.

## TECHNICAL EDITOR

Sergei Akhmin received his M.Sc. in Solid-State Physics from the Kazan State University in 1977 and his Ph.D. in 1990 in Condensed Matter Physics from the Kazan Physical-Technical Institute. His scientific interests were concentrated on EPR and ENDOR studies of ligand hyperfine and quadrupole interactions of admixture paramagnetic ions in single crystals of alkali and alkali-earth metal salts. Starting in 1990, he is involved in the activity with publishing the journal *Applied Magnetic Resonance* to become its Deputy Editor-in-Chief in 1996. Sergei Akhmin provides the prepress preparation of the journal according to the highest requirements of Springer, its publisher. In addition, he participated in the prepress preparation of various books: the monograph "Magnetic Isotope Effect in Radical Reactions" by Kev M. Salikhov (Springer), Proceedings of the XXVII Congress AMPERE, the monograph "Evgeny Konstantinovich Zavoisky: Materials to Biography", the monograph "Semen Aleksandrovich Al'tshuler: Reminiscences", to name a few.



**Sergei M. Akhmin**

He prepares the *EPR newsletter* for printers and the pdf version for the web. Please contact him if you have any questions concerning the form of submission of your materials (text and illustrations).

**S**ince many years, insiders unanimously agreed Kurt Wüthrich deserves the great prize! His and his group's innovations have changed the field of molecular biology, and the influence on the life sciences in general is immense. Before, it was impossible to study the inner workings and the interactions of biomolecules in their natural media, in aqueous solution or within membranes. Today, we have access to more secrets of nature than ever before, and our understanding of life processes and our ability to cure diseases have grown immensely.



# Nobel Prize in Chemistry 2002 to Kurt Wüthrich

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It seems to be common to all great innovations and achievements: The underlying idea is very simple, almost trivial; and over and over again colleagues ask themselves, why didn't I have that seminal idea before? – Indeed, the seminal idea of Kurt Wüthrich is very simple, and intriguing at the same time: Take two recently introduced new techniques, give them well-sounding, attractive names, combine them in an innovative, ingenious manner so that one plus one is infinitely more than two, and, finally, apply the novel methodology to a large number of highly relevant

problems of great actuality. This is, in a nut shell, Kurt Wüthrich's secret of success. – But it does not work in everybody's hands; one needs in addition his perseverance, his enthusiasm and drive, and his unbreakable belief in the ultimate success of his approach.

The two above-mentioned ingredients for determining biomolecular structures were two novel two-dimensional NMR techniques, COSY and NOESY, employing Kurt Wüthrich's catchy terminology; COSY for tracing out internuclear connectivity through chemical bonds and deter-



mining dihedral bond angles, and NOESY for measuring internuclear distances through space. And the combination of the two experiments led to his ingenious procedure for sequential assignment of the nuclear magnetic resonances of backbone protons in proteins, and later also in nucleic acids. The results became the inputs of sophisticated computer routines that, finally, calculate the best fitting three-dimensional molecular structures.

This procedure is today a standard tool, indispensable in any advanced molecular biology laboratory. Kurt Wüthrich's research group solved during the past twenty years by NMR structural questions for many proteins that could not adequately be crystallized, a prerequisite for applying X-ray crystallography.

Both experiments, COSY and NOESY, were originally invented by Jean Jeener, a brilliant Belgium physicist, without yet conceiving their final names. In 1971, Jean Jeener proposed the very first two-dimensional correlation experiment during a lecture at an AMPERE Summer School at Basko Polje in Yugoslavia. This experiment for tracing out nuclear spin systems was subsequently implemented in the author's laboratory in 1974 and introduced 1977 into Kurt Wüthrich's research group in the hope of possible biological applications. The second experiment was suggested in 1977 again by Jean Jeener during a private discussion at a Gordon conference in Wolfboro at the beautiful lake Winnepesaukee, New Hampshire. Its purpose was to trace out networks of nuclear relaxation processes. Again, the author's research group attempted its implementation, at first for elucidating chemical exchange networks, which turned out to be easier than exploring relaxation. But soon afterwards, 1980, Anil Kumar discovered in a collaborative research project, carried out in Wüthrich's research group, that the experiment works beautifully also for cross relaxation if sufficiently large molecules are used as targets.

At this moment, Kurt Wüthrich became fully alert to the possible relevance of the two independent experiments. Their marriage was soon sealed for all time to come, and their naming ceremony happened at the same time, actually to the author's dismay, being afraid of insulting the purist minds of scientists. But he soon converted also to Wüthrich's trendy nomenclature.

Although the author's collaboration with Kurt Wüthrich continued for several more

years, the seminal further development happened almost entirely within Wüthrich's group. As usual, the dry spell was long from the first conception of the idea to its truly operative implementation, and it took enormous efforts, both on the experimental spectroscopic side as well as for conceiving powerful computer data processing routines. And the first protein structure, the one of proteinase inhibitor IIa from bull seminal plasma, obtained entirely by two-dimensional NMR, could be published in 1985.

At this early stage in two-dimensional biological NMR, there was hardly any serious competition world-wide, and never any doubt occurred that the priority for the sequential assignment of proteins and their structure determination by NMR belongs to Wüthrich's research group. But rather rapidly, other research teams acquired the necessary knowledge, and serious competition arose. Nevertheless Wüthrich's group has always kept the lead until today.

A large number of exceedingly beautiful and highly relevant biomolecular structures have been determined in the mean time by his research group. Just three outstanding examples shall be mentioned: the three-dimensional structure of the complex of the peptide cyclosporin and the protein cyclophilin, of importance for the suppression of the immune response during organ transplantations; the geometry of the DNA complex of the Antennapedia homeodomain, a transcription factor from the organism *Drosophila melanogaster*; and the structures of the mouse, bovine, and human prion proteins, of major significance for understanding the inherent processes involved in BSE and CJD diseases.

Why has NMR been so successful in Zürich? First of all, certainly because Kurt Wüthrich decided in 1969 to come to the ETH, invited by the Professors Hans H. Günthard and Robert Schwyzer, after his successful postdoctoral years in the United States where he became, for the first time, fascinated by the potential of NMR as applied to biomolecules. – But in addition, NMR had already long before gained a very strong footing in Zürich. The first research in nuclear magnetic resonance was performed at the physics department of the University of Zürich. Hans Staub spent his postdoctoral years at Stanford in the group of the Swiss citizen, Nobel Laureate, and ETH alumnus Felix Bloch. After being appointed in 1949 as professor of physics, he established a very lively and successful group in NMR. Later,

in 1961, Professor W. H. Heini Gränicher employed NMR at the physics department of ETH for seminal studies on ice. The first pioneering introduction of NMR into chemistry at Zürich happened in 1957 by Professor Hans H. Günthard and especially by Professor Hans Primas who designed innovative high-resolution NMR instrumentation. This formed the major germ for the future Nobel successes at ETH Zürich, and also for the commercialization of NMR through the company Trüb-Täuber, which led to the later foundation of the internationally leading company Spectrospin, known today under the name Bruker BioSpin.

Often, serendipity is made responsible for scientific success, but we know at least as many examples where from the beginning a clearly defined goal was pursued without compromise. Wüthrich's success undoubtedly belongs to this second category. He knew his goal, the determination of biomolecular structures, already very early and was systematically looking for suitable tools, enabling him to attain the set goal. – Obviously, each scientist also requires luck in his career. And Wüthrich's luck was that the proper tools just became available when he needed them. But it is to his merit that he realized their suitability and improved them to their perfection.

Wüthrich's achievements are an excellent example for 'oriented basic research', research that is of a fundamental nature and nevertheless has clear set practical goals. Wüthrich was never caught within a detached ivory tower. His type of research can most easily be justified towards the funding agencies and towards the general public. It is also the kind of research that immediately fascinates young adventurous scientists because it is interesting, challenging, and useful, at the same time. It is not astonishing that numerous renowned scientists started their successful careers within Wüthrich's group.

Let us hope that Wüthrich's example is contagious for the entire scientific community, with the effect that university research continues to contribute significantly to solving problems of societal importance.

We would like to congratulate our colleague Kurt Wüthrich to his Nobel Prize in Chemistry.

Richard R. Ernst  
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# Zavoisky Award 2002 to Wolfgang Lubitz

The 2002 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professor Wolfgang Lubitz, Germany in a ceremony marking his outstanding contribution to multifrequency EPR spectroscopy in bacterial and plant photosynthesis.

The ceremony was preceded by the Twelfth Annual Workshop: "Modern Development of Magnetic Resonance", Kazan, 2–4 October 2002.

In the afternoon of October 2, a reception of Professor W. Lubitz by the Prime-Minister of the Republic of Tatarstan R. N. Minnikhanov took place.

The Zavoisky Award was presented October 4, 2002 in Kazan, the capital city of the Republic of Tatarstan. It was there that academician E. K. Zavoisky discovered EPR in 1944. The Zavoisky Award consists of a Diploma, a Medal and one thousand US dollars.

The Zavoisky Award was established by the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences with support from the Kazan State University, the Springer-Verlag Publishing House, the Republic of Tatarstan, the Tatarstan Academy of Sciences, the AMPERE Society and the International EPR (ESR) Society.

The Award Selection Committee consisted of well-known experts in EPR: Professors B. Bleaney (Oxford), G. Feher (La Jolla), K. Möbius (Berlin), A. Schweiger (Zurich), Yu. D. Tsvetkov (Novosibirsk), and the Chairman K. M. Salikhov (Kazan). The selection of the Awardee was made after consultations with the Advisory Award Committee which comprises: C. A. Hutchison Jr. (Chicago), and Yu. N. Molin (Novosibirsk).

Previous winners of the Zavoisky Award were: W. B. Mims (1991), B. Bleaney (1992), A. Schweiger (1993), J. R. Norris, Ya. S. Lebedev and K. Möbius (1994), J. S. Hyde (1995), G. Feher (1996), K. A. Valiev (1997), J. H. Freed (1998), J. H. van der Waals (1999), H. M. McConnell and Bruker Analytik GmbH (2000), and K. A. McLauchlan (2001).

The selection of Professor Wolfgang Lubitz was made from many nominations solicited

from international experts in EPR.

The Award Ceremony starting in the afternoon of October 4 was attended by over 200 people, among them were the scientists who had participated in the preceding Workshop.

The ceremony was chaired by Professor K. M. Salikhov. He, as the Chairman of the Award Committee, announced the decision of the Zavoisky Award Committee. The presentation was made by the Deputy Prime-Minister of the Republic of Tatarstan Z. R. Valeeva. She read the letter of congratulations from M. Sh. Shaimiev, President of the Republic of Tatarstan. The Rector of the Kazan State University, Professor M. Kh. Salakhov, the Chairman of the Presidium of the Kazan Scientific Center of the Russian Academy of Sciences, Professor A. I. Konovalov, and the Principal Scientific Secretary of the Tatarstan Academy of Sciences, Professor I. B. Khaibullin warmly congratulated the laureate. Letters of congratulations from Professor H. W. Spiess, President of the AMPERE Society, Professor J. R. Pilbrow, President of the International EPR (ESR) Society, and Professor M. Mehring, President of ISMAR, were handed to Professor Wolfgang Lubitz.

Professor Lubitz gave his Zavoisky Award lecture in which he discussed problems of



multifrequency EPR spectroscopy in photosynthesis. A concert by a string quartet preceded and followed the ceremony. After a meeting with journalists, the guests visited the museum of history of the Kazan State University. The event was concluded with a Banquet in honor of Professor W. Lubitz and his outstanding contributions to EPR. During their stay in Kazan the laureate and his spouse visited the places of historical and cultural interest in Kazan, and picturesque sites in the town Elabuga.

The Organizing Committee owes special thanks to the Ministry of Industry, Science and Technology of the Russian Federation, the Russian Fund for Basic Research and the NIOKR Fund of the Republic of Tatarstan.

## Bruker Prize 2003 to Wolfgang Lubitz

Each year the EPR Group of the Royal Society of Chemistry awards a prize in recognition of outstanding service to EPR. The prize, sponsored by Bruker, was this year awarded to Professor Wolfgang Lubitz of the Max

Planck Institute for Radiation Chemistry, Mülheim an der Ruhr, Germany. His Bruker Lecture "Signals from the Reaction Centre" on applications of EPR in photosynthesis held the audience in rapt attention.

# The Frank H. Spedding Award to Lynn Boatner

Lynn Boatner, a corporate fellow at the Department of Energy's Oak Ridge National Laboratory, has earned a prestigious award for his research on the fundamental properties and applications of rare earth phosphates and other rare earth materials.

The Frank H. Spedding Award was presented to Boatner during the Rare Earth Research Conference in Davis, California. It marks the 10th time the award has been presented in recognition of excellence and achievement in research centered on the science and technology of the rare earths.

Rare earth elements on the periodic table include cerium, gadolinium and ytterbium and lie between lanthanum and lutetium. Boatner's research in this area began in 1964,

initially focusing on fundamental spectroscopic investigations of rare earth electronic properties. He has authored or co-authored more than 440 publications, and has been awarded 13 patents, and has earned three R&D 100 awards. Boatner is a fellow of the American Physical Society, the American Ceramic Society, the American Association for the Advancement of Science, the American Society of Metals International and the Institute of Materials of the United Kingdom. He is also the review editor of the Journal of Materials Research.

In 2001, Boatner was presented the Jessie W. Beams Award for excellence in research by the Southeastern Section of the American Physical Society.



Boatner earned bachelor's and master's degrees in physics from Texas Tech University and received a doctorate in physics and mathematics from Vanderbilt University.



## The Jeol Prize 2003 to Stefan Stoll

Jeol U.K. have generously agreed to sponsor a prize for the best oral presentation by a young scientist at the conference.

The competition is restricted to 2nd and 3rd year Ph.D. students and postdoctoral fellows in their 1st year of research. Three students are selected by the scientific committee based on a submitted abstract. Each of the three students delivers a short oral pre-

sentation of 20 minutes. The student giving the best overall presentation receives an inscribed medal.

Stephan Stoll received his Jeol Prize at the 36th Annual International Meeting: Advanced Techniques and Applications of EPR, University of Manchester, of the ESR Group of the Royal Society of Chemistry.

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Last fall (2002), just as I was getting ready to take off for Las Vegas to participate in a poker tournament, I received an e-mail from Laila Mosina, the new editor of *EPR newsletter*, asking me to write about poker for her new column “Another Passion”. On the plane I mulled over the question of whether to accept such an assignment. I was reluctant because poker playing represents a rather private part of my life and, in addition, it is not a universally condoned activity. I postponed a decision. In one of Laila’s e-mails she argued that my poker playing will reveal that I

# Playing Poker

G. Feher

University of California, San Diego, La Jolla, CA 92093

am “human” and not, I suppose, a research machine. Was this a poker play to make me write the article? Actually, there are similarities between research and poker. In research, one endeavors to wrest the secrets of Nature; in poker, the secrets of your fellow players. There are, of course, basic differences: deception and bluffing, which are essential ingredients in poker, play no part in research. Further entreaties from Laila made me finally accept the task.

Poker started for me in the early 1950’s when I was a graduate student in physics at the University of California in Berkeley. During our long experimental runs at night, as we were waiting for our set-ups to cool down to cryogenic temperatures, my fellow graduate students Clarence Kooi and Ray Hoskins introduced me to the game of poker. I took to it immediately and became quite adept at it, so much so, that after a while they refused to play for money with me. When I joined Bell Labs in 1954, I was delighted to find out that there was a monthly poker game going on,



**G. Feher, third place winner in America’s Cup National Poker Championship. Las Vegas, 1992.**

which was organized by Bernd Matthias of superconductivity fame. I played with the group until I left in 1960 to join the fledgling new campus of the University of California in La Jolla. Here, again with Bernd Matthias, we quickly established a group of poker players that meets to this day twice a month. In addition, I participate 2 or 3 times a year in poker tournaments in Las Vegas and Los Angeles and we have also organized many poker games at scientific meetings. So it is fair to say that poker has been running on a parallel track (albeit, side track, to be sure) with my ~50 year long scientific career and, who knows, – it may even outrun it.

I mentioned Bernd Matthias twice in the above paragraph. I have fond memories of Bernd, who unfortunately passed away over 20 years ago. Once in the 1960’s Bernd, Walter Kohn (the developer of density function theory, DFT, for which he received the Nobel Prize in 1998) and I were flying from New York to Los Angeles. Walter was sitting between us and Bernd and I started to play poker over Walter’s seat. As Walter became more and more irritated, we suggested that he change seats. Walter refused; after all we were given specific assigned seats by the airline. As this incident shows, poker does not only bring out the character of the players but also, occasionally, of the on-lookers.



Why do I, and many other people, find poker so exciting? I find it difficult to analyze this question in detail but what I can do is describe my feelings. When I take a seat at a poker table, there is a tingling sensation, a feeling of anticipation, the thrill of taking risks, of possible surprises. It's a lot like I felt in my youth, standing on the starting block in a swim-meet, except that in poker, once the game is going, the challenges are much more multidimensional than in swimming. It's more like skiing down a treacherous slope where the terrain needs to be constantly negotiated. The terrain at the poker table are the cards you are dealt and the players at your table; the negotiations are the tactics and strategies you devise as a result of the odds you calculate for your hand and your reading of the hands of the other players. And at the end of the hand, there is the exhilaration of having done well, of having done your very best, even if you didn't win. Ultimately, poker is a lot like the game of life: You are dealt a set of cards about which you have no say (e.g. inherited traits, talents, imposed external situations) and the aim is to strategize and optimize what you can do with your hand so that, in the end, you feel that you have played to the very best of your ability.

Will we ever be able to design a computer that can effectively play poker? I don't think so. It seems to me impossible to program the reactions and psychology of the individual players, the very ingredients that make poker for me exciting. In contrast I find chess whose cold logic can be programmed into a computer to be interesting but leaving me cold.

From the above remarks you can gather that, contrary to common belief, poker is not a gambler's game (like roulette, craps, baccarat, etc.); nor is it truly a card game in the sense that the cards are not the most important part of it. It is foremost a game of psychology and keen observation of your opponents' reactions and body language. How strong is his hand? Is he bluffing or not? These are the important questions. By body language I mean the so-called "tells", the little mannerisms – tics, twitches, fiddling with ones chips, cards, fingers, rings, etc. Since we are taught from childhood that deception is a bad thing, some players cover their mouths or lower their voice when they bluff. Secondly, you have to know, of course, the statistical odds of your own hand, properly weighted by the size of the pot. This part of the game is the easiest, especially for

the analytically minded. But just knowing the odds will not make you a consistent winner.

What role does luck play in the outcome of the game? Luck, good or bad, is important only in the short run (which can take occasionally an excruciating long period of several hours). You can view periods of bad and good luck as positive and negative noise spikes which over long periods of time average to zero, analogous to the averaging of noisy traces of your EPR spectrum. This means that luck does not enter the picture if you have enough capital to withstand the negative peaks. In a tournament however, you buy in with a finite amount of money that cannot be replenished during the game. Consequently, a long negative fluctuation can wipe you out and in fact one often sees champions wiped out early in the tournament. Thus, luck plays a far greater role in tournaments than in regular games. By playing more conservatively, one can reduce the amplitudes of the peaks thereby reducing the probability of being wiped out. An additional difference between tournaments and non-tournament play is the mental stamina required to withstand the pressure over the many hours of a tournament.

Poker is probably the only card game that cannot be played without a stake, (i.e. money) since the obvious goal of the game is to get as much money from your opponents as possible. Thus, a "friendly" poker game is an oxymoron. However, a good poker player thinks of money in a rather abstract way. He does not equate it with money spent in everyday life. If you equate the size of a bet with the cost of your next vacation, you are doomed. This was brought home to me when I first started to play poker in Las Vegas. At a table where thousands of dollars passed hands, players returning from dinner griped that the price of a steak had gone up by two dollars. There clearly was a disconnect between the "real" money paid for the steak and the "funny" money used to play poker.

Let me now describe how poker tournaments are conducted. There are two to three big poker tournaments (world championships) played each year in Las Vegas in which players from all over the world participate. The most famous is the Annual World Series of Poker at Binion's Horseshoe Casino in Las Vegas. There are about a dozen different poker games played over roughly a two-week period. Some people play all games, I play only one, called "seven card stud HI-

LO split 8 or better". A typical entry fee ranges between \$1000 and \$2000 and the number of players varies between 100 and 300. As an example, let's say that 200 players enter, each paying \$2000, i.e. the total amount collected is \$400,000. This amount (minus a negligible percentage for the house) will be distributed among the winning players. The winner receives roughly half of the pot (~\$200,000), the runner-up approximately a quarter and so on. Depending on the number of players, 8–24 will receive some money.

The most exciting event of the Annual World Series of Poker in which the stake and number of participants are considerably higher than in the rest of the events, is a game called "no-limit hold them". The entry fee for this event is \$10,000 and last year (2002) about 600 players participated. The winner was Robert Varkonyi, an M.I.T. graduate who walked away with \$2,000,000. The best I ever placed in a tournament was third (see picture), good enough for them to try to interview me but I managed to escape. I imagined headlines in the San Diego Union: "U.C. Prof. Plays Poker in Las Vegas Shirking Teaching Duties". Incidentally, my poker winnings go into a research fund which, not being restricted by federal rules, has proved to be a great convenience over the years.

It is interesting how some personal traits show up in poker more crassly than in everyday life, giving insight into a person's actions and behavior patterns. Let me give you a couple of examples. On a few occasions, I played poker with Edward Teller, "the father of the H-bomb". His hawkish and far-right leanings had been difficult for me to understand. After having played poker with him, I believe that I have discovered the main driving force of his stand. It is fear. He is the most fearful (and poor) poker player that I have ever encountered. His fear of communism taking over the world was genuine and motivated his actions. Another interesting player was John Bardeen, the two-time Nobel Prize winner. No doubt, he knew the statistical probabilities cold, but was so self-contained that he had difficulties taking into account the psychology of the other players. He lost most of the time. Wouldn't it be great to understand the psyche of Saddam Hussein? I would love to play poker with him.

How about the professional poker players that I encountered in Las Vegas? One might imagine that they are an unemotional, cal-



**The home game.  
G. Feher with his  
grandson Avi, inspiring  
a new generation.  
La Jolla, June 2003.**

culating logical bunch. Far from it. Many of them display bizarre characteristics that I had never expected, such as superstition. They believe in winning and losing streaks, engendering their own self-fulfilling prophecy. Many also believe in the notion of a “hot seat” occupied by someone who had been winning for a while and clamor to occupy it when it is vacated, etc. Many of them squander their poker winnings by betting on the outcome of sporting events, elections, horse races (I can’t pass up this opportunity to give you my explanation of the origin of the phrase “horse sense”. Horses don’t bet on the outcome of human affairs.) The wife of the grand old man of poker, Johnny Moss, once confided that she surreptitiously skimmed off 10% of his winnings and put it into a savings account to enable them to live out their life in comfort.

There is one disturbing incident that took place in Las Vegas a few years ago that keeps periodically intruding on my mind. It shows the tremendous absorption, concentration and total neglect of the world outside the game. Although these traits contribute to the appeal and fascination with the game, they can as described below, on occasion, transcend the limit of decency. One of the players at a poker game in which I participated collapsed and fell to the floor. It looked like a heart attack or a stroke. The dealer called the floor manager but continued to deal the hand. Nobody stirred (except me

who left the table) and the game continued uninterrupted, except for the dealer’s shouting: “Two free seats on Table 23”. The poor man in the meantime moaned and turned more and more ashen. It took about 20 minutes for the paramedics to arrive. By that time, the man had stopped breathing and appeared dead. I was appalled, wrote a short note about it and went with it to the Las Vegas Sun. It was never published, nor was the incident mentioned. When I complained about it to the locals, they just shrugged it off with the remark: To have it publicized would be bad for business. It is, therefore, no wonder that I never met players in Las Vegas with whom I could imagine becoming friends. They, on the other hand, probably consider me an oddball and cannot understand how I can return to the “humdrum” life of academia.

Even if a friendly poker game is a contradiction in terms, there is a big difference between the bimonthly home games I’ve been playing for the past ~50 years and the games in Las Vegas that I play a few times a year. The home games with my colleagues are congenial and comfortable and I enjoy them thoroughly. Las Vegas I enjoy twice: when I arrive and when I leave. The crass (albeit picturesque) characters one plays with, the unremitting tense concentration over a long stretch of time, sometimes 24 hours non-stop, the lack of sleep add up to an experience that is exciting but draining; and

after several days, exhaustion and a desire to flee set in.

So why, in view of these derogatory remarks about Las Vegas, do I continue to go there? Simply because it is the one place where there is the challenge to measure my skills against the best in the game. I can sit at a poker table with players, whose names I have heard for years: Johnny Moss, Amarillo Slim, Doyle Bronson, Puggy Pearson, Jack Strauss – the Pauli’s and Fermi’s of Poker. I also had the pleasure of playing with the actor Telly Savalas of “Kojak” fame who was preparing for a movie depicting the legendary game at Binion’s Horseshoe in Las Vegas in 1949 between Nick The Greek and Johnny Moss. The game lasted five months and it is reputed that Nick the Greek lost two million dollars. Unfortunately, Savalas died before the film was finished.

I find that many of my academic colleagues consider my poker playing between un-understandable and despicable. Do you? Well, that’s the risk I took in writing this piece. On the other hand, if you think you will find poker exciting, or already do so, I would like to take this opportunity to invite you to join our game in La Jolla. We will be happy to give you an introductory “free” lesson.



# Anniversaries

## 95th Birthday of Evgeny K. Zavoisky

Nataliya Evgen'evna Zavoiskaya, daughter of E. K. Zavoisky, gave an interview to the *EPR newsletter* on the occasion of her father's 95th birthday.



***Nataliya Evgen'evna, 2002 was the year of your father's 95th anniversary. How is the memory about this great compatriot kept in Kazan, the birthplace of EPR?***

Yes, the Motherland of EPR, Kazan, keeps the memory about my father alive and I bow low to everybody, who remembers him and highly estimates his contributions to science. The Kazan Physical-Technical Institute (KPhTI) is named after E. K. Zavoisky, and starting in 1991, an annual International Zavoisky Award is celebrated in Kazan. The present Award holders are outstanding scientists from USA, UK, Switzerland, Germany, Russia, and The Netherlands. In 1998 KPhTI published a brochure "Materials to the Biography: E. K. Zavoisky" (in Russian), written by my mother.

Kev M. Salikhov, director of the KPhTI and corresponding member of the Russian Academy of Sciences, is a co-editor of the book "Foundations of Modern EPR". Professors Yuri V. Yablokov and Boris I. Kochelaev wrote the book "The Beginning of Paramagnetic Resonance", to mark the 50th jubilee of EPR.

At the Kazan State University, thanks to the efforts of Semen A. Al'tshuler, corresponding member of the Russian Academy of Sciences, a high relief of E. K. Zavoisky was put, Zavoisky readings were organized, memorial boards were erected, and scholarships for students were

established. Moreover, in the Museum of History of the Kazan State University there is a section dedicated to the life and activity of my father and a museum-laboratory with models of the first EPR instrumentation was opened. In the Lobachevsky Library there is a permanent exhibition of manuscripts of my father and twelve albums devoted to his scientific activity. The National Archive of the Republic of Tatarstan will soon get his archive.

The administration of the city of Kazan named one of the streets after E. K. Zavoisky.

***E. K. Zavoisky made his discovery during the hard years of World War II. What did he tell about the terms he had to work in?***

My father discovered EPR in 1944. This is the official date. However, he observed NMR and EPR much earlier. He wrote this in his "Essay of the EPR History". His first homemade setup was very simple. It contained no radar techniques, which is often mentioned in the Western scientific literature in connection with my father's discovery. At that time in Kazan there was no such technique at all.

Hardships of the wartime, inertness of our scientific authorities and also the Iron Curtain – these were the main reasons that the former Soviet Union (Russia) lost a doubtless Nobel Prize.

***Did your father ever regret that he stopped his EPR research?***

My father never stopped his EPR activity. This is evidenced by his works during the Moscow period and his reports at EPR conferences. He met his friends and colleagues, Semen A. Al'tshuler and Boris M. Kozyrev, very often and they discussed research carried out at the Kazan State University and the Kazan Physical-Technical Institute. Besides, he always read the literature in the field. Thus he was always well informed about the activities going on in EPR. At home in Moscow he had his own EPR laboratory which he built himself.

***What were the circumstances that made your father leave Kazan and move to Moscow?***

There were several reasons for this. One of them was of everyday origin: we lived in a very moist house. Judging by the windows of the ground floor, our house was in former time a storehouse. My mother fell heavily sick and my father asked the authorities to give us another flat but his request was rejected. The second reason was a scientific one. Apparently the talent of my father needed a vaster expanse. In the years after the war research in Kazan was hardly financed at all. The equipment became obsolete and new equipment was not available. Somebody recommended him to the academician Igor V. Kurchatov, and Igor Vasil'evich put him up in his laboratory (now the Russian Research Center "Kurchatov Institute"). And, finally, there was also a family reason: my father's brother and both sisters at that time already moved to Moscow. They were on very friendly terms and their families had suffered a lot at the time of terror: three members of the family were subject to repression, and only one of them returned home alive. Three kids became orphans.





Evgeny K. Zavoisky (center) with his friends and colleagues, Semen A. Al'tshuler (left) and Boris M. Kozyrev (right). Kazan, 1968.

***Was science the only passion of your father or did he have a hobby?***

My father was betrothed to physics early. It was one of his most important *raison d'être*. He was never disappointed about physics. When life forced him to participate in the creation of an atomic bomb, he wrote to my mother: "This specialty becomes nasty". But it was not physics that was nasty, it was what circumstances and people made of it. As soon as possible, he dropped the defense research and never returned to this field.

He had, of course, a hobby: it was traveling by car. My father had a car and we traveled a lot in Crimea, the Carpathian mountains, the Baltic Republics of the former Soviet Union. We visited Suzdal, Vladimir, Tver, Novgorod, and Leningrad. My father always drove a car. Moreover, he collected scientific literature and his library was rather large. He was also interested in modern painting.

***There is the saying: Behind every great man there is a great woman. Please tell us about your mother.***

On November 11, 1932 my mother submitted her documents to enter the Kazan State University. E. K. Zavoisky, Associate Professor, registered these documents. My mother told me that on this very day she fell in love with him. My mother was a charming girl, a slim blonde with big blue eyes. She was only eighteen when my parents married. My father was seven years

older. My mother told me that she was so eager to go with him to the theater, to movies, or to visit friends. But my father was so much absorbed by his interesting work that he could not find a spare minute. My parents always had an understanding. My mother took care of all daily chores, translated papers from English into Russian for my father and discussed them with him. It is my mother's merit that she kept the large archive of my father. When my father fell heavily ill, my mother stoically

fought for his life. My mother is the author of the brochure "Materials to the Biography: E. K. Zavoisky".

***What were the main characteristics of E. K. Zavoisky?***

Modesty, decency, adherence to principles, responsibility, tenderness, fidelity.

By the way, you might be interested to learn that the surname Zavoisky is rather new, it is only 200 years old. Our Vyatka ancestors had the surname Kurochkin. The clan was very large and in the family of the father's great-great-grandfather, a priest from the Rozhdestvenskoe village of the Vyatka province, three sons had the same name Nikolai, which was common at that time. In the seminary, in the beginning of the 19th century, they were given new surnames: Zakharov, Rassvetov, and Zavoisky. Our ancestor was given the surname after the river Voya.

One more piece of history: in the Peter and Paul's Cathedral in Kazan, in 1774, shortly before the Pugachev revolt, the seminarist Zakhar Stefanov Kurochkin, great-great-grandfather of my father, heartily prayed. And shortly before World War II, E. K. Zavoisky installed in this cathedral the Foucault pendulum for the museum of atheism. Jumps and grimaces of history...

## 65th Birthday of John Pilbrow

On March 28, 2003, John Pilbrow celebrated his 65th anniversary. It is difficult to find somebody in the EPR community who is not well acquainted with this outstanding man. Linn Belford gave a nice introduction of John Pilbrow as Secretary of the IES in his Editorial (*EPR newsletter*, vol. 9, no. 1, p. 2 (1997)). There is also a comprehensive entry on his research activities in the *EPR newsletter*, vol. 10, no. 3, p. 6 (1999) on the occasion of his Bruker Award 1998. From 1998 to 2002 his photograph was often in the *EPR newsletter* re IES medal presentations he made first as Secretary and then as President of the IES.

We heartily congratulate John Pilbrow and wish him and his large family all the best. In particular, good health, as he is recovering successfully from some recent heart surgery. We are looking forward to many more years of his enthusiastic activity for the benefit of the EPR community.





# 60th Birthday of Dieter Schmalbein

On 22th October 2002 Dieter Schmalbein has joined the club of the sixties. He is well known to the whole EPR community as the father of various series of commercial EPR spectrometers: ER 200, ESP 300, EMX, and ELEXSYS.

Dieter Schmalbein graduated from the Technical University in Aachen in 1969 and finished his PhD at the Ruhr University in Bochum in 1972 with his thesis "Microwave Delay Lines as Detector for Electron-Multiple-Resonance". Since 1973 he is working at Bruker starting the development of the ENDOR and TRIPLE accessory. Besides technical and scientific skills his management capabilities were evident and already in 1976 he became the division leader for EPR. Since 1990 he is one of the managing directors of Bruker Analytische Messtechnik GmbH, today Bruker BioSpin GmbH. He is an exceptional team leader of an extremely

creative EPR group including such well known scientists like the late Reinhold Biehl, Peter Höfer and Karoly Holczer. Together they developed the first commercial Pulsed EPR, Fourier-Transform EPR and Pulsed ENDOR spectrometers, as well as high-field spectrometers opening frontiers in EPR for many users. You may find Dieter Schmalbein at almost any of the leading EPR conferences, often together with his charming wife Cornelia, looking for new ideas and new challenges, as well as for new applications. He has initiated the Bruker EPR award and has received for Bruker the Zavoisky Award in 2000 in Kazan.

The EPR community is indebted to Dieter Schmalbein for many outstanding developments. We wish him health and good luck to maintain his creative spirit for the next years and are looking forward to his new developments.



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# John Pilbrow Recalls the Clarendon Laboratory in Oxford in the Early 1960's

**H**aving been introduced to EPR spectroscopy in New Zealand for my Masters degree in Physics, I left for Oxford in August 1961 to begin work on my DPhil [i.e. PhD] with the intention of working in Superconductivity! In the event I remained in EPR but that is another story.

Those of us beginning our graduate work were required to attend lecture courses by Brebis Bleaney [on EPR], Werner Wolf [on magnetism] and by John Van Vleck from Harvard, who was Eastman Visiting Professor during 1961-2. Van Vleck's lectures based on his book *The Theory of Electric and Magnetic Susceptibilities*, were both memorable and entertaining. He always came into the lecture hall with a copy of

his book and a stack of reprints of his papers about 40 cm high! In fact he spent a good deal of time searching through the stack of papers as he mostly seemed to lecture without notes. Barely legible handwritten notes were sometimes provided and I still treasure them today. What I recall particularly was the sense of history he conveyed. After all he contributed a major part of the history of the application of quantum mechanics to magnetism and this indeed was what earned him a share of the 1977 Nobel Prize in Physics. His work on paramagnetism of transition metal complexes and transition metal ions, which led to the primitive form of crystal field theory was, and remains, very insightful even today in thinking about high and low spin transition metal ions. We remain in his debt for his early contributions to spin-lattice relaxation and the Jahn-Teller Effect. These impacted on much of the early EPR spectroscopy of transition metal ions.

I worked under Bill Hayes in Lab 041 in the Townsend Building, which had been Brebis Bleaney's lab before he became Dr Lee's Professor. The long tradition of the 041

Coffee Club tradition continued. Thus, in addition to members of the Hayes group and Michael Baker's group from the next lab, another 10–15 others used to arrive every morning at about 10.30 am. Brebis Bleaney always brought important visitors for coffee. In my first year [1961-2] a regular attendee was John Van Vleck. Beginning graduate students were rostered to go into town to buy freshly ground coffee each week from a Turkish Coffee Merchant! When I first experienced a crowd of 20 or more in the lab each morning, many of whom continued their discussions until about 11:30 am, I felt somewhat annoyed because it was impossible to get started on experiments until after they had all gone. However I quickly realised that one of the reasons I had sought to go to Oxford from the small world of New Zealand was to experience the cut-and-thrust of discussion about physics, about science and about many other things. I soon learned that the experiments could wait!

Other notable memories from those days include the 10 lectures on *EPR in Semiconductors* by Anatole Abragame late in 1962. There we learned of the major contributions made by George Feher to this field which may surprise younger members of the EPR community who perhaps know only him through his work in photosynthesis. From the point of view of my general education I still value the lectures on *Optical Properties of Solids* by Roger Elliott [now Sir Roger – who with Ken Stevens introduced operator equivalents], on *Solid State Theory* by Sir Rudolf Peierls based on his book *Quantum Theory of Solids* and on *Group Theory* by Melvin Lax [Bell Labs].

In 1965 I moved my family to Australia, to Monash University in Melbourne, and again considered changing fields to Superconductivity but for several good reasons I found myself continuing in EPR – still to this day!

During 1969 it was a great privilege to have the opportunity to meet up again with Professor Van Vleck following the *IUPAC Congress* in Sydney where he had taken part in a celebration of 50 years of Quantum Chemistry. At Monash he attended the *International Symposium on Magnetic Resonance* where he gave a very memorable after dinner speech laced with fascinating historical anecdotes [*Magnetic Resonance*, Plenum Press 1970]. I knew that he had written a book on the Old Quantum Theory, *Quantum Principles and Line Spectra*, that was to have been published by Oxford University Press in 1925 or 1926, but which subsequently appeared as an NBS Monograph. So I took the opportunity to talk with him about his view as to why perhaps he, and some of his distinguished colleagues in the US, had not independently stumbled upon Quantum Mechanics. With his usual candour he replied 'I have given this a great deal of thought, but we were in the wrong philosophical climate!' What he meant was that he, at least, believed one could patch up the Old Quantum Theory. However Quantum Mechanics required a totally new approach.

The Clarendon Lab contributed the name 'paramagnetic resonance', the 'spin Hamiltonian', 'operator equivalents' as well as theory accessible for experimentalists in the field of EPR. The early 1960's saw EPR give way to other areas of research at the Clarendon Laboratory, a period in which applications to chemistry and later biology began to dominate the field elsewhere. Michael Baker's group continued the tradition and in more recent times did outstanding work on defects in diamond.. I personally owe much to my Oxford experience, friendships made and science learned and practiced.

John Pilbrow  
Monash University, February 25, 2003

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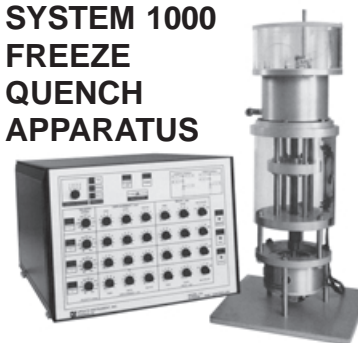
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# Lev A. Blumenfeld

## (1921–2002)

*I lived my life. I'm not to judge,  
If it was good or bad.  
But my epoch didn't manage to completely murder  
My ego in me.*

(translated from L. A. Blumenfeld, "Selected Verses", 2001)

Professor Lev A. Blumenfeld, one of the pioneers of EPR applications to biology and chemistry, passed away on 3 September 2002. He lived a bright and exceptionally intellectual life and worked actively until his last days.

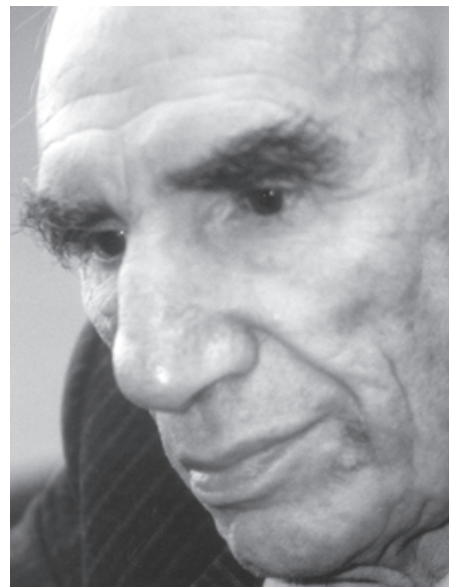
Lev A. Blumenfeld was born on 23 November 1921, in Moscow. In 1939 he became a student of the Faculty of Chemistry of M. V. Lomonosov Moscow State University. His academic carrier was interrupted by World War II. In 1941 Lev Blumenfeld volunteered in the Red Army; he participated in many battles of World War II and was wounded twice. His scientific carrier began in 1944. In the hospitals, where brave lieutenant Blumenfeld recovered after severe wounds, he began his work on the quantum chemical calculations of two-atom molecules (HF, HCl, HBr and HI). For the courage displayed during the War against fascism, Lev Blumenfeld was awarded a number of medals and orders.

In November 1945 Lev Blumenfeld was demobilized from the Army and continued his study in the Faculty of Chemistry of the Moscow University. The quantum chemical calculations carried out during the War laid the basis of his diploma work. In 1946 he successfully graduated from the University and then continued his research work in the field of quantum chemistry in the Karpov Physical-Chemical Institute. He received Ph.D. degree in 1948 for the study of electronic levels and optical properties of conju-

gated hydrocarbons. Soon after this work, Lev Blumenfeld turned to the study of physical and chemical properties of hemoglobin (Central Institute of Advanced Medical Studies, Moscow). Remarkably, as early as 1952–53, he predicted, independently of Max Perutz, the occurrence of large-scale conformational changes in hemoglobin. Lev Blumenfeld received D.Sci. degree from the Institute of Chemical Physics (1954, Moscow) for the study of hemoglobin structure and mechanisms of reversible association of oxygen with hemoglobin.

Lev Blumenfeld is well known as a pioneer of EPR applications to the study of biological systems. In 1955–56, he was the first in Europe (together with his collaborator Alexander Kalmanson and independently of Barry Commoner and his colleagues in USA) who observed EPR signals from biological samples. Professor Blumenfeld successfully continued to investigate biological and chemical systems by the EPR method together with his numerous pupils in the Institute of Chemical Physics (Moscow) and in the Department of Biophysics, Faculty of Physics (Moscow State University) for more than 45 years. In 1995 Professor Lev Blumenfeld was awarded the IES Silver medal in Biology/Medicine. In 2001 he was awarded the Voevodsky Gold Medal of the Russian Academy of Sciences.

Lev Blumenfeld also significantly contributed to the study of energy transduction in biological systems. On the turn of his 60th and 70th birthdays he put forward new ideas on the mechanisms of enzyme catalysis. Lev Blumenfeld suggested that one should consider biopolymers as molecular machines, characterized by a few selected ("mechanical") degrees of freedom. The "relaxation concept" of enzyme catalysis was experimentally substantiated by Lev Blumenfeld and his collaborators. Impressive experimental support of Blumenfeld's view on enzymes as



"molecular machines" has come from biophysical laboratories from all over the world. For his works "Physical mechanisms of energy transduction in biological membranes" Lev Blumenfeld was awarded the Lomonosov Prize (Moscow State University).

Professor Blumenfeld was Head of the Department of Biophysics (Faculty of Physics, Moscow State University) for almost 40 years. About one thousand students have graduated from this department that was founded by Lev Blumenfeld in 1959. He has personally guided more than 100 research scholars (Ph.D. and D.Sci.). His students are working now in leading academic institutions across the globe. Professor Blumenfeld was the author of 7 books and more than 300 papers published in Russia and abroad.

Lev Blumenfeld was a generously gifted and highly intellectual person. He was not only a brilliant scientist, but also a talented poet. All his life he wrote profound verses and poems, and he translated into Russian classic poetry of German and English authors (H. Heine, R. Kipling, A. Swinburne, R. Browning, K. Dixon). He also published the autobiographical novel "Two Lives".

Lev Blumenfeld continued to work until the very last minutes of his life, in spite of the fact that he was suffering from severe heart disease. Only a few minutes before his last breath he reviewed the final proof of his last book, "Solvable and Unsolvible Problems of Biological Physics".

Enno Ruuge  
Alexander Tikhonov  
Moscow State University

**In Memoriam**



# John K. Grady

## (1960–2002)

John Kevin Grady, 42, of Somersworth, New Hampshire, USA, died January 12, 2002, at Brigham and Womens Hospital, Boston, Massachusetts, after a long struggle with leukemia. Born in Manchester, New Hampshire on January 25, 1960, he was the son of the late Thomas Francis Grady Jr. and Jeannette (Charbonneau) Grady.

John earned a Bachelor's degree in Chemistry in 1983 and a Master's degree in Biochemistry in 1998 both from the University of New Hampshire.

John started working for N. Dennis Chasteen in July 1984 as a senior technician. For 16 years, John was the backbone of the Chasteen lab; he kept it running smoothly and mentored and befriended the many graduate and undergraduate students and post-doctoral fellows who came to work and learn there over the years. In his short life, John made significant contributions to our knowledge of the proteins of iron metabolism, most recently developing an important CE method for assaying the subunit composition and integrity of ferritins. John employed EPR and other physical methods to characterize the iron binding and radical

generating properties of the transferrins and ferritins. He published 15 articles, being the lead author on many of them, and was a contributor to the tips and techniques section of the *EPR newsletter*. In 2000, John assumed a senior staff position at the Center to Advance Intermolecular Science (CAMIS) at University of New Hampshire, a center devoted to studies of interactions between biological molecules and serving industry and academia. He only worked there a short while before the leukemia returned and he was again hospitalized.

John was a gifted chemist and a wonderful person of great integrity. The new EleXys 500/560 EPR/ENDOR laboratory is dedicated to John. It will be known as the John K. Grady Electron Resonance Laboratory. There will be a dedication ceremony on September 18, 2003.

On a personal note, when Reef Morse underwent surgery for prostate cancer, John began a conversation with him about cancer and how he viewed life as a result of it. John was always upbeat, humorous, supportive, and sympathetic. These conversations were important contributions to providing a perspective of cancer as a journey in life rather than a battle to win or lose. His remarkable insight, frankness, and personal generosity contributed to all those who came in contact with him.

Edited by Reef Morse  
with contributions by N. Dennis Chasteen  
and Legacy.com



Last e-mail of John K. Grady to his friends is as follows:

*Hi all,*

*Most of you know I've been pretty sick for awhile. It's pretty bad right now and if you receive this it probably means that I've succumbed to the leukemia.*

*You've all added to my life and my life was richer having known you. I love and will miss you all and my I hope your life is filled with love and happiness!!!!*

*All my love and friendship.*

*John*

# David H. Whiffen FRS

## (1922–2002)

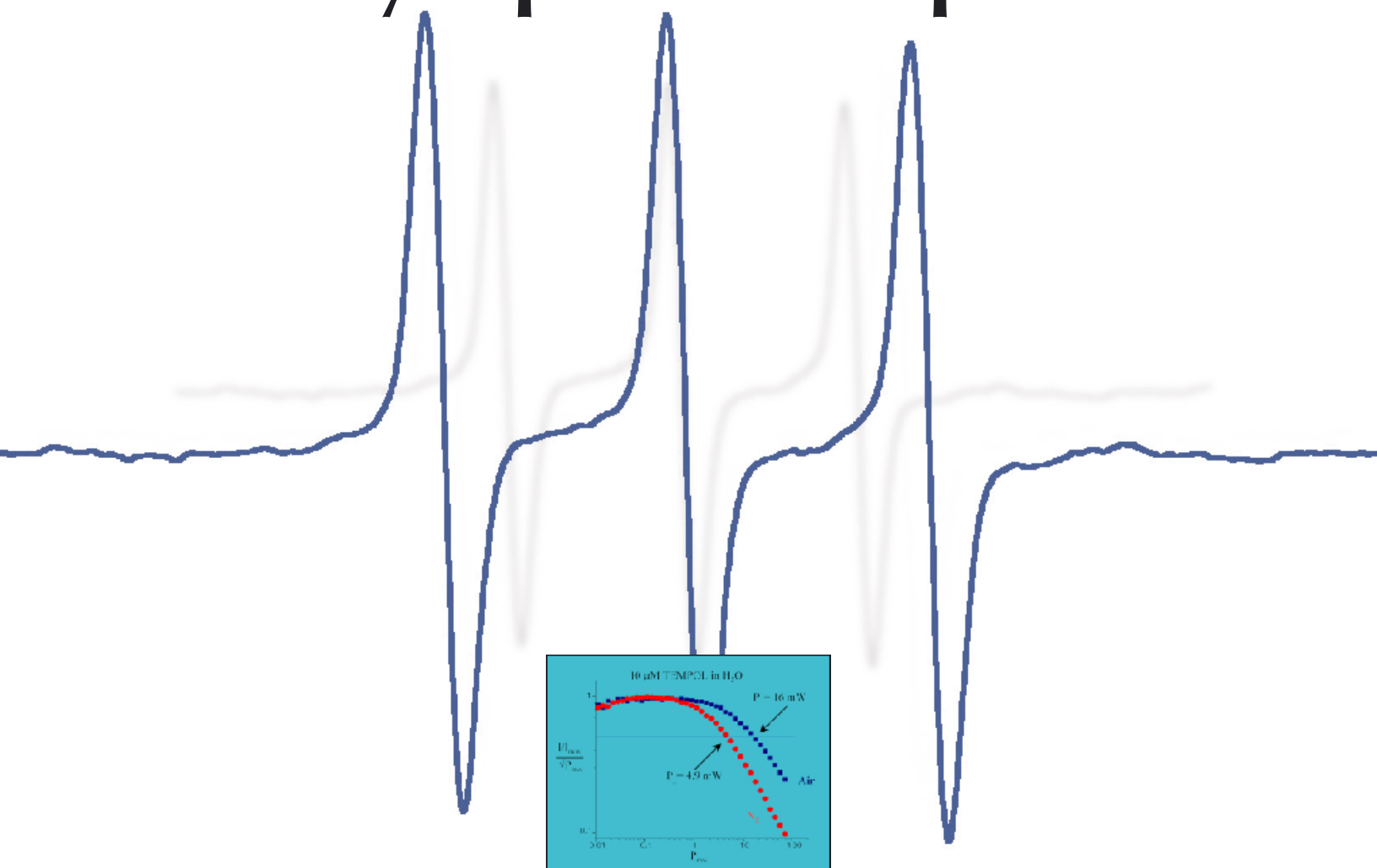
It is with regret that we record the death of David Whiffen at the age of 81. He was one of the true pioneers in the application of ESR spectroscopy to chemical systems and had a considerable influence on the development of both ESR and NMR. He was delighted when, after several years of retirement, I was able at the request of our President, to inform him that he had been elected a Fellow of the Society and to award him his

certificate. Typically modest, he was both surprised and delighted.

David graduated from Oxford in 1943 and stayed on until 1949 (with a period elsewhere) to pursue research in infra-red spectroscopy with H. W. Thompson. It was a time when researchers were becoming aware of the whole electromagnetic spectrum and David began to explore the applications of wartime RADAR equipment to the study of

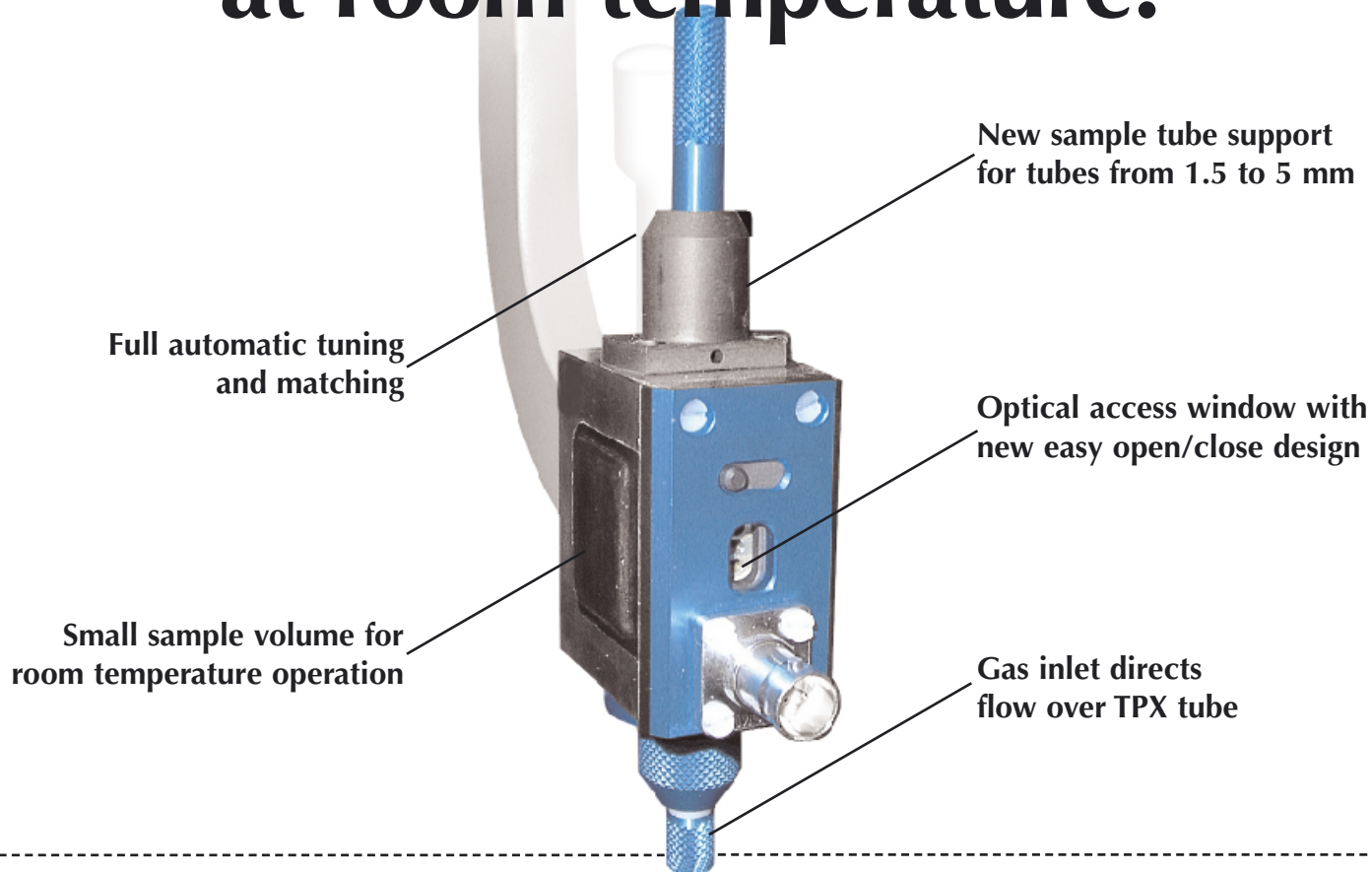


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molecules, originally in bulk. His first foray into this new field was in the area of dielectric loss phenomena at hitherto unexplored frequencies, including work done at the Bell Telephone Laboratories in Murray Hill. Returning to Oxford he demonstrated that a fundamental source of loss originated in molecular collisions and distortions.

In 1949 he became a Lecturer at Birmingham University and initially returned to the use of infra-red spectroscopy, largely in the context of structure determination with his synthetic chemistry colleagues. His contacts caused him to become interested in polymerisation, and he became aware that little direct physical evidence existed for the free radicals which were believed to occur in some polymerisation processes. He therefore built an early ESR spectrometer and had some success studying irradiated powders. But then Ubersfeld and Erb published the first study that demonstrated orientation dependence of the spectra observed from a single crystal of glycine within the magnetic field of the spectrometer. David rapidly followed this up and became the leading expert on studying such spectra and interpreting them. At the time, before the availability of digital computers, this was far from trivial and David established analytical methods for diagonalising the matrices. A large number of similar studies followed, especially when after 10 years he moved to the National Physical Laboratory at the invitation of John Pople. Neil Atherton was one of his post-graduate students in Birmingham.

These were exciting times at the NPL which rapidly became the best equipped magnetic resonance laboratory (both NMR and ESR) in Europe and which was largely staffed by post-doctoral workers, most of whom had returned from the U.S. in an

attempt to reverse the "Brain Drain". On the ESR side the early members included John Morton, Tony Horsfield, Ray Cook, Roy Brandon and John Rowlands whilst Ray Freeman, Ray Abraham, Tom Connor and Keith McLauchlan were the NMR people. Yuri Tsvetkov, now our President, came as the first Russian Exchange Visitor. David's interest in loss phenomena was continued in collaboration with Graham Williams and Brian Read. Many who joined or visited the Basic Physics Division later became at least as well known. The atmosphere was of continuous discovery and innovation, with the most stimulating atmosphere I have ever experienced.

Much of this stemmed from David himself. He set unparalleled standards for quality of results, reproducibility and depth of interpretation, and insisted on new experiments being tried continuously. Life for him was a continual intellectual challenge, with every aspect of any problem considered in depth. Lunchtimes with him were the reverse of relaxing. With Ray Freeman he published most of the work that provided the first examples of double and triple resonance in NMR studies, and contributed to the whole development of NMR spectrometers. In ESR he caused X- and Q-band spectrometers to be developed and soon extended them for very early ENDOR studies, again using both double and triple resonance. In the nine year lifetime of the Basic Physics Division at the NPL over 300 papers resulted at a time when most of the equipment was home-built and when we were all at the limits of the then understanding of magnetic resonance. David's contribution at this time cannot be over-exaggerated. He was personally original and he taught us all how to interpret our results as thoroughly as

could be done. He was a fount of knowledge, but also he encouraged us to believe that we could do *anything* either in experiment or in theory. All of us who worked with him are greatly in his debt.

Unfortunately political pressures eventually decreed that basic research had no place in UK Government Laboratories and this laboratory, which had competed with the best in the world, ceased to exist. David thereupon accepted a Chair in Physical Chemistry at Newcastle University and, although becoming active now in new techniques applied to gaseous microwave spectroscopy, never again achieved the heights he had enjoyed whilst at the NPL. Inevitably due to the progress in science many of his achievements seem less astonishing in retrospect since once he had taught us to understand them they became accepted. But at the time he shared his pre-eminence with only a few of his contemporaries. His long lasting contribution is what he taught those of us lucky enough to work with him and which we have handed down in turn to our own students. It was a genuine privilege to have had him as a supervisor and friend.

It would be remiss not to mention the non-scientist. David was a quintessential family man with four sons and several grandchildren whom he adored, and was deeply religious although not intrusively so. On retirement he had moved to a small village in Somerset and with his wife Jean entered fully into the community life, providing much assistance to old people and charities. His Memorial Service was held in the ancient church there, and it was endearing to experience the obvious sense of loss of the village congregation, quite outside that of his family and scientific friends.

Keith McLauchlan

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# Daniel Kivelson

## (1929–2003)

We are saddened to report that Professor Daniel Kivelson passed away on Wednesday, January 22, 2003. Daniel was in many ways the ideal of a UCLA professor. He was an original and deep scholar, a great teacher and a departmental and campus leader. And, above all else, he was an extraordinary friend and counselor to so many of us.

Dr. Kivelson was born in New York City in 1929. He came to UCLA in 1955 as an Instructor after completing his undergraduate and graduate studies at Harvard. His thesis research in chemical physics, under the supervision of E. Bright Wilson, was on the use of microwave spectroscopy as a tool for determining molecular structure. At UCLA he established a program in electron spin resonance. This early research had the hallmarks of his approach to science. He combined expertise in experimentation with fundamental theoretical analysis. His treatment of ESR relaxation remains one of the most highly cited papers in the field. Daniel made important contributions to the theory of molecular relaxation in fluids throughout his career and carried out complementary experimental studies by light scattering, in which he was an early leader. For the past several years he had focused on the study of supercooled liquids and glasses and brought major new insights into this important and challenging area.

Dr. Kivelson was a brilliant and charismatic teacher. He was a research mentor to many graduate students and post-doctoral fellows; he took particular pleasure in introducing undergraduates to research. In 1967 he was the recipient of the UCLA Harvey L. Eby "Art of Teaching Memorial Award" and he recently was awarded a grant from the Dreyfus Foundation in recognition of his work with undergraduates.

Daniel's record of service was also exceptional. In the department he served as chair of many committees and served as both undergraduate and graduate advisor. From 1975–78 he was departmental chair. In 1979 he was elected vice-chair of the LA Division of the Academic Senate and succeeded to the chairmanship the following year. He led many university task forces and search committees.

Dr. Kivelson was the recipient of many awards and distinctions including Guggenheim, Sloan and Fulbright Fellowships, the American Chemical Society California Section Award, and the Herbert Newby McCoy Award. In 1987 he was the recipient of the College of Letters and Science Faculty Award and in 1999 he was the winner of the American Physical Society Langmuir Prize in Chemical Physics.

Daniel is survived by his wife Margaret, his daughter Valerie and her husband Tim,



son Steven and his wife Pam, and five grandchildren. A memorial service was held in the California Room of the UCLA Faculty Center from 4 to 7 pm on Friday, January 31.

In Daniel's honor a special fund is being established for undergraduate summer research fellowships. Checks should be written to the Regents of the University of California with a notation that it is for the Kivelson Fund.

Provided by Robert R. Scott

## In Memoriam



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# **EasySpin:** *a Software Package for the Computation of EPR and ENDOR Spectra*

Stefan Stoll

During the last decade cheap and fast computers have become available. As a result, EPR spectroscopists can simulate their spectra on their desktop computer and no longer have to rely on large-scale computing facilities. This led to the emergence of several general simulation programs.

One of the first to become widely used was SimFonia for Windows, written by Ralph T. Weber (Bruker BioSpin) in the mid-1990s. Based on perturbation theory, it was not generally valid and its results had to be used with care. In 2000, Bruker BioSpin substituted SimFonia with XSophe, a significantly enhanced simulation suite now running under Linux. The program is developed by Graeme Hanson's group at the University of Queensland in collaboration with Bruker BioSpin.

Other general programs include the little known but highly useful DOS/Windows program SIM, developed by Høgni Weihe (University of Copenhagen), simpip (formerly QPOW) by Mark J. Nilges (Illinois EPR Research Center), and EPR-NMR, a long-standing project of John Weil (University of Saskatchewan) and Michael Mombourquette (Queen's University). Links to these programs and to other computational EPR software can be found on the internet at [www.esr.ethz.ch](http://www.esr.ethz.ch) or in the ESR software database (ESDB) at [epr.niehs.nih.gov/software.html](http://epr.niehs.nih.gov/software.html).

## EasySpin

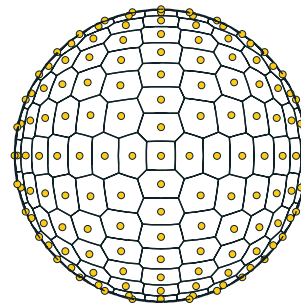
The spectrum simulation software with the most extensive functionality so far is EasySpin, developed in the EPR group at ETH Zurich (Switzerland). The software package grew out of an attempt to integrate theoretical computations, spectral simulations and data analysis on a single user platform. EasySpin consists of a collection of functions that add EPR analysis and spectral simulation functionality to the scientific computation and visualization environment Matlab ([www.mathworks.com](http://www.mathworks.com)).

The latest release of EasySpin can be downloaded from [www.esr.ethz.ch/easyspin](http://www.esr.ethz.ch/easyspin). It requires Matlab 6.0 or later

and runs on PC/Windows, PC/Linux, Sun/Solaris and SGI/IRIX. The software itself is free, but the source code is not yet available to the public.

## Powder spectra

Although it offers a host of other features, the main purpose of EasySpin is the simulation of powder EPR spectra. A powder consists of a uniform random orientational distribution of a large number of paramagnetic centres. The powder spectrum is nothing but the sum of the spectra arising from the single centres. For speedy computation, it is necessary to compute as few orientations as possible from a uniform distribution of orientations on the unit sphere. For this purpose, EasySpin uses a novel highly homogeneous triangular arrangement with octahedral symmetry (see illustration). Other programs use simple theta/phi grids (SIM), spiral arrangements (EPR-NMR) or triangular grids with  $D_{4h}$  symmetry (XSophe). For each orientation, the single-crystal spectrum is computed. Each single-crystal spectrum is multiplied by a weighting factor which is proportional to the solid angle covered by the neighborhood of the orientation (the borders of these so-called Voronoi cells are shown in the illustration below). EasySpin is the first program to include exact weighting factors for this summation.

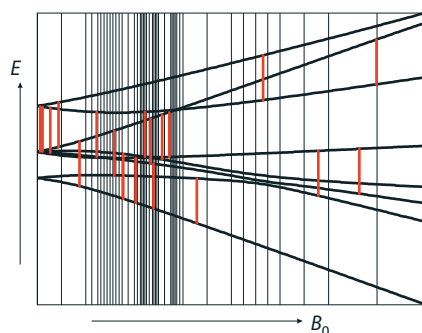


145 orientations over a hemisphere  
with their neighborhoods

## Resonance fields

For field-swept EPR spectra, resonance fields can be computed either analytically or numerically. Analytical solutions are limited in scope and exist only for small systems with one dominant interaction (e.g. the electron Zeeman interaction). Nowadays, practically all programs use entirely numerical procedures. First, state energies and vectors at one or more values of the external magnetic field are computed by numerically diagonalizing the spin Hamiltonians in their full matrix representations. These matrix diagonalizations form the most time-consuming step of the entire simulation procedure.

Second, the state energies and vectors are used to compute the resonance fields. This is the point where numerical programs differ from each other. XSophe implements a linear field segmentation scheme with second-order perturbational corrections, SIM iterates using cubic polynomials, and EPR-NMR uses a Newton-Raphson approach. EasySpin obtains the resonance fields by interpolation from an adaptively modelled cubic spline representation of the energy level diagram. This new method is accurate and very robust and needs less Hamiltonian diagonalizations than the other methods. In a complicated situation with many anticrossings (see illustration), the method needs at most three diagonalizations per resonance field (illustration: 19 resonance fields, 45 diagonalizations).



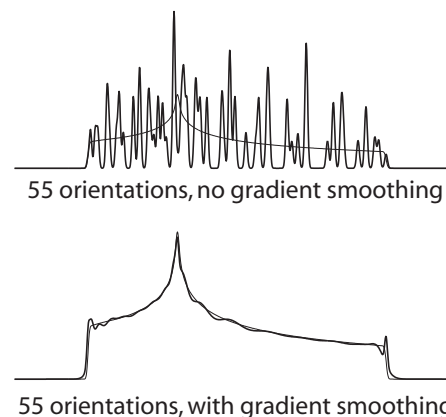
## Interpolation

The high cost of computing resonance fields can be avoided by the application of much faster interpolative procedures. Once resonance fields are known for two similar spin Hamiltonians, differing slightly e.g. in the orientation of the spin system with respect to the external magnetic field, the resonance fields of spin Hamiltonians lying in between can be computed interpolatively with only small error. Both cubic and linear interpolation can be used, depending on whether resonance fields or intensities are computed. EasySpin makes extensive use of these interpolation techniques.

## Gradient smoothing

Another feature of EasySpin's spectrum simulation algorithm that enhances performance is the use of gradient smoothing. Before combining the computed single orientation spectra into a total powder spectrum, an additional broadening is added to the intrinsic line widths in order to reduce computational noise, i.e. to bridge the gaps between the various peaks in the computed spectrum (see illustration).

In technical terms, this additional smoothing line-width is proportional to the magnitude of the gradient of the resonance field with respect to the orientation of the magnetic field in the molecular frame. The concept was first developed in a rudimentary form by Høgni Weihe for his program SIM and was later independently implemented in a more general form in both EasySpin and XSophe (where it is called "mosaic misorientation model").



## EasySpin simulation example

EasySpin's functions do not have a graphical user interface, they can only be accessed from the Matlab command line. Nevertheless, they are straightforward to use. Matlab features a full-fledged programming language, so that many specialized EPR problems can be treated by programming new functions based upon EasySpin's toolbox.

All the algorithmical improvements described above make EasySpin's cw EPR spectrum simulation function `pepper()` general and very efficient. The following lines are the input necessary to simulate a powder spectrum of a  $\text{Cu}^{2+}$  complex at X band:

```
Sys = struct('S',1/2,'I',3/2,'gn',1.484);  
Sys.g = [2 2 2.2]; Sys.A = [50 50 300];  
Par = struct('Range',[270,360],'mwFreq',9.5);  
[B,Spectrum] = pepper(Sys,Par);  
plot(B,Spectrum)
```

`pepper()` can treat parallel detection, temperature effects, higher order harmonics, systems with more than one electron, interaction matrices with arbitrary orientations and strains in  $g$ ,  $A$  and  $D$ .

Other functions provide smaller building blocks for the user. To compute only the resonance fields of an  $S = 1$  system with significant zero-field splitting, use

```
Sys = struct('S',1,'g',2,'D',[-1 -1 2]*3e3);  
Par = struct('mwFreq',10);  
Ori = [0;pi/5]; % [phi; theta]  
ResFields = eigfields(Sys,Par,Ori)
```

which returns the fields in units of mT

```
ResFields = [40.9060 238.4059 44.1146]
```



## ENDOR and Pulse EPR

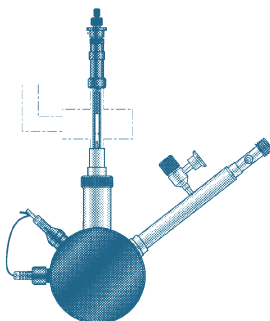
Powder ENDOR spectra are much easier to simulate than cw EPR spectra. In addition, ENDOR spectra are commonly measured selecting very few orientations and therefore yielding single-crystal like spectra even for powders. However, the situation gets more complicated if ENDOR spectra are not taken at the edges of complicated EPR spectral line shape. In this case, a full treatment of the orientation selection is crucial. EasySpin offers an ENDOR simulation routine with an accurate orientation selection procedure. Its usage is very similar to that of `pepper()`.

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A short word about pulse EPR simulations is in order. Generally applicable software is not yet available, due to the absence of a theoretically general and experimentally verified computational procedure. Current attempts are limited to special experiments and  $S = 1/2$  systems with small  $g$  anisotropy and small hyperfine couplings and include tryscore (for HYSCORE, by Daniella Goldfarb, Weizmann Institute of Science) and a program by Zoltan Mádi (ETH Zurich). Bruker BioSpin is working on an XSophe version with basic pulse EPR functionality. EasySpin is to include pulse EPR features in its next release.

## More functionality

Since Matlab's programming language is based on matrices, it is straightforward to compute spin operators and their functions. For example, the matrix representation of a  $90^\circ$  pulse on an  $S = I = 1/2$  system can be computed by the two lines

```
Sy = sop([1/2 1/2], 'ye');  
Pulse = expm(i*pi/2*Sy)
```

In addition to the usual cartesian spin operators, EasySpin provides a full set of Stevens operators for  $S > 1$ .

Among other features, EasySpin includes a function to compute the effect of field modulation in a cw EPR experiment (pseudomodulation), a time evolution function for density matrices, a database of nuclear  $g$  values, many relevant physical constants, various line shape functions, apodization functions, tools to handle rotation matrices and Euler angles, etc.

## Spectral fitting

The development and application of numerical optimization algorithms for fitting spin Hamiltonian parameters to experimental spectra is still in its infancy, mainly due to the usually exceptionally bad behavior of the error function. For powder spectra, current methods work well only when the starting guesses of the parameters are very close to the correct ones or when experimental spectra at different microwave frequencies are available. Thus, numerical fitting is mainly a tool for final refinement of spin Hamiltonian parameters. Some of the programs mentioned in the introduction have built-in spectral fitting capabilities. Matlab offers a variety of fully customizable optimization algorithms, which can be used together with EasySpin's simulation functions to write fitting programs even for multiple spectra and other complex situations.

## Further reading

- Stoll St.: Spectral Simulations in Solid-State EPR. Ph.D. thesis, ETH Zurich 2003.  
Griffin M., Muys A., Noble C., Wang D., Eldershaw C., Gates K.E., Burrage K., Hanson G.R.: XSophe, a Computer Simulation Software Suite for the Analysis of Electron Paramagnetic Resonance Spectra. Mol. Phys. Rep. 26, 60–84 (1999)

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# Error Sources in Quantitative EPR Spectroscopy

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The results obtained from international experiments, which were carried out in 1962 [1] and 1991–92 [2], clearly demonstrated the essential difficulties in quantitative EPR spectroscopy. In principle, experimental errors in quantitative EPR measurements for a given laboratory and a given EPR spectrometer may be reduced in carefully performed experiments to between 2 and 5% [3, 4]. However, in practice, quantitative analysis of the same sample in different laboratories produced results, which gave an uncertainty from 100 to 200% [1, 4], and others up to 500% [5]. No satisfactory explanation for this discrepancy has been found at present.

The main aim of this short contribution is to inform the wide EPR community about known primary and secondary error sources in quantitative EPR measurements. We believe that the tips outlined at the end of this report would be helpful in quantitative EPR praxis.

Many error sources influence the accuracy and reproducibility of quantitative EPR spectroscopy [3]. The list of instrument- and sample-associated variables, which can affect EPR measurements, is very extensive and the majority of these error sources may cause significant systematic and/or non-systematic errors in quantitative EPR experiments. Some of the most difficult problems have been selected as follows:

## Primary Error Sources

### A) Sample-associated problems

#### *Sample preparation:*

- sample material (dielectric constant),
- lossy-solvent sample,
- sample volume and sample shape,
- sample tube,
- tube wall thickness,
- lens effect,
- packing problem,
- packing density for powder and polycrystalline material.

#### *Sample insertion into the microwave cavity:*

- sample positioning and orientation,
- sample alignment procedure.

### B) Instrument-associated problems

#### *Microwave cavity:*

- microwave field profile,
- power intensity (saturation),
- cavity Q-factor change,
- filling factor,
- spectrometer sensitivity,
- single or double cavity,
- flat cell cavity.

#### *Modulation frequency:*

- modulation field profile,
- modulation coil diameter.

#### *Variable-temperature quartz Dewar:*

- presence/absence during measurement,
- sucking-in and lens effect.

## Secondary Error Sources

### C) Data processing-associated problems

- signal intensity,
- signal-to-noise ratio,
- double integration,
- base line correction,
- limits of integration.

### D) EPR standard- and calibration-associated problems

- internal or external standard,
- primary or secondary standard,
- relative spin concentration,
- absolute spin concentration,
- spectrometer calibration (microwave power, modulation amplitude, signal amplifier),
- self-calibration,
- calibration via Internet,

### E) Human factor

- absent-minded operator,
- laboratory negligence,
- interchanging of samples, parameters, data files, etc.

In order to minimize the influence of such error sources in quantitative EPR spectroscopy the most effective way would be to use the same standardized procedures for all EPR measurements and post-recording spectra manipulations. According to our theoretical computations and experimentally obtained results, it is strongly recommended that all the samples to be compared in quantitative EPR should have an identical shape [6–8]. Commercially distributed software for post-recording spectra manipulations is a basic necessity. Accurate and precise positioning of each sample in the cavity by a special alignment procedure is also essential [9, 10].

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## References

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10. Mazúr M., Valko M., Morris H.: Rev. Sci. Instr. **68**, 2514 (1997)

## **The XX1st International Conference on Photochemistry (ICP21)**

Nara-ken New Public Hall, Nara, Japan

July 26 (Sat) – 31 (Thu), 2003

<http://www.pac.ne.jp/icp21/>

**Scope of the Conference:** The conference covers diverse topics in general fields of photochemistry. The subjects include spin-mediated elementary processes in spin chemistry and time-resolved ESR spectroscopy, and organic photochemistry and reactive intermediates, from both theoretical and experimental sides. A conference report will be given in a forthcoming issue of the *EPR newsletter*.

## **1st ESR Summer School for Graduate Students on "Spin Polarization and Time-domain ESR"**

Sendai, JAPAN, August 5–7, 2003

<http://www.icrs.tohoku.ac.jp/SEST/summers.html>

This program is sponsored by the Society of Electron Spin Science and Technology. The school is open for undergraduate and graduate students to study fundamental and advanced ESR and catch an opportunity of making friends with ESR and/or non-ESR students and junior scientists. The title of the course is "Spin Polarization and Time-Domain ESR" and the subjects cover CIDEP (chemically induced dynamic polarization) mechanisms, spin-correlated radical pairs, excited states, magnetic field effects, the stochastic Liouville equation, high-field ESR, two dimensional ESR and so forth. The director of this school is Prof. Seigo Yamauchi at Tohoku University and the lecturers are Dr. Tadaaki Ikoma at Tohoku University, Dr. Akio Kawai at Tokyo Institute of Tech-

nology, and Dr. Kiminori Maeda at Tsukuba University. A conference report will be given in a forthcoming issue of the *EPR newsletter*.

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## **5th Meeting of the European Federation of EPR Groups (EFEPR)**

Lisbon, Portugal, September 7- 11 2003

<http://dequim.ist.utl.pt/EFEPR/>

The 5th meeting of the European Federation of EPR groups will be held in Lisbon, Portugal, from Sunday 7 to Thursday 11 September 2003. The meeting will provide a forum for scientists engaged in EPR spectroscopy to present and discuss recent results and developments. The scope of the meeting will cover all aspects of EPR spectroscopy, including applications in the fields of physics, chemistry, materials, biology and medicine, new techniques, instrumentation developments and theory.

### **Scientific Program**

The scientific program includes plenary/invited talks as well as oral presentations that will be selected from the submitted abstracts and poster sessions. The following colleagues have so far agreed to present plenary talks and invited lectures:

### **PLENARY TALKS**

D. Lurie (UK) Field-cycled Overhauser techniques for the study of free radicals in vivo

J. Moura (Portugal) EPR: a powerful tool for the study of metalloproteins

W. Rutherford (France) The photosystem II reaction centre: structure and function from EPR studies

A. Schweiger (Switzerland) Old wine in new bottles and new wine in old bottles

Y. D. Tsvetkov (Russia) Pulsed ELDOR and its chemical and biochemical applications

J. Freed (USA) Modern ESR methods in studies of membranes and proteins

**For more information, please contact:**

Joao Paulo Telo

5th Meeting of EFEPR

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## **Specialized Colloque AMPERE 2003**

**NMR and EPR of Broad-Line Solids Dedicated to Professor Robert Blinc on the occasion of his 70th birthday Bernardin, Portorož, Slovenia, September 8–12, 2003**

<http://ampere2003.ijs.si/>

### **Scope of the Conference**

The program of the conference is intended to cover solid-state NMR and EPR spectroscopy of solid materials with extremely broad resonance lines which in many cases cannot be measured by conventional pulsed techniques. Instead, one has to apply field-sweep and frequency-sweep techniques either in a CW mode or in a step-by-step pulsed mode. In addition, line-narrowing techniques to reduce broad spectra shall be included.

The program will focus on the following topics:

- field-sweep and frequency-sweep NMR, NQR and EPR techniques, either in CW mode or in combination with pulse techniques
- line-narrowing techniques
- ferro- and antiferromagnetic resonances in magnetic materials, nanomagnets, colossal-magnetoresistance systems
- magnetic resonances in electronic conductors, metals, semiconductors, charge-density waves, spin-density waves, superconductors
- magnetic resonance in quasicrystals
- magnetic resonance in spin glasses, proton glasses, polymer glasses, orientational glasses, relaxor systems



- detection of broad lines by novel techniques like SQUID-detection and Atomic-Force-Microscope detection
- 2D NMR and EPR techniques on very broad lines
- organic and inorganic nanotubes
- fullerene derivatives
- electronic and engineering ceramic materials

## 7th International Conference on Magnetic Resonance Microscopy

7th "Heidelberg" Conference

September 21–26, 2003

<http://www.physics.utah.edu/~icrmr/>

The 7th International Conference on Magnetic Resonance Microscopy will be held at Snowbird, Utah from September 21–26, 2003, and will be preceded by an Educational Program on September 20–21. The Chair is David C. Ailion and the Co-Chair is Robert E. Botto.

The official email address for the conference is [nmr@physics.utah.edu](mailto:nmr@physics.utah.edu)

You can address any questions to this email address. Please check this web site from time to time for further information about the Conference.

## The 8th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena

<http://www.chem.unc.edu/conferences/SCM2003/>

SCM2003 will be held September 21–26, 2003 at the Carolina Inn in Chapel Hill, North Carolina, USA. North Carolina is a mid-Atlantic state with convenient access to beautiful beaches and mountains, including Smoky Mountain National Park which borders Tennessee, and the Cape Hatteras National Seashore which contains some of the most pristine oceanfront in the United States. The University of North Carolina at Chapel Hill is the oldest public university in the country, opening its doors in 1793 and accepting its first student in 1795. The Uni-

versity is a cornerstone of the Research Triangle Park, one of the largest research and industrial parks in the world. The greater Triangle area, which comprises Chapel Hill, the state capitol Raleigh (home of N.C. State University) and Durham (home of Duke University), grew to over 1 million inhabitants in 2000. We welcome you to join us for SCM2003 in the "southern part of heaven."

## ISMAR 2004

October 24–29, 2004

<http://www.ismar.org/>

The 15th ISMAR meeting will be held in Jacksonville, Florida, USA in October, 2004, under the chairmanship of Prof. Tim Cross. It will take place near Ponte Vedra Beach outside of Jacksonville on the north Florida Atlantic coast at a beautiful time of the year. The conference will be held at the Sawgrass Marriott Resort ([www.marriotthotels.com/jaxsw](http://www.marriotthotels.com/jaxsw)). We will have the complete conference and hotel facilities at our disposal for the conference week. There will be excellent facilities for both plenary and parallel sessions, as well as lots of space for posters. Special hotel rates will be available for students and there will also be excellent locations for vendor and sponsor displays. A preconference summer school will be held at the NHMFL in Tallahassee, FL focusing on modern methodology in magnetic resonance. Buses will be available to transport attendees from Tallahassee to the Sawgrass Resort on Sunday, October 24th.

## The 42nd (2003) Annual (International) Meeting of the Society of Electron Spin Science and Technology (2003SEST)

Hiroshima University, Hiroshima, Japan

October 29 (Wed.) – 31 (Fri.), 2003

<http://home.hiroshima-u.ac.jp/sest2003>

**Scope of the Conference:** Electron spin magnetic resonance and electron-spin based science and technology in a variety of pure and applied natural sciences covering chemistry, bio-medical science, physics, materials sciences, geophysics and geology, radiology and environmental sciences, and their related

applications such as 2D-spectroscopy, spin-mediated magnetic field effects, in-vivo applications and bio-medical imaging, ESR dosimetry and archeological applications, from both theoretical and experimental sides.

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## Postponement of the APES'03 & the International School to October/November 2004

Having now received the responses from all APES Council Members as well as support and endorsement from the President of the IES, Prof. Tsvetkov, we may consider the decision to postpone the following events, originally planned as indicated below, to the period October/November 2004 as unanimously ratified and confirmed.

(1) the Asia-Pacific EPR/ESR Symposium 2003 (APES'03) originally planned to be held from November 17, 2003 to November 20, 2003 at the Indian Institute of Science, Bangalore, India

as well as

(2) the Satellite School to APES'03: International School on EPR Spectroscopy and Free Radical Research, originally planned to be held during November 11–15, 2003 at Bhabha Atomic Research Center, Mumbai

Czeslaw Rudowicz  
President, The Asia-Pacific EPR/ESR  
Society (APES)



## Twelfth Annual Workshop *Modern Development of Magnetic Resonance*

This workshop took place in Kazan in the period 2–4 October 2002 and preceded the ceremony of the Annual Zavoisky Award. The program of the Workshop was as follows:

V. E. Kataev (Kazan Physical-Technical Institute, Kazan, Russia) Magnetic resonance in low-dimensional copper oxides

W. Lubitz (MPI for Radiation Chemistry, Mülheim an der Ruhr, Germany) High-field EPR and ENDOR studies of dinuclear exchange coupled metal centers in proteins and related model systems

M. V. Eremin (Kazan State University, Kazan, Russia) Divergence of the dynamic charge susceptibility in layered cuprates as a precursor of a phase transition into the sliding orbital current state

A. A. Konovalov, V. F. Tarasov (Kazan Physical-Technical Institute, Kazan, Russia) Submillimeter EPR spectroscopy of  $\text{Ho}^{3+}$  ions in synthetic forsterite

A. N. Garroway (US Naval Research Laboratory, Washington, USA) Free induction decays and spin echoes in three-frequency NQR: Theoretical and practical aspects

A. R. Kessel, N. M. Jakovleva (Kazan Physical-Technical Institute, Kazan, Russia) Schemes of implementation in NMR of the quantum search algorithm in virtual spin representation

E. B. Feldman (Institute of Problems of Chemical Physics, Chernogolovka, Russia) Multiple-quantum NMR dynamics in one-dimensional systems in solids: Theory and computer simulations

V. A. Ulanov, M. M. Zaripov, E. P. Zheglov, E. R. Zhiteitsev (Kazan Physical-Technical Institute, Kazan, Russia) Copper impurity clusters in calcium fluoride crystals: results of EPR study

C. Corvaja (University of Padova, Padova, Italy) TR-EPR study of the interaction between photoexcited azulene and nitroxyl radical linked to a peptide template

O. A. Vasina, O. I. Gnezdilov, M. P. Tseitlin, A. A. Obynochny (Kazan Physical-Technical Institute, Kazan, Russia) Spin and molecular dynamics in course of photochemical processes. Study by EPR

Yu. I. Talanov (Kazan Physical-Technical Institute, Kazan, Russia), H. Adrian, M.

## VIth Voevodsky Conference *Physics and Chemistry of Elementary Chemical Processes*

The VIth Voevodsky Conference “Physics and Chemistry of Elementary Chemical Processes” was held in Novosibirsk (Russia) on July 21–25, 2002. The First Conference of the series took place in 1977, to honor Academician V. V. Voevodsky’s contribution to the various areas of chemical kinetics and his role in the development of physical methods in chemistry. The Conference has then become traditional and is held every five years.

The scope of the meeting included elementary processes in liquids, gases, solids, elementary processes in biology, magnetic and spin effects, development of instrumentation and methodology. A significant number of the contributions were directly related to EPR, including advanced techniques such as high-field EPR and biological applications of EPR. A number of top scientists, well known in the EPR world, took part in the Conference. It was during this meeting that the President of the IES Prof. John R. Pilbrow awarded the IES Gold Medal to Prof. Keith A. McLauchlan.

The conference was not however limited to just one particular experimental technique. Many contributors reported on the development and applications of optical methods, NMR, spin chemistry techniques, etc. The ultimate goal was investigation of elementary processes as found in chemistry and biology. Participants acknowledged this interdisciplinary approach as very interesting and stimulating.

The VIth Voevodsky Conference was attended by 180 participants, including 54 scientists from outside Russia.

Sergei A. Dzuba and Dmitry V. Stass

## 24th Discussion Meeting *Magnetic Resonance and Molecular Interactions*

Gesellschaft Deutscher Chemiker,  
Fachgruppe Magnetische Resonanzspektroskopie,  
Bremen, Germany  
September 24–27, 2002

**Conference Chairman:**  
Dieter Leibfritz, Bremen

### Tutorial

*Pulsed EPR and ENDOR spectroscopy: Methods and Applications*  
Bremen, September 23–24, 2002

**Tutorial Chairman:**  
Thomas Prisner, Frankfurt

Last year the topic of the Student Tutorial preceding the yearly meeting of the German magnetic resonance society was devoted to pulse EPR spectroscopy. Lectures were given by Marina Bennati (Frankfurt), Peter Höfer (Karlsruhe), Gunnar Jeschke (Mainz), Thomas Prisner (Frankfurt), Andreas Pöpl (Leipzig) and Jürgen Steinhoff (Osnabrück). The topic covered “Basics, Instrumentation, Simulations, ESEEM, PELDOR, Pulse-ENDOR and applications in biological systems, catalysis and polymers”. The 1½ day tutorial gave the 20 participants of the tutorial, mainly PhD students with cw-EPR background from Germany, a condensed overview of modern pulsed EPR methods and possible application areas. Most of the students also participated with poster contributions in the directly following Discussion Meeting of the GDCh which took place together with guests from the Scandinavian magnetic resonance communities. Sessions were dedicated to Protein Structures, ESR, Diffusion, Biomedical MR and Solid-State NMR with plenary talks covering the whole field of MR spectroscopy.

Thomas Prisner

Basset, G. Jakob (Johannes Gutenberg-Universität, Institut für Physik, Mainz, Germany), G. Wirth (Gesellschaft für Schwerionenforschung, Darmstadt, Germany) Non-resonant microwave absorption study of the surface barrier in ion irradiated superconductors

M. Andruh (University of Bucharest, Bucharest, Romania) Oligomeric complexes as building blocks in designing supramolecular multimetallic systems with interesting magnetic properties

M. I. Ibragimova, V. Yu. Petukhov, E. P. Zheglov, G. V. Konjukhov, A. A. Obynochny (Kazan Physical-Technical Institute, Kazan, Russia) Investigation of radiotoxin action on blood by magnetic radiospectroscopy

## 1st Annual Meeting of the Society of Electron Spin Science and Technology

The 1st annual meeting of the Society of Electron Spin Science and Technology was held in Tokyo on October 28–30, 2002. It was organized by Prof. Tokuko Watanabe at Tokyo University of Fisheries. This meeting was originally a joint meeting of the 41st ESR meeting and the 7th *in vivo* ESR meeting in Japan. As the Society of Electron Spin Science and Technology (SEST) has been founded during the meeting, the name of the meeting was modified. Now the society and the meeting cover wide areas of researches in chemistry, biology, physics, and technology. Prof. Takeji Takui at Osaka City University, the Vice President of the IES, was elected as the first President of the SEST. The title of the Society does not include the word “Japan” or “Japanese”, because they intend to evolve the activities of the society from domestic to international.

The subjects of this meeting include the representations and discussions for new findings and developments in electron spin science and technology. The meeting consists of the four sessions: invited lectures (7), oral (42) and poster (59) representations, and a symposium (2). The topics of two symposia were the present and the future in (I) *in vivo* ESR and (II) high-frequency ESR apparatus. The number of registered participants was 192 in this meeting, which far exceeded

the expectation of the organizing committee.

I was attending the ESR meeting in chemistry and was more interested in the meeting of SEST owing to various interesting oral and poster representations and animated discussions not only with the chemists but also physicists, biologists, and physicians this time. I have actually gotten valuable suggestions from them on my poster representation. Although the studies on chemical reactions and high-spin states are strong areas in Japan, the reports on materials science and life science are surely increasing. Dr. N. Mizuochi et al. at Tsukuba University reported on the structure and the electronic state of vacancies in silicon carbide, which are important to provide high-quality materials. On the basis of the hyperfine constants and nutation frequency, they discussed the vacancy of  $T_{V2a}$  in detail and assigned it as a quartet state. As I am running W-band ESR experiments, I was very interested in the symposium II. The lecture by Prof. M. Hagiwara, a physicist at RIKEN, showed clearly the merits of high-frequency ESR in the fields of magnetic materials and biological systems. Prof. H. Nojiri at Okayama University introduced a high-precision Terahertz ESR machine by use of repeating (2 s) the pulsed field (30 T) and extended his talk to applications to studies in materials science, chemistry, and biology.

We also had guests speakers from foreign countries, Dr. Y. Kotake at Oklahoma Medical Research Foundation, Dr. J. W. Chen at Harvard Medical School, Dr. P. H. Kasai at Almaden Research Center, IBM, and Dr. L. V. Mosina at Kazan Physical-Technical Institute. They also gave nice and funny talks at the conference dinner.

The SEST is planning to hold an ESR summer school for young scientists in the summer of 2003, which is organized by Prof. Seigo Yamauchi at Tohoku University. We, young scientists, are extremely delighted to have such a chance of studying electron spin science and have exchange with junior scientists and believe this will develop the electron spin science in Japan. Furthermore, we sincerely hope that some senior professor could write a modern and practical ESR textbook for young students.

The next annual meeting of this Society will be held at Hiroshima, Japan in the fall of 2003, organized by Prof. M. Shiotani at Hiroshima University.

Yohei Iwasaki

## The “Summer” School Modern EPR Spectroscopy – Methodology and Applications in Physics, Chemistry and Biology

The “summer” school Modern EPR Spectroscopy – Methodology and Applications in Physics, Chemistry and Biology took place at Retie, Belgium December 1–8, 2002. The school was an initiative of EFEP (The European Federation of EPR groups), following the one that took place in Caorle in 1999, organized by Marina Brustolon and was funded primarily by the EU commission through the High Level Scientific Conferences Program. The members of the scientific organizing committee were: D. Goldfarb, co-ordinator, Israel, K. Möbius, Germany, E. J. J. Groenen, The Netherlands, E. Goovaerts, Belgium. The local organizing committee members were: E. Goovaerts, A. Bouwen and S. Van Doorslaer, all from University of Antwerp, Belgium. There were 90 participants not including the 17 lecturers. The attendance was higher than expected and unfortunately we were not able to accommodate late registrations due to accommodation restrictions.

The scientific part of the school included three types of events. The first were lectures on topics that are central to modern EPR spectroscopy and included the basic theoretical background, experimental methods and examples of applications as follows:

- Basic EPR theory – Spin Hamiltonian and the various interactions – E. Goovaerts
- Basic EPR theory – density matrix formalism, exponential operators – D. Goldfarb
- Basic pulse EPR – G. Jeschke
- Quantum-chemical calculation of EPR observable – M. Kaupp
- Relaxation in solids and liquids – G. and S. Eatons
- CW ENDOR – K. Möbius
- FT-EPR spectroscopy – K. P. Dinse
- ODMR workshop – D. Carbonera
- ESEEM spectroscopy – S. Van Doorslaer
- Pulsed ENDOR – E. J. J. Groenen
- ELDOR spectroscopy – distance measurements – G. Jeschke
- Site directed spin labeling workshop – J. Steinhoff



- High-field EPR – K. Möbius, E. J. J. Groenen, D. Goldfarb
- Time-resolved and transient EPR – P. Hore
- EPR/ENDOR in Physics workshop – G. Denninger
- High-spin systems – D. Gatteschi
- Dynamic EPR – M. Brustolon
- Instrumentation – P. Höfer
- Pulsed EPR special – combined ESEEM/ENDOR – G. Jeschke

Each lecturer gave 2–4 lectures and emphasis was on starting with the basic such that the students who came from different backgrounds and different fields could follow. After presenting the basics and the principles the lecturers presented state of the art results on the topic, usually not limited only to their own research. There were also three workshops, each of 1 hour, which were dedicated to timely research and were aimed at stimulating the students with current problems and challenges in the field. The third event was the poster sessions (total 65 posters) where the participants presented their work and discussed it enthusiastically with their peers and the lecturers.

One afternoon was devoted to a tour in the laboratories of E. Goovaerts and S. Van Doorslaer and participants were exposed to pulse X-band EPR and high-field EPR spectrometers. The fourth workshop (2 h), that took part at the end of the school, was organized by the students and was dedicated to what they learned and experienced in the school. This was a very nice combination of science and humor.

All students were given a folder at the beginning of the meeting, which included all the lecture notes and considerable efforts were put into it. The lecturers prepared their lectures ahead of time to allow the produc-

tion of the script. In addition most of the notes were presented in a format that is very clear and after the students added their notes we hope they can be used as a good reference for years to come.

Efforts were made to promote discussions and questions during and after the lectures (this was a bit slow...) and the two students who were most active in this respect got a prize at the banquet (a bottle of special Belgian beer).

All in all we think that the school was a success, there is always room for improvement and we hope that the next school will be much better!!!

Daniella Goldfarb, co-ordinator

■ The second European EPR School took place in Retie (Belgium) from December 1, 2002 to December 8, 2002. As most of the participants can confirm, the second EU-EPR school was wonderful: funny gathering, nice tours in Lier and Antwerpen, good beer, delicious pralines and a really nice banquet. The single blind spot is that sometimes we, students, had to attend the lectures.

Joking aside: the second EPR EU-School for young investigators was a real success. It offered the opportunity of a less formal meeting between professors and students than during a conference. The level of the lectures was well tuned, growing day by day in a logical order, and giving a broad overview of EPR techniques, from the basic to the most advanced level. All topics about EPR and ENDOR spectroscopy were presented in an exhaustive way, with interesting theoretical introductions followed by well-chosen experimental examples.

This school provides further evidence that the idea, conceived and implemented for the first time in Caorle in 1999, of creating a didactic meeting for the EPR community is a winning choice. Moreover, it is clear that the organizers committee had worked with the one of the organizers of Caorle school because I noticed that some suggestions, which came from students after the previous school, were taken into account.

Actually the lectures were more didactic than they were in Caorle. This fact was more evident with younger lecturers, because they put some effort in creating an intuitive, physical description of each presented technique and in finding simple literature examples which explained when and with which samples a specific experiment is bound to be successful.

Thinking about the next school, it could be useful to plan a very informal gathering in the evening during which students can figure out what they don't latch on, discuss together and ask questions to the teachers, without any fear. Indeed, it was noticed that few students asked questions at the end of the lectures: in this way it should be easier.

The point that the EFEPR needs to focus on is: what do we really want from this type of school? I think that such schools should be *either* an informal meeting between professors and students *and* an opportunity of exchanging experience among students from different Institutions. I hope that next time the students will be less shy so that the gap between "teachers" and "students" shall be narrower and all of us, students and professors, can exploit such meetings to find out new energy to continue the hard, charming work of scientific research.

Anna M. Ferretti, student

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*Collected by Arthur Schweiger*

In this column, new books, journals and reviews on EPR, or literature closely related to EPR, are presented and briefly reviewed. The column covers material published starting from 2000 up to date; completeness is not claimed.

## BOOKS

### ***A Specialist Periodical Report: Electron Paramagnetic Resonance, vol. 17***

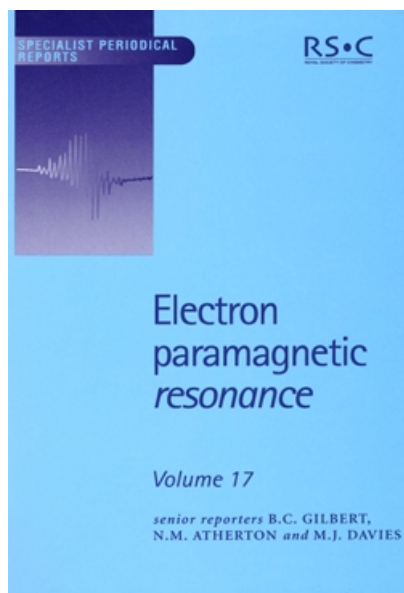
Senior Reporters: B. C. Gilbert, M. J. Davies, and K. A. McLauchlan

**Price:** £ 170 (Hardcover)

**Publication date:** November, 2000

**Publisher:** The Royal Society of Chemistry  
332 pages, ISBN 0-85404-301-1

The "Specialist periodical reports" of the Royal Society of Chemistry cover in a critical way the literature in various fields of chemistry. "Electron Paramagnetic Resonance vol. 17" is the latest issue of this popular series devoted to EPR. It contains a number of reviews written by experts in the field that are very useful in the daily work of EPR spectroscopists.



**From the back cover:** This book highlights major developments in electron paramagnetic resonance up to the end of 1999, with results being set into the context of earlier work and presented as a set of critical yet coherent overviews. The topics covered describe contrasting types of application, ranging from biological areas such as EPR and ENDOR studies of metalloproteins and evidence of free-radical reactions in biology and medically-related systems, to experimental developments and applications involving EPR imaging, the use of very high fields, and time-resolved methods. Critical reviews of applications involving bacterial photosynthesis, spin-labelling and spin-probes studies of self-assembled systems, and organo-metallic chemistry are also included.

#### **Contents:**

Biological Free Radicals

*by M. J. Davies and G. S. Timmins*

Recent EPR Studies on the Bacterial Photosynthetic Reaction Centre

*by S. Weber*

FT-EPR and Pulsed ENDOR Studies

of Encapsulated Atoms and Ions

*by K.-P. Dinse*

EPR Imaging

*by S. S. Eaton and G. R. Eaton*

Pulsed and Time-Resolved EPR Studies of Transient Radicals, Radical Pairs and

Excited States in Photochemical Systems

*by H. Murai, S. Tero-Kubota*

*and S. Yamauchi*

Progress in High Field EPR

*by G. M. Smith and P. C. Riedi*

EPR Spin-Labelling and Spin-Probe

Studies of Self-assembled Systems

*by A. Caragheorgheopol*

*and H. Caldararu*

EPR and ENDOR of Metalloproteins

*by J. Hüttermann and R. Kappl*

### ***Principles of Pulse Electron Paramagnetic Resonance***

Arthur Schweiger and Gunnar Jeschke

**Price:** £ 95 (Hardcover)

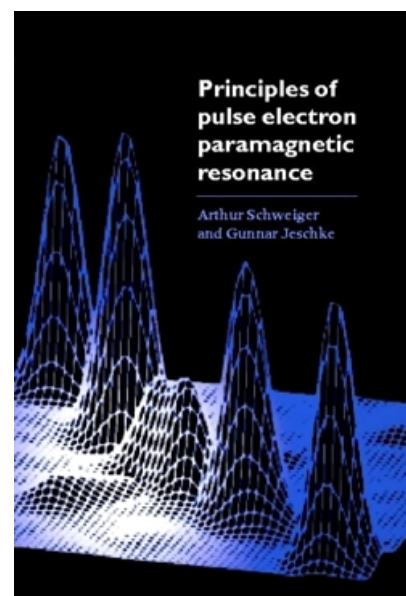
**Publication date:** July, 2001

**Publisher:** Oxford University Press

578 pages, 250 line figures, ISBN 0-19-850634-1

**List of known errors:**

[http://www.mpip-mainz.mpg.de/~jeschke/significant\\_corrections\\_240802.pdf](http://www.mpip-mainz.mpg.de/~jeschke/significant_corrections_240802.pdf)



**From the back cover:** This book explains the foundations of pulse EPR, a field of spectroscopy, which has now come of age and has found widespread application in investigations of structure, dynamics, and function of biological systems and synthetic materials. For the first time a systematic overview of the whole field is given, including coverage of Fourier-transform EPR, relaxation measurements, electron spin echo envelope modulation (ESEEM), pulse electron-nuclear double resonance (ENDOR), pulse electron-electron double resonance (ELDOR), transient nutation, and a number of advanced techniques. Researchers approaching the field will find here the basic theory as well as a description and critical evaluation of the existing methods needed for selecting the proper experiment, conducting it, and analyzing the results. The experienced researcher active in the field will find this book a useful reference and a guide to adapting EPR pulse sequences to new problems.

## Object-Oriented Magnetic Resonance: Classes and Objects, Calculations and Computations

Michael Mehring and

Volker A. Weber

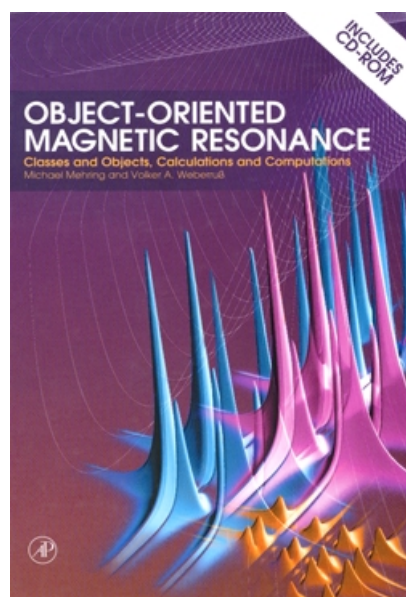
**Price:** \$ 79.95 (Hardcover)

**Publication date:** June, 2001

**Publisher:** Academic Press

560 pages, ISBN 0127406204

The structure of this book, written by one of the top experts in the field and a freelance physicist, is unorthodox and new. The book, which consists of the parts "Spin Physics", "Magnetic Resonance", and "Complementary Analytical and Numerical Methods", is based on an object-oriented analytical treatment of magnetic resonance by defining classes and objects in Hilbert and Liouville spaces. It can strongly be recommended to EPR spectroscopists who are interested in the spin physics pulse EPR is based on, and as a supplement to the book "Principles of pulse electron paramagnetic resonance" mentioned above.



**Editorial review:** This book presents, for the first time, a unified treatment of the quantum mechanisms of magnetic resonance, including both nuclear magnetic resonance (NMR) and electron spin resonance (ESR). Magnetic resonance is perhaps the most advanced type of spectroscopy and it is applied in biology, chemistry, physics, materials science, and medicine. If applied in conjunction with spectroscopy, the imaging version

of magnetic resonance has no counterpart in any type of experimental technique. The authors present explanations and applications from fundamental to advanced levels. Additionally, they pave the way to successfully simulating magnetic resonance phenomena numerically through an accompanying CD-ROM.

## Principles of Magnetic Resonance Imaging, a Signal Processing Perspective

Zhi-Pei Liang and Paul C. Lauterbur

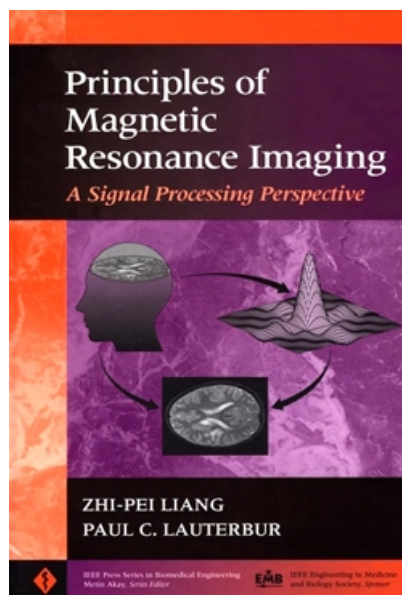
**Price:** \$ 99.95 (Hardcover)

**Publication date:** November, 2000

**Publisher:** Wiley-IEEE Press

416 pages, ISBN 0-7803-4723-4

Magnetic resonance imaging (MRI) is what makes magnetic resonance known to the man on the street. The number of books that cover the different aspects of MRI is overwhelming. However, most of these books are medically-oriented and are mainly written for physicians. Since also EPR imaging becomes more and more important, a textbook which describes the principles of MRI in a language we are familiar with is a need. Fortunately, such a textbook with Paul Lauterbur, the inventor of MRI as one of the two authors, has now become available.



**From the back cover:** The book provides a clear and comprehensive treatment of MR image formation principles from a signal processing perspective. It contains a comprehensive set of examples and homework problems.

Provides students of biomedical engineering, biophysics, chemistry, electrical engineering, and radiology with systematic, in-depth understanding of MRI.

## A Chemist's Guide to Density Functional Theory

Wolfram Koch and Max C. Holthausen

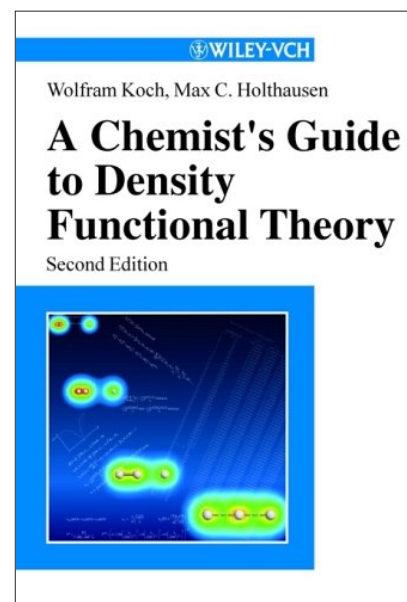
**Price:** \$ 69.95 (Paperback)

**Publication date:** July, 2001

**Publisher:** John Wiley & Sons

2nd edition, 528 pages, ISBN 3-527-30372-3

The paramouncy of density functional theory (DFT) is out of question and recent success in the prediction of EPR parameter using this theory makes DFT an indispensable tool for EPR spectroscopist. The book by Wolfram Koch and Max Holthausen is an excellent introductory text to DFT for readers who would like to make first acquaintance with the subject without getting lost in mathematical details.



**From the editorial review:** "The authors have done an excellent service to the chemical community. A Chemist's Guide to Density Functional Theory is exactly what the title suggests. It should be an invaluable source of insight and knowledge for many chemists using DFT approaches to solve chemical problems." – M. Kaupp

"The authors' aim is to guide the chemist through basic theoretical and related technical aspects of DFT at an easy-to-understand theoretical level. They succeed admirably." – P. C. H. Mitchell, Appl. Organomet. Chem.



## REVIEWS

### ***My Road to Biophysics: Picking Flowers on the Way to Photosynthesis***

George Feher

Annu. Rev. Biophys. Biomol. Struct. **31**, 1–44 (2002)

This is a highly recommended report which describes the career progression of one of our great. It is a very instructive and skillful text with a bunch of interesting scientific information and written with humor and rogue. Definitely a must!

**See also:** George Feher: Three decades of research in bacterial photosynthesis and the road leading to it: A personal account. Photosynthesis Research **55**, 1–40 (1998)

### ***Parametrization of ESR Spectra in Disordered Solids: Measurement Aspects***

L. Cugunov, p. 1–30

### ***Computer Aided Analysis of EPR Spectra of Copper Complexes***

R. Basosi, G. Delle Lunga, and R. Pogni, p. 169–210

### ***Applications of EPR Spectroscopy in Solids***

A. B. Vassilikou-Dova, p. 405–440

### ***Two-Dimensional ESEEM Spectroscopy***

S. A. Dikanov, p. 523–568

in: New Advances in Analytical Chemistry by Atta-Ur-Rahman (Editor)

**Price:** \$ 264 (Hardcover)

**Publication date:** September, 2000

**Publisher:** Taylor & Francis

1272 pages, ISBN 9058230317

This book about recent developments in spectroscopy contains four reviews related to EPR. The review by L. Cugunov is devoted to computer simulations of EPR spectra, a field with ongoing research activity. In the review by R. Basosi, G. della Lunga and R. Pogni, the analysis of copper complexes in solutions and in solids is described. The interest in this type of compounds goes like a threat through the EPR literature and has recently underwent a revival in studies related to catalysts and metalloproteins. The contribution of A. B. Vassilikou-Dova is an introductory text about EPR and its applications to defect centers. Finally, S. A. Dikanov describes the power of HYSCORE spectroscopy, the most popular two-dimensional pulse EPR experiment. He highlights the basic concepts and illustrates the poten-

tial of the technique by a number of applications on transition metal complexes.

**From the editorial review:** This book presents recent developments in various spectroscopic techniques such as NMR spectroscopy and mass spectroscopy in the form of 30 reviews. Papers dealing with NMR include the structural elucidation of polysaccharides, isotope effects in NMR spectra as a structural tool for organic molecules, solid state NMR studies of carbohydrates and their analogues, application of the Z-COSY technique for the analysis of NMR spectra of oriented molecules, and two-dimensional ESEEM spectroscopy. Other papers discuss computer aided analysis of EPR spectra of copper complexes, and nuclear quadrupole resonance studies of electron density distribution and molecular dynamics.

### ***Electron Spin Echo Envelope Modulation (ESEEM) Spectroscopy as a Tool to Investigate the Coordination Environment of Metal Centers***

Yiannis Deligannakis, Maria Louloudi, and Nick Hadjiliadis

Coord. Chem. Review **204**, 1–112 (2000)

ESEEM spectroscopy in one and two dimensions is one of the corner stones of pulse EPR spectroscopy. This review gives the reader a first access to the field, and describes recent applications of ESEEM to elucidate the structure of active sites in metalloproteins.

### ***Spin-Hamiltonian Formalisms in Electron Magnetic Resonance (EMR) and Related Spectroscopies***

Czeslaw Rudowicz and Sushil K. Misra

Appl. Spect. Rev. **36**, 11–63 (2001)

This is an extensive review about one of our main tool, the spin Hamiltonian. It explains the nature of the spin Hamiltonian, introduces fictitious spins, calls the readers attention to misconcepts related to the zero-field splitting, and tries to put things straight with respect to notations. The text can highly be recommended for those who work with tran-

sition metal and rare-earth ions, in particular with spin systems  $S > 1/2$ .

### ***Electron Paramagnetic Resonance (EPR) Biodosimetry***

Marc Desrosiers and David A. Schauer

Nucl. Instr. and Meth. in Phys. Res. B **184**, 219–228 (2001)

This short review is mainly focused on dosimetry of tooth enamel. It describes sample collection and preparation, as well as dose reconstruction and the interpretation of the EPR data.

### ***New Methods in Electron Paramagnetic Resonance Spectroscopy for Structure and Function Determination in Biological Systems***

Thomas F. Prisner

in: Essays in Contemporary Chemistry: From Molecular Structure towards Biology by Gerhard Quinkert and M. Volkan Kiskäurek (Editors)

**Price:** 149 (Hardcover)

**Publication date:** October 2001

**Publisher:** Wiley-VCH

472 pages, ISBN 3-906390-28-4

In this brief account the rapidly increasing impact of modern EPR techniques for the determination of local structures and dynamics of disordered systems is emphasised. The review is written for a broader audience and mainly concentrates on ENDOR and multifrequency EPR.

**From the book description:** In this volume, internationally renowned chemists recount their roles in the progress of chemistry research toward elucidation of biological processes. Beginning with a historical perspective on the development of X-ray crystallography, the reader is regaled with first-hand accounts of research milestones. The contributors, who number among the finest scientists in the world, including two Nobel Prize winners, are Peter B. Dervan, Jack D. Dunitz, Christian Griesinger, Jean-Marie Lehn, Thomas F. Prisner, Gerhard Quinkert, Peter G. Schultz, Helmut Schwarz, Dieter Seebach, and Ahmed Zewail. Additionally, there is a prologue by Albert Eschenmoser, for whom this collection was conceived, and an epilogue that contains facsimiles of notes from his landmark lecture 'Synthesis of Co-Enzyme B12: A Vehicle for Teaching Organic Synthesis'.



## Spin Chemistry in Japan

A special issue of *Applied Magnetic Resonance*  
edited by Seigo Yamauchi and  
Masaharu Okazaki

The studies of the magnetic field effect were started in Japan in the middle of the 70's and rapidly developed in the 80's and early 90's. This is considered to be the first Golden Age of spin chemistry in Japan. Thereafter, various kinds of magnetic field effects and their mechanisms have been found and discussed extensively in a variety of systems till the middle of the 90's. Another field related to spin chemistry which employed EPR techniques was opened in Japan in the early 80's. Although the Japanese groups working on the magnetic field effects in chemical reactions took the leadership in competition with foreign groups, the Japanese EPR chemists were left behind for several years. However, as many groups made continuous efforts in their studies, spin chemistry flourished in our country in the middle of the 90's, making a second Golden Age. The studies were mostly made of photochemical reaction intermediates such as radicals, radical pairs, and excited triplet states, by means of time-resolved EPR and unique methods of product-yield-detected magnetic resonance. Since the late 90's, spin chemistry is still developing and extended over new aspects of photochemistry and to the related areas, such as materials science, physics, and biochemistry. In this special issue of *Applied Magnetic Resonance*, we present a selection of our community's recent achievements.

### Part I: Photochemistry

**H. Murai, S. Yamauchi, A. Kawai, K. Obi, N. Hirota:** Developments of Magnetic-Resonance-Related Spin Chemistry in Japan  
**Y. Kobori, T. Yago, S. Tero-Kubota:** Diffusion-Model Analysis of Effective CIDEP Distance in Solvent-Separated Radical-Ion Pair  
**H. Yonemura, S. Moribe, K. Hayashi, M. Noda, H. Tokudome, S. Yamada, H. Nakamura:** Photoinduced Intramolecular Electron-Transfer Reactions in Carbazole-Fullerene and Phenothiazine-Fullerene Linked

Compounds in Benzene and Benzonitrile as Studied by Fluorescence, Transient Absorption, Time-Resolved EPR, and Magnetic Field Effects

**M. Horiuchi, K. Maeda, T. Arai:** Magnetic Field Effect on Electron Transfer Reactions of Flavin Derivatives Associated with Micelles

**Y. Sakaguchi, J. R. Woodward:** Pulse-Shift Measurement: a Direct Observation of Radical Pair Dynamics in a Micelle

**K. Hansongnorn, T. Fukujū, H. Yashiro, K. Maeda, T. Azumi, H. Murai:** Time-Resolved EPR Study of the Photoreduction of Phthalic Anhydride and Chlorinated Phthalic Anhydrides in 2-Propanol

**A. Kawai:** Dynamic Electron Polarization Created by the Radical-Triplet Pair Mechanism: Application to the Studies on Excited State Deactivation Processes by Free Radicals

**K. Ishii, T. Ishizaki, N. Kobayashi:** Time-Resolved EPR Studies on Magnetic Interactions between Excited Triplet (Tetraphenylporphyrinato) Zinc and Doublet Nitroxide Radical

**Y. Iwasaki, K. Katano, Y. Ohba, S. Karawasa, N. Koga, S. Yamauchi:** On the  $g$ -Value Shift and Intersystem Crossing in Photo-Excited Radical-Triplet Systems

**M. Asano-Someda, N. Toyama, Y. Kaizu:** Time-Resolved EPR Spectra of a Photo-excited Phenanthrene-Linked Copper(II)-Free-Base Porphyrin Dimer: An Intermediate-Coupling Case in a Triplet-Doublet Spin System

**Y. Kamata, K. Akiyama, S. Tero-Kubota, M. Tabata:** Two-Laser Two-Color Time-Resolved EPR Study on Higher-Excited-State Triplet-Singlet Intersystem Crossing of Porphyrins and Phthalocyanines

**M. Yagi, I. Yamamoto, R. Sasase, K. Seki:** Optical and Time-Resolved Electron Paramagnetic Resonance Studies of the Excited States of Para-Methylcinnamic Acid and Para-Methylcinnamate Anion

### Part II: Material Science, Methodology, Biochemistry

**M. Okazaki, K. Toriyama, N. Sawaguchi, K. Oda:** The Solution Flow through the

Nanochannel of MCM-41: a Spin-Probe Study

**T. Ikoma, S. Okada, S. Tero-Kubota, H. Nakanishi, T. Kato, P. Höfer, A. Kamłowski, K. Akiyama:** Angle-Selective Measurements of Spin Soliton in Ladder Polydiacetylene by Pulsed 94 GHz EPR

**S. Kuroda:** ESR and ENDOR Studies of Solitons and Polarons in Conjugated Polymers

**Y. Matsuda:** Encapsulation of Atomic Hydrogen into Silsesquioxane Cages and ESR of Encapsulated Hydrogen Atoms

**S. Okubo, T. Kato:** ESR Parameters of a Series of  $\text{La@C}_n$  Isomers

**D. Shiomi, C. Kaneda, T. Kanaya, K. Sato, T. Takui:** Hyperfine Structure of ESR Spectra as a Probe for Heisenberg Exchange Couplings in Nitroxide Triradicals Serving as Building Blocks for Molecule-Based Ferromagnets

**H. Morikawa, S. Karasawa, N. Koga:** Magnetic Properties after Irradiation of Tetakis[4-( $\alpha$ -diazobenzyl)pyridine]copper(II) in a Frozen Solution

**H. Matsuoka, K. Sato, D. Shiomi, T. Takui:** 2-D Electron Spin Transient Nutation Spectroscopy of Lanthanoid Ion  $\text{Eu}^{2+}$  ( $^8\text{S}_{7/2}$ ) in a  $\text{CaF}_2$  Single Crystal on the Basis of FT-Pulsed Electron Spin Resonance Spectroscopy: Transition Moment Spectroscopy

**Y. Ohba:** Application of Two-Dimensional Pulsed EPR Nutation Spectroscopy to a Disordered System with Large  $g$ -Anisotropy

**A. Kawamori, N. Katsuta, H. Hara:** Structural Analysis of Three-Spin Systems of Photosystem II by PELDOR

**H. Mino, T. Ono:** Applications of Pulsed ELDOR-Detected NMR Measurements to Studies of Photosystem II: Magnetic Characterization of YD Tyrosine Radical and  $\text{Mn}^{2+}$  Bound to the High-Affinity Site

**K. Kasazaki, K. Yasukawa, H. Sano, K. Yamada, H. Utsumi:** Application of In Vivo ESR Spectroscopy to Pharmaceutical Sciences: Evaluation of In Vivo Inhibitory Mechanism of Antigastric Lesion Drugs

A copy of this double issue (*Applied Magnetic Resonance* vol. 23, nr. 3–4) costs EUR 332.- (excl. VAT and carriage charges). The issue can also be obtained as part of a subscription to the volumes of 2002, 22 and 23, which is offered at a special rate of EUR 146.- (excl. VAT and carriage charges) to members of the IES ordering directly from Springer-Verlag in Vienna, Austria.

Seigo Yamauchi  
Masaharu Okazaki

## ***EPR of Free Radicals in Solids. Trends in Methods and Applications***

edited by Anders Lund and Masaru Shiotani

**Price:** 148.00 EUR / 145.00 USD / 93.00 GBP (Hardbound)

**Publication date:** May 2003

**Publisher:** Kluwer Academic Publishers  
606 pages, ISBN 1-4020-1249-7

The purposes of this book are to present *methods* and *applications* of modern EPR for the study of free radical processes in solids. The first part is concerned with trends in experimental and theoretical *methods*. In the first chapter by A. Lund and W. Liu continuous wave (CW) EPR and ENDOR methods for studies of radical structure in single crystals and powders are reviewed. Most of the following seven chapters give accounts of novel developments that so far are only available in the journal literature. The chapter by M. Brustolon and A. Barbon describes the different pulsed techniques as applied to radicals and spin probes in solid matrices. Methods to extract dynamical parameters from CW and pulsed EPR are summarized in the chapter by N. P. Benetis, which also contains an account of relaxation phenomena. The chapter by M. Shiotani and K. Komaguchi deals with quantum effects in isotopically labelled radicals, which are especially manifested in high resolution EPR at low temperature. The theoretical interpretation of measured parameters, *i.e.* the *g*- and hyperfine coupling tensors in terms of electronic properties is treated in two chap-

ters by R. J. Boyd and his coworkers, and by M. Kaupp. The trend is towards *ab initio* and density functional methods even for the biological systems. The new experimental methods to determine accurate *g*-tensors with high-field EPR have been reviewed elsewhere but the modern theoretical treatment described here is probably less well known. Single crystal measurement is the most straightforward but not always applicable method for complex systems, where often only powder spectra can be obtained. For these systems analysis by simulation techniques based on exact diagonalization are beginning to replace the previously used perturbation methods, as described in the chapter by G. R. Hanson and coworkers. Furthermore, myon spin resonance provides new means to considerably lower the detection limit in heterogeneous systems as described in a chapter by C. J. Rhodes.

In terms of *applications* there is a trend both towards simplification by using matrix isolation in frozen noble gas matrices with accompanying increase of resolution as illustrated in two chapters and towards studies of complex systems treated in the chapters by T. Takui and his coworkers, M. Baumgarten and A. Kawamori. In the former case H. Kunttu and J. Eloranta give an overview the matrix isolation technique for studies of atoms embedded in solid rare gases and V. Feldman presents recent development in the EPR studies of reactive intermediates from irradiation of moderately large organic molecules using matrix isolation. In the latter case two chapters address the issue of high-spin systems, the one by M. Baumgarten in organic systems, the other by T.

Takui and his coworkers in metal-based molecular clusters, which are fields that have strongly developed toward molecular magnets recently. The chapter by A. Kawamori describes studies of plant photosystem II by pulsed EPR and dual mode CW EPR, and pulsed electron-electron double resonance, the latter to obtain distances between radical pairs trapped after illumination. For EPR dosimetry and other kinds of quantitative EPR, the problem of calibration is an important issue that is addressed in the chapter by N. Yordanov and V. Gancheva. Recent developments of optical detection to lower the detection limit and to obtain time-resolution in the characterization of defect centers in semiconductor materials are presented in the chapter by W. Chen.

Provided by Takeji Takui

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# Positions

## Available & Wanted



### PRINCETON UNIVERSITY DISTINGUISHED POSTDOCTORAL FELLOWSHIPS IN EPR SPECTROSCOPY

HFSP, NIH and the Dreyfus Foundation are funding a pair of research projects at [Princeton University](#), which supports the application of EPR spectroscopy to understanding fundamental questions in biological chemistry and materials science. Applications for a postdoctoral position are invited for an **EPR spectroscopist** with experience in pulsed EPR methods and data analysis. This person will join a [team](#) of biochemists and materials chemists in the [Chemistry Department](#) under the supervision of [Charles Dismukes](#).

#### Projects:

- I Distance Measurements in Proteins using ELDOR and Double Quantum Coherence ESR. This project aims to advance knowledge of the structure of biomolecules where XRD is not available. Applications to multi-sub-unit proteins, photosynthetic reaction centers and other biological materials.
- II The Structure and Function of Enzymes and Inorganic Materials using Electron-Nuclear Double Resonance (ENDOR) and 2D-Hyperfine Sublevel Correlation Spectroscopy (HYSCORE). To determine the electronic and magnetic environments surrounding the nuclei in coordination complexes and enzymes which determine their catalytic properties.
- III Functional Dynamics of Proteins and Material by Time Resolved FT-ESR. To study transient structural changes in the photochemistry of photosynthetic reaction centers and inorganic materials related to catalysis and solar energy conversion and internal dynamics with proteins.

The postdoctoral fellow will have access to two [Bruker EPR spectrometers](#) (EleXsys 585 FT-EPR/ENDOR; ESP-300 series; ENDOR and TRIPLE accessories; fitted with

Oxford helium cryostats) and major research resources in the Princeton Materials Institute and the Department of Chemistry. PhD applicants are invited with training in physics or chemistry. Send your CV, list of publications and names and contact information for three referees who have first hand knowledge of your work to Ms. Lynn Mendenko ([mendenko@princeton.edu](mailto:mendenko@princeton.edu)), Princeton University, Hoyt Laboratory, Department of Chemistry, Princeton, NJ, USA 08544. Posting Date: September 30, 2003. A further description of the criteria for selection, benefits, and the project can be found at <http://www.princeton.edu/Siteware/Administration.shtml>.

#### Research Group links:

[Professor G. C. Dismukes](#)  
<http://www.princeton.edu/~catalase/>

### POSTDOCTORAL POSITIONS AVAILABLE, UNIVERSITY OF DENVER

Two positions are available immediately for postdoctoral research associates.

**Position 1:** Measurement of Interspin Distances via Relaxation Times.

The goal of the project is to use electron spin relaxation times to measure interspin distances and as probes of oxygen concentration. As part of these projects we are studying relaxation times for a range of samples under various conditions and as a function of microwave frequency to understand the mechanisms of relaxation and factors that influence the relaxation rates. Relaxation times are then used to measure interspin distances in biological molecules. The work is funded by the National Institutes of Health

**Position 2:** EPR at 250 MHz.

EPR spectroscopy at 250 MHz is being developed for in vivo spectroscopy and imaging. In this project we are developing rapid scan and spin echo methods for imaging at 250 MHz. The project involves technique development and comparison of methods to optimize signal-to-noise. The work is funded by the National Institutes of Health.

**Job Requirements:** Ph.D. in Chemistry or related field. Experience with EPR is required. Experience with pulsed EPR is preferred.

#### For further information please contact:

Professors Sandra or Gareth Eaton  
[seaton@du.edu](mailto:seaton@du.edu) or [geaton@du.edu](mailto:geaton@du.edu)  
Department of Chemistry and Biochemistry,  
University of Denver  
Denver, CO 80208  
phone: 303-871-3102

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<http://www.jeol.com/esr/fa100.html>

## POSTDOCTORAL POSITION

A postdoctoral position is presently available in the physics department of the University of Dortmund for the study of metalloproteins with optically detected EPR techniques. In this project, we use advanced optical/microwave double resonance techniques to investigate the electronic structure of the metal ion and its ligands.

The successful candidate should have experience in EPR spectroscopy and/or laser spectroscopy. He/she is expected to further develop the existing instrumental basis as well as the methodology and apply them to the investigation of biologically relevant samples.

The University of Dortmund is an equal opportunity employer. Preference will be given to women and candidates with disabilities.

**Please contact:** Dieter Suter  
[dieter.suter@physik.uni-dortmund.de](mailto:dieter.suter@physik.uni-dortmund.de)  
Fachbereich Physik,  
Universität Dortmund  
D-44221 Dortmund, Germany  
phone: (+49 231) 755 3512,  
(+49 231) 755 3652  
<http://e3.physik.uni-dortmund.de>

## POSTDOCTORAL POSITION: PULSED EPR OF METALLOPROTEINS AT UNIVERSITY OF ILLINOIS

An NIH-funded postdoctoral position is available in the Illinois EPR Research Center at the University of Illinois (Urbana, USA) for research work in pulsed EPR and ENDOR spectroscopy of metalloproteins. There is a focus on ESEEM theory and on structure-function relationships in Rieske and related proteins.

Expected education: PhD or equivalent in a discipline such as chemistry, biochemistry, molecular and cellular biology, physics, or biophysics. Background should include (1) experimental and/or theoretical magnetic resonance (preferably pulsed) and/or (2) experience with protein preparations and analysis.

Interested individuals should contact Prof. R. L. Belford ([rbelford@uiuc.edu](mailto:rbelford@uiuc.edu)). The successful candidate will report directly to Dr. S. I. Dikanov ([dikanov@uiuc.edu](mailto:dikanov@uiuc.edu)) and may collaborate with other faculty groups. Salary will be comparable to the usual NIH postdoctoral scale. The University of Illinois is an equal-opportunity employer.

**Please contact:** Prof. R. Linn Belford  
Illinois EPR Research Center,  
Department of Chemistry,

University of Illinois  
Box 18-6 CLSL, 600 S. Mathewa  
Urbana, IL 61801 USA  
phone: 217-333-2553  
fax: 217-244-3186

## POSTDOCTORAL POSITION IN PRION RESEARCH AT UC SANTA CRUZ

Recent results suggest that the prion protein's normal function is related to its ability to bind copper. Through a widely collaborative effort, the Millhauser lab has determined the features of the copper sites and is now moving on to examine potential function and how function may be lost in prion diseases. Current work has made extensive use of EPR, protein expression and protein synthesis. Although EPR, both CW and pulsed, will be key for continued work, the research will expand by moving into cellular assays, proteomics and perhaps transgenic experiments. The Millhauser lab is looking for an enthusiastic, recent PhD who is comfortable with EPR and interested in learning new biophysical and biological techniques.

**Please contact:** Prof. Glenn L. Millhauser  
[glenm@hydrogen.ucsc.edu](mailto:glenm@hydrogen.ucsc.edu)  
Department of Chemistry &  
Biochemistry, UC Santa Cruz  
Santa Cruz, CA 95064  
phone: 831 459 2176  
fax: 831 459 2935  
[http://chemistry.ucsc.edu/millhauser\\_g.html](http://chemistry.ucsc.edu/millhauser_g.html)

## JUNIOR NMR SPECTROSCOPIST NEEDED – USAMRICD

A junior NMR spectroscopist is needed at the U.S. Army Medical Research Institute of Chemical Defense (USAMRICD), Aberdeen Proving Ground, MD. Position is only open to U.S. citizens. Qualified candidate must have a strong background in NMR spectroscopy.

The successful candidate will provide guidance on the operation of a Varian 600 MHz INOVA NMR and will obtain liquid and solid-state NMR spectra to aid principal investigators in studying chemical warfare (CW) agents and pharmacological countermeasures for CW agents. As NMR administrator for the Institute, the candidate will be responsible for maintaining and troubleshooting the instrument, user training, and managing the instrument in areas of biochemistry, organic, inorganic, and protein chemistry.

**Please contact:** Dr. Carmen M. Arroyo  
[carmen.arroyo@amedd.army.mil](mailto:carmen.arroyo@amedd.army.mil)  
USAMRICD, 3100  
Ricketts Point Rd, APG, MD 21010  
phone: 410-436-4454

## MAGNETIC RESONANCE POSTDOCTORAL POSITIONS AVAILABLE IN EUROPEAN UNION

For information on postdoctoral research opportunities in projects funded by European Union organizations, try these websites:

<http://www.uio.no/~kkan/EUTMR.htm>  
and  
<http://improving-rtn.sti.jrc.it/default/>

## GRADUATE SCHOLARSHIPS IN CHEMISTRY AVAILABLE AT THE UNIVERSITY OF ILLINOIS IN URBANA-CHAMPAIGN

Predocorral Graduate Scholarships are available for highly qualified new applicants to the PhD program in the University of Illinois Department of Chemistry. Specialty areas in this department are Physical, Analytical, Organic, and Inorganic Chemistry as well as Materials Chemistry, Chemical Biology, and Chemical Physics. Magnetic resonance is one of the traditional strengths of our department.

These Scholarships carry excellent full-year stipends and exemption from tuition and most fees. Graduate Scholars are guaranteed continued financial support until completion of the PhD degree as long as satisfactory progress toward the degree is maintained.

Applicants whose native language is not English should take the TSE as well as TOEFL and GRE tests. I can provide information and application forms if you send me an e-mail.

**Please contact:** Prof. R. Linn Belford  
[rbelford@uiuc.edu](mailto:rbelford@uiuc.edu)  
Department of Chemistry,  
University of Illinois  
Box 18-6 CLSL, 600 S. Mathewa  
Urbana, IL 61801 USA  
phone: 217-333-2553  
fax: 217-244-3186



## FOR SALE – NMR MAGNETOMETER

Sentec Model 1001, including 3 standard probes covering the range of 1 to 10 kG. In good working order, this 1981 model (uses NIM bin!) includes 7-digit display, 0.01 Gauss resolution, accuracy:  $10^{-6}$  relative,  $10^{-5}$  absolute, has automatic peak search feature, BCD output, etc. Can be bought with or without NIM bin and CRT display. Make an offer!

**Please contact:** Prof. E. J. Knystautas  
[ejknyst@phy.ulaval.ca](mailto:ejknyst@phy.ulaval.ca)  
 Physics Department, University Laval  
 Quebec City (Quebec) G1K 7P4  
 phone: 1-418-656-5569  
 fax: 1-418-656-2040

## FOR SALE: VARIAN EQUIPMENT

Resonance Instruments has available:

- 1 replacement Klystrons for Varian EPR Bridges (at reduced prices) and other klystrons,
- 2 Varian V4500-41A low/high power microwave bridge with new klystron – excellent condition.

For more information on these units **please contact:**

Clarence Arnow, President  
[rii1@earthlink.net](mailto:rii1@earthlink.net)  
 Resonance Instruments  
 phone: 1-847-583-1000  
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## AVAILABLE: USED VARIAN EPR EQUIPMENT

- 1 Two Varian E-3's are now being refurbished. They will meet factory specifications and will come complete with a one-year warranty. The units may also include some upgrades.
- 2 Varian ENDOR accessory, with Varian ENDOR cavity.
- 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  
[janderson36@wi.rr.com](mailto:janderson36@wi.rr.com)  
 1030 S. Main St.,  
 Cedar Grove, WI 53013, USA  
 phone/fax: 1-920-668-9905

## CAVITY NEEDED

We need urgently an X-band TE-102 cavity for use with Varian E112 EPR equipment, either free or for a reasonable modest price.

**Please contact:** Prof. P. T. Manoharan  
[ptm@rsic.iitm.ernet.in](mailto:ptm@rsic.iitm.ernet.in)  
 RSIC, Indian Institute of Technology  
 Chennai 600 036, India  
 fax: 91 44 2350509 (or 2352545)

## DO YOU NEED HELP IN 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-band, C-band, S-band, L-band, or Megahertz versions.

Complete microwave/RF bridges from 150 MHz to L-band, S-band, or C-band are available from designs previously built and tested at the University of Denver.

**Please contact:** Richard W. Quine  
[rquine@du.edu](mailto:rquine@du.edu)  
 phone: 1-303-871-2419

## AVAILABLE: ISOTOPE-CONTAINING SPIN PROBES

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[maxx@nioch.nsc.ru](mailto:maxx@nioch.nsc.ru)  
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 Novosibirsk 630090, Russia  
 In the US **please contact:**  
 Dr. Sergei Dikanov  
[dikanov@uiuc.edu](mailto:dikanov@uiuc.edu)



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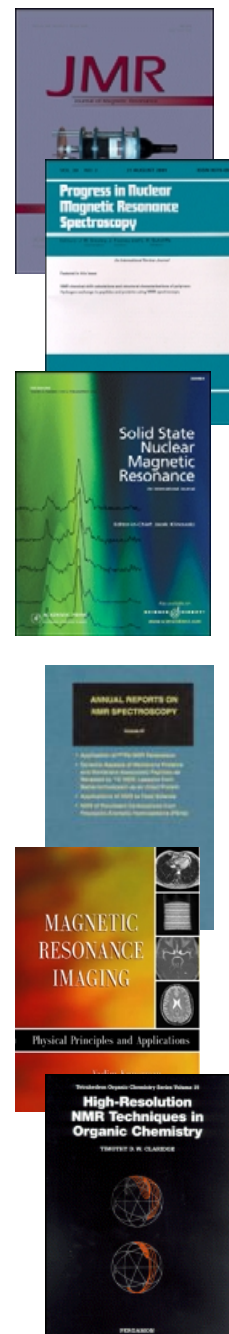
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This title focuses on all aspects of experimental and theoretical solid state NMR, including advances in instrumentation and technique development.

### Books

- **Annual Reports on NMR Spectroscopy**, *Webb*  
Annual Reports on NMR Spectroscopy has established itself as a means for the specialist and non-specialist alike to become familiar with new applications of NMR Spectroscopy in all branches of chemistry.
- **Magnetic Resonance Imaging**, *Kuperman*  
This book is intended as a text/reference for students, researchers, and professors interested in physical and biomedical applications of Magnetic Resonance Imaging (MRI). Both the theoretical and practical aspects of MRI are emphasized.
- **High-Resolution NMR Techniques in Organic Chemistry**, *Claridge*  
In this book, emphasis is on the more recently developed methods of solution-state NMR applicable to chemical research, which are chosen for their wide applicability and robustness. These have, in many cases, already become established techniques in NMR laboratories, in both academic and industrial establishments. A considerable amount of information and guidance is given on the implementation and execution of the techniques described in this book.



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