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The Publication of the International EPR (ESR) Society

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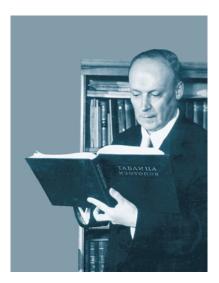
Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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**The cover picture** shows E. K. Zavoisky, the pioneer of electron paramagnetic resonance. Moscow, April 1957.

Taken by M. Red'kin (TASS). From the archives of N. E. Zavoiskaya.



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19 Market Place



# Editorial

Dear colleagues,

Hope all of you who had a look at or even read my editorial in the *EPR newsletter* 17/1 immediately recognized the man on the cover of this issue. Yes, this is Evgeny Konstantinovich Zavoisky, the pioneer of electron paramagnetic resonance. I have to confess that this is my favorite photo of him and I could not stand the temptation to share it with you. I think that even not knowing who this man is, one easily recognizes the extreme intelligence hidden by the high brow, his self-control and dedication to the cause of science.

To mark the 100th anniversary of E. K. Zavoisky, many columns of this issue are Zavoisky-oriented. Just check how many times you saw his name in the list of contents! To remind you, in previous issues of the *EPR newsletter* you could have found several articles that recognize the father-founder of EPR, E. K. Zavoisky (13/1-2, pp. 13–14 and 14/4, pp. 6–7 and 12–13).

In the course of his life he courageously moved from one new field of science to another and in each field he made important discoveries. To quote academician V. I. Ginzburg, Nobel Prize laureate: "...The discovery of EPR – electron paramagnetic resonance (Kazan, 1944), a very sensitive method to study the structure of matter, a method that gave birth to a new field of physics, radiospectroscopy, and found application in physical chemistry, biology, medicine, techniques; the creation with a collective of collaborators of electron optical converters, enabling one to 'see' separate photons and to measure super-short time intervals (Moscow, 1953); studies in the field of thermonuclear synthesis, leading to the discovery of the anomalous increase of the resistance and turbulent heating of plasma by electric current (Moscow, 1961) – this is far from being a complete list of works in which his talent of an experimenter manifested itself brightly and fruitfully."

Information about Zavoisky's involvement in the Soviet atomic bomb project (p. 7) threw a bomb into the opening ceremony of the "Zavoisky Week" (p. 14). Reports about the activity of E. K. Zavoisky after his discovery of EPR disclosed a research less known to the EPR community.

It is great to realize that the 100th anniversary of E. K. Zavoisky gave occasion for summing up the state of the art in the relevant fields of science so nicely demonstrated at the International conference "Modern Development of Magnetic Resonance" (p. 15) and other numerous magnetic resonance conferences. We witness how new pulse EPR methods and their applications develop. Sabine Van Doorslaer presented a brilliant review of pros and cons of hyperfine sublevel correlation spectroscopy (p. 09).

I have to add a sad note: Dietmar Stehlik, Zavoisky Award laureate 2004, passed away (p. 8). His research can be continued by his colleagues and collaborators but the loss of a man and a friend is irreplaceable...

Laila Mosina

PS: Not to forget, Wayne Hubbell covered the IES membership dues for his young collaborators who were interested in its activities. Please feel free to follow him!

### ★ IES BUSINESS ★ IES BUSINESS ★

### Out-of-date Email Addresses and Mailing Address

Please go to the IES webpages and check that your mail and email addresses are current. Many are out of date and the emails are returned or the shippers are unable to deliver printer copies. If you have forgotten your username, email the Secretary.

## **IES Annual Meeting**

The 2008 IES Annual Meeting will be held during the 6th Asia-Pacific EPR/ ESR Symposium which will be held in Cairns, Australia from July 13 to July 18 in 2008.

The Annual Meeting timing has yet to be confirmed. Please send any Agenda items to the IES Secretary as soon as possible.

The New IES Executive will be announced at the 6th Asia-Pacific EPR/ ESR Symposium and will take office on 1st October 2008.

## Membership Dues

Membership dues for 2008 are now due. If your membership is over a year in arrears, your membership will shortly be de-activated and this may be the last members issue of the Newsletter you receive.

# The Bruker Prize 2008

**Edgar Groenen** University of Leiden, Leiden The Netherlands

# The IES Gold Medal 2008

**Jan Schmidt** University of Leiden, Leiden The Netherlands

# Fellows of the IES 2008

Sandra S. Eaton and Gareth R. Eaton University of Denver, Denver USA

The 2007 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professor Brian M. Hoffman, Northwestern University, Evanston, Illinois, USA, in a ceremony marking his outstanding contribution to fundamental magnetic resonance studies of metalloenzymes, their catalytic intermediates, and electron transfer between proteins.

The ceremony preceded the International Conference "Modern Development of Magnetic Resonance", 25–29 September 2007 (see also p. 14).

The Zavoisky Award was presented on September 24, 2007 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 a cheque (in 2007, for 1500 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 Society. The Award Selection Committee consisted of well-known experts in EPR: Professors G. Feher (La Jolla), D. Gatteschi (Florence), H. M. McConnell (Stanford), K. A. McLauchlan (Oxford), K. Möbius (Berlin), and the Chairman, K. M. Salikhov (Kazan). The selection of the Awardee was made after consultations with the Advisory Award Committee which comprises Yu. N. Molin (Novosibirsk), and Yu. D. Tsvetkov (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), K. A. McLauchlan (2001), W. Lubitz (2002), W. L. Hubbell (2003), K. M. Salikhov and D. Stehlik (2004), H. M. Swartz (2005) and J. Schmidt (2006).

The selection of Professor Brian M. Hoffman was made from many nominations solicited from international experts in EPR.

The Award Ceremony was chaired by Professor M. Kh. Salakhov. Professor K. V. Salikhov, the Chairman of the Award Committee, announced the decision of the Zavoisky Award Committee. The presentation was made by R. F. Muratov, the First Deputy Prime Minister of the Republic of Tatarstan. Professor M. Kh. Salakhov, RecFrom left to right: B. M. Hoffman, M. Kh. Salakhov, and K. M. Salikhov.

tor of the Kazan State University, Professor A. M. Mazgarov, President of the Tatarstan Academy of Sciences, and Professor W. Lubitz, President of the International EPR Society, warmly congratulated the laureate. Academician K. A. Valiev congratulated the laureate on behalf of the Russian Academy of Sciences. Letters of congratulations from Professor B. H. Meier, President of the AMPERE Society, and Professor A. Bax, President of ISMAR, were handed to Professor B.M. Hoffman by Professor Ch. Griesinger, member of the ISMAR Council and the AMPERE Committee.

A concert by a string quartet preceded and followed the ceremony. The event was concluded with a Banquet in honor of Professor B. M. Hoffman and his outstanding contributions to EPR. During their stay in Kazan the laureate visited the museum of history of the Kazan State University and places of historical and cultural interest in Kazan.

The Organizing Committee owes special thanks to the Russian Academy of Sciences, Russian Foundation for Basic Research, and the Ministry of Education and Science of the Republic of Tatarstan.







# 100th Anniversary of E.K.Zevoisk

Ceptember 28th, 2007 marked the100th Janniversary of Evgeny Konstantinovich Zavoisky, Laureate of the Lenin Prize, Hero of Socialist Labor, Full Member of the Academy of Sciences of the USSR. This date has been largely celebrated in Kazan, the Birthplace of EPR. In Kazan, several International Conferences and Youth Schools were held. Ceremonial meetings took place in Kazan and in Moscow (in the Russian Scientific center "Kurchatov Institute"). The Kazan Zavoisky Physical-Technical Institute participated in all these activities and their organization. This anniversary was celebrated not only by the scientific community but by many other people as well, and also well-presented in the mass media A special issue of a local popular magazine, "Kazan", devoted to the 100th anniversary of E. K. Zavoisky was published.

The worldwide recognition of E. K. Zavosiky is related to his discovery of the phenomenon of electron paramagnetic resonance (EPR) in 1944 when he was Associate Professor at Kazan State University. The discovery of EPR remains an outstanding scientific event. Today EPR is widely applied to research covering various fields of science, from molecular properties, spin and chemical dynamics in the nanosecond time scale, to dating archeological objects, electronic structure of paramagnetic particles, phase transitions, measurement of electron density distribution in quantum dots, dosimetry, quality control of tea, beer and wine, etc. With the development of pulse EPR methods, high-frequency and high-field EPR, new opportunities for the EPR method continue to abound.

In 1969, to mark the 25th anniversary of the EPR discovery the International scientific conference took place in Kazan. From the rostrum of the conference, A. Kastler, Nobel Prize laureate, an outstanding French physicist, said the following: "The river Volga starts from a little spring, grows more and more and finally transforms into an enormous stream, as full as the sea. The same happened with paramagnetic resonance. It started with a modest experiment carried out here at the Kazan University 25 years ago. In the years that have passed it transformed into an enormous field of investigations and resulted in thousands of experiments and publications".

The International Society of Magnetic Resonance posthumously conferred to Professor E. K. Zavoisky the International Society of Magnetic Resonance Award for the year 1977 in recognition of his discovery of the electron paramagnetic phenomenon in Kazan, USSR, in 1944. The Award was signed by Alfred Kastler, Chairman, Prize Committee; Daniel Fiat, Chairman, International Society of Magnetic Resonance. At the Sixth International Symposium on Magnetic Resonance, Banff, Alberta, Canada, May 1977, Professor Karl Hausser gave the Award Address. He said: "We are here in memory of a great scientist and his important discovery, Professor E. K. Zavoisky and electron paramagnetic resonance... The full impact of Zavoisky's discovery together with the independent discovery of nuclear magnetic resonance by Purcell and Bloch becomes clear at this meeting, to which, 30 years later, so many scientists – physicists, chemists, and biologists – have come together from many countries in order to discuss the different aspects of magnetic resonance".

How was it that the discovery of EPR was a major scientific event? Electrons have spin magnetic moments which undergo certain motions in magnetic fields, i.e., electrons have a spin degree of freedom. There are two aspects related to the spin degrees of freedom of electrons. On the one hand, the electron spin state and its motion in a magnetic field in many cases is important in itself. For example, it is well known that the state of electron spins is crucial for the formation of covalent chemical bonds, the occurrence of magnetic properties of substances, luminescence, etc. EPR is important for it provides a means to control systems by influencing the motion "along" the spin degrees of freedom. This has led to new fields of science and technology: spin physics, spin chemistry and spin technology. On the other hand, spin dynamics sensitively reacts to the state and motion of molecules along non-spin degrees of freedom. These facts make EPR a unique tool for scientific research. By means of EPR one can study electron structure of paramagnetic particles, molecules, local defects, structure of proteins, molecular and spin dynamics of particles, kinetics of chemical reactions, electron transfer, spin transfer, energy transfer, etc.

E. K. Zavoisky also achieved remarkable success in the field of plasma research. He developed a method of turbulent heating to obtain thermonuclear plasmas. The Zavoisky-Fanchenko method to study fast processes based on the use of electron-optical transducers is an outstanding scientific contribution. By means of this method photography with femtosecond resolution is already achievable.

The 100th anniversary of E. K. Zavoisky and the relevant activities were significant cultural events in the life of Kazan and the Republic of Tatarstan.

It turned out that I saw E. K. Zavoisky and listened to him lecture only once. It was during the International EPR conference dedicated to the 25th anniversary of the EPR discovery held in Kazan in 1969. In 1988, when I was working in the Institute of Chemical Kinetics and Combustion of the Siberian branch of the Academy of Sciences of the USSR in Akademgorodok, I was invited to participate in the competition of the position of Director of the Kazan Physical-Technical Institute of the Academy of Sciences of the USSR. In accepting this proposal, I was impressed that this institute bears the name of E. K. Zavoisky. The prospect of working in the Zavoisky Institute strongly excited and inspired me. I thank my lucky stars that for about twenty years I have had the privilege to work in this institute founded by E. K. Zavoisky and bearing his name. The Zavoisky Physical-Technical Institute was and remains one of the leading world centers for developing EPR and its applications.

> Kev M. Salikhov Kazan Zavoisky Physical-Technical Institute

### Evgeny K. Zavoisky (28.09.1907–09.10.1976)

### **Curriculum Vitae**

### Education

1926–1930 Student, Kazan State University, Kazan, USSR 1930–1933 Post-graduate Student, Kazan State University, Kazan, USSR

### Degrees and academic status

1933 – Defense of the Candidate dissertation on "The study of super-regenerative effect and its theory", Kazan State University, Kazan, USSR

1945 – Defense of the Doctor of Sciences dissertation on "Paramagnetic absorption in perpendicular and parallel fields for salts, solutions and metals", Lebedev Physics Institute of the Academy of Sciences of the USSR, Moscow, USSR

1953 – Elected Corresponding Member, The Academy of Sciences of the USSR

1964 - Electedf Full Member, The Academy of Sciences of the USSR

### Professional carreer

1933–1947 Head, Chair of Experimental Physics (Associate Professor from 1935; Professor from 1945), Kazan State University, Kazan, USSR

1946–1947 Head, Physics Department, Kazan Physical-Technical Institute, Kazan Branch of the Academy of Sciences of the USSR, Kazan, USSR

1947–1951 Participation in the Soviet atomic bomb project, Arzamas-16, USSR

1951–1971 Sector Head, Kurchatov Institute of Atomic Energy, Moscow, USSR

### Awards

1949 – Stalin Prize and Order of Lenin

1954 – Order of Lenin

1957 – Lenin Prize

- 1969 Hero of Socialist Labor
- 1975 Order of the Red Banner of Labor

1977 - Prize of the International Society of Magnetic Resonance (posthumously)

# Nominations Open for the Zavoisky Award 2008

The Zavoisky Award 2008 will be presented at the Annual Symposium "Modern Development Magnetic Resonance" to take place in Kazan in September 2008.

This prestigious award is given in recognition of an outstanding contribution to the development of electron paramagnetic resonance. It is presented by the Kazan Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, Kazan State University, the Tatarstan Academy of Sciences, and Springer-Verlag Wien New York. The lecture of the award-winner will be published in the journal *Applied Magnetic Resonance*.

Nominations are being sought from the EPR community worldwide. A brief presentation of the applicant covering 1-2 pages is expected. The final decision is made by the Award Selection Committee which

comprises G. Feher (La Jolla), D. Gatteschi (Florence), H. M. McConnell (Stanford), K. A. McLauchlan (Oxford), K. Möbius (Berlin), and the chairman, K. M. Salikhov (Kazan). The selection of the Awardee is made after consultations with the Advisory Award Committee which comprises Yu. N. Molin (Novosibirsk), and Yu. D. Tsvetkov (Novosibirsk).

Nominations should be submitted to Dr. Laila V. Mosina, Executive Secretary of the Zavoisky Award Committee, Zavoisky Physical-Technical Institute of the Russian Academy of Sciences Sibirsky trakt, 10/7 Kazan, 420029 Russian Federation E-mail: mosina@kfti.knc.ru

E-mail: mosina@kfti.knc.r Fax: 7-843-2725075

The deadline for submission of nominations is May 1, 2008.



# 15th anniversary of EFEPR, and more to come!

The idea of a European Federation of EPR groups (EFEPR) was first put forward during a joint conference organized in August 1991 in the historic town of Padua by the British ESR group, the oldest one in Europe, and the then more newly formed Italian ESR group. The need was felt for a forum gathering the researchers dedicated to the development EPR methods and their application in physics, chemistry, biochemistry, medicine and materials sciences. The next year, the European federation was founded. Klaus Möbius (Berlin) was elected in 1994 as its first president and was succeeded consecutively by Marina Brustolon (Italy) and Daniella Goldfarb (Israel), and by Etienne Goovaerts (Belgium) in charge since September 2003. The four presidents are pictured on a photo, happily meeting at the 40th anniversary meeting of the ESR Group of the Royal chemical Society held in March 2007 in Oxford.

EFEPR (see also www.physics.ua.ac.be/ EFEPR) is a non-formal organization, which at presently gathers 14 regional EPR groups from European countries and others in the region. EFEPR is devoted to the interchange of information between the different



groups. Its activities include a triennial conference (Paris 1994, Leipzig 1997, Norwich 2000, Lisbon 2003, Madrid 2006, and the upcoming one in Antwerp 2009) that provides a forum for scientists engaged in EPR spectroscopy to present and discuss recent results and developments. Since 1999, it also regularly organizes EPR schools that disseminate modern EPR methodology to the community through its young researchers. In line with its mission, EFEPR is actively involved in the International EPR (ESR) Society together with the Asia-Pacific EPR Society.

EPR research in Europe has expanded in this period in many directions. This is nicely illustrated by the successful activities of the EU COST Action P15 on 'Advanced paramagnetic resonance methods in molecular biophysics' which is supporting network activities between research groups developing new EPR instrumentation and

From left to right: Daniella Goldfarb, Marina Brustolon, Klaus Möbius, and Etienne Goovaerts.

methods and applying them to specific classes of biomolecules. The upcoming EPR school (St.-Andrews, August 2008) and conference (Antwerp, September 2009) will be co-organized with COST P15, as were the respective previous editions. We hear that researchers in other European countries are declaring their interest to either join with a new regional group or to be associated in other ways with EFEPR, while recently the Greek group has been joining the federation.

We heartily congratulate all members of the regional groups in EFEPR with this anniversary and wish them success in their research, and besides also good health and all the best!

> Etienne Goovaerts President of EFEPR





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# Evgeny Konstantinovich Zavoisky – A Participant of the Soviet Atomic Project\*

# Yu. N. Smirnov

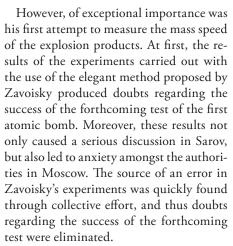
Leading researcher, Russian Scientific Center "Kurchatov Institute"

In August 1947 I. V. Kurchatov sent E. K. Zavoisky to Sarov (Arzamas-16) for what should have been a short visit. Therefore Zavoisky did not take his family with him, leaving them in Moscow. But in fact, he worked in Sarov more than four years. During this period the first three Soviet nuclear bombs (with the assistance of Evgeny Konstantinovich) were created. He also participated in

the first stage of the development of A. D. Sakharov's Sloika design (RDS-6s) – the first Soviet thermonuclear bomb.

At that time in Sarov together with E. K. Zavoisky were Dr. K. I. Schelkin – Sector Head; three corresponding members of the Academy of Sciences of the USSR: Ya. B. Zeldovich, I. E.Tamm, and N. N. Bogolyubov, and six Drs. Sci. V. G. Kuznetsov, G. N. Flerov, D. A. Frank-Kamentskii, Yu. A. Pomeranchuk, S. Z. Belenky and A. F. Belyaev; A. D. Sakharov was one of 15 Candidates of Sciences.

During his time in Sarov, Zavoisky developed a method for the registration of extremely short and weak light signals. As a result of this work, multi-cascade electron-optical converters were produced which allowed one to measure signals of duration from  $10^{-12}$ –  $10^{-14}$  s. Due to the development of these devices our country became the world leader in the creation of electron-optical converters and super-high-speed recorders. Zavoisky also proposed and constructed the first luminescent chamber for studying nuclear processes and also developed a method of nuclear polarization by using the Lamb shift.



Already on April 15th 1949, Yu. B. Khariton and K. I. Schelkin reported to L. P. Beria about work carried out under the guidance of L. V. Altshuler, V. A. Zukerman, and Prof. E. K. Zavoisky: "...The above works gave confidence in obtaining a considerable reduction in the device during the explosion of the compound charge and, accordingly, in obtaining a satisfactory coefficient of efficiency. These works are an outstanding scientific achievement." Thus, the main obstacles were removed.

In this history, which ended on August 29th, 1949 through the successful test of the first Soviet atomic bomb, it is necessary to emphasize the great courage demonstrated by Zavoisky. In fact, the very idea of how to measure the mass speed was his discovery and he was absolutely sure that it was correct. In spite of everybody's hope for the success of the first test at the nuclear test site nothing could stop him from alerting the authorities about his concerns given the failure of his first experiments on measuring the mass speed of explosive products and his view of the likely failure at the test site. This was made known in spite of I. V. Stalin's optimistic assurances in the mass media. On February 9th 1946, Stalin said: "I do not doubt that if we help our scientists, in the near future they will manage not only to catch up but also to surpass achievements of science outside our country." Undoubtedly, under 'achievements of science outside our country' he meant nuclear weapons.

In the Sarov Nuclear Weapons Museum. From left to right: RDS-1, RDS-3 and RDS-6s.

E. K. Zavoisky as the Head of the electromagnetic laboratory and a talented physicistexperimenter participated directly in the creation of the first sample of the Soviet bomb RDS-1. Documents testify that he made measurements concerned with the development of RDS-3 tested successfully on 18 October 1951. At last, before his departure from Sarov to Moscow in October 1951, E. K. Zavoisky participated in several experiments on the device RDS-6s, in particular, used his electron-optical method of highspeed photography to study the flight of shells, their crushing and their form ...

<sup>\*</sup> An extract from the report at the International conference "Modern Development of Magnetic Resonance", 25–29 September 2007, Kazan, Russian Federation to be published elsewhere.



# Dietmar Stehlik (1939–2007)

For those who knew Dietmar Stehlik it is still inconceivable: On August 8, 2007 Dietmar Stehlik passed away at the age of only 68. He was on one of his favoured bicycle trips with his wife Brigitte, enjoying the beautiful landscape of the Orkney Islands, when suddenly he had a cardiac arrest. Dietmar Stehlik's much too early death means a tragic loss for his family and friends. Also his colleagues at the Free University Berlin and of the German and international magnetic resonance community grieve for him, they have lost an outstanding scientist and admirable human being.

Throughout Dietmar Stehlik's scientific activities there were two main subjects: The interactions of electron and nuclear spins in magnetic fields and the interactions of light with organic molecules, both in molecular crystals and photosynthetic proteins. In 1962 he started his undergraduate work on spin echo phenomena in the group of Karl Hausser at the Max-Planck-Institute for Medical Research in Heidelberg. After his diploma degree he continued to work on coherent spin physics in the Hausser group and received his PhD in 1966. From 1967-1969 he was a post-doc in Erwin Hahn's group at Berkeley. The scientific and personal experiences he made there, interacting with famous professors and insubordinate students alike, has coined his social and professional way of thinking, and he remained true to the principles of scientific honesty and so-



cial responsibility ever since. After returning to Heidelberg, he invented methods to generate optical nuclear spin polarization in organic molecular crystals. With this work he habilitated in 1975.

In1976 he accepted an offer for a professorship at the Physics Department of the Free University Berlin. In the new environment he gradually shifted his scientific interest to biophysics. He focussed on the primary processes of photosynthesis, both in bacteria and plants, taking advantage of his expertise in spin physics. He applied time-resolved EPR methods on delicate protein preparations he had obtained from cooperation partners around the globe. His tenacity in trying to understand the underlying principles of light-induced charge separation in photosynthesis was just admirable. It stimulated generations of students and visiting scientists to work with him on transient donor-acceptor radical pairs and on the concept of spin dynamics.

In all the years in Berlin, Dietmar Stehlik was strongly involved in creating and cultivating the scientific openness of mind indispensable for interdisciplinary research on fundamental photoprocesses in proteins. Scientific face-to-face cooperation with physicists, chemists and biologists was Dietmar Stehlik's key strategy for scientific success, personal delight and satisfaction. Consequently, over the years he was strongly involved in five Collaborative Research Centers of the Deutsche Forschungsgemeinschaft. For two of them he served as their speaker and, thanks to his fairness and balancing character, he always managed to solve emerging difficulties, be it with the administration or with participating scientists.

Extremely important for Dietmar Stehlik was international cooperation, most of all with scientists from the US, Israel and Russia. What started as scientific cooperation often turned into personal friendship, and mutual visits over weeks, sometimes months, were like heaven on earth for him. Just to mention a few long-term visitors representative for many more: Ken Sauer and Mel Klein from Berkeley, John Golbeck from Penn State, Haim Levanon from Jerusalem, Kev Salikhov, first from Novosibirsk, later from Kazan.

Dietmar Stehlik never accepted political barriers, such as the Iron Curtain or the Berlin Wall, to impede scientific contacts and personal friendships. He always was very creative in tunnelling such barriers, very much to the delight of his cooperation partners and friends on the other side. Together with them we are now in mourning for Dietmar Stehlik. We miss him as a dear friend and stimulating colleague.

> Klaus Möbius Ludger Wöste



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# Hyperfine Sublevel Correlation Spectroscopy

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### Introduction

The idea of Peter Höfer et al. [1] to insert a  $\pi$  pulse between the second and third  $\pi/2$ pulse of the well-known three-pulse ESEEM experiment was both simple and brilliant: simple, because it was the obvious step to take for the NMR-inspired scientists from Stuttgart, and brilliant, because it opened a new area for ESEEM spectroscopy. Indeed, the  $\pi$  pulse will transfer the nuclear coherence created by the first two  $\pi/2$  pulses from one  $m_S$  manifold to another. Independent variation of the two time intervals  $t_1$  and  $t_2$  and subsequent two-dimensional Fourier transformation then gives rise to cross peaks linking nuclear frequencies of the different  $m_{\rm S}$  manifolds (see Figure). In this way, the rich spectral information hidden in many broad features observed in three-pulse ESEEM spectra can be revealed. Höfer et al. named this two-dimensional four-pulse-ESEEM technique hyperfine sublevel correlation (HYSCORE) spectroscopy.

Twenty years after the introduction of HYSCORE, many applications of this technique can be found in the EPR literature. Nevertheless, the interpretation of HYSCORE spectra remains non-trivial and there lie many pitfalls in the use of this technique. Rather than to focus on specific examples of HYSCORE applications, I will give here my personal view on the advantages and disadvantages of the technique and present some hints how to get the most out of this method.

#### **Advantages and Pitfalls**

As is the case for all ESEEM methods, the HYSCORE technique allows for a good detection of the smaller nuclear frequencies, particularly in the frequency area where the ENDOR methods are performing badly (i.e. frequencies below 5 MHz). As a rule of thumb, ESEEM techniques are usually applied to study small hyperfine couplings, whereby ENDOR is the method of choice to trace the more strongly coupled nuclei [2]. However, the application regions strongly overlap and new developments in pulsed EPR and ENDOR are even increasing this overlap (see further).

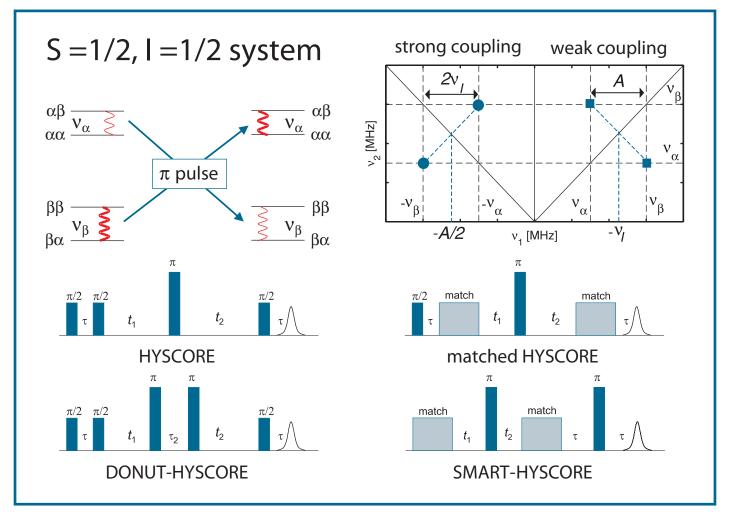
From the introduction, it should be clear that the specific advantage of the HYSCORE technique lies in the fact that it allows to correlate nuclear frequencies from different  $m_s$ manifolds, as is shown for the simple case of an S = 1/2, I = 1/2 system in the accompanying Figure. Furthermore, the appearance of the dominant cross peaks in a specific quadrant already gives clues about the size of the hyperfine interaction. In case of a weakly coupled nucleus (i.e. the hyperfine coupling smaller than twice the nuclear Zeeman frequency), the dominant cross peaks will be observed in the (+,+) quadrant of the spectrum, whereby the strongest cross peaks are found in the (-,+) quadrant for the strong coupling case. Moreover, when the unpaired electron(s) is (are) interacting with several nuclear spins, the observation of specific combination frequencies can reveal the relative sign of the hyperfine couplings, since only nuclear frequencies within one  $m_{\rm s}$  manifold can combine (product rule) [2]. Indeed, assume a hypothetical case of an electron spin S = 1/2 weakly interacting with two nuclear spins  $I_{1,2} = 1/2 (g_{n,1}, g_{n,2})$ 0), whereby the basic nuclear frequencies  $\nu_1 < \nu_2$  and  $\nu_3 < \nu_4$  belong to the interaction with  $I_1$  and  $I_2$ , respectively. If both hyperfine couplings are positive, the nuclear frequencies  $\nu_1$  and  $\nu_3$   $(\nu_2$  and  $\nu_4)$  belong to the  $\alpha$ (β) manifold. Consequently, cross peaks involving the combination frequencies  $v_1 \pm v_3$ and/or  $\nu_2 \pm \nu_4$  will be observed, whereas the combination frequencies  $\nu_1 \pm \nu_4$  and  $\nu_2 \pm \nu_3$ can only be found in case the two hyperfine interactions have opposite sign. Note that the HYSCORE cross peaks involving these combination frequencies are often very weak and are not always observable.

Unfortunately, the HYSCORE technique has also many drawbacks. Since the technique involves the variation of two time intervals, the recording of a single HYSCORE experiment can take from 45 min up to many hours depending on the echo intensity, spin system and spectrometer type. Furthermore, the individual cross-peak intensities depend on the time interval  $\tau$  between the first two pulses and some of the spectral features can be fully suppressed for certain values of  $\tau$  (socalled blind-spot effect) [2]. Hence, several HYSCORE spectra with different  $\tau$  values should be recorded for each magnetic-field setting in order to minimize the blind-spot effect [3]. This makes HYSCORE spectroscopy extremely time-consuming (and thus expensive).

Since the  $\pi$  pulse needs to induce a transfer of nuclear coherence from one  $m_{\rm s}$  manifold to another, a short and strong  $\pi$  pulse with sufficient bandwidth needs to be applied in the HYSCORE experiment. This is technically easy to achieve at the lower microwave frequencies (S- to Q-band), but at high microwave frequencies (95 GHz and higher), this is no longer trivial. Hence, W-band HYSCORE is currently not feasible on the commercial Bruker spectrometers, except for very special cases such as high-electron-spin systems with high effective g values [4]. It should be noted that this technical problem may be overcome by a new generation of Wband EPR spectrometers, such as the ones currently constructed in St-Andrews (HIPER project, Graham Smith) or the Weizmann Institute (Daniella Goldfarb).

One of the hidden pitfalls of HYSCORE (and standard ESEEM experiments in general) was recently revealed in an article by S. Stoll et al. [5]. In this paper, it is shown how the contributions of weakly modulating nuclei (e.g. weakly coupled protons) can be fully suppressed by the contributions of strongly modulating nuclei (e.g. <sup>14</sup>N nuclei). This cross-suppression effect may lead to serious misinterpretations of the experimental data.

Finally, there are a number of additional complicating factors of a more general nature. First, no HYSCORE (or ESEEM) spectrum can be obtained at room temperature for paramagnetic systems in low-viscosity solutions, since the modulation depth is zero for an isotropic hyperfine coupling [2]. Similarly, the modulation depth be-



comes zero for the principal orientations of the hyperfine tensor [2]. Second, the example in the accompanying Figure presents the simplest case that can be encountered. For interactions with higher nuclear spins, the amount of potential cross peaks increases dramatically. In this case, also multi-quantum nuclear transitions ( $|\Delta m_1| > 1$ ) can be observed. For example, for an S = 1/2, I = 1system, up to 18 cross peaks per quadrant can be obtained, whereas for an S = 1/2, I = 3/2 system already 72 potential cross peaks per quadrant can be expected [6]. Although not all cross peaks will be observed in practice, HYSCORE spectra of high-spin nuclei are complex. This explains why only few HYSCORE studies of I > 1systems are found in literature. Furthermore, in most practical cases, the electron spin is interacting with several nuclear spins which evidently increases the complexity of the HYSCORE spectra. Moreover, for disordered systems, such as frozen solutions, the cross peaks are no longer sharp features, but broad ridges stemming from the sum of the individual contributions of all molecular orientations excited at a certain observer position.

All of this makes that the interpretation of HYSCORE spectra can still be quite challenging, despite the advantage of the second dimension.

### Getting the most out of the HYSCORE technique

From the above section it should be clear that standard HYSCORE experiments should always be performed at different  $\tau$  values in order to avoid misinterpretations due to blind-spot effects. Furthermore, a strong  $\pi$ pulse should be used at all times, otherwise the HYSCORE spectra will be dominated by strong features on the diagonal stemming from incomplete transfer of nuclear coherence. It is advisable to use small time increments (usually 8 ns) for the first HYSCORE spectrum that one records of a sample. From this spectrum one can then determine the highest observed nuclear frequencies and hence deduce the optimal highest time increment that can be used (Nyquist criterion [2]). It is clear that doubling the time increment will reduce the recording time with a factor

of four, and that a lot of valuable time can be saved in optimising this parameter. In a first step, a small set of HYSCORE spectra should be recorded at observer positions spanning the full *g*-anisotropy. For systems with low symmetry, the best observer positions to start with are usually the ones corresponding to the principal *g* values. For systems with high symmetry, e.g. defects in cubic crystals, the pincipal *g* axes are likely to coincide with the principal hyperfine directions and are thus bad choices to perform initial HYSCORE experiments.

Starting from this first set of standard HYSCORE spectra, one can start to think of a second series of HYSCORE-based experiments in order to enhance the spectral information. In a number of very nice papers [7–9], Gunnar Jeschke and Arthur Schweiger provided us the tools to target specific interactions. Indeed, by the use of matched pulses, the signal intensity of cross peaks linked to a specific hyperfine interaction can be selectively increased. For this, the second and fourth pulse in the HYSCORE spectra need to be replaced by high-turning-

angle (HTA) pulses, of which the  $B_1$  field will determine the type of interaction that will be enhanced and the length is tuned experimentally (via the related matched threepulse ESEEM scheme) to give the optimal enhancement [9]. In order to enhance weakly coupled nuclei, the  $B_1$  field should match the nuclear Zeeman interaction, whereby an optimal enhancement of the strong couplings is usually achieved by the maximum microwave-field strength. In this way, stronger hyperfine couplings (20-40 MHz region) can be observed that are generally thought to be only accessible by ENDOR-type techniques [9]. It is my experience that Q-band HYSCORE experiments benefit hugely from the use of matched pulses. It often provides the only way to observe a decent HYSCORE spectrum at this microwave frequency.

Alternatively, matched pulses can be used in a SMART (single pulse matched resonance transfers) HYSCORE experiment [10], which combines the advantage of the specific enhancement with the fact that the replacement of the nuclear-coherence generator ( $\pi/2$ - $\tau$ - $\pi/2$ ) by a single HTA pulse makes the method virtually blind-spot free.

The matched HYSCORE and SMART-HYSCORE experiments can help to overcome the earlier mentioned cross-suppression effects [5]. In an on-going analysis of cyanide-ligated ferric globins, we observed a nice example of this. In these ferric globins, the unpaired electron is strongly coupled to the heme nitrogens and weakly coupled to the surrounding protons, but the standard HYSCORE spectrum reveals only the cross peaks related to the interaction with the histidine nitrogen, which happens to be in exact cancellation and therefore gives rise to very deep modulations that suppress all other contributions. Using specifically matched pulses, clear proton ridges and strong cross peaks stemming from the heme nitrogens can be regained. In a very recent work, B. Kasumaj and S. Stoll showed that a six-pulse ESEEM scheme can also provide a valuable alternative to avoid the cross-suppression effects [11]. This method may be especially important in cases where little is known about the nature and magnitude of the nuclear interactions, and where it is thus difficult to select the appropriate matching conditions.

If possible, HYSCORE experiments should be performed at different microwave frequencies. Multi-frequency HYSCORE allows you to circumvent some of the cross-suppression effects. By changing the microwave frequency (and hence the external magnetic field), the ratio of the hyperfine versus the nuclear Zeeman interaction is altered with a linked change of the modulation depth. In this way, you can selectively drive one or the other nucleus into the strong or weak modulation case and hence reveal many features that would remain hidden in a single microwave experiment. Combination with the above-mentioned matching schemes can allow you to fully unravel the whole set of nuclear interactions. Of course, I am aware that only a minority of groups have a pulsed EPR facility spanning a larger range of microwave frequencies and that the above approach is time- and money-consuming. For this reason, I have always been an ambassador of (inter)national collaborations.

Note also that many experiments derive from the HYSCORE scheme. Combination-peak (CP) experiments [12] and the DEFENCE (deadtime free ESEEM by nuclear coherence-transfer echoes) method [13] use the same four-pulse sequence as HYSCORE, but now  $t_1$  and  $t_2$  are stepped simultaneously (CP) or  $t_2$  is stepped with constant  $t_1$  (DE-FENCE). The CP experiment allows the analysis of the combination frequencies in detail, whereby the DEFENCE spectrum gives in essence a three-pulse-ESEEM-like spectrum that is undistorted by deadtime artefacts. Although each HYSCORE spectrum includes a CP spectrum (Fourier transform of the diagonal of the time-domain matrix) and many DEFENCE spectra (Fourier-transform of individual columns of the time-domain matrix), it may be of interest to perform separate CP or DEFENCE experiments whereby the  $\tau$  value is varied in a second dimension. Summation over all  $\tau$  values will give a blindspot free CP or DEFENCE spectrum and, in cases of sufficiently long phase-memory time, two-dimensional Fourier-transformation may lead to extra information [14]. In some cases, time can be saved by performing HYSCORE experiments for a number of carefully selected observer positions and recording DEFENCE spectra at some intermediate magnetic-field positions.

In a DONUT (double nuclear coherence transfer) HYSCORE experiment, the mixing  $\pi$  pulse of the standard HYSCORE experiment is replaced by the DONUT mixer,  $\pi$ - $\tau_2$ - $\pi$  [15]. In case of an S = 1/2, I = 1/2system, such an experiment is of course useless, because the first  $\pi$  pulse will transfer  $\nu_{\alpha}$  ( $\nu_{\beta}$ ) to  $\nu_{\beta}$  ( $\nu_{\alpha}$ ), after which the second  $\pi$ pulse will transfer it back to  $\nu_{\alpha}$  ( $\nu_{\beta}$ ), and only uninformative cross peaks on the diagonal (( $\nu_{\alpha}$ ,  $\nu_{\alpha}$ ) and ( $\nu_{\beta}$ ,  $\nu_{\beta}$ )) will be visible. However, when the unpaired electron is interacting with a high-spin nucleus or is interacting with several nuclei, cross peaks linking basic nuclear frequencies within one  $m_s$  manifold will be observed. In combination with the corresponding HYSCORE spectrum, these peaks can give an idea about the relative sign of the observed hyperfine interactions. If we go back to the hypothetical three-spin system that was introduced earlier (S = 1/2,  $I_{1,2}$  = 1/2), the same sign of the hyperfine value will lead to cross peaks at  $(\nu_1, \nu_3)$  and  $(\nu_2, \nu_4)$ in the DONUT-HYSCORE spectrum. An opposite sign of the hyperfine coupling will result in  $(\nu_1, \nu_4)$  and  $(\nu_2, \nu_3)$  cross peaks. In principle, this technique also allows to differentiate the above three-spin system from two two-spin systems (S = 1/2,  $I_1 = 1/2$  and S = 1/2,  $I_2 = 1/2$ ) for the case of two species with overlapping EPR spectra (e.g. two radicals). In the latter spin system, the off-diagonal cross peaks will not be visible. Where the observation of the off-diagonal cross peaks is conclusive for the three-spin system, the inability to see them may unfortunately also result from technical reasons. Note that, due to the extra microwave pulse, DONUT-HYSCORE spectra may be less intense than their HYSCORE counterpart. In cases of very small spin-echo intensity, you should take into account that a DONUT-HYSCORE experiment may be impossible within a reasonable time scheme.

Until now, I have focussed on the experimental side of optimising the HYSCORE outcome. However, in many cases, one of the biggest bottlenecks is the interpretation and simulation of these spectra. As frustrating as it may sound to young EPR scientists, one of the most important factors that facilitates the simulation of HYSCORE spectra (or any EPR/ENDOR spectrum for that matter) is experience. Trying to be an EPR spectroscopist is sometimes a bit like trying to be an art specialist. There is nobody who will contest that you need to look at many art works in order to be able to differentiate for instance the cubist paintings of Bracke and Picasso, and equally, the importance of the pattern-recognition mechanism of the human mind should not be underestimated in spectroscopy. I can therefore strongly advise to read as many HYSCORE papers as possible, to simulate different HYSCORE spectra for hypothetical cases and, most importantly, to try to understand how the different spin-Hamiltonian parameters influence the observed patterns. Having said this, let me nevertheless try to outline some general guidelines to facilitate HYSCORE simulations. Make a list of all types of nuclei that potentially can be observed with their nuclear spin and the nuclear Zeeman frequency at the observer position. Use this list to identify the peaks that stem from the I = 1/2 nuclei (weak coupling: signals in (+,+) quadrant, centred around the nuclear frequency; strong coupling: cross peaks in the (-,+) quadrant separated by twice the nuclear Zeeman frequency). Then, check whether the remaining peaks can be explained in terms of the highspin nuclei that are on your list. Focus first on the most intense peaks and ask yourself the question whether these peaks belong to the single-quantum or multi-quantum transitions. It will help to look how these peaks evolve when the magnetic-field settings are changed. Use the simple first- or second-order expressions for the nuclear frequencies to get an idea about the magnitude of the hyperfine and nuclear-quadrupole tensor. In this way you can get starting values to perform the simulations. In order to save time, you can best first concentrate on reproducing the peak positions (without intensities). This can in principle be done using any of the programs that can compute nuclear frequencies for a given spin system. I tend to use EasySpin for this, since it allows the custommade manipulation of the frequency data via Matlab [16]. Once you get satisfying results using this approach (i.e. you are nearing the optimal parameters), you can start the more time-consuming simulations that include the full intensity reproduction (e.g. via a timedomain simulation as is done by [17]).

Reproducing the exact peak intensities observed in the experiment is virtually impossible. The peak intensities are governed by many factors: pulse shape and bandwidth, tuning of the pulses, g, A and Q strain effects, relaxation times, and last but not least, the cross-suppression effect. The latter effect makes that, even if we would have the ideal experiment, we can only reproduce the correct intensities if we take into account all the interactions with the surrounding nuclei. The size of our spin system would then be simply too high to handle. Note that the inability to correctly reproduce the peak intensities is also one of the reasons why an automatic fitting procedure for HYSCORE simulations is not (yet) feasible and why errors on the simulated parameters are hard to quantify in a correct manner. I sometimes get the question whether it is then at all helpful to invest time in simulating the peak intensities, and the answer is yes. Focussing on the peak positions alone has several drawbacks: you can not estimate the effect of the blind-spots, you do not see the areas that have zero intensity because you hit a principal hyperfine direction and you do not differentiate between the most intense and the less intense peaks. For higher nuclear spins, the frequency approach sometimes results in a zoo of spots of which many have quasi-zero intensity in practise. It is in that case very hard to obtain sensible parameters without including the peak intensities.

### **Conclusion and outlook**

The many applications of HYSCORE that can be found in literature prove that the technique has a large potential. In this text I have tried to point out that, nevertheless, one has to be very careful when performing and interpreting these experiments and hope I have provided some useful guidelines. Furthermore, I would like to stress that one should never consider the HYSCORE technique as an isolated method, but use it as part of a package of different EPR techniques, such as CW-EPR, ENDOR, ELDOR-detected NMR, other ESEEM experiments and even DFT computations, that allow the full characterization of a paramagnetic system.

Besides the intellectual pleasure of translating experimental outcomes in mathematical terms and back again into the molecular knowledge, examination of a HYSCORE spectrum sometimes also offers an esthetical pleasure, which brings me back to the art specialist <sup>©</sup>.

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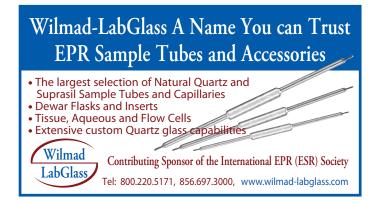
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### EUROMAR 2007 Terragona, Spain, July 1–5, 2007

EUROMAR brings together the Europe-an magnetic resonance community. In 2007, there were 11 plenary talks; and 64 lectures divided into two parallel sessions, including two EPR sessions, one of them sponsored by COST P15 Action: Advanced Paramagnetic Resonance Methods in Molecular Biophysics. Additionally there were 408 posters. At the end of the conference on the 6th of July, there were three satellite meetings in parallel: the II Ibero-American NMR meeting; New NMR pulse sequences for protein, nucleic acids, and protonless NMR; and Electron-Nuclear Spin Interactions, sponsored by EU-DNP and attended by a mixed group of EPR and NMR scientists.

EPR and related fields were well represented at the conference. W. L. Hubbell of UCLA gave a comprehensive plenary talk on

the EPR-based method of Site Directed Spin Labeling applied to signal transduction in the visual system. R. G. Griffin of MIT gave a splendid plenary talk on high-frequency Dynamic Nuclear Polarization and its application to solid-state NMR on biomolecules. Using high-power gyrotrons to excite a range of single- and bi-radicals, DNP enhancements ranging from 40-300 are now routinely available. B. E. Bode from the Goethe-University in Frankfurt received the MRC Young Scientist Award for his contribution on "Counting the Monomers in Nanometer-Sized Oligomers by PELDOR".

Distance determination using EPR is a field with a growing interest; there were interesting talks on this topic by M. Huber, G. Jeschke, and Th. Maly. High-field EPR on molecular nanomagnets was covered by D. Gatteschi. S. Van Doorslaer gave a good talk on the analysis of highly anisotropic low-spin ferric heme proteins using X-band (matched) HYSCORE and pulsed ENDOR. The effect of spin relaxation on pulsed ENDOR experiments (W-band) on frozen solutions of Copper(histidine)2 were presented by D. Goldfarb and N. Domracheva gave a talk on Copper(II) dendromesogenic complexes using CW-EPR. On the hardware side, G. Smith discussed the latest advances in achieving sub-nanosecond dead-times and pi/2 pulses at W-band, and P. Blümler reported on the development of portable EPR (and NMR) force-free magnets for S- and X-bands, allowing magnetic resonance techniques to come out of the laboratory into nature.

It would not be possible to report on EU-ROMAR 2007 without mentioning the warm reception we all received from local organizing committee and naturally the fantastic weather. There was an excellent social program, including a city tour and wine tasting. If that was not enough, most evenings were supplied with local foods, music and more wine tasting organized by the different sponsors. At the Conference Dinner we were treated like royalty at the La Boella Restaurant. And finally, by coincidence in Tarragona there was an international fireworks competition; every night a different display from a different county.

Mark Prandolini



celebrated in Kazan by the "Zavoisky Week" which included the ceremonial meeting dedicated to this anniversary, the International Zavoisky Award 2007 ceremony (see also p. 3), the presentation of the Kazan Zavoisky Award for young researchers, the International conference "Modern Development of Magnetic Resonance" (Zavoisky100), and the International Youth Scientific School "Actual Problems of Magnetic Resonance and Its Applications".

The main organizers of the "Zavoisky Week" were the Government of the Republic of Tatarstan, Russian Academy of Sciences (RAS), Kazan State

> University, and Kazan Zavoisky Physical-Technical Institute of the Kazan Scientific Center of the Russian Academy of Sciences. Nataliya E. Zavoiskaya, daughter of E. K. Zavoisky, participated in the "Zavoisky Week". On the initiative and support of the Russian Scientific Center (RSC) "Kurchatov Institute" where E. K. Zavoisky worked in the period from 1951 till 1971, she published a book "A history of one discovery". The following talks were given during the opening of the "Zavoisky Week": Prof. B. I. Kochelaev (Kazan State University) "The Discovery of EPR by E. K. Zavoisky and Its Significance for Modern Physics"; full mem-

At the monument to E. K. Zavoisky. From left to right: K. Möbius, B. I. Kochelaev, K. M. Salikhov, N. E. Zavoiskaya, A. V. Aganov, W. Lubitz, B. M.

ber of RAS V. P. Smirnov (Director, Institute of Nuclear Synthesis, RSC "Kurchatov Institute", Moscow) "E. K. Zavoisky in the Kurchatov Institute: from EPR to Plasma Physics"; leading scientific researcher Yu. N. Smirnov (Institute of Nuclear Synthesis, RSC "Kurchatov Institute", Moscow) "E. K. Zavoisky and Soviet Atomic Bomb Project"\*

The International conference "Modern Development of Magnetic Resonance" was one of the main events of the "Zavoisky Week". It took place in the period from 25 to 29 September 2007. The Organizing Committee was

headed by Kev M. Salikhov, corresponding member of RAS. 32 scientists from 17 countries: Australia, Belarus, Brazil, Czech Republic, Germany, India, Israel, Italy, Japan, Kazakhstan, Moldova, Poland, Slovenia, Switzerland, Ukraine, and USA, and more than 100 Russian scientists participated in the conference. There were presented 166 reports demonstrating the current level of the development of magnetic resonance and its applications in physics, chemistry, biology, medicine, geology, materials science, etc. Reports of the participants were presented at the plenary sessions and ten scientific sections:

Low-dimensional systems and nanosystems; Chemical and biological applications of magnetic resonance; Bio- and Medical physics; Strongly correlated electron sys-

See also an extract from this report on p. 7.



tems; EPR of doped materials; Clusters and supramolecular systems; NMR problems; Minerals; Other applications of magnetic resonance; Modern methods of magnetic resonance and related phenomena.

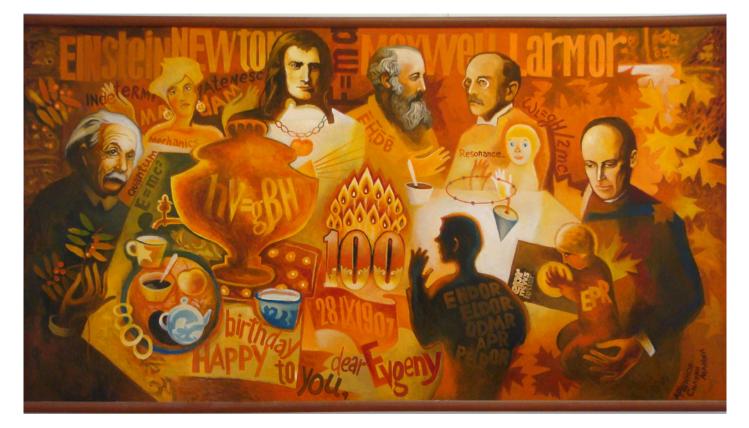
A special session was devoted to the presentations of instrumentation manufacturers Bruker BioSpin GmbH, Varian, Tokyo Boeki Ltd, and RTI Cryomagnetic Systems. Representatives of these firms participated in discussions at the round table as well.

Plenary lectures reflected the current directions of the development of magnetic resonance and its applications: "Pulse EN-DOR of Short-Lived Triplet States in Photosynthesis" (W. Lubitz, J. Niklas, S. Prakash, A. Marchanka, M. van Gastel, Max-Planck-Institut für Bioanorganische Chemie, Mülheim an der Ruhr, Germany); "Dynamical Transition in Disordered Media and in Proteins as Detected with Electron Spin Echo Planting trees in the Zavoisky alley. From left to right: M. S. Tagirov, G. Kothe, G. R. Hanson (behind the tree), B. Eichhoff, S. Yamauchi, U. Eichhoff.

of Molecular Spin Probes" (S. A. Dzuba, Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia); "Tunable High-Frequency EPR Spectroscopy of Non-Kramers Impurity Ions in Solids" (V. F. Tarasov, A. A. Konovalov, G. S. Shakurov Zavoisky Physical-Technical Institute, Kazan, Russia); "Use of Spin Labels for Investigation of Membrane Proteins with High-Frequency ENDOR Spec-

troscopy" (S. B. Orlinskii, I. V. Borovykh, V. Zielke, E. J. J. Groenen, H.-J. Steinhoff , Kazan State University, Kazan, Russia, Huygens Laboratory, Department of Physics, Leiden University, Leiden, The Netherlands); "EPR Studies of Nitrogenase Intermediates: Towards the Mechanism of N<sub>2</sub> Reduction" (B. M. Hoffman, Northwestern University, Evanston IL, USA); "Towards Single Spin Detection: the Role of Scanning Probe Microscopy Techniques" (M. Martinelli, Istituto per i Processi Chimico-Fisici, Consiglio Nazionale delle Ricerche, Pisa, Italy); "Spin-Dependent Recombination in Systems with Semiconductor Nanocrystals: ODMR" (N. G. Romanov, P. G. Baranov, Ioffe Physical-Technical Institute, St. Petersburg, Russia); "The Evolution of Spectral Interpretation - From Spin Systems to Molecular Structure and Beyond" (Ch. Noble, S. Benson, G. R. Hanson, Center





Nikolai Silkin conceived the idea of this painting spontaneously when he wrote an article for the magazine "Kazan" about Zavoisky's passion for art. He wanted to pay tribute to this outstanding man whom he met as a PhD student in 1971. This painting is strongly influenced by Russian lubok (popular print), the surrealism of Salvador Dali, paintings of the St. Petersburg's Mit'ki group, and socialist art. It features Einstein, Mme Quantum Mechanics, personified as a lovely woman, and the Heisenberg uncertainly principle, Newton, Maxwell, Larmor and Zavoisky. A kid on Zavoisky's lap, "EPR", holds in her hands the Nobel issue of the *EPR newsletter* (14/1-2). Other kids at the table personify various advanced EPR methods. This painting is a collective creation. The idea and composition are Nikolai Silkin's; Georgii Mamin did supplementary computer design; the oil painting is by Victor Arshinov's, a professional painter. This painting was demonstrated at the closing of the "Zavoisky Week".

for Magnetic Resonance, the University of Queensland, St. Luchia, Australia).

There was a total of 66 oral lectures. The poster session featured 89 presentations. Young participants of the International Youth Scientific School "Actual Problems of Magnetic Resonance and Its Application" presented 55 reports and listened to the lectures of the leading experts in magnetic resonance.

We will never forget the delight of the concert for flute and clarinet with orchestra given by U. Eichhoff (flute, Bruker BioSpin, Karlsruhe, Germany), J. Forrer (clarinet, ETH, Zurich, Switzerland), and the string orchestra "New Music" (Conductor Anna Gulishambarova, Kazan, Russia).

The closing of the conference was marked by planting trees in the E. K. Zavoisky alley at the university campus.

Valery F. Tarasov, Deputy Chairman of the Zavoisky100 Conference Violeta K. Voronkova, Scientific Secretary of the Zavoisky100 Conference

### A Joint Conference of the International Symposium on Electron Spin Science and the 46th Annual Meeting of the Society of Electron Spin Science and Technology (ISESS-SEST2007)

Shizuoka, Japan, November 6–9, 2007

The 46th Annual Meeting of the Society ▲ of Electron Spin Science and Technology (SEST) was held as a joint conference with the International Symposium on Electron Spin Science (ISESS) in the period from November 6 till 9, 2007, at Shizuoka Granship, Shizuoka, Japan. This conference was planned to celebrate the 5th anniversary of the establishment of SEST in 2002. SEST took over the former domestic EPR meeting started from 1962 as the Annual Meeting of SEST. The conference was cosponsored by the Chemical Society of Japan, the Physical Society of Japan, the Pharmaceutical Society of Japan, Shizuoka University and supported by Inoue Foundation for Science and many

other organizations. The number of the registered scientists was 205 including 27 oversea attendants (Germany, USA, Russia, Australia, England, China and other countries).

This conference was designed for the exchange of information in different fields of electron spin science and technological applications, including medical, electronic devices and so on. Seventeen invited lectures were presented. The lecturers were P. Kuppusamy (Ohio State University), H. J. Halpern (University of Chicago), K. Möbius (Free University Berlin), W. Lubitz (Max-Planck-Institut für Bioanorganische Chemie), K. Maeda (University of Oxford), J. R. Norris (University of Chicago), G. R. Hanson (The University of Queensland), T. Arata (Osaka University), Y. Li (Tsinghua University), G. Kothe (University of Freiburg), M. Wohlgenannt (University of Iowa), H. Ohta (Kobe University), E. Bagryanskaya (International Tomography Center, Novosibirsk), J. R. Woodward (University of Leicester), T. Ikoma (Niigata University), M. R. Wasielewski (Northwestern University), and K. M. Salikhov (Kazan Physical-Technical Institute of the Russian Academy of Sciences). Six Award lectures of SEST members were also presented. Another important function of this conference was the encouragement of young electron spin scientists and also students. Five young oversea scientists were chosen as the speakers by their applications, and financial supports were given. In the second day afternoon a special minisymposium on advanced instrumentation of EPR was also held by Prof. Y. Shimoyama. During the conference, the SEST General Meeting by the SEST members took place for the approval of the new council members and the budget, new rules and awarded scientists. At this meeting Prof. Anzai and Prof. Ohta were appointed as the President and the Vice-President of SEST, respectively, for the next term (2008-2009).

All the attendants really enjoyed scientific discussion and the exchange of friendship and information amicably. Shizuoka is a famous place of agricultural production of green tea leaves and tasty green tea was served at the tea break. In the second day evening a mixer was held at the restaurant in the conference building. In the third day evening a banquet took place in the hall of the building. In the banquet, five senior professors were congratulated by becoming honorable members of SEST. After the conference, about 25 attendants including their spouses joined the excursion to Nippon-daira and Mihonomatsubara.

The organizers would like to thank all the speakers, the poster presentations and the session chair persons. The enthusiastic jobs of organizing committee members and all the staff who worked hard before and during the conference were so wonderful. Especially the job of Prof. Yasuhiro Kobori, secretary and treasurer, was excellent. All of them made the conference successful and very memorable. Hisao Murai, Chairman

### My impression about ISESS-SEST2007 in Shizuoka and Workshop at Kobe University

I am excited with the scientific results presented at the ISESS-SEST2007 conference in Shizuoka by Japanese colleagues. They do a lot to further develop methods of the electron paramagnetic resonance spectroscopy and to extend its applications to different problems. In principle, I knew about that also before my visit to this meeting but what I have seen was much more than I expected. And it is remarkable how intensively scientists in Japan are focused to cover all the way from the basic research to the actual applications. This important aspect is explicitly specified in the title of their "Society of Electron Spin Science and Technology". After this exciting and big conference it was good to participate on the compact Workshop organized by Prof. Ohta and Prof. Tominaga at Kobe University during November 11–12. There were interesting discussions and excursion to see faculty facilities. In between we got the nice experience about Japanese style of life and have learned a little bit of Japanese history.

I would like to express my sincere thanks to all organizers of the ISESS-SEST2007 meeting in Kobe Workshop, in particular to Prof. Murai, Prof. Kobori, Prof. Nakamura, Prof. Ohta, Prof. Tominaga, Dr. Furukawa and Dr. Fujisawa for everything they did to make these meetings greatly successful from the point of view of the high level of science and of the social aspects: everything was just excellent, thanks and congratulations to our Japanese colleagues.

Kev Salikhov Kazan Physical-Technical Institute of the Russian Academy of Sciences, Kazan



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### Collected by Candice Klug

If you have recently become a new Assistant Professor in EPR spectroscopy, or know someone who has, please contact an Associate Editor for inclusion in future newsletters. Thank you.



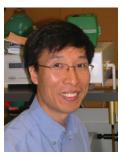
Shojiro Kimura Osaka University

Shojiro Kimura became an Assistant Pro-fessor of KYOKUGEN, Osaka University in May 2005. His training includes a postdoctoral fellowship in high field ESR with Koichi Kindo at Osaka University. He received his PhD in physics in 1998 from Kobe University in the laboratory of Hitoshi Ohta where he studied the Haldane and one dimensional S = 1 alternating-bond systems using high field ESR. His undergraduate degree is in physics from Kobe University. He recently received the Young Investigator Award from the Society of Electron Spin Science and Technology (SEST) in Japan for the development of a high field/high frequency ESR system and for ESR studies on quantum spin systems.



Linda Columbus University of Virginia

Linda Columbus became an Assistant Professor of Chemistry at the University of Virginia in August 2007. Linda received her undergraduate degree in chemistry from Smith College and her PhD degree in Molecular Biology and Biochemistry from the Chemistry and Biochemistry Department at UCLA in 2001. Her graduate work was carried out in the laboratory of Wayne Hubbell where she trained in the fields of EPR spectroscopy and protein dynamics. Linda continued her training in magnetic resonance as a postdoctoral fellow at The Scripps Research Institute under the direction of Keith Wuthrich, where she gained experience in NMR spectroscopy techniques. Her current research focuses on determining the structure and conformational changes of membrane proteins involved in bacterial infection using a combination of SDSL and EPR spectroscopy, NMR spectroscopy, and X-ray crystallography methods, as well as characterizing protein detergent interactions to aid in more efficient protein structure determinations.



Kyoung Joon Oh Rosalind Franklin University of Medicine and Science

✓young Joon Oh became an Assistant Kyoung Joon On Decar Professor of Biochemistry & Molecular Biology at the Rosalind Franklin University of Medicine and Science in April 2007. Joon received his PhD degree in chemistry from the California Institute of Technology in 1993 under the guidance of John D. Baldeschwieler. He then continued his training as a postdoctoral fellow in the laboratory of Wayne Hubbell at UCLA until 1997 and with R. John Collier at Harvard Medical School. In 1999, he joined the laboratory of Stanley J. Korsmeyer at the Dana-Farber Cancer Institute to study apoptosis, where he became a Research Scientist and an Instructor at the Harvard Medical School. Upon Korsmeyer's death in 2005, after briefly serving as the Director of the Structural Biology Core at the Cancer Vaccine Center at Dana-Farber until spring of 2007, he moved to Illinois to become a faculty member at Rosalind Franklin University. Joon's current research focuses on understanding the mechanism by which the poreforming BCL-2 proteins become activated by other pro-apoptotic BCL-2 members and how they are organized within the membrane using various methods, including EPR spectroscopy.



Eiji Ohmichi Kobe University

Eiji Ohmichi became an Associate Pro-fessor of Physics at Kobe University in October 2006, and develops highly sensitive ESR techniques using microdevices such as microcantilevers and microcoils in collaboration with Professor Hitoshi Ohta at Kobe University, Japan. He was a Research Associate at the Institute for Solid State Physics (ISSP), University of Tokyo during 2000-2006, and experimentally studied electronic and magnetic properties of condensed matter using the strong pulsed magnetic field. He belonged to the group of Professor Takehiko Ishiguro at Kyoto University, where he studied magnetic field effects on two-dimensional organic and oxide superconductors, and earned a doctoral degree in physics in 2000. His undergraduate degree was also in physics from Kyoto University in 1995. He received the Miura Encouragement Award in 2005 from the High Magnetic Field Forum of Japan for his development on microcantilever magnetometry in strong pulsed magnetic fields.



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



## Collected by Candice Klug

This is a new column highlighting young EPR faculty members who have recently moved around.



Marumoto University of Tsukuba

Kazuhiro

Kazuhiro Marumoto recently moved to the University of Tsukuba and became an Associate Professor of Institute of Materials Science in January 2006. From 1997– 2005 he was employed as an Assistant Professor of Applied Physics at the Nagoya Uni-



POSITIONS

### The University of New Hampshire invites

The Department of Chemistry at the University of New Hampshire welcomes inquiries from PhD scientists at any rank regarding research, and graduate and undergraduate teaching opportunities, in the area of Experimental Physical or Biophysical Chemistry. Candidates with research interests in electron resonance are particularly encouraged. Facilities include Bruker ELEXSYS E500/E560 with X-band CW-ENDOR, and Varian Xand Q-band CW-EPR/ENDOR spectrometers with dispersion and absorption mode detection and temperature capability from 2 to 300 K. The electron resonance lab has a variety of microwave components, bridges, cavities and electronic measuring equipment for instrument construction as well as facilities for biochemical research. Inquiries should include a cover letter explaining the type of research and teaching opportunities desired, a CV, research plans and teaching goals, and should identify three people as references. Send to: Christopher F. Bauer, Chair, Department of Chemistry, University of New Hampshire, Durham, NH 03824 (603) 862-1550 (fax 4278), cfb@cisunix.unh.edu. Inquiries will be reviewed as they are received. UNH supports diversity and strongly enversity and performed EPR studies of organic solids such as conducting and electroluminescent polymers with Professor Shin-ichi Kuroda at the Nagoya University. In 1997, he received his PhD in physics from the Osaka University in the laboratory of Yoshihito Miyako where he studied the magnetism of uranium- and rare-earth-based heavy-fermion systems. He received his undergraduate degree in physics from the Hokkaido University in 1992. Kazuhiro recently received the Young Investigator Award from the Society of Electron Spin Science and Technology (SEST) in Japan for his development of a new method for studying microscopic properties of organic devices by EPR.

courages women and minority candidates to send an inquiry.

## Research Positions - Advanced EPR of Bioinorganic Systems

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

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

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

# Discount AMR subscription rate for IES members

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

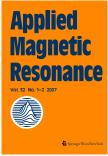
Please send your application to Prof. Dr. Wolfgang Lubitz, Max Planck-Institute for Bioinorganic Chemistry, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany

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

### The National Biomedical Research Center for AdvanCed ESR Technology (ACERT) at Cornell University invites applications for two Postdoctoral positions

Applications are encouraged from individuals who can contribute strongly to areas of: (1) ESR Microscopy. This position is for the further development of ESR-Microscopy to provide true micron resolution at very high spin sensitivity, and for its application to the study of small biological samples such as single cells. (2) Pulsed ESR and Molecular Dynamics. This position is for the study of molecular motions of membranes and proteins by multi-frequency 2D-FT-ESR techniques at 9, 17, 35, and 95 GHz. Experience in pulsed ESR techniques and/or ESR spectral simulation is highly desirable.

Interested qualified candidates should direct their inquires to acert@cornell.edu. Applicants should provide a cover letter and most recent CV. Two or three letters of rec-



ommendation are also required. Additional information about the ACERT may be found at www.acert.cornell.edu.

#### Postdoctoral or Research Associate position

A position on pulse EPR at the postdoctoral or research associate level depending on qualifications is available at the CNR-INFM MDM National Laboratory, in Agrate Brianza (Milano, Italy). The research activity is related to the pulse EPR/ENDOR investigation of impurities in semiconductors for quantum information processing. The successful candidate must have experience on the pulse EPR/ENDOR techniques possibly connected with the study of semiconductors or insulators, excellent knowledge of solid state physics and quantum mechanics, and good experimental skills. The position is initially for one year, but can be renewed up to five years. For additional information please contact: Prof. Marco Fanciulli, marco.fanciu lli@mdm.infm.it, tel. +390396036253 (direct), +390396037489 (secretary).

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

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

### Postdoctoral position at the University of Illinois at Urbana-Champaign

A postdoctoral position for research supported by US NIH and DOE funding is available at the University of Illinois at Urbana-Champaign. A significant component of the work would include multifrequency ESEEM and ENDOR characterization of the iron-sulfur clusters and semiquinone radicals in membrane proteins. An expertise in the area of biochemistry for work with proteins, and familiarity with freeze-quench techniques for protein sample preparations would also be desirable. Interested individuals should contact: Prof. Antony Crofts (a-crofts@life.uiuc.edu) or Prof. Sergei Dikanov (dikanov@uiuc.edu).

Applicants should send a compete CV, and ask for two letters of recommendation to be sent by e-mail independently.

### EQUIPMENT

#### **Design and construction of EPR electronics**

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

Please contact: Richard W. Quine, e-mail: rquine@du.edu, phone: 1-303-871-2419

### Available: EPR accessories and supplies

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

Gareth R. Eaton geaton@du.edu

#### For sale: Varian and ESR equipment

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

#### Please contact:

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

### Available: Used Varian EPR equipment

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

Please contact: James Anderson, Research Specialties, 1030 S. Main St., Cedar Grove, WI 53013, USA.

phone/fax: 1-920-668-9905 e-mail: janderson36@wi.rr.com

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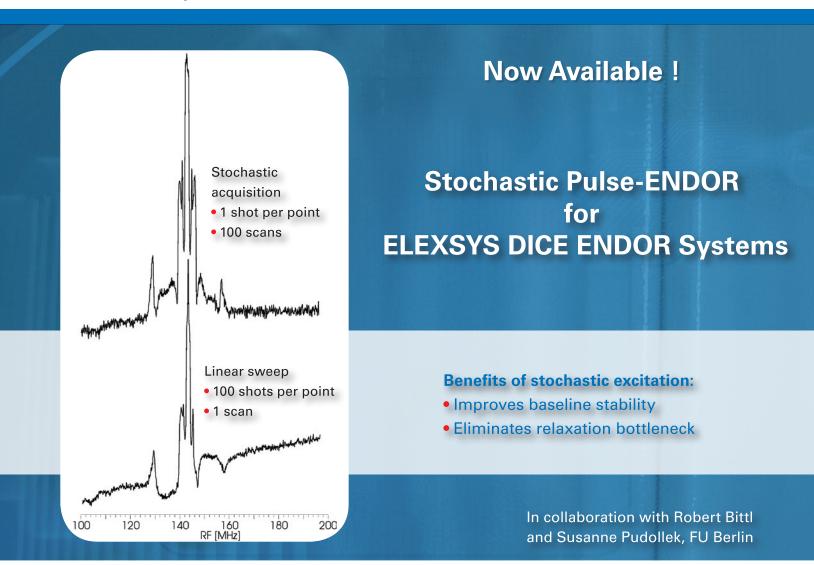
Our group used the magnet now and then at 10000 G, cooling with raw water. The system worked fine as of December 2007.

There is also a 9-inch diameter Varian magnet with a gap of about 1.75 inches. This 'little brother' weighs 1800 pounds. It too is a 1/4 ohm design, but the maximum current is 160 A.

Please contact: Mark Conradi at msc@wuphys.wustl.edu or by phone at 314-935-6418 (office + voicemail) or 314-935-6292 (lab).



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## think forward

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