2004 volume 14 number 3

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The Publication of the International EPR (ESR) Society

ENQOR



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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 an aspect of the research carried out in the group of Michael Bowman, recipient of the IES Silver Medal for Chemistry 2003. It shows the conformation of the symmetric trityl radical in frozen solution as determined from pulsed ENDOR and quantum chemical calculations of hyperfine tensors. The central methyl carbon is colored green to illustrate how it is shielded from solvent by the rest of the radical. The ENDOR and ENQOR spectra are of ¹³C in natural abundance bridging the two sulfurs on each aryl group. The ENQOR pattern shows that the hyperfine coupling of the bridging carbon and the parallel hyperfine coupling of the methyl protons have opposite signs.



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

photo of the issue see page 20



Take our quiz!

Send an e-mail message to the editor telling what kind of sound the microphone records. Deadline: March 30, 2005. The most humorous answers will be published in one of the next *EPR newsletter*. The readers of the *EPR newsletter* may vote by e-mail messages to the editor to decide who is the prize winner to get this photograph signed by Erwin Hahn. His/her name will be announced in the *EPR newsletter*.

Editorial

Dear colleagues,

This time you will come across columns that were delayed by the Nobel special issue. These are new columns as well as those you might have already gotten used to. Thomas Prisner starts a new column "Pro & Contra" in which "... the author of ... a mini-review of a specific EPR method or application area would not only stress in short terms his personal view of the advantages and perspectives of this method, but would also frankly and open address his concerns on their drawbacks, limitations and bottlenecks". To introduce the style he has in mind he presents his article on pulsed high-field EPR. Gareth and Sandra Eaton revive the "Reader's Corner" column with their note about Nobel Laureates in magnetism and kind words concerning our Nobel issue 14/1-2. Sandy and Gareth, thanks a lot! Hopefully their contribution will let this column go the same as the delightful picture of Sandy gave a start to the "Photo of the Issue" column. Looking back, August Maki tells us a thrilling story of "a totally obscure chemistry graduate student at the University of California, Berkeley", who became one of our greats. Reef Morse discloses the mystery of the EPR list server and hopefully this will result in an increase of subscribers to this other "resource and means of communication for the EPR community".

In 2001, for the first time I heard the silver flute of Uwe Eichhoff and was completely charmed... its sound tasted like ripe, juicy grapes. Since then I always look forward to his performances, the same as anyone who has heard his flute before. In the "Another Passion" column Uwe shares with us the story of how music came into his life and stayed with him. The minutes of the General Meeting of the IES held in August 2004 (a letter from the President, the Secretary's Report, and the Treasurer's Report) provide detailed information about the current condition of the IES affairs. It may become a boring old tune but I have to emphasize that by paying your dues promptly you ensure the general stability of the society and the soundness of its finances. As they say in commercials, "pay your dues and sleep like a baby!". We all join in to congratulate George Feher, Yuri Molin and Aleksandr Milov on their birthday. We owe special greetings to George. He gave the *newsletter* his support from the very beginning of its new stage and we are most appreciative of it. His article "Playing Poker" (*EPR newsletter* 13/1-2, 10–12 (2003)) is a profound study of poker being a lot like the game of life.

I am a bit hesitant if I should end this editorial as I intended. Well, let it be! I am sure that every column of our *newsletter* but one finds its readers. This very 'one' column is the editorial. You see, before I became an editor, I very rarely read editorials. I could start reading a journal or a newsletter from the beginning to the end or was jumping from one column to another, and it happened very often that I never found time to read the editorial. Since I am writing editorials myself, I am anxious to know if anyone reads them. My dear reader, you, who reads these lines, could you please send me a short confirmation?! Thanks a lot in advance for your troubles.

> Laila Mosina mosina@kfti.knc.ru

IES Annual Meeting 2004

Held at the 27th EPR Symposium at the Hyatt Regency, Denver USA on August 3rd 2004. The meeting was chaired by Ron Mason, Vice-President Americas and opened at 17:11.

1 Attendance (25)

Members: R. Mason, C. Felix, J. Pilbrow, K. Madden, S. S. Eaton, G. R. Eaton, C. P. Scholes, J. L. Zweier, M. Brynda, K. Victor Babu, M. Peric, E. Hustedt, E. Goovaerts, L. Kispert, A. Smirnov, T. Smirnova.

Non-members: N. Nusair, J. I. Jutson, V. Lau, J. Koscielniak, E. Erden, J. Harmer, C. Calle, A. Ruuge, M. A. Voinov.

Apologies were received from Yu. Tsvetkov, S. A. Fairhurst, M. Brustolon and T. Takui.

2 The Report of the General Meeting held on 29th July 2003 was accepted without comment

3 There were no matters arising from the 2003 General Meeting Report

4 President's Report

(read by R. Mason, Vice-President Americas)

Dear Colleagues,

On behalf of the IES Executive Committee, I wish to welcome all participants to the 2004 General Meeting of the IES and the 27th International EPR Symposium in Denver. I would like to express my gratitude to Professors Sandra and Gareth Eaton for again allowing our General Meeting to take place during this Symposium. For the last 27 years this Symposium has provided an excellent forum for presenting progress made in our discipline, for exchanging views, for meeting our colleagues and for making new links both scientific and of friendship. I am certain that year will be no exception. I regret that I will not be able to join you this year.

During this IES General Meeting we will present the results of our activities during the past year. Chris Felix, our Treasurer, will report on the first year of secure online credit card payment via the society web site: www.eprs.org. Chris has news of new features on this site and will also present details of our current finances. The Executive Committee has to deal with the general stability of the society and with the soundness of its finances. We cannot live beyond our means and even though the Executive all work on a voluntary and unpaid basis we are not yet in a strong financial situation. I am hopeful that in the near future we will be able to introduce some form of sponsorship or bursaries, particularly to help younger members attend conferences and workshops. Please help us do this by paying your dues promptly.

I am delighted to mention the ongoing success of our Newsletter following its transfer to Kazan. I am sure that you will agree with me that Laila Mosina has proved an excellent and tireless Editor. The new format of the Newsletter is extremely good both in terms of the wide range and high standard of the content and in the high quality of the publishing. I want to take this opportunity to thank Laila and her team of Associate Editors: Graham Timmins (Americas), Thomas Prisner (Europe) and Takeji Takui (Asia-Pacific);



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. B

and our Technical Editor Sergei Akhmin for their work. Please remember to contact them if you have any news or views you want to share with your colleagues via the Newsletter. I would also like to express special thanks on behalf of the Society to Bruker for covering the cost of the Newsletter's color hard cover and their help in posting the Newsletter to all paid up members. There have been some delays in delivery of the latest issue of the Newsletter by post. This arose through delays at the mailing house and we are hopeful that such delays can be avoided in future.

Thanks too must go to Professor Arthur Schweiger and his group at the ETH in Zurich for both maintaining and hosting the Newsletter website: www.epr-newsletter.ethz.ch. I commend this site to you all. As well as electronic copies of the Newsletter, you will find information about the Society, details of upcoming conferences and links to many EPR groups and details of our sponsors plus much more.

I wish to congratulate Professor Harry Kurreck (Free University, Berlin) who received our Fellowship. I had the great pleasure of presenting Harry with his Fellowship certificate in April at the Colloquium for Prof. Stehlik and Prof. Möbius at the Free University in Berlin.

This year in Denver we are presenting a special medal to Professor John Pilbrow, IES President (1999–2002). Under John's leadership the society gained a new constitution, a Society logo was designed and much more. It is a pleasure to acknowledge the debt the society owes to John for his untiring work on our behalf.

In 2004 we have presented no other Medals but I want to remind you all that in 2005 we will present the Gold Medal, the Silver Medal for Instrumentation and the Young Investigator Medal. Nominations for all three categories should be sent direct to me by the closing date of December 15th 2004. Visit the IES website to the full Call for Nominations.

On behalf of the Society I want to express thanks to our corporate sponsors:

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I would like to also thank the Executive Committee of the IES: our Vice-Presidents: Ron Mason (Americas), Marina Brustalon (Europe), and Takeji Takui (Asia-Pacific); our Immediate Past President: John Pilbrow; our Secretary: Shirley Fairhurst, and our Treasurer: Chris Felix, for all their efforts on our behalf.

Finally, I hope that all the participants of this 27th EPR Symposium in Denver find it to be both stimulating and rewarding and wish you all success.

Prof. Yuri Tsvetkov, IES President

5 Secretary's Report (Shirley Fairhurst)

International EPR(ESR) Society Awards 2005 *Call for Nominations*

Nominations are invited for: Gold Medal, Silver Medal (Instrumentation) and Young Investigator Awards and Fellowship of the Society (see extract from by-laws below or visit ieprs.org for full constitution and by-laws).

All nominations must be accompanied by a 100–150 word citation in support of the nomination and, in the case of the Young Investigator Award, nominees will be asked to provide copies of two recent published papers which in their judgment represents their best work. No nomination can be considered without a citation. Additional supporting material may be included.

Nominations are to be sent to the President by email to: tsvetkov@kinetics.nsc.ru in word or pdf format (preferred method), or by mail to: Prof. Yu. D. Tsvetkov, Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Institutskaya St. 3, Novosibirsk 630090, Russian Federation.

The closing date for nominations for Awards in 2005 is 15th December 2004.

By-laws

A *Gold Medal* shall be awarded for distinguished contributions to EPR (ESR) Spectroscopy.

A *Silver Medal* shall be awarded for significant contributions to EPR (ESR) Spectroscopy in the area of Instrumentation.

A *Young Investigator Award* shall be made for outstanding contributions to EPR (ESR) Spectroscopy by a young scientist. Nominees should be under the age of 35 years on

Yu. D. Tsvetkov (right) presents Harry Kurreck (left) with his Fellowship certificate



the 1st of July of the year of the award. The date of birth of the nominee must be included in the nomination. The nominee will ordinarily be at the post-doctoral level. Only in exceptional circumstances will either doctoral candidates or junior faculty members be considered for this Award.

A *Fellowship of the Society* may be conferred on individuals who have made influential and distinguished contributions to the practice of EPR (ESR) Spectroscopy and its welfare over a long period.

IES Awards Schedule 2005-2009

- 2005 Gold + Instrumentation + Young Investigator
- 2006 Biology/Medicine + Chemistry
- 2007 Physics/Materials Science + Young Investigator
- 2008 Gold + Instrumentation
- 2009 Biology/Medicine + Chemistry + Young Investigator

Table. Report on the IES finances.

Year 2003. Full Year Accounts (u.	naudited)		
Balance January 1, 2003		\$ 15234.98	
Income		\$ 4904.00	
Expenses:		\$ (8376.44)	
Bank & credit card fees	\$ 414.12		
Web design & fees	\$ 2113.32		
Newsletter	\$ 5444.00		
Travel support	\$ 400.00		
State of Illinois	\$ 5.00		
Balance December, 31 2003		\$ 11762.54	
Year 2004. Half Year Accounts (unaudited)			
Balance January 1, 2004		\$ 11762.54	
Income		\$ 2687.76	
Expenses		\$ (8843.57)	
Balance June 30, 2004		\$ 5606.73	
Income Expenses Balance June 30, 2004		\$ 2687.76 \$ (8843.57) \$ 5606.73	

From left to right: Ron Mason, Susan Pilbrow, John Pilbrow, Sandy Eaton and Gareth Eaton at the 27th International EPR Symposium

6. Treasurer's Report (Chris Felix)

Chris presented the report on the society's finances (see Table) and announced that e-mails regarding outstanding dues payments would be sent soon.

Society (official) Website

Our official Society website: ieprs.org

- is a secure professional website providing:
- Instant online payment (active soon)
- Online membership records (unique username/password for all members coming soon)
- Link to Newsletter website for newsletter online
- · For officers: direct database access for queries

7. Computer Special Interest Group Report

Members were reminded that the EPR-LIST remains active. To join send an e-mail to majordomo@xenon.che.ilstu.edu in the body of the e-mail, put only the words: subscribe epr-list. Contributions to the 'Computer Corner' in the Newsletter are welcome. Send them to Reef Morse. Members interested in EPR JCAMP-DX standard should contact Reef Morse: reef@scientific-software.com

8. Any Other Business

Ron Mason thanked Yuri Tsvetkov (President), Shirley Fairhurst (Secretary), Marina Brustolon and Takeji Takui (Vice Presidents), Chris Felix (Treasurer), John Pilbrow (Past President), Arthur Schweiger for the Newsletter website, Reef Morse for the 'Computer Corner', and Laila Mosina and her team for the excellent Newsletter. Thanks go to Sandra and Gareth Eaton for allowing us to hold this meeting at their Symposium, to our Corporate Sponsors, to Bruker (for covering the cost of the Newsletter's color hard cover and distributing the Newsletter), to Keith Madden of the Notre Dame Radiation Laboratory for taking notes at this meeting.

Special thanks to all paid up members for without you we would have no society and to all who attended the meeting.

The meeting closed at 17:30.



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The Zavoisky Award 2004 to Kev M. Salikhov and Dietmar Stehlik

The 2004 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professors Kev M. Salikhov (Kazan Physical-Technical Institute, Russian Academy of Sciences, Kazan) and Dietmar Stehlik (Free University Berlin, Berlin) in a ceremony marking their outstanding contributions to the theory of EPR and its application to problems of chemistry and biochemistry.

The ceremony took place at the opening of the International Scientific Forum dedicated to the 200th anniversary of the Kazan State University and 60th Anniversary of EPR, 15–20 August 2004. The Forum comprised two conferences, "Nanoscale Properties of Condensed Matter Probed by Resonance



Phenomena" and "Modern Development of Magnetic Resonance".

The Zavoisky Award was presented 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, Springer-Verlag Wien, 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: G. Feher (La Jolla), D. Gatteschi (Florence), H. M. Mc-Connell (Stanford), K. Möbius (Berlin), A. Schweiger (Zurich), and the chairman, K. A. McLauchlan (Oxford). The selection of the awardee was made after consultations with the Advisory Award Committee which comprises B. Bleaney (Oxford), C. A. Hutchison Jr. (Chicago), 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

The Bruker Prize 2004 to Wayne L. Hubbell

In 2004, at Warwick University this award sponsored by Bruker BioSpin went to Professor Wayne Hubbell of the University of California Los Angeles, CA, USA for his outstanding work on the technique of sitedirected spin labeling, a powerful tool for the study of protein structure and dynamics, in particular his work on light-activated rhodopsin, the visual pigment in photoreceptor cells of the retina. Wayne Hubbell became the 19th Bruker Lecturer.

From left to right: John Walton (ESR Group President), Wayne Hubbell, Dieter Schmalbein (EPR Division, Bruker BioSpin GmbH)



(2001), W. Lubitz (2002), and W. L. Hubbell (2003). The selection of Professors Kev M. Salikhov and Dietmar Stehlik was made from many nominations solicited from international experts in EPR.

The Award Ceremony starting in the morning of August 16 was attended by about 400 people, among them were the scientists who participated in the Forum.

The decision of the Zavoisky Award Committee was announced by K. Möbius, member of the Zavoisky Award Committee. The presentation was made by the Deputy Prime Minister of the Republic of Tatarstan Z. R. Valeeva. The Rector of the Kazan State University, M. Kh. Salakhov, the Chairman of the Presidium of the Kazan Scientific Center of the Russian Academy of Sciences, A. I. Konovalov, and the Vice-President of the Tatarstan Academy of Sciences, I. B. Khaibullin, warmly congratulated the laureates. Letters of congratulations from H. W. Spiess, President of the AMPERE Society, Yu. D. Tsvetkov, President of the International EPR Society, and M. Mehring, President of ISMAR, were handed to Kev M. Salikhov and Dietmar Stehlik.

A concert by a string quartet preceded and followed the ceremony. The event was concluded with a Banquet in honor of Kev M. Salikhov and Dietmar Stehlik and their outstanding contributions to EPR. The Zavoisky Award lectures of the laureates were included in the program of the conference "Modern Development of Magnetic Resonance".

The Organizing Committee owes special thanks to the Russian Academy of Sciences, the Russian Foundation for Basic Research, the NIOKR Fund of the Republic of Tatarstan, Bruker BioSpin GmbH (Karlsruhe) and the firm MELT (Kazan).

The Jeol Young **Investigator Prize** 2004 to Dariush Hinderberger

Jeol UK have generously agreed to sponsor a prize awarded for the best oral presentation by a young scientist at the conference. The competition is restricted to 2nd and 3rd year PhD students and postdoctoral fellows in their 1st year of research. In 2004, Dr. Dariush Hinderberger (Max-Planck-Institut Mainz, Germany) received his Jeol Prize at the 37th Annual International Meeting of the RSC's ESR Group.



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Playing Flute

Uwe Eichhoff

ooking through the concert schedule of Moscow you may find the name of the German flutist Uwe Eichhoff, mainly with the Ensemble of "Ancient Music Da Camera e Da Chiesa". In 2001–2002 they were performing a cycle of six concerts "Music at the Prussian Court" comprising trio sonatas and flute concertos of C. Ph. E. Bach, J. J. Quantz, the Royal flute player King Friedrich II and his sisters Princess Anna Amalia and Markgräfin Wilhemine, and others. In December you find him playing flute concertos by Vivaldi, Mozart, Haydn, Cimarosa* and J. S. Bach with leading Moscow symphony orchestras. His name may sound familiar to you. At his concerts you may find a significant part of the Moscow EPR and NMR community.

Yes, it's me, the same guy, that is giving lectures on NMR and EPR at various conferences!

After school I devoted myself to physics and chemistry. Later, I was an exchange scientist at the Moscow State University and then started to work at Bruker. Together with my wife Barbara, working at that time on her PhD on Russian literature, we built up the Bruker representation in Moscow, selling in 25 years several hundreds EPR, NMR, IR and MS spectrometers. In my leisure time I was still playing the flute but not performing in the public for about 35 years.

The silver flute I am playing is closely connected with EPR, because it was bought at Yamaha in Tokyo by my EPR colleague Karoly Holczer. By mistake he chose a much better and much more expensive instrument than I wanted. After starting to perform in the public it turned out to be just the right choice.

The beginning of my musical education dates back to 1950, the 300th anniversary of J. S. Bach, when I was 10 years old. All over the year my father, a professor for chemistry at Mainz University, took me to the concerts in the various protestant churches of Wiesbaden, my hometown. He explained to me the different musical forms and I began to love classical music and to listen carefully to understand what is behind the beautiful sound.

Anyway, at that time this was a passive attitude to music and it changed four years lat-

er, when my schoolmates interested in playing an instrument were asked to come together in the music room to meet potential teachers. I told this to my father and he gave me an old flute, which was played centu-

> Uwe Eichhoff (left) and Vladimir Stachinski (right)

ries ago by one of my ancestors and kept as a family relic. I took it to school and the flute teacher burst into laughter. This instrument was built in such an old system that almost nobody could play it these days, it was even tuned half a tone higher than the usual pitch of today, as it was common centuries ago.

I went home quite disappointed and told this to my father, who probably had expected something like that, but he asked me to tell him about the flute teacher. It turned out that this was the solo flutist of the Wiesbaden symphony orchestra, which my father had admired all his childhood, when he was singing in a chorus performing oratories and Mahler symphonies together with this orchestra. It was always the flutist who fascinated him most. So, I went back to chamber virtuoso Franz Danneberg, this was his name and title. He was a charming elderly man in the age of almost 80 years. During the lessons in his home I met the famous conductor Karl Schuricht, he showed me letters of the composers Richard Strauss and Camille Saïnt-Saens. And most important, he was an excellent teacher and a fascinating person. I loved him and I always worked hard to satisfy him. He owned a silver flute, which was donated to him by Adolph Goldberg, a famous rich Jewish flute lover. The other two instruments were donated to the solo flutists of the Berlin and the Vienna Philharmonic orchestra. He himself preferred to play an old wooden instrument, which Barbara donated to me later as a present for my PhD. Some years later she presented me a facsimile of Goldberg's book with pictures and portraits of the most famous flutists of all times, starting with the Greek and Indian gods Pan and Krishna and ending with Franz Danneberg, my teacher.

When I was just playing for one and a half year, our school orchestra lost its first flutist during the rehearsals of J. S. Bach's 4th Brandenburg concerto with two solo flutes. I told this to my teacher and he put the score in front of me and asked me to play the first



^{*} The first movement of the Sinfonia concertante for 2 flutes and orchestra, G major, by Domenico Cimarosa, eprnl.org/eichhoff.mp3.

part. I thought he was crazy, but I tried. Some months later I was performing successfully with our school orchestra. This was the starting point of my public musical performances. Together with my sister playing violin and a classmate playing piano, harpsichord and organ we met weekly for chamber music. The highlight of my yearly musical career was playing the solo flute in St. John's passion in various cities with the chorus and chamber orchestra of the Luther-Kirche in Wiesbaden.

This was during school and the very first years at the university. In the following more than 30 years I did not find the time for daily exercise and was just lucky to play for some hours during the weekend.

My second musical career started in Moscow and it was due to a quite unexpected telephone call at the end of 1996. Once working in our office in the Institute of Chemical Physics of the Russian Academy of Sciences, I got a call from somebody introducing himself as the conductor Vladimir Stachinski. He asked me if our company could sponsor a concert devoted to the 110th birthday of the famous German conductor Wilhelm Furtwängler. It turned out that he just began to call all representations of German companies following the alphabet. We told him that our small company could not afford such a patronage, especially as he intended to perform the requiem of Johannes Brahms with big chorus and orchestra. We gave him the recommendation to go at least one character further in the alphabet and he would find Deutsche Bank, Dresdner Bank, and Daimler Benz. They hopefully would be able to help him. Two months later he called us again. He did not get any support from any German company but had the impression that we were the only real music lovers among them. I finally wanted to get rid of him and continue my daily work. So, I told him that all my life I had the dream once to play with an orchestra the concert for flute and harp by W. A. Mozart. If he could arrange this, I might think of some support. He did not know, how I was playing and I was not quite serious woth my proposal at that moment. Anyway, after about one month he invited me to play with the excellent harpist Natalya Svadkovskaya and the Big Russian State Radio and Television Concert Orchestra. At the first moment I was shocked, I even did not have my best instrument at hand. Anyway, everything was



Franz Danneberg, my flute teacher, as portrayed in the book of Adolph Goldberg

arranged and for the first time after 35 years I played again with an orchestra. It was not that bad for the first time and I thought my dream to be fulfilled. I had enjoyed it and was happy about it. Surprisingly the musicians asked me, why we do not play in an official concert. I started practising daily for one hour and on March 6th 1997 we performed together in the Moscow House of Scientists in front of a big auditory, mainly friends and colleagues, but also open to the public. Everybody encouraged me to continue. So in our yearly pre-Christmas concerts in Moscow I have performed with various orchestras all the flute concertos by Mozart as well as by Telemann, Haydn, Stamitz, Vivaldi, and J. S. Bach. One of our customers recommended me to the Moscow Ensemble of "Ancient Music Da Camera e da Chiesa" and I became their regular partner for many concerts. Altogether we have performed at various places in Moscow in about 40 chamber concerts. I introduced to the Russian auditory many composers of the baroque and classic periods almost unknown in Russia, and our concerts got quite a good reputation. I performed as well at conferences in Moscow, St. Petersburg, Tver, Kazan, Azov, Kiev, Minsk, and Tallinn.

Of course, I am still an amateur and I realized during my concerts what makes the difference. A professional also has his good and bad days, but he never plays below a certain level. I had at least one performance which was so bad that I decided no longer to show up in the public. But there was still a concert announced in the press with the same program, which could not be cancelled, and it went very well. So I still continue... Sometimes I get tired, but then my friends call me asking for the next concerts and I know, they really like it and are waiting for it.

Time went by since my early days, when Barbara looking at me called me the young Mozart. Now she claims that I sometimes remind her the old grumbling King Friedrich.

I have performed with different musicians in various cities. Often we had just one rehearsal to get acquainted with each other and with the music to play. It is always surprising, how step by step we begin to understand each other, and with this continuing understanding the music comes to life. This is the same as in science, when common interest turns into mutual understanding and that is why, I believe my profession as a scientist fits together with this other passion.



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Anniversaries

80th Birthday of George Feher



On May 29th 2004 George Feher celebrated his 80th birthday in La Jolla, California. 137 (the reciprocal of the fine structure constant, a number close to George's heart) invited guests joined the party, mostly family, close friends, and present and past students, postdocs and collaborators from many different countries. The celebration took place under the motto "The Man and his Science" in the beautiful settings of the Birch Aquarium overlooking the Pacific Ocean near the Scripps Institute of Oceanography, on whose premises UC San Diego was started in 1960 with George Feher as one of the founding fathers of the Physics Department.

A presentation was made which included 23 speakers illuminating different periods of George's life. This covered his childhood in Bratislava (Slovakia), his time in Palestine as a teenager and young man, undergraduate and graduate days at UC Berkeley, his years as research scientist at Bell Telephone Laboratories, New Jersey, and as professor at Columbia University, New York, and at UC

George Feher and his wife Elsa

San Diego. The many personal stories and anecdotes told by his friends, fellow scientists and former students and postdocs made this meeting an unforgettable event for all participants.

Among the many interesting stories of his life was the secret design of an apparatus for the Ha'agana in 1945 to unscramble the telephone conversations between the British High Commissioner in Jerusalem and the Prime Minister at 10 Downing street in London during the British occupation of Palestine.¹ His lifelong close connection to Israel, where his older sister Erika and her family is living, and his many contributions to science in Israel were highlighted by several speakers. Special ties also exist to Argentina, the home country of his wife Elsa. His passion for sports, story telling and for playing poker² were addressed as well as his numerous important scientific contributions to solid state physics, biophysics, photosynthesis and spectroscopy during the last 50 years.³

George Feher contributed strongly to the early development of EPR spectroscopy. In 1956 he invented ENDOR, which was the first double resonance technique combining both EPR and NMR to sensitively detect and resolve the hyperfine interaction with magnetic nuclei in complex paramagnetic systems. ENDOR was first applied in solid-state physics, later extended to metal complexes and radicals/radical ions both in chemical and biological systems, as demonstrated by the elegant work of Feher's group. He also built the first solid-state MASER (in 1957), described the paraelectric resonance phenomenon (1966) and invented fluctuation spectroscopy (1973), to name a few of his major early achievements.

Application of EPR techniques to problems of photosynthetic charge separation in the late sixties marked the start of Feher's work in biophysics and the beginning of his life-long dedication to elucidate the structure and function of the photosynthetic reaction center (RC). In the seventies biochemical and molecular biology techniques were introduced in the laboratory and several fundamental experiments were performed on the crystallization of proteins. This laid the foundation for the crystallization of the RC of Rhodobacter sphaeroides and the elucidation of the X-ray crystallographic structure, which to his regret was only finished after the work of Michel, Deisenhofer and colleagues in Munich on the RC from a different bacterium, which earned them the Nobel Prize in Chemistry in 1988.

Feher's group contributed fundamentally to the functional understanding of the RC both with respect to electron and proton transfer. Many of his papers have become citation classics. For his work George Feher received numerous honors and awards, including the American Physical Society Prize (1960) and the O. E. Buckley Prize (1976), the APS Biophysics Prize (1982), the Gold Medal of the International EPR Society (1991), the Rumford Medal (1992), the Bruker Prize (1992) and the Zavoisky Award (1996). He is a member of the National Academy of Sciences, the American Academy of Arts and Sciences, and a Fellow of the AAAS and the Biophysical Society. In



¹ Abramovich S. in: Yediot Achronot, 23 April 1992.

 ² Feher G.: EPR Newsletter 13 (1-2), 10–12 (2003)
 ³ Feher G.: Annu. Rev. Biophys. Biomol. Struct. 31, 1–44 (2001)

1994 he received an honorary doctorate of the Hebrew University of Jerusalem.

The students and postdocs of George Feher profited enormously from the work in his laboratory and many of us stayed in the sciences and became university professors. George told us how to select a scientific problem, design the experiments, keep notebooks and analyze the data, which was followed by the often painstaking long procedure of writing a paper: "Every published word stays on your scientific record forever!".

We all owe you a lot, George. You always had an open ear not only for our scientific but also for our personal problems. We wish you a Happy Birthday – and may you have many more.

Wolfgang Lubitz

70th Birthday of Yuri N. Molin

Full Member of the Russian Academy of Sciences, Fellow of the IES, Professor Yuri N. Molin recently celebrated his 70th birthday.



Yu. N. Molin started his research under the supervision of Professor V. V. Voevodsky in 1957, when he joined his laboratory at the Institute of Chemical Physics (Moscow). Soon, together with other Moscow young scientists he moved to Novosibirsk, to the newly founded Institute of Chemical Kinetics and Combustion. Yuri Molin was the Director of this institute in the period from 1971 till 1993.

Yuri Molin made outstanding contributions to the development of chemical radiospectroscopy. Already in the Moscow period of his work (1957-1961), he and A. G. Semenov created a unique device for studying EPR spectra under the effect of an electron accelerator, which was used for many years to study primary radical stages of radiationchemical reactions. After moving to Novosibirsk, the main scientific interests of Yu. N. Molin were concentrated on the search for weak interactions due to distant delocalization of the spin density in complexes and radicals and the interpretation of their role in spin and charge transfer. To this end, new original approaches to study the distribution of the spin density by contact shifts in nuclear magnetic resonance spectra were developed and realized. The role of this delocalization in electron spin exchange was studied. On the basis of these results, the monograph "Spin Exchange. Principles and Applications in Chemistry and Biology" by Yu. N. Molin and coauthors (Springer 1980) was written. Up to now, it is the only monograph in this field. Interesting phenomena, such as chemical nuclear and electron polarization and the influence of magnetic fields on radical pair reactions discovered in the end of the sixties and the beginning of the seventies of the 20th century were a brilliant illustration of the role of weak interactions in chemical reactions. In these reactions the magnetic interactions with an energy many orders of magnitude less than the thermal energy of molecules control the mutual orientation of the electron spins in a pair and consequently the elementary chemical act in solutions. Therefore it was natural that Yuri Molin concentrated on the research in this field, which was later called "spin chemistry".

The results of the first stage of the development of spin chemistry were summarized in the monograph "Spin Polarization and Magnetic Effects in Radical Reactions" by Yu. N. Molin et al. (Elsevier 1984).

Recent research of Yuri Molin is concentrated on the development of actual problems of spin chemistry. He works in several directions including the search for and study of new aspects of magneto-spin effects, the development and improvement of high-sensitivity methods on the basis of the principles of spin chemistry, and the application of these methods to study short-lived intermediates which cannot be registered by any other methods.

Yu. N. Molin was a member of many editorial boards and international committees. He was awarded the prestigious Lenin Prize (1986) for his contributions to the development of spin chemistry. He also got four national medals and an "Outstanding Scientists of Russia" grant (2001).

We wish Yuri further success in his scientific research and good health for the years to come!

> Sergei A. Dzuba Kev M. Salikhov

60th Birthday of Aleksandr D. Milov

The friends and colleagues of Aleksandr Milov extend to him the warmest greetings and congratulations on his 60th birthday this year. His scientific career has centered



around spin relaxation in condensed phases. He joined the laboratory of Professor V. V. Voevodsky in the Institute of Chemical Kinetics and Combustion after graduation and began measuring the dielectric properties of organic solutions at low temperature in the group of Professor V. A. Tolkachev. In 1971 he joined the Tsvetkov Laboratory for postgraduate studies which included applications of the newly constructed electron spin echo (ESE) spectrometer. He published some of the earliest papers on ESE of free radicals in the liquid phase and on the phase relaxation of hydrogen atoms in irradiated solids. From that time, his work has focused on the effect of dipolar interactions on ESE signals. His detailed experimental work helped establish the general laws of phase relaxation in different types of samples. In 1977, he started using phase relaxation to investigate the spatial distribution of paramagnetic species in solid samples. His work was important for the development of ESE spectroscopy from a tool for solid-state physics into a general method applicable to the fields of chemistry, biophysics and biochemistry.

Aleksandr Milov served as the scientific secretary of the Institute for 10 years, but in 1984 he took off this neckline to devote his full efforts to the development of Pulsed ELDOR or DEER. In 1984 he published the fundamental paper showing that PELDOR can directly measure electron dipole interactions in a model disordered system. This work forms the basis for PELDOR measurements of protein structure using site-directed spin labeling that is becoming a very important method today. His work was honored with the prestigious state Prize in 1988 for pulsed EPR methods. Since 2000, he has focused on the application of PELDOR to peptide secondary and quaternary structures where his careful and detailed work provides a basis for the detailed interpretation of all such PELDOR measurement today. His friends and colleagues congratulate him for his scientific achievements and wish him the Best on his 60th.

> Rimma Samoilova Michael Bowman



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n 1956, chemists were adopting EPR with the idea of applying it to chemical problems. Research on organic free radicals was being carried out by C. A. Hutchison Jr., S. I. Weissman, G. K. Fraenkel, their students and colleagues. H. M. McConnell had provided a theoretical basis for connecting the rich hyperfine structure of aromatic free radicals in solution to the π -electron spin density distribution. At that time the Department of Chemistry at Harvard University had no one on its faculty trained in EPR or NMR spectroscopy. Directly across Oxford Street from Mallinckrodt Chemistry Laboratories,



Looking Back

August H. Maki

however, the Lyman Laboratories of Physics was home to such notables of magnetism and magnetic resonance as J. H. van Vleck, N. Bloembergen, E. M. Purcell, R. V. Pound, and N. F. Ramsey. Casting about for someone to introduce EPR to Chemistry, Harvard settled on a totally obscure chemistry graduate student at the University of California, Berkeley, who was hard at work finishing his PhD dissertation under the guidance of B. R. McGarvey.

Sometimes the brashness of youth prevents one from being totally cowed by the reality of a situation, and I think that this was the case when I arrived in Cambridge, Massachusetts in the Fall of 1957 as Instructor of Chemistry at Harvard. If providing funds sufficient for setting up a new laboratory was customary at this time, neither the Chemistry Department nor I were aware of it. Since I had rebuilt much of the EPR spectrometer I used at Berkeley, I set about to build one at Harvard using such funds as were provided. These were not sufficient to purchase a magnet with a current-regulated power supply, but a large electromagnet with no power supply was found. Unregulated power was available from a DC line in Mallinckrodt Labs that was a relic from a previous age. A huge rheostat was obtained to set the magnetic field (it also helped warm the laboratory); sweep and modulation coils were added that made it possible to obtain rather poorly resolved EPR spectra after the magnet had stabilized for some time. It was clear, however, that this behemoth had to be replaced if any serious work was to be done.

It had by now become easier to obtain grant funds from federal agencies for the support of research (thanks in part to Sputnik that was visible throughout the world in 1957). With the support of several distinguished faculty colleagues, a proposal to the National Science Foundation was successful, and a 6 inch electromagnet with current-regulated power supply was purchased eventually from Varian, Inc.

It was the intervention of Professor E. Bright Wilson Jr. that led to my association with our colleague David Geske, who was an analytical electrochemist and Instructor of Chemistry. Wilson informed me that Geske was investigating the electrochemistry of organic compounds and that free radicals were likely products. Since I had constructed an EPR spectrometer, perhaps Geske and I could collaborate on some joint research. Good thought. Geske and I decided to work together and use EPR to study electrochemically generated radicals. Out of our discussions originated the idea of introducing a small polarizable electrode into the microwave cavity. We adopted a cylindrical design that worked well with our cavity. We called the method intra muros electrochemical radical generation for EPR. (Varian, Inc. soon produced a commercial flat cell version for their rectangular cavity). Our first "intra muros" paper was published in 1959 and featured the EPR spectrum of a radical, probably ClO₂, generated at a Pt anode in an acetonitrile solution of an alkylammonium perchlorate. Miraculously, this spectrum was obtained with the original magnet system described above. A year earlier, D. J. E. Ingram and coworkers had published spectra of radicals collected during controlled potential electrolysis that were subsequently frozen for EPR. Their work was important in demonstrating the presence of radicals at the electrode, but the spectra were featureless because the samples were frozen. With the substitution of a Hg cathode for the Pt anode (and the introduction of the new Varian magnet and power supply), we were able to generate well resolved spectra of a number of anion radicals. Since the anions are generated in a high dielectric constant solvent with bulky alkylammonium counterions, the spectra are simple since ion pairs, frequently present in alkali metal reduced aromatics, do not form.

I later had occasion while at Harvard to collaborate with my inorganic chemistry colleagues, Professors Richard H. Holm and Alan Davison. Noting that stable bis-dithiolate complexes of Ni had been synthesized with Ni in both the II and IV formal oxidation states, Holm and Davison thought it might be possible to obtain stable Ni(III) bis-dithiolate complexes which should have a d⁷ configuration. Would I be interested in examining the EPR of such complexes? I did not know of any previous EPR studies of Ni(III), and thought this would be a great opportunity to learn about the electronic structure of these complexes. We found from our work that square-planar Ni(III) bis-dithiolate complexes are low-spin with the unpaired electron occupying one of the $d\pi$ metal orbitals that was extensively (ca. 50%) delocalized over the π system of the ligands. In my mind, there is no other interpretation of the EPR data, but this contradicted the position of Professor Harry B. Gray who favored a "cation-stabilized anion free radical" model. This model places the unpaired spin entirely onto the ligands. Sadly, this disagreement developed into a lively battle in the journals between the Gray forces and the Holm forces and I was caught up in it. But I was able eventually to escape to other EPR problems.

I don't remember when and how the importance of applying ENDOR to free radicals in solution occurred to me; ENDOR would lead to improved resolution and a great simplification of analysis since each set of nonequivalent protons would produce only two signals. I remember discussing the idea with Weston Anderson of Varian, Inc. at a Magnetic Resonance Gordon Conference in 1961. Anderson suggested that if I could get away from Harvard for a while, this would be a good project for me to try at Varian in Palo Alto, California. He pointed out the excellent technical resources there, etc. The opportunity came in the Fall semester of 1963 when I was allowed a sabbatical leave, and was appointed Visiting Professor at Varian. James Hyde welcomed me into his EPR development lab and we worked together on modifying a Varian cylindrical cavity for ENDOR measurements. I was sure that the experiment would work provided electron spin-lattice relaxation took place to a significant extent via cross-relaxation with protons, and that rf-induced transitions in the nuclei could be driven rapidly enough to compete with natural relaxation. For free radicals in solution, this would obviously require large rf fields. Hyde and I had a limited amount of time to work together, since I was due back in Cambridge for the Spring Semester to lecture Chemistry 60, the physical chemistry course. The system we put together was not very refined, but it was effective enough to produce ENDOR signals from the two sets of nonequivalent protons of Coppinger's radical in liquid n-heptane. (We originally thought we had three sets of nonequivalent protons, but Jack Freed later showed that one set of signals was split in two due to coherence effects.) Although I did not know it then, A. Cederquist, a graduate student in Sam Weissman's lab, had carried out an analogous experiment on free electrons in liquid ammonia in which distant ENDOR was observed. Hyde went on to improve the crude ENDOR spectrometer after I returned to Harvard. It was later developed at Varian, Inc. into a commercial ENDOR attachment. A more successful ENDOR cavity was developed later at Bruker, Inc., and is in wide use today.

I left Harvard in the Summer of 1964 to accept an Associate Professorship at Riverside, one of the new campuses of the University of California. Alvin Kwiram, meanwhile, arrived at the Harvard Chemistry Department to keep EPR alive there. One of my highest priorities was to continue with solution ENDOR, so I set about to construct an ENDOR spectrometer at Riverside similar to the one I left behind at Varian. Because of the help and encouragement of some remarkable visiting scientists, Klaus Möbius and Hans van Willigen, and a talented postdoctoral fellow, Robert Allendoerfer, some of the early papers in solution ENDOR originated at Riverside. Allendoerfer and I developed and tested a simple model for solution ENDOR. Möbius and van Willigen did some fine work on ENDOR of cyclopentadienyl radical derivatives, and made several improvements on the rf circuitry. (I recall walking into the laboratory one morning and spying an empty wine bottle wrapped with heavy copper wire



near the ENDOR cavity. It had been added by Möbius and van Willigen as an inductance to improve the impedance match. I wondered what had become of the original contents of the bottle.) Jan Kommandeur was invited to Riverside as Visiting Professor to give a course in magnetic resonance from which my students benefited tremendously. We became good friends, and Kommandeur was of particular help to my graduate student, Luis Alcacer, who was studying EPR and electrical conductivity of metal bis-dithiolate-perylene crystals.

In 1967, Kwiram, at Harvard, published one of the two original papers on ODMR of phosphorescent triplet states. The other independent paper by Mark Sharnoff appeared at the same time. Both experiments were done at fixed microwave frequency by sweeping an external field in the traditional EPR manner. In 1968, Jan Schmidt and Joan van der Waals reported the first ODMR of a triplet state in zero field. The microwave frequency was swept through resonance with the sample held in a slow wave helix. This was a very significant advance in ODMR, since Zeeman broadening is avoided and well-resolved spectra can be obtained in randomly oriented samples. It happened that Mostafa El Sayed, Charles B. Harris, and I got to talking about these experiments at the Western Spectroscopy Conference at Asilomar, California early in 1969. El Sayed was then studying high resolution phosphorescence of aromatic molecules at low temperature; we agreed to get together and measure ODMR of individual vibronic bands in zero field to determine their spin sublevel activities. We decided to pool our equipment and to meet in El Sayed's lab at UCLA to add ODMR to his phosphorescence spectrometer. Harris flew down from Berkeley, and I made the short drive from Riverside. Dino Tinti, then a postdoctoral fellow in El Sayed's group, completed our quartet. The experiment succeeded on 2,3-dichloroquinoxaline almost immediately; we were able to map the spin sublevel activity of individual vibronic bands and thus determine their assignment from symmetry considerations. We called the method PMDR, phosphorescence-microwave double resonance, when ODMR is applied to individual vibronic bands. We also managed to measure optically detected ENDOR of a triplet state simultaneously with similar experiments done independently at Leyden by I. Y. Chan, J. Schmidt, and J. H. van der Waals. The meetings at UCLA working on PMDR were an enjoyable mixture of work and play. With the experiment well under weigh, Harris, and I would occasionally leave El Sayed and Tinti in charge and depart to one of the many piano lounges in Los Angeles where we sometimes convinced the piano player to let us take over for a while. El Sayed joined us on one or more occasions. Harris improvised piano jazz pretty well, and I always brought my snare drum and high-hat to the experimental sessions, in case they were needed. However, no one has ever suggested that we change our professions to music.

The ODMR "quartet" eventually went their separate ways, and worked individually on various advances in optical-microwave spectroscopy. I built an ODMR spectrometer at Riverside, and have remained closely involved with applications and development of ODMR for the remainder of my professional career. Working with me at Riverside, was Chris Winscom, a postdoctoral fellow who developed a useful "microwave-induced phosphorescence transient" method for obtaining kinetic and radiative properties of triplet sublevels. David Kearns and I collaborated on ODMR of triplet states of conjugated enones, and showed that the zfs of these 3π , π^* states was strongly influenced by spin-orbit coupling.

I realized that zero-field ODMR would be an ideal method for investigating biological samples that are difficult to obtain in single crystal form. Working on this project in my group were Joseph Zuclich and Dieter Schweitzer, postdoctoral fellows who in 1971 succeeded in obtaining our first ODMR spectra of a protein, bovine serum albumin. Jost von Schütz soon joined our group, and the three made much progress in ODMR, especially in applications to proteins. Kwiram was leading an active program in ODMR of proteins in the early 1970's, as well. We began studying nucleic acids using ODMR, and employed external heavy atom effects of bound ions such as Ag⁺ and CH₃Hg⁺ to enhance ODMR intensity.

In 1974, I moved my research group to Davis, a campus of the University of California near San Francisco. We were heavily involved by this time in studying proteins and nucleic acids using ODMR. A graduate student, Tiao-te (Rochester) Co, was the first to detect ODMR of tryptophan residues in an enzyme by monitoring fluorescence of a bound dye molecule sensitized by triplet-singlet energy transfer. This remains one of my favorite OD-MR experiments. Klaus-Peter Dinse joined my group for a short time in 1975, and using a clever time-resolved method observed ODMR from duplex DNA for the first time. This work solidly confirmed earlier evidence of Eisinger, Lamola and coworkers that duplex DNA phosphorescence originates from neutral thymine. The ODMR spectroscopy in my group at Davis was carried out initially on both simple aromatic molecules and on biological molecules, but in the 1990's the emphasis shifted largely to the study of proteins and nucleic acids. A large part of our efforts eventually focused on the application of ODMR to study protein-nucleic acid interactions, including the binding of quinoxaline peptide antibiotics to DNA and nucleic acid binding of single stranded DNA binding proteins where we investigated base stacking interactions with tryptophan. We often used the effects of a heavy atom-derivatized base on the tryptophan ODMR to prove that a close interaction occurs. We became interested in a small peptide, the nucleocapsid protein (NCp7) of HIV that carries a single tryptophan and binds to specific RNA hairpins of the genetic material and whose integrity is essential for the assembly of an intact virus. We found that stacking interactions with bases of RNA in the absence of heavy atoms produce effects on tryptophan ODMR that vary with the base identity, and thus could be used as a structural tool in the study of protein-nucleic acid interactions that involve tryptophan.

Most recently, we also have worked on improving ODMR methodology. One of the problems with steady state ODMR, especially of long-lived triplet states such as tryptophan, is the line-shape problem. Unless one traverses an inhomogeneously broadened ODMR band impossibly slowly, the band shape is distorted by passage effects. I developed an algorithm to account for these passage effects that was written into a computer code by my former postdoctoral fellow, Jie Q. Wu. Using this program, the true band center, and bandwidth can be extracted from the ODMR slow-passage and delayed slow-passage data regardless of passage rate. Andrew Ozarowski was the last postdoctoral fellow to work in my lab. Ozarowski's expertise was in transition metal EPR, gained in McGarvey's lab, but in spite of this background he is largely responsible for several advances in ODMR, including an important improvement in microwave-induced delayed phosphorescence (MIDP) methodology. Using global analysis by computer of complete sets of MIDP responses (tens of thousands of data points) we were able to show that a simulation is not possible if spin-lattice relaxation is omitted from the kinetics. Thus, global analysis of MIDP data sets allows the individual determination of spin-lattice relaxation rate constants and sublevel vertical decay rate constants of the triplet state. This method led to our discovery that spin-lattice relaxation of triplet states in glass matrix is heterogeneous at the low temperatures of ODMR experiments. The tryptophan triplet state consists of a subpopulation coupled to tunneling, or disorder modes, that relaxes too rapidly to produce ODMR signals, and an uncoupled population responsible for the ODMR, that relaxes slowly as in a crystal.

One of my last conversations with Arnold Hoff was in 1998 at the Annual Biophysical Society Meeting in Kansas City, Missouri. I congratulated him on his upcoming appointment as Fellow of the American Physical Society. Hoff was active in ODMR research, mainly its applications in photosynthesis. He stated and I agreed that it was becoming increasingly difficult to obtain funding of ODMR research in biology. As a structural method in biology, ODMR lacks the general applicability of X-ray crystallography, or NMR (as exemplified, for example, by the work of Kurt Wüthrich, see EPR newsletter 13/1-2, p. 6). Also, it has a rather small following.

Continuation of my research funding from the National Institutes of Health was not recommended in 2001, and I chose not to reapply. After all, I have grandchildren to play with.

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Horia Caldararu (1937–2003)

It is with great regret that we tell about the death of Dr. Horia Caldararu, one of the pioneers and leading Romanian scientists in the application of EPR spectroscopy to organic radicals, colloid and interfacial chemistry and catalysis. He was not only the author of over 70 scientific papers, several book chapters and review articles who devoted most of his time and life to science, but also a good friend, full of passion and interest in politics, jazz, paintings and skiing. For almost 40 years his scientific carrier was connected with the Center of Physical Chemistry transformed, after 1990, into the I. G. Murgulescu Institute of Physical Chemistry, where he was employed first as a chemist, then as a researcher, a senior researcher and finally, since 1989, he became the head of the Laboratory of Quantum Chemistry and Molecular Structure. Despite the unfavorable circumstances and financial difficulties, Horia Caldararu was able to keep the laboratory running, carry out top-level research and provide sufficient support to buy new equipment including his last purchasing a new EPR spectrometer. He was also a mentor for his younger coworkers, always providing



a bright example of scientific frankness and personal generosity.

Horia earned his BSc degree in Physical Chemistry in June 1959 from the University of Bucharest and a PhD in May 1978 from the Institute of Physical Chemistry in Bucharest, Romania. The title of his dissertation "Contributions to the Study of the Structure of Some Organic Radicals" determined to a great extent his scientific interest in the future, which was related with investigations of the structure, stereochemistry, molecular motion and reactivity of σ -radicals. Paramagnetic surface sites and materials of catalytic interest constitute another domain of his EPR activity. He became an expert in studying the nature of electron donor-ac-

ceptor sites in oxides and zeolites, valence, coordination and redox properties of transition metal ions dispersed in multicomponent phosphate, molybdate and scheelite catalysts, as well as electrochemically generated paramagnetic intermediates. The third important field of Horia's fascination was undoubtedly related with spin probes, spin labeling and spin trapping studies. Aggregation of nonionic surfactants, local polarity, microviscosity and order in reversed micelles, structure of hydrophobic gels, dynamics of spin-trapped and spin-labeled proteins and more recently investigations into the structure of surfactant aggregates within the mesoporous silica and alumina should be mentioned among many other topics of his judicious EPR studies. Horia Cardararu collaborated worldwide with many scientists and research institutions, including Germany (Jena and Berlin), USA (Prof. DeArmond, North Carolina State University), Scandinavia (Prof. Lemmetyinen, University of Helsinki, Prof. Almgren, University of Uppsala and Prof. Lindman, University of Lund). In the last ten years he had been regularly joining the group of Prof. Gilbert from the University of York in UK, and we had a pleasure of welcoming him at the Jagiellonian University in Cracow (Poland) several times.

What Horia left on the scientific side is remarkable, but what he left on human ground is even more valuable as all who had the pleasure of meeting him could personally experience.

> Zbigniew Sojka and Krystyna Dyrek Jagiellonian University in Cracow

Carl Lagercrantz (1917–2004)

Carl Lagercrantz, Professor in Medical Physics at University of Gothenburg, Sweden, passed away March 4th 2004 after a long time with a slowly weakening heart. He is survived by three daughters, Agneta, Henriette, and Caroline with husbands and grandchildren and great grandchildren.

Carl Lagercrantz (Calle Lager) was born in Uppsala (50 miles North of Stockholm), Sweden, November 17, 1917, the son of Otto Lagercrantz, Professor in Greek language and President for Uppsala University, and artist Siri Lagercrantz, nee Magnus. He grew up in the middle of the academic life of



Uppsala, where the university and the archbishop's dome were the main institutions, and anything else but an academic career was almost impossible. Thus he educated in medicine and graduated as a physician during WWII. After serving in the military forces for some time he began his postgraduate studies in medical chemistry with Professor Gunnar Blix at Uppsala University. His first research paper 1944 was about electrophoresis which recently had been developed by Swedish Nobel laureate Arne Tiselius. Even if Sweden did not take part in the war, resources were limited and contacts with the surrounding world difficult. Much of the equipment had to be made by PhD students themselves. In 1948 Carl Lagercrantz published his first paper in Nature describing such a "homebuilt" device for counting microscopic cells. He developed the equipment further and in 1952 he graduated as an MD with a thesis "On the Theory of Counting Individual Microscopic Cells by Photo-Electric Scanning. An Improved Counting Apparatus."

In 1955 Carl Lagercrantz and family moved to Gothenburg, where he took up a position as Assistant Professor in Medical Physics at the university. In 1972 he was appointed Full Professor. His interest had now switched into more pure research in molecular physics and chemistry. His tools were microwave spectroscopy and nuclear magnetic resonance spectroscopy, with which he among other things studied the Overhauser effect. However, from about 1960 his main research interest was free radical chemistry studied by electron spin resonance spectroscopy, which resulted in a steady flow of research papers during four decades. In 1967 a breakthrough came, when he developed a method to trap short-lived free radicals with small nitroso compounds transforming them into more stable nitroxide radicals. It was

Philip H. Rieger (1935–2004)

Philip H. Rieger, Professor Emeritus of Chemistry, Brown University, passed away on April 17th 2004. Besides his wife Anne (Nancy) Rieger, he leaves a daughter, Christine Conklin of Clermont, Florida, two grandchildren, Stephen and Ashley, a brother, Frederick Rieger of Port St. Lucie, Florida, and numerous nieces and nephews.

He was the son of Otto and Carla Rieger of Portland, Oregon, and attended Reed College, graduating Phi Beta Kappa in 1956. He then attended Columbus University and received a PhD in Chemistry published in Nature the following year. Similar techniques were more or less simultaneously explored by E. G. Janzen, Athens, Georgia, and M. J. Perkins in UK. It was later called "spin trapping".

However, Carl Lagercrantz, did never continue the development of spin trapping. He created new ideas all the time and continuously went on to new projects. He was very well informed of what was going on in a broad area of research and many were those weekends, when - after reading a recently published paper - he just had to test a new idea in his lab. During the years he has worked together with people from many parts of the world. Nevertheless, Carl Lagercrantz always went his one way and often worked alone in his lab. And it is typical that he was the single author of almost half the number of his research papers. He was one of the last of his kind, who during the decades after WWII had the favor of exploring virgin ground, which then still was possible for a lone gifted researcher.

In 1982 Carl Lagercrantz retired, but he continued his research as emeritus for many years. His last paper appeared in 1999, when he was 82. A few years later he lost his wife Ulla, which made him much isolated, as his bad hips did not allow him to move far. However he continued to communicate with his friends via telephone and e-mail until his very last days. Late 2003 his heart got worse and in March 2004 it did not manage any longer.

We are happy to have had Calle Lager as our mentor and friend and we remember gratefully many stimulating discussions and also more relaxed and humoristic moments with storytelling etc. His philosophical view of life, science and research has given us a very good start in our own careers.

> Göran Adevik Sahlgrenska University Hospital, Gothenburg, Sweden Stig E. Forshult Karlstad University, Karlstad, Sweden

in 1962. Phil Rieger joined the faculty of Brown University in 1962, where he rose to the rank of Full Professor in 1977. During his forty years of active service at Brown, Professor Rieger taught more that 10000 undergraduates in a variety of chemistry courses. He also made major contributions to the Educational Testing Service of Princeton, New Jersey. In research at Brown University, Philip Rieger specialized in electron spin resonance spectroscopy and organometallic chemistry. In both areas he made seminal scientific discoveries, and published over one hundred research articles along with a highly successful textbook entitled "Electrochemistry". He and his wife spent sabbatical years in Australia, New Zealand, England and Vermont.



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11 Dearborn Road, Peabody, MA 01960, USA Phone: 1-978-535-5900; Fax: 1-978-536-2205 e-mail: dipas@jeol.com http: www.jeol.com/esr/fa100.html When Laila asked me some time ago to edit a new column in the *EPR newsletter* I immediately thought on something similar like Arthur Schweiger's former column *Specialist Vignette*. I always enjoyed these articles, because they had the style and purpose of a review article but were, on the other hand, much shorter and compact! This forced the authors to concentrate on the main story, without the chance to dwell on specific details or do any detours, as many of the usual journal review articles do! In the same way the citation list was not extensive

and comprehensive, but more personal and specific. Therefore these short *mini-reviews* serve a quite different purpose: instead of giving an extensive overview of a method with proper credit to the methodological developments and past applications it will – because of its shortness – emphasize a much more personal and subjective view on the topic. This is somewhat similar to the introductory articles in *Nature* or *Science*, only that not a single new research article is described in this case but, more general, a special new method or application.

This was the concept that I had in mind, when I agreed to follow this line and edit a column. I also thought that it would be really interesting, if the author of such a *minireview* of a specific EPR method or application area would not only stress in short terms his personal view of the advantages and perspectives of this method, but would also frankly and open address his concerns on their drawbacks, limitations and bottlenecks. Therefore I choose as title for this mini-review *Pro&Contra*.

I thought the best way to introduce the style I have in mind for this column is to start with the first contribution - hopefully this article can serve as a loose layout for the upcoming contributions. I choose the same topic for this article that I was invited by Arthur years ago to write about in his column: pulsed high-field EPR. Clearly this article is different from this article more than 6 years ago, firstly because, since that time, quite a lot of scientific progress was achieved and secondly because the slightly changed emphasis of the new column – if you kept the old issues of the EPR newsletter (as I do) you can do this comparison. I am also happy about any feedback about your opinion on this topic or column.



Pulsed High-Field EPR An Expert View

Thomas Prisner

Center of Biomolecular Magnetic Resonance, Goethe University Frankfurt, Germany

Introduction

To clarify this point immediately: this will be a personal view on pulsed high-field EPR (pulsed HF-EPR) and *not* on high-field EPR in general. From the methodology and technical point of view, both can easily be distinguished, despite the fact that most of the cw-EPR results can also be obtained by the pulsed methods (but not vice versa!). There is also a discussion on the term high-field: here it is defined as the most common definition in the community, that means magnetic field values of higher than 3 Tesla.

The history of pulsed HF EPR spectroscopy is for me combined inevitable with Jan Schmidt in Leiden. He published the first pulsed HF EPR paper in 1989 [1]. Brave enough, but clearly in his scientific tradition, he started immediately with the construction of a pulsed HF spectrometer, without the detour of first developing a cw-HF-EPR spectrometer. Not only that: his spectrometer was not even capable to perform cw-EPR experiments (as most other spectrometer do), because of the injection locked pulsed IMPATT amplifiers involved. It was a seminal paper, encouraging many other EPR groups to follow these steps and go in the same direction. On the other hand, he also keeps the most recent benchmark with his impressive 280 GHz pulsed EPR spectrometer [2]. In this span of 15 years some dozens other pulsed HF EPR spectrometers have been constructed in laboratories around the world.

Technical Aspects

Commercial pulsed HF-EPR spectrometers are available at 95 and 140 GHz microwave frequency. Above this frequency only two homebuilt pulsed EPR spectrometers exist at the moment at 180 and 280 GHz [2, 3]. The highest-frequency pulsed EPR experiments were performed with two far-infrared laser sources at 604 GHz [4].

The requirements on the main magnet are identical to HF cw-EPR methods. Typically a wide bore solid-state NMR magnet can be used. It is convenient if a secondary sweep coil is available to allow for field sweeps with the main coil in persistent mode. The requirements on the HF microwave source are much less stringent with respect to source noise compared to cw-EPR applications. On the other hand, higher powers are required to achieve sufficiently short microwave pulses (shorter than 100 ns). This can be achieved by a high-power microwave source or by microwave amplifiers. In many cases the microwave switching is achieved at lower microwave frequencies and then transferred in a last step via higher harmonic generators to the final excitation frequency. In these cases the power handling of the final frequency doubler limits the maximum achievable power.

For pulsed experiments a microwave resonance structure is mandatory to achieve large enough microwave field strengths at the sample. At the same time the microwave cavity strongly increases the absolute sensitivity of the spectrometer (this holds also for cw-EPR). Fundamental mode resonance structures become very tiny (submillimeter sizes), difficult to build and handle at high microwave frequencies. In the same way the sample handling (0.1–0.5 mm quartz capillaries) becomes more troublesome. This holds for both pulsed- and high-sensitive HF cw-EPR experiments with a cavity. Microwave transmission is typically done via quasi-optical microwave transmission [5, 6]. This allows for very low microwave power losses in the transmission to the microwave cavity and to the receiver unit. It also allows one to mimic microwave components as circulators and phase shifters, which are not available in classical microwave technology at this high frequencies, by quasi-optical analogues.

The microwave receiver system for pulsed HF-EPR is typically different from cw-EPR spectrometers and consists of a sensitive mixer detector. In many cases a heterodyne system is used, resulting in an intermediate frequency in the low gigahertz frequency range, where the signal can be conveniently amplified, filtered and phase-sensitive detected.

A good overview of the instrumentation part of pulsed HF-EPR spectroscopy is given in several review articles [7–9].

Specific Advantages and Limitations

Pulsed HF-EPR shares the typical advantages of the high magnetic field with the cw-EPR method, as:

- enhanced spectral resolution
- separation of radicals with different *g*-values
- resolution of *g*-tensor anisotropy
- enhanced sensitivity for small samples like single crystals
- detection of high-spin transitions with large zero-field splitting
- narrow lines for the central transition of half-integer high-spin systems

(as, for example, Mn^{2+}).

Unfortunately, this is not in the same way true if the advantages of pulsed EPR at typically lower fields and frequencies (typically 0.3 T and 9 GHz) are compared with HF pulsed EPR applications! One of the big advantages of pulsed EPR spectroscopy, the possibility to resolve small hyperfine couplings by ESEEM spectroscopy, is only working in very rare cases at high magnetic fields, because of the strongly reduced mixing of the nuclear hyperfine

levels at high magnetic fields. On the other hand, this missing of modulation effects can be of advantage if the echo decay function is under study. Technically it is much more demanding to achieve short pulses (because of the very expensive microwave power) and phase switching, limiting the application of multi-pulse sequences severely. Even with these limitations, pulsed HF-EPR has several advantages:

- it is extremely sensitive, because the quality factor *Q* of the cavity has not to be reduced, compared to cw-experiments
- it is much more stable and reliable, compared to HF cw-EPR spectroscopy, because the requirements on a critical matching of the resonant structure are much less stringent
- it is the basis for pulsed HF-ENDOR, a very powerful spectroscopical tool, which has strong stability advantages compared with HF cw-ENDOR, as mentioned above
- it allows one to detect or suppress the field calibration lines of the typical used MnO standard in field-swept echo-detected spectra by their relaxation properties and allows therefore a sensitive detection of g values
- it allows for the determination of the transversal and longitudinal relaxation properties at high magnetic fields and their orientational anisotropy if the *g*-tensor anisotropy is resolved

The last point allows to extrude the frequency or field dependence of the relaxation rates; this may help to understand the physical origin of the dominant relaxation mechanism. For many mechanisms the relaxation rates will differ with respect to the orientation of the molecule with respect to the external magnetic field. Because HF-EPR usually resolves the g-tensor anisotropy spectrally, this



relaxation anisotropy can be measured and correlated to the molecular axis system, allowing one to achieve a more unique determination of the dominating mechanism and its molecular details.

Other advantages, often mentioned with HF-EPR, are the potential high time reso-

lution (large cavity bandwidth) and, related to that, the extremely short instrumentation dead time. The later argument will only get its full strength if high-power coherent microwave sources will be used in such setups - such spectrometers are in the stage of development at Cornell University and St. Andrew's University (both at W-band frequencies). In these cases special care has to undertaken to avoid that the high pulsed excitation power saturates the sensitive detection channel, which would again lead to extended dead time. One way to do so is to use the perpendicular linear polarization component for the detection, as can be easily achieved with a Fabry-Perot resonator. With such a setup, a dead time of 20-50 ns (including the 14 ns $\pi/2$ pulse) has been realized at 140 GHz with a 300 W extended interaction klystron source [10].

Applications

The majority of the HF applications are still performed in a cw mode of operation, similar to the situation many years ago at X-band frequencies. In most cases where pulsed HF-EPR applications are described, field-swept echo-detected spectra were taken and different pulse separation times were chosen to separate different overlapping radicals and to assign them. In some rather rare cases ESEEM effects on strongly coupled nitrogens were observed. Stimulated echo experiments, performed as a function of *T* and τ , were used to examine the dipolar

> coupling in a nitroxide biradical. In a number of pulsed HF-EPR the spectrally resolved anisotropy of the transverse relaxation time T_2 was related to small angle librational motion of the molecule. The transversal relaxation rate in this case for a certain temperature range is dominated by the modulation of the effective g-tensor value induced by the librational motion. Because the relaxation rate could be measured for all mean orientations of the molecule with respect to the magnetic field separately, a detailed picture of the

anisotropy of the librational motion of the molecule could be deduced. Measurements at different high fields allow one to test the motional regime of the librational motion and the validity of fast motional analysis of the data. As an example, the anisotropic T_2 relaxation of a nitroxide radical measured

photo of the issue



Erwin Hahn playing Rossini

in frozen solution at low temperatures by a pulsed Hahn-echo sequence at 180 GHz is shown. The resolved 2-D spectrum nicely shows that the relaxation time is strongly correlated to the anisotropy of the *g*- and hf-tensors, as expected for a librational motion of the molecule.

Outlook and Perspectives

If the transmission pathways from the source to the cavity and to the receiver are designed carefully, a time resolution on the order of 1 ns can be envisaged. This will allow one to observe paramagnetic species with at least one order of magnitude faster relaxation times or lifetimes. For example, short-lived photoexcited transient states that could not be observed so far by pulsed or transient EPR methods at X-band frequencies will be accessible by these setups. Also this new generation of pulsed spectrometers will give additional information to investigate the motional dynamics of paramagnetic molecules.

Further technical improvements can be foreseen for HF-EPR in the near future. Low-noise and high-power solid-state highfrequency amplifier will improve the performance of such spectrometers and therefore allow one to approach the theoretical possible advantage of HF-EPR with respect to time resolution, excitation bandwidth and sensitivity. Especially the very high absolute sensitivity of HF-EPR could extend the application range to new areas.

Pulsed HF-EPR is the prerequisite for pulsed HF-ENDOR, a very successful method that will further gain in importance in the future. Recently Bruker BioSpin has demonstrated that PELDOR (pulsed electron double resonance) can be performed also at high magnetic fields successfully. On the one hand, there is a loss in pumping efficiency at high magnetic field strengths because of the increased spectral width, but on the other hand, this could lead to additional angular information on the dipolar axis with respect to the molecular g-tensor axis frames. This might be even more important for aromatic organic radicals which have no resolved spectra at X-band frequencies.

Existing high-resolution magnets would still allow one to extend HF-EPR up to 600 GHz. Because there is no possibility to sweep the magnetic field at these values cw-EPR applications cannot be performed. On the other hand, because pulsed EPR experiments are typically performed at a fixed magnetic field value, a pulsed very-high-frequency EPR spectrometer, where the microwave and the resonance structure frequencies are tuned to the right spectral position once before the experiment, seems possible.

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Reef Morse

Computer

One of the better-kept secrets of the EPR community is the EPR list server. As of this moment, there are only 167 subscribers to this list. Because it can act as a resource and means of communication for the EPR community (with occasional incursions from the NMR community announcing conferences and other important events), and because of the possibility of knitting the EPR community together through the list server, I thought it was timely to tell everyone about it. Here goes!

The epr-list runs on a Sun workstation maintained by the Chemistry Department at Illinois State University. Even though I am no longer at ISU, they have kindly agreed to keep the list on their computer. I (Reef Morse) provide all the maintenance of the list.

The EPR list server is a moderated list that means that people who are approved to be on the list can send messages to the list. A message sent to the list goes out to all members of the list. Messages from email addresses that are not on the list are sent to me and I either post them to the list, or delete them. Thus, there is no spam on this list - all such messages are filtered out manually before they get to you. I also handle messages of the type "I'm writing a paper on EPR and I wondered if you could tell me anything about it" (I advise the sender to go to the library, see what they can find, and get back to me). Thus, the content of the list is limited to actual EPR-related information and questions, requests for post-docs, graduate positions, and fellowships, EPR-related sales information (spectrometers, cavities, etc.), conference notifications, availability of resources, and the like.

Joining the list is easy. Send the line

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Side Bar

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This is your list. My job is to make sure that everyone with a legitimate need can join the list and to keep illegitimate messages (spam) out. Help this list to achieve its potential to keep us all in contact.

If you forget all this, you can get this information again by sending mail to majordomo @xenon.che.ilstu.edu with a line saying

help epr-list

and you will receive considerable information about the list from this help message. However, there are no files associated with the list at this time and you cannot find out who is on the list for privacy reasons.

If you have further questions about the list, feel free to contact me at

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Introduction to the basic principles of EPR and EPR instrumentation. Participants will learn how to acquire EPR spectra and how to optimize the parameters as well as to use the acquisition and evaluation software. **Topics:**

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- Single crystal simulation
- Power simulation
- Lineshape models

Introduction to FT-EPR:

Introduction to FT-EPR instrumentation. Participants will learn to run FT-EPR spectra and to use the FT software. **Topics:**

- Spin echo techniques
- Fourier transform EPR
- Xepr software package
- ESEEM experiments
- 2D EPR ESEEM
- Variable temperature experiments

Introduction to EPR at 94 GHz (W-Band):

Introduction into high-frequency/high-field EPR at 94 GHz. The participants will acquire CW-EPR data as well as pulse EPR data including cold field sweeps.

Topics:

- Introduction to W-Band instrumentation
- Running supercon sweeps

- CW-EPR
- Pulse EPR
- Xepr software package

The 38th Annual International Meeting *Advanced Techniques & Applications of EPR*

University of Bath, Bath, UK March 20 (Sun) – 24 (Thu), 2005 www.esr-group.org.uk/Bath/index.html

This meeting will follow the now familiar pattern.

Starting on *Sunday* with registration, supper and a reception by the ESR Group.

Monday starts with two plenary lectures in the morning, then the JEOL student lectures in the afternoon, followed by a poster session after tea. There will be a reception by JEOL in the evening.

On *Tuesday* morning there will be two more plenary lectures, and the session will be dedicated to the memory of the late Professor Phil Rieger. *Tuesday* afternoon has an excursion – where else but to the town of Bath! On *Tuesday* evening after supper this year's Bruker Lecture (the 20th) will be given by Professor Klaus-Peter Dinse of Darmstadt University. To be followed by a reception hosted by Bruker SpectroSpin.

Wednesday sees three more plenary lectures, with the ESR Group AGM just after teatime in the afternoon. In the evening there will be a Banquet.

The meeting finishes with two more plenary lectures on *Thursday* morning, and after lunch delegates depart.

The 9th International Workshop Electron Magnetic Resonance of Disordered System

Bulgarian EPR Society, Sofia, Bulgaria June 8–15, 2005

Scientific program

EMARDIS-Fundamental

The aim of this section is to cover all qualitative (structural-reactivity, kinetics, etc.) aspects of recent development in theory, experiment, methodology, instrumentation, etc. of EMR (EPR, ENDOR and ESE) spectroscopy of disordered systems (powders, glasses, liquids).

EMARDIS-Applied

The topics planed to be discussed are: Fundamental aspects of Quantitative EPR (standards, calibration, metrology and methodology of quantitative measurements, instrumentation – new methods, advanced techniques, automation, etc.); EPR dosimetry (monitoring of high energy radiation, high-energy radiation processing control in food preservation, pharmaceutical sterilization and materials science, dating of archaeological and geological samples, etc.); EPR in biology, medicine (clinical and biomedical studies); EPR in life science; EPR in the environmental control; EPR in petrol industry; EPR and fossil fuels; EPR in polymer chemistry, etc.

Presentations

Main lectures (40 min), oral (25 min) and poster presentations of original contributions are planned. The program will also include round-table discussions. In addition there will be plenty of time for free evening discussions.

Abstracts preparation

One page abstract of every presentation will be published in the Proceedings of the meeting. Abstracts must be received before January 31, 2005.

Second circular

Second circular of the EMARDIS meeting with more details will be distributed in the beginning of March, 2005. It will be available also at the web page of the European Federation of the EPR Groups.

Address for correspondence:

N. D. Yordanov (Convenor) Laboratory EPR, Institute of Catalysis Bulgarian Academy of Sciences 1113 Sofia, Bulgaria tel: (+359 2) 979-2546 or 724-917 fax: (+359 2) 971-2967 or 870-5024 e-mail: emardis@ic.bas.bg

A Joint Conference of the 11th *In Vivo EPR Spectroscopy and Imaging* and the 8th *International EPR Spin Trapping*

The Ohio State University College of Medicine and The Dorothy M. Davis Heart and Lung Research Institute, Columbus, Ohio, USA September 4–8, 2005

The meeting (EPR 2005) sponsored by the National Institutes of Health will present cross-sections of the most recent advances in the areas of EPR spectroscopy, as applied to biological systems. This includes instrumentation, software, spin probes (for the detection of oxygen free radicals, nitric oxide and oxygen), spin-labeling, and imag-



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ing. This will maximize the cross-fertilization of ideas, allowing experts in each area to exchange information and catalyze rapid advances. The organizers will promote this by integrating plenary talks from different areas and by designing symposia that address interfacial topics.

The oral sessions will highlight the following areas:

- Spin-trapping applications reactive oxygen radicals, and protein radicals
- Spin labeling protein structure/ function
- In vivo imaging applications spatial, spectral-functional imaging

- Oximetry/dosimetry applications including clinical developments
- Hardware/software/methods resonators, data acquisition, image reconstruction, and simulation
- Development of probes redox, oximetry, spin labels, spin-traps
- Emerging technologies PEDRI/ OMRI, Pulse, EPR Microscopy, MFM, and MRFM

See you in Columbus in 2005!

You may use epr2005@medctr.osu.edu for contacts. The conference website heartlung.osu.edu/epr will be ready in a couple of weeks.

The 28th International EPR Symposium University of Denver, Denver, Colorado, USA July 31 – August 4, 2005

The 28th International EPR Symposium will be held at the Hyatt Regency Denver hotel. **For further information, please contact:**

Profs. Sandra Eaton or Gareth Eaton Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80208, USA e-mail: seaton@du.edu



Magnetic Resonance Workshop Development and Application of Magnetic Resonance Methods

Hirschegg, Austria February 14–18, 2004

NMR, ESR and SKI were the topics of interest in a recent joint workshop between the Graduate College on Advanced Magnetic Resonance Type Methods in Materials Science in Stuttgart and the EPR and NMR groups of A. Schweiger and B. Meier from the ETH Zürich which was held in Hirschegg, Austria, from 14 till 18 February 2004.

The funding agency of Graduate Colleges, the Deutsche Forschungsgemeinschaft, wants PhD students to take more responsibility for their own education and research and expose them to experts on an international level. In the spirit of these principles the workshop was organized entirely by PhD students and young postdoctoral coworkers. The chairman of the organizing committee, Alexander Panchenko from Stuttgart, less than 25 years old, was actually the youngest participant. I am pleased to acknowledge that these people did a perfect job and put together a multinational and truly stimulating meeting with close to 50 students, postdocs, and group leaders, originating from about 20 different countries. This of course reflects the international composition of the involved groups.

The program consisted of invited and contributed lectures and a poster session. It covered instrumental and methodological developments and their application to the determination of structure and dynamics in various contexts, ranging from molecular magnets over spider silk to spin dynamics and quantum computing of defect centers in diamond. It was complemented by theoretical contributions on spectral simulation and on relativistic calculations of EPR parameters. Details about the program as well as pictures are found on the homepage of the Graduate College under www.uni-stuttgart.de/gkmr/ news/Hirschegg_2004.html

The free afternoons benefited from the fresh air, the sun, the perfect snow conditions and the impressive mountain scenery around Hirschegg. Here is where the third discipline came in: SKI, both down hill and cross-country, and snow walking. Amazing analogies to magnetic resonance were discovered: while some people demonstrated undamped FID traces in the snow, others developed techniques to cope with T_2 dephasing of their skis or experimented with inversion-recovery sequences or nonmagic angle spinning. Nevertheless, despite all spikes and singularities we are glad to report that all participants returned home relaxed and safe.

Emil Roduner, organizer, Stuttgart

The magnetic resonance workshop "Development and Application of Magnetic Resonance Methods" was held in Hirschegg, Austria in the period 14-18 February 2004. I would say (and I am sure other co-participants have the same comment) it was a wonderful and exciting opportunity to learn about many advanced methods in magnetic resonance spectroscopy and how they are applied to real systems. The workshop, jointly organized by the Graduate college on Advanced Magnetic Resonance type methods in materials in Stuttgart, and the EPR and NMR groups of ETH, Zürich, is a paradigm for future workshops of similar nature. Good beer, nice climate, fresh air, enchanting Alpine mountains covered with snow, informative and interactive scientific sessions, and even more exciting afternoon sessions for skiing. Moreover, the organizers had worked with a spirit, which gave the workshop a touch of being homely.

It offered a real opportunity to meet and mingle with the pioneers in the field of EPR and NMR. The lectures were tuned in such a way that each day was interesting and exciting giving a broad overview of advanced spin resonance techniques. The entire workshop was like a test cricket match for me, as it kept the enthusiasm and thrill from the dawn to dusk and beginning to end. The first innings was opened by Arthur Schweiger, the soul of the EPR group at ETH. After a small and crispy introduction about magnetic resonance methods, when the lecture turned to advanced pulse methods in EPR, the words from the preface of the book "Principles of Pulse Electron Paramagnetic Resonance" by A. Schweiger and G. Jeschke came into my mind: "Pulse techniques have been considered as a play ground for a few eccentrics...". Being part of a community of such an eccentric, it was interesting to hear how EPR spectroscopy has grown to its heights now when it is celebrating its 60th year of birth. The following sessions took the audience through the advanced magnetic resonance methodologies, and their real-time applications

ranging from biological systems like metalloenzymes to the world of materials science and fuel cells. The sessions were didactic and youngsters were given a special privilege to ask questions and discuss at the end of each talk. The different group leaders presented a pedagogical overview of what the group was doing, followed by the lectures of group members who explained their projects. The contributory lectures were centered around EPR and NMR methodologies, such as hyperfine decoupling, transparency, spin polarization transfer methods, computational and instrumental developments for the spectral simulation and universal probe-heads, application aspects to transition metal complexes, enzymes, homogeneous catalysts, molecular magnets, fuel cells, solid-state NMR characterization from the spider silk to metal hydrides and diamonds, DFT in the calculation of EPR and NMR parameters, muon spin resonance and their applications and, finally, an amazing world of beautiful pictures as an introduction to MRI.

Besides these lectures, there was a poster session and a movie. The poster session benefited from mutual one-to-one interactions and prolonged discussions and comments. I think that the real target of this workshop, which was aimed at the information exchange between the different groups, was fulfilled to the greater extent and I once again take this opportunity to thank the organizers for giving us such a splendid week of science and skiing.

Sreekanth Anandaram, student, Zürich

The 27th International EPR Symposium Denver, Colorado, USA August 1–5, 2004

The Symposium was preceded by an EPR Imaging Workshop on Sunday, August 1, at the University of Denver. The Workshop was sponsored by Bruker BioSpin and the University. Topics discussed during the Workshop include:

- Introduction Insights from imaging

 a. In the beginning
 - b. Applications to materials science
 - c. Electrochemistry
 - d. Diffusion
 - e. Application to biological systems animals
 - f. Microscopic imaging
- 2. Methods of EPR imaging
 - a. Fundamentals
 - b. Definition of projections

- c. Spectral-spatial imaging
- d. What to image
- e. What information is in the image
- f. How to obtain an image
- g. Relation between MRI and EPR imaging
- h. Pulsed EPR imaging
 - i. Pulse shaping
 - ii. Single-point imaging
- 3. Magnets
- 4. Magnetic field gradients
 - a. Static gradients
 - b. Stepped gradients
 - c. Modulated gradients
 - d. Rotated gradients
 - e. Pulsed gradients
 - f. Some practical matters about gradient coils
 - g. Concomitant gradients
- 5. Resonators
- 6. Other detection techniques rapid scan, DNP, LODESR, etc.
- 7. Image reconstruction
 - a. Missing angle algorithm
 - b. Portions of spectra
 - c. Resolution
- 8. Microscopic imaging
 - a. Magnetic force microscopy
 - b. Single spin imaging
- 9. Instrumentation for imaging in more detail
 - a. Gradient coil design
 - b. Commercial instrumentation
- 10. References
 - a. Glossaries
 - b. General reviews on imaging
 - c. Cited references
 - d. Selected bibliographies from several labs

All attendees received a booklet on EPR imaging prepared especially for the Workshop.

The research reports during the 2004 EPR Symposium on the following four days included oral and poster sessions covering all aspects of EPR. A session on spin labels as reporters for protein conformational change was organized by Hassane Mchaourab, Vanderbilt University, and Y.-K. Shin, Iowa State University, and there was a related session entitled "provocative discussion" on spin labeling. A session on EPR imaging was organized by Shulamith Schlick, University of Detroit, and Howard Halpern, University of Chicago. A session on computation of metal EPR parameters was organized by Sarah Larsen, University of Iowa.

Jay Zweier, Ohio State University, presented the Lawrence Piette Memorial Lecture "EPR Imaging of Free Radicals: Applications from Mouse to Man". Bruker demonstrated a new L-band imaging spectrometer. There was also a meeting of the International EPR Society. Thirteen students were awarded partial travel support, sponsored by the Jules Stein Professorship Endowment (UCLA) and the Iowa State University.

Gareth and Sandra Eaton

The International Conference *Modern Development of Magnetic Resonance* (EPR₆₀) Kazan, Russian Federation

August 15–20, 2004

This conference was organized as part of the International Scientific Forum dedicated to the 200th anniversary of the Kazan State University and the 60th anniversary of EPR discovered by E. K. Zavoisky. The conference was successful both in scientific and social aspects. The scientific program of the conference consisted of plenary lectures, invited talks, oral presentations and poster sessions covering recent achievements in various fields of paramagnetic resonance, in particular electron paramagnetic resonance, including the development of modern methods and their applications to studying structure and dynamics of condensed matter and applications of radiospectroscopy in chemistry, biology, materials science, etc. in the following sessions:

- Modern EPR methods (pulse methods, time-resolved EPR spectroscopy, highfrequency EPR spectroscopy, indirect methods of EPR detection)
- EPR of doped materials
- Chemical and biological applications of magnetic resonance
- Magnetic resonance in geology
- Magnetic resonance imaging (physical basics)

157 scientists from different countries (Byelorussia, Georgia, Germany, Italy, Japan, Kazakhstan, Moldova, Poland, Russian Federation, Switzerland, Turkey, Ukraine, and USA) participated in the conference. All attendees received a book of abstracts. Full original papers submitted by the participants of the conference are being refereed and will be published in a special issue of Applied Magnetic Resonance. Detailed information can be found on the conference website www.kfti.knc.ru/epr60: the program, a list of participants and a photo session. The 2004 Zavoisky Award was presented during this conference (see this newsletter, p. 6). The social part of the conference included an exciting concert (Mozart and Danzi played by Uwe Eichhoff, Bruker BioSpin, (flute), Jörg Forrer, ETH, (clarinet), the string quartet "Kantilena" and the orchestra "New Music"), a boat trip on the river Volga, and site-seeing excursions.

Kev Salikhov, Chairman



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Recent Achievements in Fundamental and Practical Aspects of EPR

A special issue of *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* edited by Nicola D. Yordanov

This special issue of *Spectrochimica Acta Part* A (vol. 60, no. 6, 1239–1410 (May 2004)) contains 21 papers with contributions presented at the EMARDIS-8 June 2003 workshop. The studies cover a wide range of applications of EPR:

- B. Rakvin, D. Žilić, N. S. Dalal, J. M. North, P. Cevc, D. Arčon, K. Zadro: An EPR Method for Probing Surface Magnetic Fields, Dipolar Distances, and Magnetization Ffluctuations in Single Molecule Magnets
- D. Zayachuk, Ye. Polyhach, E. Slynko, O. Khandozhko, C. Rudowicz: EPR and NMR in Powders of Doped and Undoped IV-VI Crystals
- Z. Sojka, P. Pietrzyk: Paramagnetic Species on Catalytic Surfaces – DFT Investigations into Structure Sensitivity of the Hyperfine Coupling Constants
- H. Yahiro, A. Lund, M. Shiotani: Nitric Oxide Adsorbed on Zeolites: EPR Studies

- D. Mustafi, J. E. Hofer, W. Huang, T. Palzkill, M. W. Makinen: Chromophoric Spin-Labeled β-Lactam Antibiotics for ENDOR Structural Characterization of Reaction Intermediates of Class A and Class C β-Lactamases
- B. Jeliazkova, A. Dimitrova, M. Doicheva: Charge-Transfer Photolysis of Copper(II) Dithiocarbamate Mixed-Ligand Complexes in Toluene/Alcohol Solutions
- M. A. Doytcheva, B. G. Jeliazkova: Structure of Copper(II) Dithiocarbamate Mixed-Ligand Complexes and Their Photoreactivities in Alcohols
- N. D. Yordanov, E. Georgieva: EPR and UV Spectral Study of γ -Irradiated White and Burned Sugar, Fructose and Glucos
- K. Nakagawa, Y. Sato: ESR Investigation of Sucrose Radicals Produced by Particle Irradiation.
- E. Lund, H. Gustafsson, M. Danilczuk, M. D. Sastry, A. Lund: Compounds of ⁶Li and Natural Li for EPR Dosimetry in Photon/Neutron Mixed Radiation Fields
- B. Ciesielski, K. Schultka, M. Penkowski, E. Sagstuen: EPR Study of Light Illumination Effects on Radicals in γ-Irradiated L-Alanine
- S. Talbi, J. Raffi, S. Aréna, J. Colombani, P. Piccerelle, P. Prinderre, J.-M. Dolo: EPR Study of γ-Induced Radicals in Amino Acid Powders
- H. Masmoudi, C. Rebufa, J. Raffi, A. Permanyer, J. Kister: Spectroscopic Study of Bituminous Oxidative Stress
- D. Gourier, L. Binet, A. Scrzypczak, S. Derenne, F. Robert: Search for EPR Markers of the History and Origin of the Insoluble Organic Matter in Extraterrestrial and the Terrestrial Rocks
- U. Ulusoy: ESR Studies of Anatolian Gypsum
- N. D. Yordanov, I. Najdenova: Selective Estimation of Soot in Home Dust by EPR Spectrometry

- M. B. Kadiiska, A. J. Ghio, R. P. Mason: ESR Investigation of the Oxidative Damage in Lungs Caused by Asbestos and Air Pollution Particles
- M. Šentjurc, M. Čemažar, G. Sersa: EPR Oximetry of Tumors *in vivo* in Cancer Therapy
- F. Czechowski, I. Golonka, A. Jezierski: Organic Matter Transformation in the Environment Investigated by Quantitative Electron Paramagnetic Resonance (EPR) Spectroscopy: Studies on Lignins
- N. D. Yordanov, R. Mladenova: EPR Study of Free Radicals in Bread
- C. J. Rhodes, T. T. Tran, H. Morris: A Determination of Antioxidant Efficiencies Using ESR and Computational Methods

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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 Charless Dismukes.

Projects:

• 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-subunit proteins, photosynthetic reaction centers and other biological materials.

- 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.
- Functional Dynamics of Proteins and Materials by Time Resolved FT-ESR. To study transient structural changes in photochemistry of photosynthetic reaction centers and inorganic materials related to catalysis and solar energy conversion and internal dynamics with proteins.

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Ms. Lynn Mendenko mendenko@princeton.edu Princeton University Hoyt Laboratory Department of Chemistry Princeton, NJ 08544, USA A further description of the criteria for

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Gareth R. Eaton geaton@du.edu

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Nobel Laureates in Magnetism

Dear Laila,

Thank you for the excellent issue on Nobel prizes. About ten years ago, while we were preparing the book *Foundations of Modern EPR* with Kev Salikhov, Professor B. Bleaney (Oxford) sent us a list of Nobel prizes for work that he considered foundations of magnetic resonance. This list may be of interest to other EPR spectroscopists.

- 1902 H. A. Lorentz and P. Zeeman (magnetism and radiation)
- 1913 H. Kamerlingh Ohnes (low temperature physics)
- 1936 P. Debye (dipole moments)
- 1943 O. Stern (molecular beams and magnetic moment of proton)
- 1944 I. I. Rabi (resonance method for nuclear moments)

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- 1945 W. Pauli (exclusion principle)
- 1949 W. F. Giauque (chemical thermodynamics and low temperatures)
- 1952 F. Bloch and E. M. Purcell (NMR)
- 1955 W. E. Lamb (fine structure of the hydrogen atom) and P. Kursch (magnetic moment of electron)
- 1970 L. Neel (antiferromagnetism and ferrimagnetism)
- 1977 P. W. Anderson, N. F. Mott, and J. H. Van Vleck (magnetism and disordered systems)
- 1989 N. F. Ramsey (masers and atomic clocks)
- 1991 R. R. Ernst (high resolution NMR)

Since this list was prepared in 1994, it does not include the prizes to Kurt Wüthrich, Paul Lauterbur, and Peter Mansfield, all of which were highlighted in your recent issue.

Gareth and Sandra Eaton

Our quiz of EPR newsletter 14/1-2

We got the following three versions of a dialog between Niels Bohr (N.B.) and Wolfgang Pauli (W.P.) from our readers:



1

N.B.: Look! This time I was fortunate and the top jumped upside down.

W.P.: Really, one-axial body interacting with the gravitation field can rotate around its axis and jump upside down too. Spinning of the sphere is a good model for this unique feature of the electron. After H. E. Uhlenbeck and S. Goudsmit we call it spin.

N.B.: Let us talk to Wojciech Rubinowicz who worked out the theory of electric quadrupole radiation. Perhaps a two-axial body (ellipsoid of revolution) model in the gravitation field can illustrate his equations describing nuclear spin?

W.P.: Good idea, I think these simple mechanical models will stimulate people for EPR, NMR and NQR inventions.

N.B.: I am sure, successful experimentators will be awarded the Nobel Prize.

2

N.B: Have you any idea, buddy, why the heck it doesn't fall down?

W.P.: This is a good question...

3

N.B.: Wolfgang, do we need the Pauli's principle to describe how this thing moves?W.P.: No, Niels, we even do not need Bohr's principles here.

4

It is Chanuka, **N.B.** and **W.P.** are playing the traditional dreidel game and singing:

- Dreidel, dreidel, dreidel, Spin, spin, spin,
- Spin up, spin down,
- Who do you think will win?

Please, vote via e-mail to the editor, which of these dialogs is the one which is most to the point. We keep the names of the authors incognito to ensure an independent choice. The winner will be announced in one of the next EPR newsletter and will get a nice tippe top.

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