

EPR NEWSLETTER

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Page 1

Summer/Fall, 1997

BUCHACHENKO WINS VOEVODSKY AWARD

Anatole Buchachenko of the Semenov Institute of Chemical Physics (Moscow) has won the Voevodsky Award for 1997. The officers of the International EPR (ESR) Society and the editorial staff of the Newsletter extend our hearty congratulations to Professor Buchachenko, who was honored for his outstanding contributions to the understanding of chemical reaction mechanisms and both structure and properties of free radicals by use of radiospectroscopic methods.

Information transmitted by Prof. Yu. D. Tsvetkov, Chairman of Voevodsky Award Committee

IN MEMORIAM: JOHN EDWARD WERTZ (1916-1997)

John Wertz, a pioneer of EPR spectroscopy, passed away quietly on 8 August 1997 after a lengthy illness.

John was born on 4 December 1916 in Denver CO, received his BSc in Chemical Engineering from the University of Denver in 1937, an MSc in 1938, and a PhD in Chemistry (T.F. Young, Supervisor) in 1948 from the University of Chicago. He started his academic career in 1941 at Augustana College in Rock Island IL, moved on in 1944 to Gustavus Adolphus College in St. Peter MN, and then to the University of Minnesota in 1947, where he remained until his retirement in 1981. One of John's early interests was surface chemistry, e.g., the magnetic susceptibility of adsorbed layers. When he started at the University of Minnesota, he acquired some surplus Navy equipment, including a bank of submarine batteries which he used to provide dc current for the magnet of his home-built EPR spectrometer. He polished his EPR spectroscopic expertise as a Fulbright Scholar and Guggenheim Fellow at the Clarendon Lab, Oxford UK in

1957-8. A fire in the Chemistry Building in the early 1960s destroyed this spectrometer, but led to the opportunity to purchase a new Varian EPR spectrometer (but only the essential core). John had drawers full of microwave parts and loved to construct special "add-ons." He was interested in many aspects of EPR spectroscopy, from the spectra of semiquinones in solution to those of point defects in solids. A major review article "Nuclear and Electronic Spin Magnetic Resonance" [Chem. Rev. 55, 829 (1955)] by John enhanced his fine reputation. His work on the EPR and optical spectroscopy of such defects in MgO is undoubtedly his most important research legacy, and is summarized in the book "Defects in the Alkaline Earth Oxides" co-authored by R. Henderson and J.E. Wertz, Halsted Press, New York NY 1977.

In 1970, John was instrumental in encouraging Jim Bolton to come to the University of Minnesota as an Assistant Professor. He kindly gave up part of his large lab so that Jim could start his EPR work there. The two

ANNOUNCEMENT: *Nominations are welcome for the IES Awards. See pages 3 & 4 of this issue for full details.*

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FELLOWS OF THE INTERNATIONAL EPR(ESR) SOCIETY

- | | |
|-----------------------|-----------------------|
| • Anatole Abragam | • George Feher |
| • Brebis Bleaney | • Ralph Hahn |
| • Clyde Hutchison | • J. H. van der Waals |
| • Aleksandr Prokhorov | • Samuel Weissman |

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shared EPR equipment and became friends, but each maintained their own research projects. In 1967, the American Chemical Society asked John to organize a "Short Course on EPR." John invited Jim to join him in this effort and together they presented at least 5 such courses, all over the USA. The "course notes" from these grew and grew, and it became obvious that they represented the core of a book on EPR. Over the next two years, John and Jim spent many weekends and evenings working together on writing "Electron Spin Resonance: Elementary Theory and Practical Applications" by J.E. Wertz and J.R. Bolton, published by McGraw-Hill in 1972. Notable innovations were an extensive series of problems after each chapter and appendix, and a series of background tutorial appendices taking up 22% of the book's pages. This book quickly became recognized as the premier textbook in the field.

Toward the end of John Wertz's academic career, he became very involved in the Metric Commission and tried fervently to push America toward the use of metric units in schools and society.

In 1989, John and Jim decided that the time had come to prepare a revision to their text, and invited John Weil from the University of Saskatchewan to join them as a third author. The three arranged several extended visits where they planned and discussed, but sadly it became apparent that John Wertz's Parkinson's disease had taken its toll and he had to bow out of active participation. The revised textbook appeared in 1994 as "Electron Paramagnetic Resonance: Elementary Theory and Practical Applications" by J.A. Weil, J.R. Bolton and J.E. Wertz, published by John Wiley & Sons, reprinted in 1995.

John Wertz is survived by his wife Florence, sons John A. and Byron A. and daughter Kristin M. He will be remembered warmly by his friends as a quiet pioneer of EPR spectroscopy, a fine researcher, a wonderful teacher, and a kind gentle person who always laid out the welcome mat for visitors from near and far.

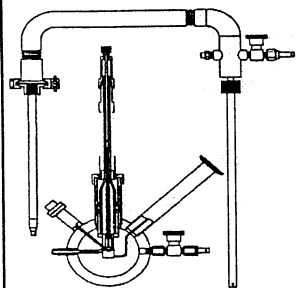
Jim Bolton, Professor Emeritus
University of Western Ontario

John Weil, Professor Emeritus
University of Saskatchewan

FROM THE EDITOR

As I write this, I am both sad and cheered. Sad to mourn the passing of EPR pioneer John Wertz (page 1 story) and cheered by the acceptance by another EPR pioneer, Professor John Pilbrow of Monash University, as Secretary of the IES. John Pilbrow is not only my good friend and colleague, but brings enormous energy, enthusiasm, and sense of community to this position. He will be a worthy successor to Arthur Schweiger, a tall order for anyone indeed! I got to know John especially well over two decades ago, when he spent a sabbatical with me in Urbana. He and wife Susan arrived on site with a family seemingly large enough to constitute a whole baseball team or both sides of a basketball game, and they were incredibly well organized and in great good cheer. He took on organizing and teaching a whole university course in physical chemistry, gave my research group an extensive and well-organized series of lectures on details of EPR theory and practice, and spent what seemed like full time engaged in very productive collaborative research work on theoretical topics in EPR spectroscopy of transition metal ions. His too-brief stay here was wonderful for me and my research group; it was marked by ebullience, fine organization, sound judgement, excellent productive intellectual efforts, and the joy of discovery. These qualities have marked John's career since then, and they will serve us all well in his role as IES Secretary. John Pilbrow is currently Vice-President of the Australian Institute of Physics and a Member of the National Committee for Physics in Australia (the National Committee interacts with IUPAP and other such bodies). He has been selected to receive the 1998 Royal Society of Chemistry ESR Group Bruker Prize in Manchester in April, 1998 and to present the Bruker Lecture. In this, he follows a succession of illustrious IES colleagues including Keith McLauchlan, Brian Hoffman, Jack Freed, Jim Hyde, and George Feher.

The time is nearing for an updated Directory issue, which many readers tell us is particularly useful to them. But it is not very useful if it is riddled with errors and omissions. So we ask you, please, to check it over and inform the editorial office of errors. We know that several E-mail addresses, especially, are wrong or out of date, but we have no way of correcting them unless you tell us the new information. Also, perhaps you know of some other



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people who are active or interested in some variety of EPR and who ought to be represented in our directory. I have been asked why there are interest codes for some persons in the directory but not for others. Usually, these interest codes come from the IES members' application forms or updates. If you notice colleagues whose entries show no interest codes, they probably are not members; please urge them to join! Membership is inexpensive and carries a high benefit/cost ratio. Only with a substantial membership can we publish your Newsletter, provide the information you frequently request of us, offer highly subsidized IES member subscription rates (ca. 90% discount!) to *Applied Magnetic Resonance*, maintain an effective official presence for the EPR community at key international conferences, give international awards to recognize distinguished scientists and encourage especially talented and promising young scientists in our field, and work in many other ways to promote the interests of our field and facilitate interactions among us all. Information can be obtained from any officer, by E-mail to ierc@uiuc.edu, and from the Society's Web page -

<http://ierc.scs.uiuc.edu/IES.html>.

Of course, joining once and then lapsing doesn't help much either. Need to check your dues status? Check the Web page (<http://ierc.scs.uiuc.edu/payment.html>) for a record of your dues payments. You can now pay by credit card as described on a link from the Society's Web page.

◆ IES AFFAIRS ◆
ANNOUNCEMENTS AND
REPORTS FROM THE INTERNATIONAL
EPR (ESR) SOCIETY

From the President—

I prepare this letter with considerable enthusiasm. August 24-25 I was in Leipzig, Germany to attend the III European ESR Meeting and, along with outgoing Secretary Arthur Schweiger, to represent the IES for our annual award ceremony. For the first time, the society is presenting its awards in a location other than the EPR Symposium of the Rocky Mountain Conference held annually in Denver, USA. This change in location for this 1997 is to foster an international spirit for the IES.

After considerable discussions and on the advice of five committees, the 1997 recipients of recognition from our Society are as follows:

Gold Medal for Biology/Medicine: Harden McConnell, USA; Silver Medal for Chemistry: Hanns Fischer, Switzerland; Silver Medal for Instrumentation/Physics: Roger Isaacson, USA; Silver Medal for Biology/Medicine: Anatole Vanin, Russia; Young Investigator: Robert Bittl, Germany.

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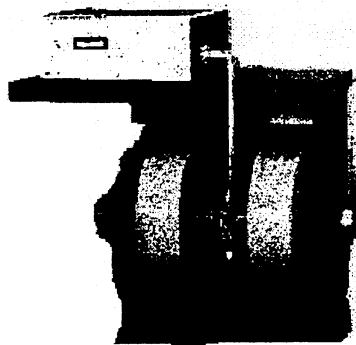
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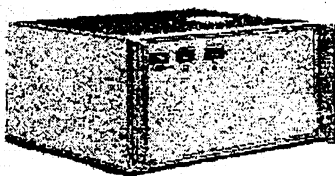
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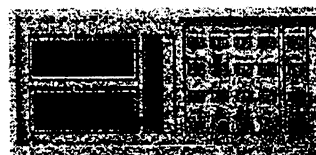
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The achievements of this group are well known to many of us. In forthcoming issues of this Newsletter, we will be describing their accomplishments in EPR. Also, independent of Arthur and me, I hope everyone extends congratulations to these well-deserved awardees.

Our awards not only serve to recognize outstanding contributions, but they also maintain interest in the field of EPR. To achieve these goals, the International EPR (ESR) Society must maintain its membership. Therefore, I urge you to keep your membership current so that we can continue to operate as a Society. Please check on the World Wide Web for your current membership status. To update your membership please contact your local treasurer or Balaraman Kalyanaraman, our Treasurer. Presently, we are operating in the red financially and need your help. We will be unable to function as a Society unless we are financially sound.

Sincerely, Jim Norris

From the Secretary—

John Pilbrow, new Secretary of the IES for a three-year term - to September, 2000 (see EPR Newsletter, v. 7 #4 and the Editor's column above) - writes "I shall count it an honour to work with my friends at Illinois and with Jim Norris and Raman Kalyanaraman." All IES members should feel free to contact John about any matter of Society policy or practice. John's E-mail address is: john.pilbrow@sci.monash.edu.au.

IES Awards —

Previous IES Awards Winners

IES Gold Medal: 1992-George Feher; 1993-James Hyde; 1994-Jack Freed; 1995-Sam Weissman (Chemistry); 1996-Kev Salikhov (Physics & Instrumentation); 1997-Harden M. McConnell (Biology & Medicine). **IES Silver Medals/Biology/Medicine:** 1994-Hal Swartz; 1995-Lev Blumenfeld; 1996-Ron Mason; 1997-Anatole Vanin. **IES Silver Medals/Chemistry:** 1994-Keith McLauchlan; 1995-Clyde Hutchison; 1996-Klaus Möbius; 1997-Hanns Fischer. **IES Silver Medals/Physics/Instrumentation:** 1994-Wojciech Froncisz; 1995-Jan Schmidt; 1996-Johann-Martin Spaeth; 1997-Roger Isaacson. **Young Investigator Awards:** 1994-Devkumar Mustafi (Univ. Chicago); 1995-R. David Britt (Univ. California); 1996-Gunnar Jeschke (Univ.

Bonn); 1997-Robert Bittl (Techn. Univ. Berlin). A listing of the Fellows of the Society appears on page 1.

Nominations for Each Year Due by Jan. 1 of That Year.

We repeat here the Society's award policies: Awards are not restricted to IES members, but the committees may take membership into account when deciding on the award winners. Each year, three major awards, the IES Gold Medal, the Bruker Prize, and the Zavoisky Prize, are devoted to the recognition of outstanding achievements in EPR. By agreement between the British and Russian Groups and the IES, we co-operate in the award of the Bruker and Zavoisky Prizes and our Gold Medal Award each year. Each group is invited to make input into the selection of each, but the final choice is left to each group. The area of research interest rotates among the groups each year, with the three following loosely-interpreted categories: chemistry, physics and instrumentation, and biological sciences (including medicine). These categories are to be interpreted very liberally.

Prof. Larry Berliner is the continuing Chair of the IES Gold Medal Award Committee.

Gold Medal: Send nominations for the annual Gold Medal, recognizing benchmark contributions to EPR spectroscopy, to Prof. Larry Berliner, Chairman of the Gold Medal Committee. (Send E-mail to berliner@chemistry.mps.ohio-state.edu.) The Gold Medal will stress contributions in Chemistry for 1998, and in Physics and Instrumentation for 1999; send nominations to Prof. Berliner by January 1.

Silver Medals: Three annually, i.e., one each for outstanding EPR work in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine. Please send your suggestions, preferably prepared as full nominations, to the appropriate Silver Awards Subcommittee(s): *For Chemistry* - Bruce Gilbert, Chair (bcg1@york.ac.uk), N. Hirota, Jim Bolton, and Kev Salikhov. *For Physics and Instrumentation* - John Pilbrow, Chair (john.pilbrow@sci.monash.edu.au), George Feher; and Jan Stankowski. *For Biology/Medicine* - Harold M. Swartz, Chair (harold.swartz@dartmouth.edu), Marjeta Sentjurc, Hideo Utsumi, and Tadeusz Sarna.

Young Investigator Awards: One Young Investigator award each year; "young" means being under 35 on January 1 of the award year. Send nominations to Prof. James R. Norris, Jr. (E-mail to j-norris@uchicago.edu).

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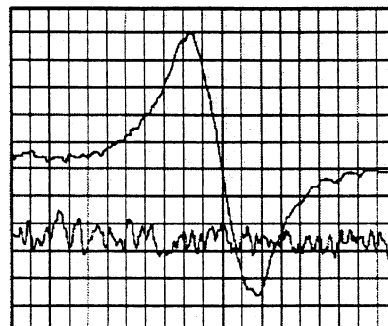
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Fellows of the Society: The IES Fellowships recognize truly outstanding contributions and achievements in electron paramagnetic/spin resonance among distinguished scientists (hopefully, IES members) who are either retired or are close to retirement. As the highest international standards are to be applied to the recognition of those worthy of this distinction, their formal connection with the Society will enhance its own image. Send confidential nominations for the Committee's consideration by January 1 of each year to Prof. James R. Norris, Jr., Univ. Chicago, Dept. Chemistry - Searle 133, 5735 S. Ellis Ave., Chicago, IL 60637 USA; ☎: 1-312-702-7864; FAX: 1-312-702-0805; E-mail: j_norris@uchicago.edu.

THE COMPUTER CORNER

*Edited by Keith P. Madden, Reef (Philip D., II) Morse,
Graeme Hanson, Dave Duling & Richard Cammack*

The EPR Computer Corner is a regular feature of the EPR Newsletter. It is managed and edited by:

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Items for this column may be sent to any of the above authors. Submissions may be edited for publication.

EPR-List Server Upgrade

by Reef Morse

Xenon, our trusty VAXStation 3100, will be replaced with an SGI server. We haven't chosen our new list server software yet and so procedures for joining the EPR list aren't determined as of the date of publication. However, if you want to join the list, contact me at reef@xenon.che.ilstu.edu and I'll put you on it. As soon as we determine our list server software, we'll publish new information about how to subscribe to and unsubscribe from the list.

EPR Software Database

by Yang C. Fann

We are currently updating the software database established by Richard Cammack to ensure that it contains the most useful programs in the most accessible format. The present list of 180 programs will be put into an archive that will be accessible through the web at the site of the Illinois EPR Research Center. We will have a more up-to-date list of programs which are frequently accessed by users. At this stage we'd also like anyone who has contributed to the software database to contact Yang C. Fann (fann@niehs.nih.gov). NIH/NIEHS, P.O. Box 12233, Research Triangle Park, NC 27709, USA; FAX: 1-919-541-5737. Programs submitted will be installed on

the web and ftp sites at the Illinois EPR Research Center (<http://ierc.scs.uiuc.edu> or direct to <ftp://ierc.scs.uiuc.edu>).

Computer Simulations - XSophe - Sophe

by Graeme Hanson and Kevin Gates

Computer simulation of EPR spectra provides a quantitative method for the determination of Spin Hamiltonian parameters which are required for the elucidation of structural information from paramagnetic materials. With the advent of true multifrequency (200 MHz to 250 GHz) EPR spectroscopy, characterisation of more complex multi-electron spin systems is achievable. Unfortunately EPR spectra from these multi-electron spin systems can exhibit energy level anticrossings, looping transitions and significant state mixing. A consequence of these effects is that the use of perturbation theory for the analysis of these systems is no longer valid and thus matrix diagonalisation becomes the preferred method.

Development of Sophe and XSophe involves a collaboration between the Centre for Magnetic Resonance and the Department of Mathematics at the University of Queensland and the EPR Division of Bruker Analytik. The software suite provides scientists with an easy-to-use research tool for the analysis of isotropic, randomly orientated and single crystal continuous wave electron paramagnetic resonance spectra.

Sophe is a sophisticated computer simulation software suite, written in C++ using the most advanced techniques, including the SOPHE partition and interpolation schemes and the segmentation algorithm. The functionality of *Sophe* is shown below.

Experiments

- Energy level Diagrams
- Transition Surfaces
- Continuous Wave EPR Spectra
- Pulsed EPR Spectra (under development)

Spin Systems

- Isolated
- Magnetically Coupled
- Supports an unlimited number of electron and nuclear spins
- Each nucleus can have multiple isotopes

Continuous Wave EPR Spectra

- Solution Spectra
- Randomly Orientated Spectra
- Single Crystal Spectra
- Symmetries:
 - Isotropic
 - Axial
 - Orthorhombic
 - Monoclinic
 - Triclinic

Methods

- Matrix Diagonalisation
- Sophe Interpolation
- Homotopy (under development)
- Perturbation (1st, 3rd Order for Superhyperfine

Interactions, 3rd order under development)

Optimisation (Direct Methods)

- Hooke and Jeeves
- Simplex
- Simulated Annealing
- Spectral Comparison

Raw Data

Fourier Transform

Sophe employs matrix diagonalisation and overcomes lengthy computational times through the use of a novel partition scheme for partitioning the unit sphere (Figure 1a),^{1,2} an interpolation scheme involving a combination of cubic spline (for calculating B_{res} and $1_{\mu ij}$ ^{1,2} along the edges of the spherical triangle) and linear interpolation (for calculation of the points within a triangle, Figure 1b) and a segmentation method for handling multiple resonances between a given pair of energy levels.² The Sophe package can be used to simulate a variety of EPR spectra arising from isotropic organic radicals to complex coupled spin systems described by the spin Hamiltonian:

$$H_{Tot} = \sum_{i=1}^N H_{A_i} + \sum_{i,j=1, j \neq i}^N H_{A_i, j}$$

$$H_{A_i} = \underline{S}_i \cdot \underline{D}_i \cdot \underline{S}_i + \beta \underline{B} \cdot \underline{g} \cdot \underline{S}_i +$$

$$\sum_{k=metal, ligand} \underline{S}_{i,k} \cdot \underline{A}_k \cdot \underline{I}_k + \underline{I}_k \cdot \underline{Q}_k \cdot \underline{I}_k - \gamma_k \underline{B} \cdot \underline{I}_k$$

$$H_{A_i, j} = J_{A_i, j} \underline{S}_{A_i} \cdot \underline{S}_{A_j} + \underline{d}_{A_i, j} \cdot \underline{S}_{A_i}$$

$$\times \underline{S}_{A_j} + \underline{S}_{A_i} \cdot \underline{D}_{A_i, j} \cdot \underline{S}_{A_j}$$

An example of the computational efficiency of Sophe is shown in Figure 2, which displays spectra for a Cr(III) spin system, $g_e = 1.990$, $D = 0.1 \text{ cm}^{-1}$, $E/D = 0.25$, $g_n = 1.50$, $A_x = A_y = 120 \times 10^{-4} \text{ cm}^{-1}$, $A_z = 240 \times 10^{-4} \text{ cm}^{-1}$, $\nu = 34 \text{ GHz}$.

XSophe provides an X windows Interface for Sophe allowing the creation of multiple input files for Sophe, and the display of sophelog and input files. XSophe allows transparent transfer of EPR spectra and spectral parameters between XSophe, Sophe and Xepr, using state of the art

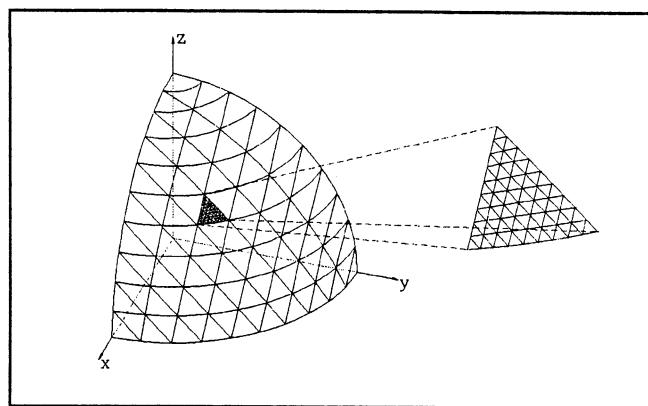


Figure 1: (a) Sophe Grid; (b) Sophe Interpolation Scheme.

platform independent Corba libraries. This interactivity allows XSophe to run and interact with Sophe on the same computer or on remote hosts located on the same subnet or across the world. XSophe can run Sophe interactively or in batch modes (foreground, background and queues).

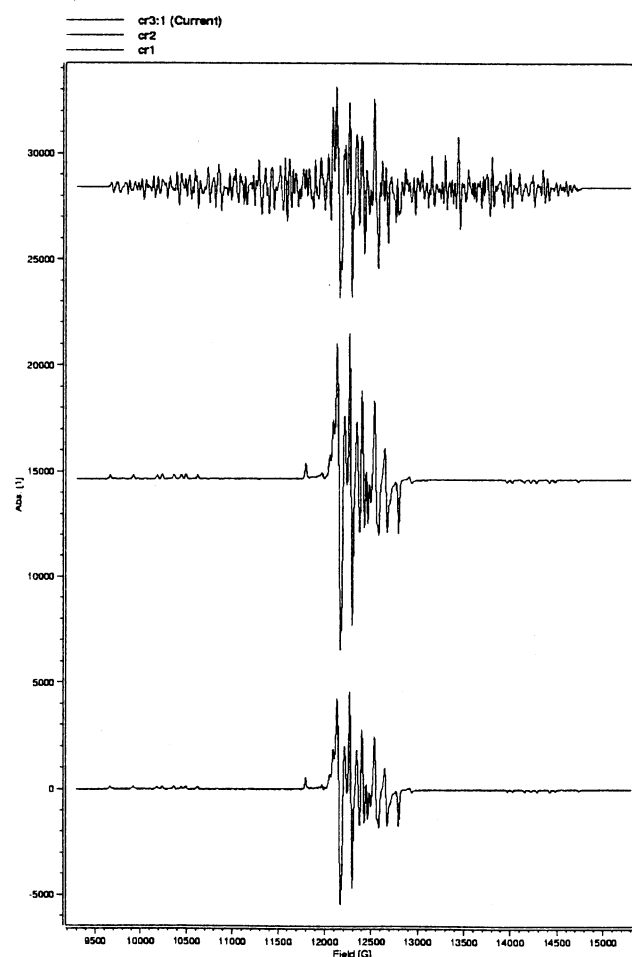


Figure 2: (a) without Sophe interpolation, $N=18$, time = 32 sec; (b) with Sophe interpolation, $N=18$, time=1.3 min; (c) without Sophe interpolation, $N=200$, time=58 min. Run on a Silicon Graphics Solid Impact R10k. Computational times increase by a factor of 2 for a Silicon Graphics O2 workstation.

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1. Wang, D. and Hanson, G.R., J. Magn. Res. A, 1995, 117, 1.
2. Wang, D. and Hanson, G.R., Appl. Magn. Res., 1996, 11, 401.

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Programming with Pictures

by Ray C. Perkins, Resonance Technologies, Inc.
and Bill Leece, IERC, University of Illinois at Urbana

The Paradigm

For those of us with a little or a lot of gray around the temples, computer programming requires the creation of "instructions" formed from a limited though precise "language." These "instructions" are assembled in a sequence of logical steps which, when "executed," provides the desired calculation or communication. Though effective, this "code" paradigm leaves much to be desired. Its reliance on arcana, namely the "language," and non-intuitive structure makes its use the purview of experts. Meshing code from multiple programmers (or the same programmer over time) into a single, coherent whole is difficult in the best of cases. Indeed, programming styles are sufficiently personal as to render one person's code indecipherable by others. Finally, and perhaps a corollary to the previous statement, the interface between the code's function and the operator who seeks to exploit that function has to be layered on, largely as an afterthought. How many thousands of line of code sit unused since the day of departure of the graduate student who wrote them? The door is left open, then, for a fundamentally different programming paradigm which makes up for these shortcomings without loss of effectiveness. Our experience suggests that "G" for "Graphical" programming is that paradigm, particularly for instrument control.

"G" programming, as the name implies, consists of selection, placement and connection of graphical objects into the logical assembly demanded by the task at hand. The "object" might be as simple as a numeric input (or output) or as complex as a multi-dimensional array. It might be a "button" designated as a control element or "light" used as an indicator of task completion. Much, of course, depends on the depth of the object library (The development software used in this project, LabView from National Instruments, has a well-rounded collection of object libraries.). The objects, specifically those which interact with the operator, can be moved and grouped in logical patterns, e.g. all the input controls for a specific device can be grouped together. Likewise, output graphs and charts can be positioned as desired. Numerous tools such as matrix mathematics, iterative or conditional operators and sequential execution are also provided as graphical objects. To the point of this project, communications tools such as serial and GPIB objects are included as libraries as well.

One advantage of this approach is immediately

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obvious: *the operator interface, that is, the presentation of the software to the operator, must be created as the software is written.* If for no other reason, this apparent stricture is a huge benefit in the development of operator-friendly "code." Some examples will be provided in the next section which describes the project itself.

The Project

We, Res-Tech, and the Illinois EPR Research Center collaborated on the development of precision field control of superconducting magnets, especially for the multi-Tesla scans required for transition metal research. For this project, we controlled and/or monitored two magnet power supplies and four magnetic field and current measurement devices. LabView-based software was developed which incorporated these devices into a variety of experiments ranging from simple device testing to step-by-step control of drive current and "automatic" reading from four measurement devices. Device readings were displayed graphically and numerically in "real time." Data was organized and "stored" in formats compatible with most database software. The results of our work were quite interesting, but are the subject of another day. The G-Programming "code" is the grist for today's mill.

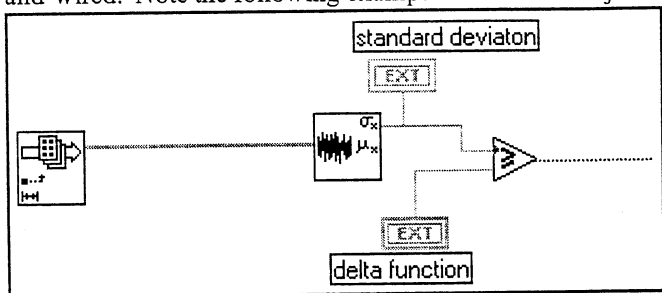
The "Code"

Below is the section of the "code" developed for operator interaction with one of the magnet power supplies:

Hopefully, the various input parameters are self evident (this particular supply has a soft-settable maximum current, "Vmax"). The important point, the crucial point, is that *this display is the code*, one portion of it. Having selected and

Scan & Power Supply Input	
Scan Time (Min.)	<input type="text" value="2.00"/>
# Data points	<input type="text" value="10"/>
Drive Voltage	<input type="text" value="10.00"/>
V Max	<input type="text" value="10.00"/>
Current Start	<input type="text" value="0.0000000"/>
Current Stop	<input type="text" value="0.0000000"/>

positioned the object it must subsequently be "wired" (LabView jargon for making inter-object connections) into the object for which it is a control. For example, the "#Data Points" is the index on a graphically-selected-and-wired "For" loop. "Current Start" and "Current Stop" are boundaries of the magnet drive current to be tested and are inputs in a GPIB command icon, also graphically-selected-and-wired. Note the following examples of "wired" objects:



In this example, the standard deviation of a segment of an array formed by successive readings of the magnet drive current (the leftmost object) is compared to an operator preset value, the "delta function." If the "standard deviation" is equal to or less than the "delta function," we know that the drive current has stabilized. The array object and the mathematical operator are both selected objects from the library. The central object is a "canned" routine specifically designed to perform statistics. Lastly, though it may not be obvious from the display as reproduced, the "wires" differ, depending on data type. Here, the thicker line from the array object to the statistics object indicates that array data "passes" along this path. The thinner wires represent single numbers.

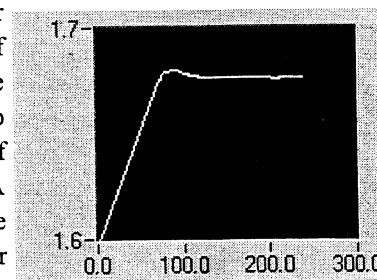
Hopefully, a small sense of the power of G-programming begins to emerge. An enormous range of selectable objects virtually (no pun intended, National Instruments calls software developed with LabView, "Virtual Instruments") defines the operator interface as the programming occurs. Another library of operators are available to "wire" the control inputs into the requisite control and data collection objects. Finally, graphical and numeric output is provided through yet other objects. Powerful editing and debugging tools round out the developers arsenal.

So far, so good. "Code" is developed that almost insists on concurrent creation of the operator interface. Wide-ranging libraries of tools allow objects to be "wired" in logical fashion. However, the resulting planar structure of the "code" can itself create problems, one of which we had to overcome in the course of our work.

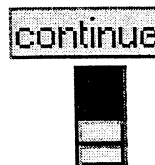
Thorns Among The Roses

G-Programming is at least two-dimensional (the use of the G-Programming analog of "subroutines," the "subVI," effectively adds further dimensions to the "code" and its

operation). "Code" is created through the "wiring" of objects in a "plane" as opposed to the linear nature of more traditional programming approaches. Therefore, one of the tricky aspects is the determination of "when" an operation occurs, particularly in relation to another. For example, one experiment type required the tuning of a measurement device following a current ramp. Only then could reasonable data be collected. We discovered, however, that our stabilization monitors (a portion of which is shown above) and data acquisition from other measurement devices attempted to execute 6 "concurrently." Our solution was the use of real-time display of the drive current coupled to soft-button initiation of data acquisition. A typical display of drive current during and after a ramp is shown here:



For each current ramp initiated, this display of drive current versus time popped up - that is, replaced the "front panel" display with this image. As the drive current was measured, statistical calculations were performed to insure settling. Upon successful convergence of the drive current, the display popped down, replaced by the front panel graphics. This pop-up/pop-down cycle told us that the current had indeed stabilized and that we were free to adjust tuning or perform other tasks as required. Pressing a soft-button initiated simultaneous acquisition of data from all devices prior to starting a new current ramp.



One other potential problem is execution speed, particularly in the interpretive mode. However, the code can be compiled and speeds comparable to those of more traditional programming modes achieved.

One Bottom Line

Perhaps one of the most telling observations we can pass along is how little time it took us to program the software for this project: 120 person-hours! Start to finish, top to bottom, 120 hours total. In less than three weeks we'd successfully written and debugged routines comparable to those required for simple spectrometer control. For me (Ray Perkins) this is astonishing efficiency as compared to my experience at several instrument companies. Despite its noted shortcomings and cost (this stuff is not cheap) G-Programming is a remarkably efficient and effective collection of tools — even for gray haired programmers like some of us!

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EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

MAGNETIC RESONANCE ON SINGLE MOLECULES

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Introduction

Most EPR and NMR experiments make use of a direct detection of the magnetic resonance signal. This has the advantage of a wide applicability; however, it notoriously lacks sensitivity since low energy microwave or radiofrequency photons have to be detected. One thus is limited to a minimum number of 10^{10} - 10^{12} spins in an EPR experiment and 10^{16} - 10^{18} spins in an NMR experiment. It has been known for almost two decades that optical magnetic resonance detection techniques (ODMR: optically detected magnetic resonance) yield a considerable increase in sensitivity mainly due to the higher photon energy in the optical regime. On the basis of this technique, experiments on as low as 10^5 electron and nuclear spins have been reported in literature. There is, however, no physical reason why this should be a minimum number by principle since it is known that optical photons can be counted individually. In 1993 two groups demonstrated independently the feasibility of an ESR experiment on a single molecule -

i.e., the probing of an individual electron spin (1,2). It is the purpose of this contribution to give a brief introduction into the technique.

Optical Selection and Detection of Single Molecules

A prerequisite for a magnetic resonance experiment on single electron spins is the isolation and detection of individual molecules. In the present case this is done by optical means (3). Several ways have been accomplished in the past five years to detect individual chromophores. Most notably, it is possible to detect individual molecules by microscopic techniques (near-field and confocal microscopy) on surfaces at room temperature (see Fig. 1). In this technique, highly fluorescent dye molecules like the laser dye Rhodamine 6 G are detected in thin solid films on surfaces with highly efficient fluorescence detection (4,5). An alternative way opens up at low temperature ($T < 10\text{K}$) where a special class of dye molecules embedded in certain matrices allows a spectroscopic selection of individual chromophores. A typical such system is pentacene (PC) embedded in a p-terphenyl (PT) single crystal. In this system the homogenous line width of the strongest allowed optical transition between the singlet ground state (S_0) and the first excited singlet state (S_1) reaches 10 MHz and is totally determined by the (radiative) relaxation rate to the ground state (i.e. by T_1). Usually at low temperature the optical line shape of an ensemble of PC molecules is determined by the inhomogeneous broadening caused by the guest-host interaction. In low-concentration samples when the number of molecules is such that on average only one molecule is found in a frequency interval larger than 10 MHz it is thus possible to isolate individual chromophores by narrow band laser excitation. Usually the technique of fluorescence excitation is used since tunable narrow band dye lasers ($\nu_{1/2} < 1\text{MHz}$) have been commercially available for a decade (6). If such a laser is tuned in resonance with the S_0 - S_1 transition of a particular molecule (see Fig. 2), this molecule is able to absorb

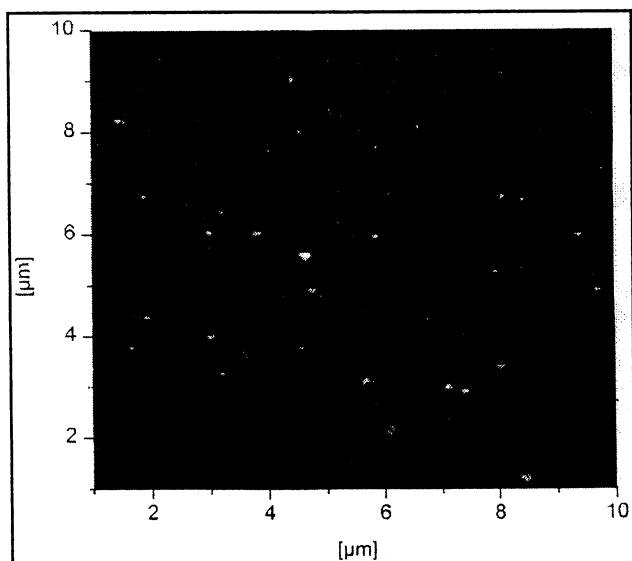


Figure 1. Confocal image of individual Sulforhodamin 101 molecules on a silica surface. The image is recorded at room temperature. Each fluorescence spot represents one molecule. The size of the spots is given by the resolution of the microscope to be roughly 300 nm. The different brightness of the spots is due to a different orientation of the molecules on the surface.

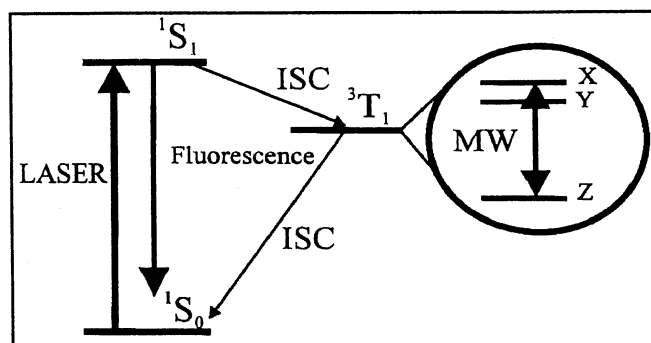


Figure 2. Basic energy level scheme of a pentacene molecule. S_0 and S_1 are the singlet states of the molecule, T_1 is the triplet state. The separation between the singlet states is roughly $17,000\text{ cm}^{-1}$. The energy separation between the singlet and the triplet state is not exactly known. The splitting in the triplet state is 1.4 GHz. The ISC probability from S_0 to T_1 is 0.5%.

photons from the laser field. Usually the molecule relaxes to the ground state via emission of a fluorescence photon. In many cases (controlled by the Franck-Condon factor) this relaxation populates one of the vibronically excited states of S_0 and is thus shifted to longer wavelength with respect to the excitation. This spectrally shifted emission is recorded as a function of the excitation wavelength. Fig. 3 depicts such a fluorescence excitation spectrum of 23 different PC molecules. As expected, each molecule exhibits an individual Lorentzian-shaped peak of 10 MHz width. This is one indication that the experiment indeed shows the optical signal of a single molecule. Other indications are the observation of quantum jumps of single molecules (7) or certain characteristics in the statistics of the photon emission.

ODMR

The detection of the electron spin resonance signal of a single molecule follows well known schemes of the optical detection of magnetic resonance. Upon being excited to S_1 there is a certain probability for the molecule to undergo an intersystem crossing process (ISC) to the lowest excited triplet state 3T_1 (see Fig. 2) instead of a relaxation to S_0 . In contrast to the singlet states S_0 and S_1 , 3T_1 is a paramagnetic state with a total spin angular momentum of $S=1$. Even without the application of an external magnetic field, the threefold degeneracy of the spin sublevels (which will be termed x,y and z hereafter) in this state is lifted due to the anisotropic dipolar interaction of the two unpaired electron spins. The ISC process from S_1 to 3T_1 is due to spin-orbit coupling, which is sensitive to the symmetry of the spin sublevels. This is why the population rates of the three sublevels usually are highly different. The same is generally true for the depopulation rate of these levels. For PC the situation is such that the x-level shows the highest population rate (150 kHz) and also has the highest depopulation rate (25 kHz), whereas the z-level hardly shows any population probability and has the longest lifetime. If now a microwave source is tuned in resonance with the transition between these sublevels (see Fig. 2), the population probability of the long lived z-level is increased. Consequently, the mean residence time of the molecule in 3T_1 is increased. Since the molecule does not emit photons during its residence in 3T_1 , a lengthening of the 3T_1 interval is equivalent to a reduction in the fluorescence intensity since the molecule is shelved for a longer time from the fluorescent S_1 - S_0 transition. This reduction in fluorescence intensity can be easily calculated on the basis of the known photophysical parameters of PC to be on the order of 20% of the fluorescence.

Fig. 4a shows an ODMR spectrum of a fully protonated PC molecule ($PC_{H_{14}}$) in PT at a small external magnetic field B_0 of 8 mT. As is evident from the figure,

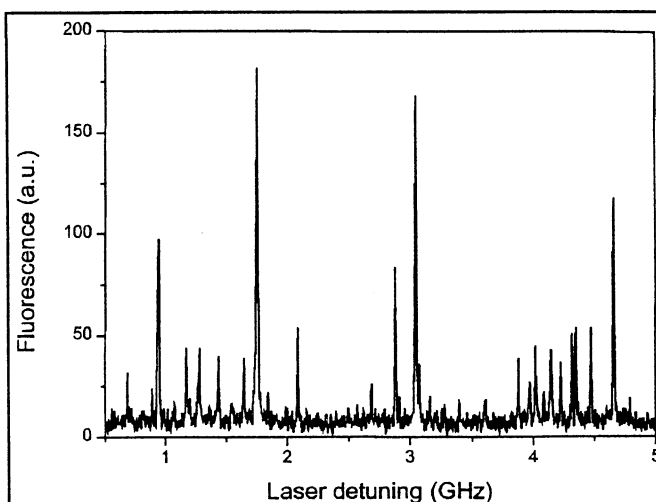


Figure 3. Fluorescence excitation spectrum of 23 pentacene molecules under high resolution laser excitation at $T=1.5K$.

two transitions are observed which can be attributed to two of the three possible transitions in 3T_1 (see Fig. 2). Both transitions are broad Gaussian-shaped resonance lines (line width 30 MHz for the x-z transition). Upon performing experiments on PC molecules where all but the central two positions of the molecule are deuterated, (Fig. 4b) a threefold-split ESR line is observed. The threefold splitting of the ESR line arises because of the hyperfine coupling (hfc) of the electron spin with the two proton spins which acquire their four possible configurations in the course of the experiment. The residual line width of the hyperfine components is given by the hfc of the deuterons. Obviously the experiment probes not just a single nuclear spin configuration in the vicinity of or at the molecule, but a large number of different configurations. The experimental result is that one observes the same ODMR line shape as if a large number of electron spins each probing a particular nuclear spin configuration is used in the experiment. The reason for the observation of a large number of nuclear spin

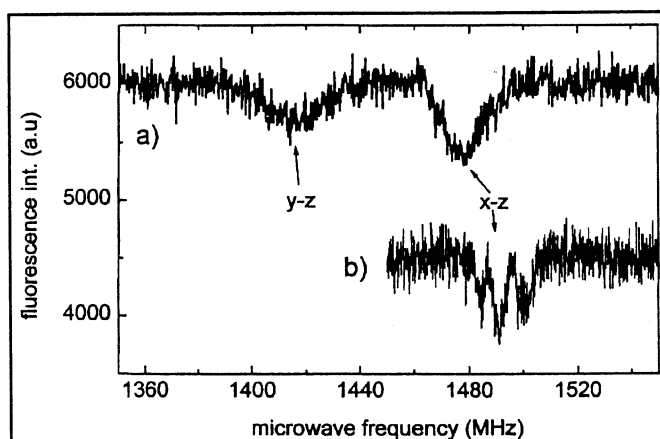


Figure 4. ODMR spectrum on single pentacene molecules. Trace a) shows the spectrum of a fully protonated molecule. The external field B_0 is 8 mT. Trace b) shows the x-z transition ($B_0=8mT$) of a pentacene molecule which is completely deuterated except for the central two positions. The splitting observed is due to the hfc of the electron spin with the two protons.

configurations in a single molecule ESR experiment is the nuclear spin diffusion process together with the long averaging time necessary to achieve a sufficient signal-to-noise ratio. This diffusion arises because of the dipolar coupling of the nuclei among each other. When the molecule is in 3T_1 , the strong hfc of the nuclei close to the molecule shifts these nuclei out of the dipolar spectrum of the nuclear spin reservoir in the bulk. These nuclei form a so called frozen core around the electron spin which contains nuclei that do not participate in the spin diffusion

process. The two H nuclei at the PC molecule (see Fig. 4b) belong to this core. As soon as the molecule resides in the singlet state these nuclei are free to participate in the spin diffusion process. On the average, a PC molecule resides for 20 μ s in the singlet interval under the experimental conditions chosen. Since the timescale on which the nuclear spin diffusion of protons takes place is on the order of some tens of μ s the duration of a singlet interval is long enough to allow for a nuclear spin flip. During the 10 min it takes to record the spectrum in Fig. 4 the molecule passes roughly 10^6 times to the singlet state such that a similar number of nuclear spin configurations is sampled. This is long enough to observe the complete inhomogeneously broadened ODMR line shape.

In order to get access to a nuclear magnetic resonance signal on a single molecule, an ENDOR type of experiment is necessary. Recently the first ENDOR signals have been successfully detected. In these experiments a Davies type pulse sequence is used. In contrast to conventional microwave detected ENDOR experiments no echo detection of the ENDOR signal has to be used since the response of the molecule to the microwave pulses can be detected without dead time problems. The ENDOR signal is a 15% change in the ESR signal intensity which requires long averaging times to achieve a sufficient signal-to-noise ratio (8).

A straightforward way to decrease spin diffusion times is to completely deuterate the guest-host system, which however still yields a too high a diffusion rate. More promising is the selection of molecules with a single ^{13}C nucleus (9). The natural abundance together with its low magnetic moment yields a spin diffusion time in the order of some seconds. Even in such systems the single molecule EPR experiment shows an inhomogeneous ODMR line shape.

Coherence

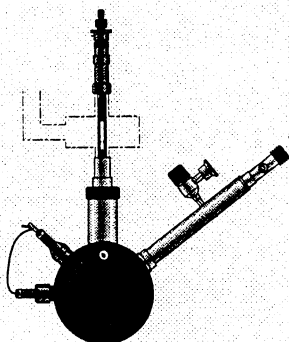
In quantum mechanics the most widely spread description of coherence is the density matrix representation. The density matrix, on the other hand, is the representation of a classical ensemble (Gibbs ensemble) in quantum mechanics. The notion of coherence and experiments on single electron spins seems thus to be contradictory. This, however, is by no means true. Every two-level system can be in one of its eigenstates or in a coherent superposition of these eigenstates. Literally coherent superposition means that it is in an "as-well-as" superposition of states. If the coherence in such a single two-level system has decayed, it is in an "either-or" superposition of eigenstates. There are distinct differences between the two forms of superposition that can, for example, be observed via the

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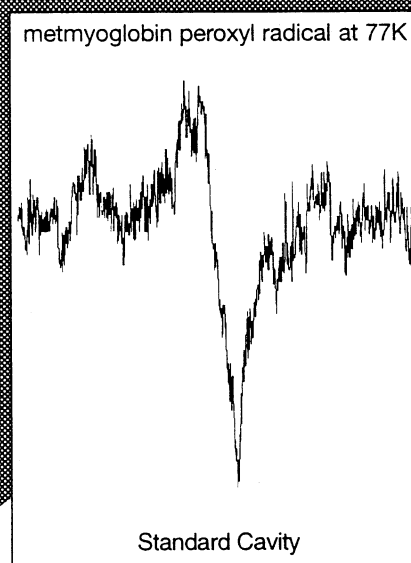
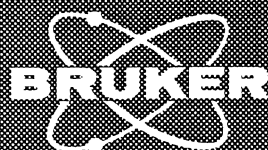
You are cordially invited to witness a major paradigm shift in EPR:

Bruker is once again raising the sensitivity threshold for solids and liquids in EPR spectroscopy. On February 6th, 1998 a public contest was held at the Oxygen Club of California (OCC) 1998 World Congress in Santa Barbara, CA to test the sensitivity of the Bruker EMX (equipped with SHQ cavity and matched bridge) versus that of other manufacturers. Initiated by Dr. Ronald Mason, the contest was refereed by Dr. Yang Fann. The premise: "There has been no advance in aqueous sample sensitivity since Varian introduced the TM₁₁₀ cavity in 1978."

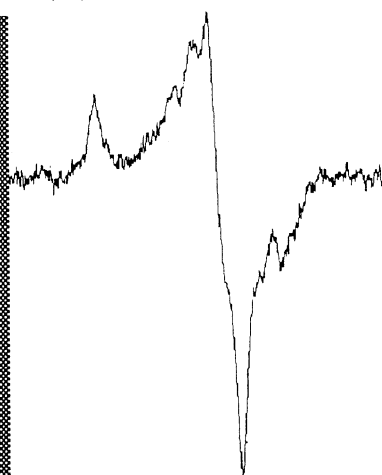
Results: The Bruker team demonstrated on that day the superior sensitivity of the EMX spectrometer with an SHQ cavity. In short: An order of magnitude greater sensitivity in the Standard Weak Pitch test. The Frozen Sample test yielded an increase in sensitivity by a factor of six. And the Aqueous Sample at Room Temperature test showed an improvement by a factor of four. (The details for each test of this contest are available, of course!)

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appearance or disappearance of interference fringes in the famous two-photon experiments in a Young double slit experiment. In addition to that, the ergodic theorem allows one to use the ensemble representation in single molecule electron spin resonance experiments as long as only time averages over periods longer than the relaxation times are taken into account.

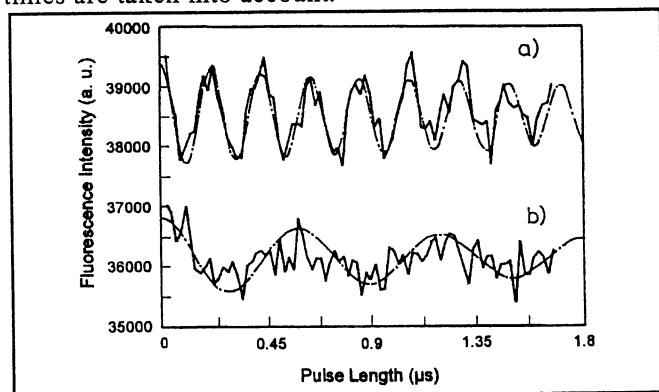


Figure 5. Transient nutations of a single electron spin. The solid curves are experimental traces and the dotted curves are the result of a simulation. Curve b) is recorded with a microwave power attenuated by 10 dB with respect to curve a).

The classical example for a coherent interaction between microwave (radiofrequency) irradiation and matter is the observation of transient nutations. Fig. 5 shows such an experiment carried out on a single molecular triplet electron spin (10). The experiment is the result of a time average over roughly 10 min equivalent to some 10^6 triplet events. In the experiment, the microwave pulse length is increased gradually. The microwaves are irradiated in resonance with the transition between the x- and z-spin sublevel. When the molecule undergoes an ISC process to 3T_1 , it populates the x-sublevel with highest probability. Since this level is short lived its occupation results in a high fluorescence intensity. Upon irradiation with MW pulses of increasing length the population probability of the long lived z-level gradually increases, as is evident from Fig. 5 by the initial decrease in fluorescence intensity. For a pulse length longer than a π pulse the reduction is gradually reversed. From Fig. 5 it becomes apparent that the single molecule experiment is equivalent to the classical ensemble experiment. The important thing to note here is that a coherent superposition of states is created upon applying a microwave pulse of proper length. However, upon measurement the superposition is projected into one of the eigenstates. The probability of being projected in one particular state is given by the square of the expansion coefficient of that particular eigenstate in the coherently superposed state. One thus measures projection probabilities instead of populations, which is the notion in ensemble experiments. Time-averaged projection probabilities, however, yield the same physical results as

measuring population numbers, as ensured by ergodicity. Differences between single molecule experiments and ensemble studies only arise when no temporal average is carried out. If for example in a nutation experiment no temporal average is carried out, the cease of coherence after for example a $\pi/2$ pulse can be detected as an increase in the fluctuation of the observable of the experiment, i.e. the fluorescence intensity. The reason is that for a $\pi/2$ pulse, the projection probability into the x-state and thus the measurement of a high fluorescence intensity and the probability to be projected into the z-state is equal. This means that each time after a $\pi/2$ pulse has been applied, either a low or high fluorescence intensity and thus a maximum variance is measured. It is this point where single spin experiments and ensemble studies yield completely different results.

Outlook

A variety of different magnetic resonance experiments on single molecules have been performed. Among these are pulsed experiments like echo studies on single electron spins (11), the detection of the hyperfine interaction of a single electron spin and a single nuclear spin (9), as well as ENDOR experiments on single molecules. All such experiments have been carried out on one system: pentacene in p-terphenyl. It is thus one of the major tasks to introduce new systems to the technique. It is expected that due to the high constraints with respect to the photophysical properties, there will only be a very limited number of systems accessible to single spin ESR. However, experiments on basic properties of quantum mechanic can be performed very well with the system used for the present experiments and the detection of the quantum projection noise shortly mentioned in the last paragraph is one example of this class. Investigations on the spinor properties of single spin $1/2$ nuclei could be another field of interest. However, it is the personal belief of the authors that the true potential of the technique lies in the combination with microscopic techniques (see Fig.1). Experiments on single molecules at room and liquid helium temperatures have already been performed with near-field optical microscopy i.e. with a lateral resolution on the order of 50 nm (12). By use of magnetized near-field apertures, extremely high magnetic field gradients can be created in the vicinity of the molecule. With such an experimental arrangement, magnetic resonance imaging with Å resolution is feasible (13). This is not limited to single molecules, but defect centers in semiconductor, quantum dot and well structures will be accessible by this technique. The combination of magnetic resonance spectroscopy and microscopy will finally build the bridge between experiments on single quantum systems addressing fundamental properties of

quantum mechanics and spectroscopy on technically relevant materials.

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Building the Perfect Beast

by Chris Bender

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LOOP PROBE COUPLERS AND COPING WITH MICROPHONICS

Various EPR sample resonator designs are facilitated by coupling to coaxial transmission lines via probes or loops, which are typically some variant of a grounded wire loop or exposed inner conductor of a coaxial transmission line. For prototyping work, it is quite easy to fabricate a probe by exposing a section of the center conductor in sem-rigid coax cable and then form the desired probe from that. But crude approach is not always suitable for the spectrometer because of microphonics (the wire is exposed) or non-optimal geometry (impedance factor). Some useful construction hints may be revealed by dissecting some old coaxial klystrons.

Figure 1 depicts the inductive coupler of a klystron oscillator. One of the first design features that is striking is that the loop is embedded in a dielectric material that ensures rigidity. This feature will reduce the possibility of microphonic noise that arises from minute movement of the wire. A suitable dielectric plug can be made from Rexolite rod that is cut in half, inner face milled to accept the wire (a Dremel tool with milling accessory and small

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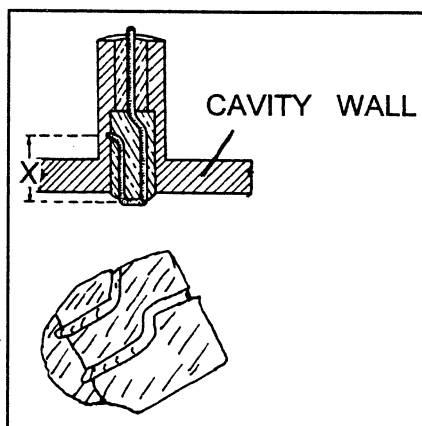
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round bit works well; Figure 1, bottom), and then glued back together.

An interesting point may be made regarding the length of the loop. According to Huggins *et al.*, if the length corresponds to $\frac{1}{4}\lambda$

the loop will behave as a probe (i.e. exposed inner conductor of milled to accept the wire loop; a second piece of coaxial line), whereas a length of $\frac{1}{2}\lambda$ will enable magnetic coupling (a grounded loop). The difference between the two modes of operation has to do with the resultant impedance, and the surface area covered by the loop dictates the tuning range (*i.e.* effective bandwidth) of the coupler.

Reference: Huggins, W.H.; Zeidler, H.M.; Manning, L.A. in *Very High Frequency Techniques*, Volume 2. Radio Research Laboratory Staff. McGraw-Hill, New York 1947. p878ff.



CONFERENCE REPORT

EPR METHODOLOGIES — WAYS OF LOOKING AT ELECTRON SPINS

by

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<http://www.du.edu/~seaton/eprsym.html>

There was a time within the memory of most spectroscopists (and almost all people who control funding!), when almost all EPR was CW, linear, and X-band. The image was that expressed by a colleague who, in a different context, dedicated his book to WOCP

(wiggles on chart paper). Today, EPR is a much different field. There are unpaired electron spins in most samples, from materials science to biology, and one or another of the EPR methodologies is the technique of choice for using the physics of spins to peek into the secrets of nature.

The 20th International EPR Symposium, Denver, CO, USA, August 3-7, 1997, emphasized the many ways to look at spins. Since it was the 20th year we hoped to have at least 20 ways represented in the papers at the Symposium. Actually, there were close to 40 different EPR techniques presented in the papers at the Symposium.

Even some people at the Symposium were surprised to be reminded of the richness of the field, and urged us to make available the list we presented at the opening of the Symposium. We do that here, with a few references, and with the addition of the techniques our colleagues presented with "here is another for your list!" We hope this list will be stimulating, and maybe even useful in expanding the perspective of those whose view of the future influences the resources available to use the power of EPR.

Some of the EPR methods that have been published are listed below. Here we focus entirely on ways to manipulate the spins to obtain information, not the chemical or biological methods of performing studies, such as spin trapping or site-directed-spin-labeling. Any such list is arbitrary in so far as distinction is made or not made between two methods, but the primary message is that many methods have been used to study electron spins. The "normal" method, first on the list, is the most common, but is not necessarily the most powerful way to answer a particular question. We invite colleagues to tell us about recent developments in methodology and how these methods give special insights into nature.

We thank Professor Arthur Schweiger for assistance in preparing this list.

References:

Rather than give a specific reference for each technique, we provide reference to a few recent books and reviews that collectively provide a modern view of EPR.

1. Pulsed EPR: A new field of applications. C. P. Keijzers, E. J. Reijerse, and J. Schmidt, eds., North Holland, Amsterdam, 1989.
2. Advanced EPR: Applications in Biology and Biochemistry, A. J. Hoff, ed., Elsevier, Amsterdam, 1989.

3. Modern Pulsed and Continuous-Wave Electron Spin Resonance, L. Kevan and M. K. Bowman, eds., Wiley, New York, 1990.
4. A. Schweiger, Pulsed Electron Spin Resonance Spectroscopy: Basic Principles, Techniques, and Examples of Applications. Angew. Chem. Int. Ed. Engl. 30, 265-292 (1991).
5. C. Gemperle and A. Schweiger, Pulsed Electron-Nuclear Double Resonance Methodology. Chem. Rev. 91, 1481-1505 (1991).
6. Electron Spin Echo Envelope Modulation (ESEEM) Spectroscopy, S. A. Dikanov and Yu. D. Tsvetkov, CRC Press, Boca Raton, FL, 1992.
7. Proceedings of National High Magnetic Field Laboratory Workshop on Nuclear Magnetic Resonance. E. R. Andrew, T. Mareci, and N. S. Sullivan, eds., published by the Division of Sponsored Research, University of Florida, 1992.
8. A. Schweiger, Excitation and detection schemes in pulsed EPR. Pure & Appl. Chem. 64, 809-814 (1992).
9. New Applications of Electron Spin Resonance: Dating, Dosimetry, and Microscopy. M. Ikeya, World Scientific, Singapore, 1993.
10. A. Schweiger, Concepts for the Measurement of Hyperfine Structure in EPR Spectroscopy. Appl. Magn. Reson. 5, 229-264 (1993).
11. A. Ponti and A. Schweiger, Echo Phenomena in Electron Paramagnetic Resonance Spectroscopy. Appl. Magn. Reson. 7, 363-403 (1994).
12. Handbook of Electron Spin Resonance. Data Sources, Computer Technology, Relaxation, and ENDOR. C. P. Poole, Jr., and H. A. Farach, eds., American Institute of Physics Press, New York, 1994. A second volume is in press.
13. S. S. Eaton and G. R. Eaton, The Future of EPR. Bull. Magn. Reson. 16, 149-192 (1995).
14. Electron Spin Resonance. A Specialist Periodical Report, The Royal Society of Chemistry, annual publication.

A partial list of EPR techniques:

linear CW, absorption, magnetic field modulation
absorption
adiabatic rapid passage
Carr-Purcell-Meiboom-Gill
Chirp ENDOR (electron nuclear double resonance)
Chirp hyperfine spectroscopy
COSY (correlation spectroscopy)
CW, non-linear
coherence transfer ENDOR
coherent Raman beats (CRB)
DECENT (decoupled ESEEM correlated to nuclear transition frequencies)
DEFENCE (deadtime free ESEEM by nuclear coherence transfer echoes)
direct detection



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 echo-detected, with sample rotation
 echo modulation echoes
 electron-Zeeman resolved EPR
 ELDOR, CW (electron-electron double resonance)
 electrically detected EPR
 electron spin echo (ESE) decay
 electron spin transient nutations
 electron-Zeeman-resolved EPR
 ENDOR, CW (electron nuclear double resonance)
 ENDOR-edited-ESEEM
 ENDOR-induced EPR
 ESEEM, 2-pulse (electron spin echo envelope modulation)
 ESEEM, 3-pulse
 ESEEM, 4-pulse
 ESEEM, 5-pulse
 ESR-Josephson junction
 EPR-detected nuclear transient nutations
 EXSY (exchange spectroscopy)
 extended time excitation
 fast passage
 FID (free induction decay)
 FID-detected hole burning
 field-swept-echo-detected
 field-swept-FID-detected
 force microscopy
 forbidden-transition-labeled EPR (FORTE)
 FT-EPR
 FT-EPR-detected NMR
 FT-hyperfine spectroscopy
 HYEND (hyperfine correlated ENDOR)
 high-field/high-frequency EPR
 hole burning
 hyperfine decoupling in EPR
 hyperfine-selective ENDOR
 hyperfine spectroscopy
 HYSCORE (hyperfine sublevel correlation spectroscopy)
 HYSCORE, 6-pulse
 imaging, spectral spatial
 improved modulation depth
 inversion-ELDOR
 inversion recovery
 inversion-recovery-detected EPR
 in vivo EPR
 linear CW, absorption, magnetic field modulation
 linear electric field effect
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 magic-angle spinning EPR
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 multiple-quantum ENDOR
 non-linear CRB
 nuclear coherence transfer echo
 nuclear-Zeeman-resolved ESEEM
 optically detected EPR
 orientation-modulated EPR
 parallel mode ($B_1 \parallel B_0$)
 PEANUT (phase-inverted echo-amplitude detected nutation)
 PEDRI (proton-electron double resonance imaging)
 phase cycling
 phase-shifted excitation
 probe-pulse-detected HYSCORE
 progressive saturation
 pulsed ELDOR
 pulsed ELDOR detected NMR
 pulsed (Mims) ENDOR
 pulsed (Davies) ENDOR
 pulse-train-detected ESEEM
 quantum beats
 Raman heterodyne
 rapid passage
 reaction-yield detected EPR
 remote echo detection
 right-angle-spinning EPR (RAS-EPR)
 RF-driven ESEEM
 RF EPR (radio frequency)
 sample heating detection of EPR
 saturation-ELDOR
 saturation recovery
 saturation-recovery detected EPR
 saturation-transfer (ST-EPR)
 scanning tunneling microscopy-ESR
 SECSY (spin echo correlated spectroscopy)
 SEDOR-ENDOR (spin echo double resonance)
 spin-dependent recombination

spin-locked ESEEM
 soft ESEEM
 stochastic ENDOR
 strain-modulated EPR
 superheterodyne
 thermal modulation
 time-resolved
 transient nutations
 Triple
 2-D combination peak (2D-CP)
 2D-ELDOR
 2D-FT-EPR
 2D sum-combination peak ESEEM
 2+1 pulse train ESE
 zero-field EPR
 zero-field ESEEM
 zero-field pulse ENDOR

A version of this will be on our Home Page. We invite updates and comments, and especially examples of problems solved with combinations of modern methodologies.

NOTICES OF MEETINGS

NOTICE: NOTICES AND UPDATES ABOUT SOME MEETINGS ARE NOT PRINTED IN THIS COLUMN IF THE INFORMATION ARRIVES TOO LATE OR IF SPACE IS LIMITED. BUT SUCH MEETINGS MAY BE ANNOUNCED ON THE EPR NEWSLETTER WEB SITE WITH LINKS TO DETAILED CONFERENCE INFORMATION WHERE POSSIBLE. PLEASE CONTACT IERC@UIUC.EDU TO HAVE YOUR MEETING ADDED-

<http://ierc.scs.uiuc.edu/news.html>

Xth INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE IN CHEMISTRY, to be held during June of 1998, Suzdal, Russia.

For more information on this meeting, contact Dr. A. Goloschapov, Russian Acad. Sci., Inst. Biochemical Physics, Moscow, Russia (e-mail: mol@chph.ras.ru).

INTERNATIONAL CONFERENCE on BIODOSIMETRY and 5th INTERNATIONAL SYMPOSIUM on ESR DOSIMETRY and APPLICATIONS, June 22-26, 1998, Medical Radiological Research Center, Moscow/Obninsk, Russia.

The Medical Radiological Research Center of the Russian Academy of Medical Sciences (MRRC RAMS) is pleased to announce the International Conference on Biodosimetry and the 5th International Symposium on ESR Dosimetry and Applications. The Conference and Symposium are being organised by the MRRC RAMS in co-operation with the World Health Organization, the European Commission, the International Atomic Energy Agency, the Radiation Effects Research Foundation, the US Department of Energy, the Chinese Academy of Medical Sciences, GSF - National Research Center for

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Environment and Health, the German Federal Office for Radiation Protection and the Russian Academy of Sciences.

The scope of the Conference is broad but bound coherently by the themes of biodosimetry and electron spin resonance (ESR) spectrometry applied to absorbed dose measurement and analysis of a variety of radiation effects in organic and inorganic matter.

Full information on the Conference can be found at the Conference website:

<http://www.gsf.de/ESR/index.html>

or by contacting the Programme Chairman and Vice President, Dr. D. Regulla, GSF-Forschungszentrum, Institut für Strahlenschutz, Postfach 11290, D-85764 Neuherberg, Germany; ☎: 49-89-3187-2224; FAX: 49-89-3187-2517; E-mail: regulla@gsf.de OR the Conference President, Prof. A. Tsyb, or Co-President, Prof. L. Ilyin, Russian Academy of Medical Sciences, MRRC, 249020 Obninsk, Kaluga oblast, Russian Federation; ☎: 7-095-956-1441; FAX: 7-095-956-1440; E-mail: mrcc@obninsk.ru.

TWENTY-FIRST INTERNATIONAL EPR SYMPOSIUM at the 40th Annual Rocky Mountain Conference, July 26-30, 1998, Denver, CO, USA.

This traditional annual event for EPR scientists worldwide features plenary lectures, talks, extensive poster sessions, presentation of IES awards, and a manufacturers-vendors exposition as well as social events. See Web site <http://www.du.edu/~seaton/eprsym.html> for details and program. Or you may contact Prof. Sandra S. Eaton and Gareth R. Eaton, Dept. of Chemistry and Biochemistry,

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29th AMPÈRE — 13th ISMAR INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE & RELATED PHENOMENA, August 2-7, 1998, Technische Universität Berlin, Berlin, Germany.

You are cordially invited to participate in the joint 29th Congress AMPÈRE on Magnetic Resonance and 13th Conference of the International Society of Magnetic Resonance. Both conferences are part of a series of international conferences which were held successively in major cities. It is the aim of the joint conference in Berlin, 1998, to provide a forum for physicists, chemists, and biologists working in the fields of EPR and NMR and related phenomena. Junior scientists are particularly encouraged to participate.

Inquiries and further mailings: Contact Dr. F. Lendzian, Secretariat, AMPÈRE/ISMAR-98, Max-Volmer-Institut, TU Berlin, FB 5, PC 14, Straße des 17. Juni 135, D-10623 Berlin, Germany; ☎/FAX: 9-30-314-21122; E-mail: ISMAR-CA98@echo.chem.tu-berlin.de.

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XVIIIth INTERNATIONAL CONFERENCE ON MAGNETIC RESONANCE IN BIOLOGICAL SYSTEMS (ICMRBS), August 23-28, 1998, Hachioji, Tokyo, Japan.

The conference will be organized by a committee consisting of representatives of the magnetic resonance community within Japan. The organizers, Yoji Arata, Yoshimasa Kyogoku, and Masatsune Kainosho, will formulate the committee and be responsible for the program and the conference organization. The program committee will represent all major fields of magnetic resonance applied to biological systems.

At this preliminary stage it is proposed that the conference will be organized such that there are 100 lectures (including 10 plenary lectures) divided into three or four parallel sessions with the remainder of the presentations being given as posters.

For further information on the XVIIIth ICMRBS, please contact Prof. M. Kainosho, Dept. Chemistry, Tokyo Metropolitan Univ. (TMU), Hachioji, Tokyo, Japan; ☎: 81-426-77-2544; FAX: 81-426-77-2525; E-mail: kainosho@raphael.chem.metro-u.ac.jp.

WORKSHOP ON EPR STUDIES OF VIABLE BIOLOGICAL SYSTEMS (ESPECIALLY IN VIVO) AND RELATED TECHNIQUES (ESPECIALLY OXIMETRY), September 13-18, 1998, Hanover, NH.

The EPR Center for the Study of Viable Biological systems at Dartmouth Medical School, Hanover, NH, USA (Hal Swartz, PI) is pleased to announce the scheduling of the approximately 7th meeting in the series on In Vivo EPR and related studies (previous meetings include: L'Aquila #1 1989), workshop at University of Illinois (1990), Dartmouth #1 (1993), Yamagata #1 (1994), L'Aquila #2

(1995), and Yamagata #2 (1997). The meeting will take place on September 13-18, 1998 and be carried out as part of the activities of the EPR Center for Viable Systems at Dartmouth, an NIH-supported resource center.

The aim is to bring together all active researchers in this field to present the latest results and concepts in the field. The meeting will include coverage of the following general topics:

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 - C. Overhauser Imaging
 - D. Pulse Methods
 - E. Resonators
2. In Vivo Oximetry
3. In Vivo Measurements of Nitric Oxide
4. Use of In Vivo EPR for Pharmacology
5. In Vivo Measurements of Reactive Species
6. EPR Studies of Viable Cell Systems

The program, as in the previous meeting at Dartmouth, will emphasize opportunities for scholarly and personal interactions, similar to the atmosphere of a Gordon Conference. There will be oral and poster presentations, with a focus on discussions.

The anticipated logistical/financial arrangements are to have a single registration fee to cover all meals and hotel for the evening of September 13 through lunch on September 18. Financial assistance will be available for some young investigators. We estimate the total cost per person, including registration, rooms, and meals, at about \$400 for those who stay at the Hanover Inn and share a room.

If you are interested in attending, please fill out the

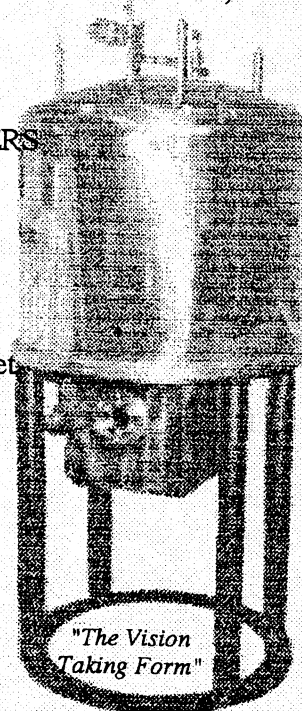
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**2nd ASIA-PACIFIC EPR/ESR SYMPOSIUM,
November 15-19, 1999, Zhejiang University, Hangzhou,
Peoples Republic of China.**

The 1st Asia-Pacific EPR/ESR Symposium was held at the City University of Hong Kong, January 20-24, 1997. The Asia-Pacific EPR/ESR Society will provide the logistic support and coordination for the organization of the future Symposia. The President of the Asia-Pacific EPR/ESR Society has recently conducted a search for an Asia-Pacific EPR/ESR group willing to host the next Symposium. After consultations with the potential hosts it has just been decided that the 2nd Asia-Pacific EPR/ESR Symposium will be held at Zhejiang University, Hangzhou, P.R. China, 15 -19 November 1999. Prof. Yuanzhi Xu, the Chairman of the Local Organizing Committee (LOC), is the member of Magnetic Resonance Special Committee, Chinese Physical Society.

Continuing with the spirit of the 1st Symposium, the future Asia-Pacific EPR/ESR Symposia is aimed primarily at the Asia-Pacific countries but will be open to participants from all over the world. The 2nd Symposium (APS'99) aims to cover all subareas of EPR/ESR. Contributions dealing with any aspects of recent developments in Theory, Methodology, Instrumentation, and Experimental Techniques are invited. The focus will be on recent applications of the EPR/ESR spectroscopy, e.g., conventional EPR/ESR, high-frequency and high-field EPR, ENDOR, ESEEM, MRI, ELDOR, CIDEP, ODMR, OPEPR. Four parallel topical sessions are planned: (1) Biology, Life and Medical Sciences, (2) Chemistry, Earth and Environmental Sciences, (3) Physics and Materials Science, (4) New Developments and Crossdisciplinary Areas.

Nominations (including self-nominations) are invited for up to eight invited speakers to deliver the plenary lectures dealing with the current most important topics. Please provide us with a short abstract of the lecture and a brief CV of the potential speaker. Make the nominations immediately (preferably by E-mail or Fax) to the President of the Asia-Pacific EPR/ESR Society or the Chairman of the Local

Organizing Committee. A selection committee will announce its decisions by the end of June 1998.

The host city, Hangzhou, is a beautiful location, especially in autumn. A famous idiom in China is: "We have Su & Hang in the Earth as well as Paradise in the sky." It means that Suzhou & Hangzhou are as beautiful as Paradise. You can directly fly from Singapore or Hong Kong to Hangzhou, and it can also be easily reached via Shanghai. From Shanghai to Hangzhou it is only 180 km, and it takes about 2.5 hours by train or by car on highway.

The Second Announcement and Call for Papers will be circulated early in 1998. If your name is not on the list of the 1st Asia-Pacific EPR/ESR Symposium participants, please provide us with your name and full address, as soon as possible.

For more information contact: Prof. Yuanzhi XU, Chairman, LOC, The 2nd Asia-Pacific EPR/ESR Symposium (AP EPR/ESRS'99), Department of Chemistry, Zhejiang University, Hangzhou 310027, P. R. China ☎: 86-571-7984095/86-571-7951352; Fax: 86-571-7984095/86-571-7951895; E-mail: xyz@public.hz.zj.cn or Prof. Czeslaw Rudowicz, The President, The Asia-Pacific EPR/ESR Society, Department of Physics and Materials Science, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong SAR, P. R. China; ☎: 852-2788-7787 Fax: 852-2788-7830; E-mail: apsepr@cityu.edu.hk.

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Contact Dr. Louis-Claude Brunel, ☎: 1-904-644-1647, FAX: 1-904-644-1366; **E-mail: brunel@magnet.fsu.edu**, for further information. Send CV and arrange for 3 letters of support to be sent to: Dr. Louis-Claude Brunel, National High Magnetic Field Laboratory, 1800 E. Paul Dirac Dr., Tallahassee, FL 32310, USA.

Position Available in the EPR Center at Dartmouth for Instrumentalist. The theme of the EPR laboratory is the use of EPR in viable biological systems, with a particular emphasis on EPR spectroscopy in vivo. This laboratory has recently been awarded a five year grant from NIH for the development of instrumentation for in vivo EPR, including development of resonators suitable for use in large animals and human subjects. Within this effort there is a need for an individual with a strong background in instrumental development and an interest in pursuing such developments on a full time basis as part of a multidisciplinary team. The principal duties will be in connection with the development of a low-field multi-quantum EPR spectrometer for in vivo spectroscopy, in collaboration with the National Biomedical EPR Center in Milwaukee. The position will involve locating in Milwaukee for much of the period of the initial appointment. Hands-on experience in instrument development is essential. The initial appointment will be for 1-2 years with the possibility of renewal.

Candidates should submit a complete CV including a description of prior experience and areas of research interests, and arrange for 3 letters of reference to be sent directly to Professor Harold M. Swartz, Dartmouth Medical School, 7785 Remsen, Hanover, NH, 03755 USA; **E-mail: harold.swartz@dartmouth.edu**; FAX: 1-603-650-1717.

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Research Assistant Professor, DNA Radiation Chemistry. A non-tenure track faculty position supported by a grant from NIH/NCI and the University of Rochester Medical Center is available. The research project is on direct damage in DNA produced by ionizing radiation. Methodologies include EPR, ENDOR, crystallography, NMR, and a variety of chromatographic techniques. Strong expertise in the application of chromatography to oligoDNA and low molecular weight derivatives of DNA components is desirable. The initial appointment will be for one year and is renewable while funding is available, currently four to five years beginning in the spring of 1998. Salary will be commensurate with experience.

Send, preferably by E-mail, a complete curriculum vitae, short summary of research interests, and names and addresses of 3 references to William A. Bernhard, Univ. Rochester Medical School, Dept. Biochemistry & Biophysics, P.O. Box 712, Rochester, NY 14642 USA. (The University of Rochester is an Affirmative Action/Equal Opportunity Employer.)
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Postdoctoral Position Available immediately or in the very near future at the University of Florida. Research requires strong background in ESR spectroscopy (CW, Bruker 300, ENDOR) to be applied to matrix-isolated species at 4 K, analysis, and interpretation of magnetic parameters. Familiarity with FT-IR and FT-Raman would be helpful. Salary \$27,000 for a year with extension to two years possible

by mutual agreement. Send CV and arrange for two letters of reference to be sent directly to Professor William Weltner, Jr., Department of Chemistry, University of Florida, Gainesville, FL 32611-7200, USA. FAX: 352-392-0872.

Postdoctoral Position for a chemist/biophysicist with background in EPR and interest in biomedical research applications available in my laboratory in the Radiation Biology Branch of the National Cancer Institute in Bethesda, MD. Send CV to Dr. Peter Riesz, Bldg 10, Rm B3B69, NIH, Bethesda, MD 20892-1002, USA. ☎: 301-496-4036; FAX: 301-480-2238.; E-mail: sono@helix.nih.gov.

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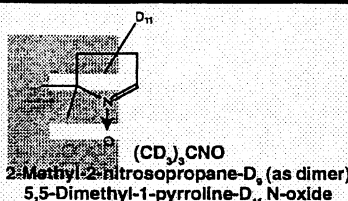
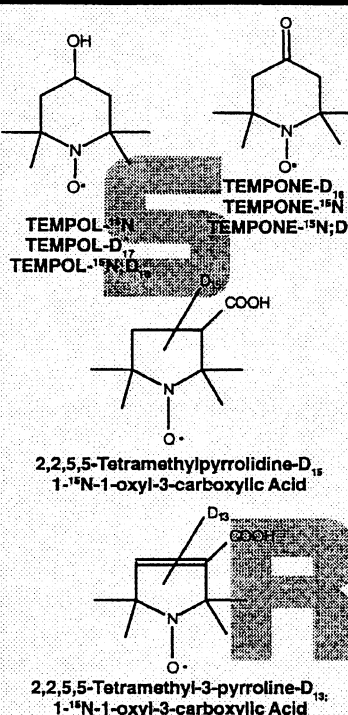
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EPR NEWSLETTER

Volume 9, Number 2

Directory Issue - Page 1

Winter, 1997-8

DIRECTORY OF MEMBERS OF THE INTERNATIONAL EPR (ESR) SOCIETY AND OF OTHERS INTERESTED IN ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY

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E-mail has become a pervasive means of communication, so having correct e-mail addresses is vital. While the directory issue published each year helps, we receive changes almost every day as e-mail systems are upgraded. To assist in communications among EPR researchers, we have put e-mail addresses on the IES WWW. This list is updated monthly. Please check your own e-mail address on the Web to see if we have the correct one. The WWW address is:

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EPR NEWSLETTER

Volume 9, Number 3

Page 1

Summer/Fall, 1998

From the Editor

With this issue of your Newsletter, we are continuing our campaign to provide for our readers citations of all significant awards and honors received by IES members and of awards made by the IES and other organizations in the general area of electron magnetic resonance. The awards have been announced here, but frequently no statement appropriate for publication has been transmitted to us introducing the awardee and explaining the reasons for the award. I applaud the IES officers, and especially John Pilbrow, the current Secretary of the Society, and Arthur Schweiger, past Secretary, for taking action to secure the missing award citations from 1995 to 1997 so that we can make them available to our readers. This issue contains eleven such citations. The citations for the 1998 IES awards (see box to the right) and others will be published in the next issue. Henceforth, all nominations for IES awards must include brief citations appropriate for delivery at the award ceremonies and for publication in the EPR Newsletter. Please note the IES Logo Competition announcement on page 5.

R.L. Belford

Awards Profiles & Announcements

Möbius Wins 1998 Ampère Prize—

Congratulations to Klaus Möbius (Free Univ. Berlin) on winning the 1998 Ampère Prize. More information will be provided in the next Newsletter.

Freed Wins Zavoisky Award 1998—

Following an extensive round of nominations from the international community of EPR scientists, the International Zavoisky Award Committee is delighted to announce that the Zavoisky Awardee for 1998 is Prof. Jack H. Freed (Cornell

1998 IES AWARD WINNERS ANNOUNCED



ARTHUR SCHWEIGER—

GOLD MEDAL

WILLIAM B. MIMS—

SILVER MEDAL

FOR PHYSICS/INSTRUMENTATION

RICHARD W. FESSENDEN—

SILVER MEDAL
FOR CHEMISTRY

EDWARD G. JANZEN—

SILVER MEDAL
FOR BIOLOGY/MEDICINE

ALEXEJ I. SMIRNOV—

YOUNG INVESTIGATOR AWARD

Univ., Ithaca, New York). He was awarded the Prize at the annual Workshop "Modern Development of Magnetic Resonance" held in Kazan 22-26 September 1998. The laureate, Prof. Freed, is distinguished for work in electron paramagnetic resonance and, in particular, his contribution to multifrequency EPR studies of molecular motion in liquids and restricted media. A more extensive citation of his work will appear in a forthcoming issue of "Applied Magnetic Resonance."

Prof. Kev M. Salikhov
Chairman, Zavoisky Award Committee

(Awards continued on page 3)

- Newsletter Editor: R. Linn Belford, Urbana, IL
- Assistant Editor, Becky Gallivan, Urbana, IL
- Typography: Martha Moore, Urbana, IL.
- This, the official newsletter of the **International EPR(ESR) Society**, is supported by the Society, by corporate and other donors, and by the National Center for Research Resources in the U.S. National Institutes of Health. For additional information including how to contact the editor, see "About This Publication" on p. 33.

FELLOWS OF THE INTERNATIONAL EPR(ESR) SOCIETY

- | | |
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IN MEMORIAM: JOHN TURKEVICH (1907-1998)

JOHN TURKEVICH, Professor Emeritus of Chemistry at Princeton University, died peacefully in his sleep in Lawrenceville, NJ on March 25, at the age of 91. Born in Minneapolis in 1907, he was educated at Dartmouth (B.S., M.S.) and Princeton (M.S., PhD). In 1930, he taught organic chemistry at Dartmouth for a year before coming to Princeton for his Ph.D. to study catalytic chemistry with Sir Hugh Taylor. After his Ph.D. work, he did postdoctoral research in quantum chemistry with J. E. Lennard-Jones (Cambridge University) and K. Bonhoeffer (Leipzig University). He was appointed to the Princeton faculty in 1936 and remained associated with Princeton throughout his career. He retired from full-time teaching at Princeton in 1975 as the Eugene Higgins Professor of Chemistry, but continued an active research career at Princeton for another 20 years. He delivered his last lecture at Princeton on October 9, 1997 at the age of 90, in his 7th decade of teaching and lecturing.

John Turkevich was a multi-faceted individual who made major contributions to several fields of human endeavor. He was a renowned teacher and lecturer at Princeton extending over 65 years. He taught for many years a popular freshman chemistry course. With his wife Ludmilla, they introduced the teaching of Russian at Princeton and the first national guide to translations of the Russian scientific periodical literature. He taught a seminar on government and science at the Woodrow Wilson School.

His contributions to public service were extraordinary. He was an expert in Soviet science and frequent advisor to the US government, giving expert testimony to congressional committees on Atomic Energy, Foreign Affairs and Government Operations. He served on the Manhattan Project for the development of atomic energy, providing the first measurement and analysis of the infrared spectrum of uranium hexafluoride, which enabled both its purification from contaminants and prediction of its thermal properties critical to isotopic enrichment. During World War II Princeton was a center for research on deuterium enrichment. With Hugh Taylor, he developed a method using catalytic exchange of heavy water. With G. Joris, Turkevich built an early isotope ratio mass spectrometer and later, he was the first to apply the new technique to the study of isotope distributions in chemical reaction mechanisms. In 1941 following the Japanese blockade of shipment of natural rubber to the U.S., he was enlisted to head a research team that developed a catalyst for preparation of synthetic rubber by dehydrogenation of butane to butadiene. He taught extensively at the National War College, Army War College, Air University, the Armed Forces College, and the Imperial Defense College (London). He was advisor to the Commanding General of the Strategic Arms Command, and the Department of State. Following the war, he founded, with R.W. Dodson, the Chemistry Department at Brookhaven National Laboratory. He was an active proponent for the peaceful uses of atomic energy, serving as U.S. delegate to the first and second U.N. Conferences in Geneva on Peaceful Uses of Atomic Energy. He founded the Office of Scientific Attaché in the U.S. Embassy in Moscow following the Stalin era, where he was a member of the executive committee. As

Chairman of the first U. S. Delegation of University Professors to the Soviet Union, he initiated the first scientific exchanges and later served as mentor for five Soviet scientists and organizer of three US-Soviet scientific conferences.

Prof. Turkevich led a distinguished research career. His research at Princeton was immediately successful, starting with the discovery in 1936 of the first process for catalytic rearrangement of inert hydrocarbon molecules—commonly found in petroleum in the form of linear chains of carbon atoms—into branched chains and rings that were far more useful. Turkevich's process proved to be critical in World War II, as it enabled synthesis of high-octane fuels that permitted a higher ceiling to be reached by the British Air Force than the Luftwaffe, and to the munitions works that needed toluene for production of TNT. This discovery was followed by the synthesis and characterization of many other catalysts for controlling the rate and course of various chemical reactions. In the late 1940s-50s, he pioneered the first and currently used method for preparation of platinum and gold micro-particles called colloids, possessing the most uniform size and catalytic properties then known. He developed the first method for obtaining high-resolution images of the surfaces of catalysts by introducing a technique known as electron microscopy. He introduced the first spectroscopic methods for the determination of the number and chemical identity of the active species on catalytic surfaces. These discoveries provided the conceptual and practical knowledge for the modern process now used for creation of high-octane anti-knock fuels (branched and ring type hydrocarbons) from low octane gasoline (linear hydrocarbons), and for hydrocarbon cracking. Platforming—a platinum reforming catalytic process—employs Turkevich chemistry for the commercial production of high-octane gasoline on a global scale. After retiring in 1975, he continued active research but moved to a new application of catalytic chemistry. He synthesized new platinum-containing molecules that are derivatives of the same family known as cis-platinum, which was discovered (by accident) to have anti-tumor activity by Barnett Rosenberg in 1969. Turkevich's candy-coated cis-platinum derivatives, as he called them, were also useful clinical agents in cancer chemotherapy. When he died, experiments were still being planned with colleagues in PMI and Chemistry. Professor Turkevich attracted many students and foreign scholars to Princeton University, and expanded its reputation as a world center for catalysis research.

As a devout Orthodox priest, Rev. Prof. Turkevich served the spiritual needs of the University for 25 years as the Orthodox chaplain and the Princeton community throughout his life. He was a spiritual father, counselor, and master of the three-minute sermon. He was loved by his colleagues, students, and parishioners, who also saw him as a role model for uniting the spiritual and scientific worlds.

John Turkevich was a loyal son of Princeton and keen Princeton sports fan. Among our last memories will be a story from a colleague who visited him the evening of the Princeton-Penn basketball game a few weeks before his death. After an hour of scientific discussions, John announced that it was time to watch the game on TV, as the outcome would determine whether Princeton kept its

undefeated record and national ranking intact. Not to be deterred by the unanticipated TV blackout of the game, he found instead a portable radio with earphones. His eyes sparkled with every Princeton basketball as he proudly announced to his visitor each new score.

Prof. G. Charles Dismukes, Prof. Walter Kauzmann,
and Prof. Donald McClure, Princeton University

Awards Profiles Continued from page one...

Profile of Anatoly Buchachenko, 1997 Voevodsky Award Winner—

It is a great pleasure for us to congratulate our colleague and friend, whose name is really well known among the radiospectroscopists, Anatoly Buchachenko (Inst. Chemical Physics, Moscow, Russia), who was recently named as the first winner of the new and prestigious Award dedicated to the memory and name of famous Russian scientist academician Vladislav V. Voevodsky.

A. Buchachenko's name is firmly associated with EPR and NMR spectroscopy and spin chemistry. His life in science always rotated around the electron and nuclear spin. The first EPR spectrum he recorded was in 1960 with the assistance of the great EPR spectroscopist Jacob Lebedev. This spectrum of a stable phenoxyl radical began two lines in Buchachenko's life: to his friendship with Jacob Lebedev, Yuri Molin, Renad Sagdeev, Yuri Tsvetkov, Nikolay Bubnov, Kirill Zamaraev and other brilliant scientists of Voevodsky community, and to his deep attachment to the electron spin. His works on EPR spectroscopy and physical chemistry of stable radicals, especially nitroxide radicals, are very well known. He was the first who suggested use of nitroxides as spin probes and spin labels. He proposed the idea of spin exchange interactions in nitroxide polyradicals via intramolecular encounters of the radical fragments, which allowed interpretation of the wonderful EPR spectra of these polyradicals. Of course, now it has mainly historical interest, but in those years it was really great. In the 1970's, Buchachenko moved into the NMR spectroscopy of paramagnetics - organic radicals and their labile, short-lived complexes with organic molecules. He has studied (in co-operation with N. Sysoeva) the paramagnetic shifts and nuclear relaxation, and found the regularities, peculiarities, and mechanisms of the spin density delocalization along the chemical bonds. He has also identified the main types of complexes of organic radicals and molecular oxygen with organic ligands. He presented criteria on how to discriminate among these complexes and how to determine which orbitals of a radical and a ligand combine to form the complex.

Prof. Buchachenko pioneered in spin chemistry; he is one of the leaders and creators of this new field of modern chemistry. He was the first to observe CIDNP ^{13}C and ^{31}P in chemical reactions. In the 80's, in cooperation with V. Berdinsky, he developed the theory of the radiowave maser with chemical pumping, and experimentally found the chemically induced radiowave emission of benzene and quinone molecules with inverted population of nuclear Zeeman levels. In 1976 he published the first paper on the experimental observation of the magnetic isotope effect. His outstanding contribution to the chemical physics of this remarkable phenomenon was summarized in his brilliant paper "MIE Versus CIE: The Comparative Analysis of

Magnetic and Classical Isotope Effects" which appeared in *Chemical Reviews*, 1995.

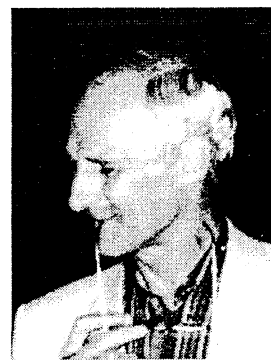
A new phenomenon in spin chemistry – the radio-induced magnetic isotope effect, when the radio frequency pumping of electron spins stimulates selective chemical reactions of the radicals with magnetic nuclei and results in the isotope separation, had been predicted and then experimentally observed by him. In recent years, Buchachenko together with V. Berdinsky has been developing the theory of spin catalysis, which implies the triplet-singlet conversion of the radical pairs induced by the presence of a third spin (a radical or an ion). This phenomenon was experimentally discovered by Buchachenko in co-operation with E. Step and N. Turro. Molecular ferromagnets and organic ferromagnetism are also priorities of Buchachenko's interests.

A. Buchachenko is known to many people from the scientific community as a very nice and friendly man, as an active, talented person consumed in science. He was recently elected (according to recommendation of the late Ya. Lebedev) the Chairman of the Russian group of the International EPR/ESR Society. We should like to wish to Professor Anatoly Buchachenko new ideas and further successes in his beloved science of spins, as well as in his hobby: the modelling of old wooden Russian churches.

A. Kokorin, A. Wasserman
Inst. Chemical Physics, Russian Acad. Sciences
Moscow, Russia

Keith McLauchlan, 1997 Bruker Prize Winner—

The 1997 Bruker Prize was awarded to Keith McLauchlan (Oxford Univ., UK), a past President of the International EPR/ESR Society. It was made for his pioneering work on flash-photolysis ESR in which he obtained the first high-resolution spectra from very short-lived radicals, providing the means for their identification in solution. Simultaneously with Barry Smaller's group in the U.S. he developed a new technology based upon a sampling principle in which the spectrum was built up from information obtained from a multitude of flashes which occurred as the magnetic field of the spectrometer was incremented, rather than trying to extract it from a single radical creation event. This led to the recognition of electron spin polarization (known as Chemically Induced Dynamic Electron Polarization, CIDEP) in radicals observed shortly after their creation. This was exploited by the Oxford group to investigate photophysics and photochemistry in solution and a wide range of kinetic processes including degenerate electron transfer, proton transfer and site exchange. McLauchlan continues to contribute to this research field, along with wider aspects of Spin Chemistry including the investigation of the effects of extremely low static and radiofrequency magnetic fields on chemical and biological processes.



John Pilbrow, Monash University
Clayton, VIC, Australia

Hanns Fischer, 1997 IES Silver Medalist in Chemistry—



Hanns Fischer (right) accepting the Silver Medal from Jim Norris

Hanns Fischer (Univ. Zürich, Switzerland) was awarded the 1997 IES Silver Medal (Chemistry) in recognition of his outstanding contributions to the application of EPR spectroscopy to the study of short-lived organic free radicals in solution. He has brought innovations and new analytical insights, both practical and theoretical, into a wide range of chemical applications including photochemical generation of radicals, CIDEP and CIDNP phenomena, kinetic studies of radical termination, and a detailed analysis of steric and polar effects, for example in addition reactions.

Bruce Gilbert, Univ. York, UK

Roger Isaacson, 1997 Silver Medalist in Physics & Instrumentation—

Roger Isaacson has been working in EPR for over three decades, joining the group of G. Feher at the University of California at San Diego in 1962, where he is still actively engaged in research.

Roger has distinguished himself in two areas. One is instrumentation; the other is the use of EPR to solve problems in solid state physics (1962-1970) and more recently problems of biological importance, e.g. the electronic structure of heme proteins and the identification and characterization of the primary reactants in bacterial photosynthesis.

In the area of instrumentation, Roger pioneered several cavity designs and detection schemes, not all of them published. Many in the EPR community turn to him for blueprints, which he generously supplies. Among his published innovations are the early use of a boxcar integrator to measure T_1 (1968), the observation of broad EPR lines using temperature modulation (1969), a novel plastic ENDOR cavity to study biological samples (1976), a new microwave coupler (1976), and a coaxial coupler for 9 GHz EPRI/ENDOR.



John Pilbrow, Monash University
Clayton, VIC, Australia

Profile of Kamil A. Valiev, Winner of the 1997 Zavoisky Award—

The Annual 1997 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professor Kamil A. Valiev (Institute of Physics & Technology, Russian academy of Sciences, Moscow) in a ceremony marking his outstanding contribution to the development of the theory of spin relaxation. The ceremony was preceded by the Sixth Annual Workshop: "Modern Development of Magnetic Resonance" 23-26 September 1997. The program of the Workshop is in meeting

The Zavoisky Award was presented September 25, 1997 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.

Previous winners of the Zavoisky Award were: W.B. Mims (1991), B. Bleaney (1992), A. Schweiger (1993), J.R. Norris, and Ya.S. Lebedev and K. Möbius (1994), J.S. Hyde (1995), G. Feher (1996).

Professor Kamil A. Valiev was selected from many nominations solicited from international experts in EPR.

In the morning of September 25, a reception for Professor Valiev by the Prime Minister of the Republic of Tatarstan, F. Kh. Mukhametshin, took place. The Award Ceremony in the afternoon was attended by over 200 people, among them were the scientists who had participated in the preceding Workshop.

K.A. Valiev gave his Zavoisky Award lecture in which he discussed problems of the theory of spin relaxation and molecular motion in liquid. A concert by a string quartet preceded and followed the ceremony. After a meeting with journalists, the guests visited the museum of history of the Kazan State University. A choral concert followed to mark the event, which was concluded with a Banquet in honor of Prof. Kamil A. Valiev and his outstanding contributions to EPR.

Profile of Johann-Martin Spaeth, Silver Medalist 1996, Physics/Instrumentation—

On the occasion of his election as the 1996 IES Silver Medal Awardee, it is a great pleasure for me to write some words about Johann-Martin Spaeth (Univ-GH Paderborn, Germany), my thesis advisor and mentor for a long time.

His scientific career started at the University of Munich where he finished his diploma work in 1962 on the topic of ferromagnetism. He then joined the group of Prof. Pick (coming from the color centre school of Hilsch and Pohl in Göttingen) at the University in Stuttgart. Martin Spaeth's Ph.D. thesis (1965) already gives witness of the magnetic resonance technique he is famous for – electron nuclear double resonance (ENDOR) on interstitial hydrogen centers in alkali halides. He continued on this subject (after marriage with an Australian girl – his wife Anne and a one year stay as post-doc in Australia) and in his habilitation in 1969 he documented a brilliant theoretical analysis of the measured superhyperfine interactions of atomic hydrogen centers using the concept of orthogonalized wavefunctions.

In 1976 he took the chair for experimental physics at the newly founded Paderborn University where he combined magnetic resonance with optical spectroscopy into what is now known as optically-detected magnetic resonance (ODMR). While at that time there were strong contributions using ODMR with luminescence detection, he and his group particularly worked on the detection via absorption – to be specific, via the magnetic circular dichroism of absorption. But also the ENDOR technique developed into more sophisticated applications like ENDOR-induced EPR (some call it field-stepped ENDOR) and stochastic ENDOR. Until 1983 defects in ionic systems were still a main research topic (including applications for tunable solid state lasers). However, in the following years his interests shifted more

Logo Competition—

The officers of the IES have announced a competition to design a logo for the Society. The prize will be one year's free subscription (for members) and a copy of *Foundations of Modern EPR* [edited by Eaton, Eaton and Salikhov].

Submissions are to be sent to the Secretary of the IES, Prof. John Pilbrow, Dept. Physics, Monash University, Clayton, Victoria, Australia 3172, to reach him by January 11, 1999. The competition will be judged by the members of the IES Executive Committee and the winner will be announced in the next possible *EPR Newsletter* and on the IES web site.

towards defect identification in semiconductors – thermal donors in silicon and intrinsic defects (EL2) in III-V compound semiconductors, to mention only some.

1987 marked the year where the full potential of magnetic resonance was combined with optical spectroscopy by optically-detected ENDOR (ODENDOR).

Taking advantage of a quantum transformation, i.e., detecting low-energy microwave quanta on high-energy optical quanta, this is not the ultimate gain in sensitivity and selectivity. Electronic devices operate in the micro-AMPÈRE range and detection of nano- and even femto-AMPÈRES is by no means impossible with state-of-the-art measurement techniques. It was, therefore, quite logical to apply magnetic resonance to actual devices and detect EPR/ENDOR via changes in the current flow or in the applied voltage. The acronym is now EDMR for electrically-detected magnetic resonance, at present one of the major activities in Martin Spaeth's group.

In the last 10 years he contributed, by various modifications of magnetic resonance, to defect identification in semiconductors, but he never forgot about his first love – defects in ionic systems – and some rumors say that the pendulum swings back towards this early research topic. Color centers useful for X-ray storage brings magnetic resonance into the area of applied physics.

Martin Spaeth, with his co-authors Niklas and Bartram, has written a well recognized book on the analysis of point defects. In his spare time he enjoys classical music, especially if it is played by his two daughters both already in academic positions.

Bruno K. Meyer
Justus-Liebig University
Giessen, Germany

Brian Hoffman, Bruker Prize Winner 1996—

Brian Hoffman got his PhD at Caltech with Harden McConnell, from whom he developed an interest in magnetic resonance while doing very little of it. After a postdoctoral year with Alex Rich at MIT he assumed a faculty position at Northwestern University, where he now is Professor in the Chemistry and Biochemistry, Molecular Biology and Cell Biology Departments.

Brian Hoffman has had a long-standing commitment to the development of advanced paramagnetic resonance techniques (ENDOR and its junior partner, ESEEM) and their application to bioinorganic chemistry. One major effort

has been to develop methods by which the structure of a paramagnetic center in frozen solution can be determined by use of ENDOR (and ESEEM) based on the electron-nuclear hyperfine and nuclear quadrupole coupling tensors of interacting nuclei. When Brian Hoffman began his work, there simply was no overall conceptual framework for characterizing the ENDOR patterns that arise in such cases. His group showed how these tensors can be determined for a frozen solution sample by analyzing the orientation-selective 2D pattern generated by collecting ENDOR spectra at multiple fields across the entire EPR envelope. They further showed how this goal can be reached by a combination of multi-frequency, multi-nuclear continuous wave and pulsed ENDOR measurements.

In another development that combined both conceptual and technical advances, his group dramatically expanded the applicability of ESEEM and ENDOR to non-Kramers doublets in an integer-spin system. Although it has been known for over forty years that such systems frequently are EPR active, recently there has been a resurgence of interest in them because they are widely exhibited by metallo-biomolecules, yet no ESEEM or ENDOR study of any type had been reported previously.

The methodological developments from Hoffman's Lab all have been in aid of his overriding goal of working to solve key problems in the structure and function of enzyme systems. These have involved: monometallic sites, such as the blue-copper centers as well as both heme and non-heme iron enzymes; binuclear sites such as the Rieske and carboxylate-bridged diiron centers, sulfite reductase, which exhibits coupling between a heme and an [4Fe-4S] cluster; the CuA, all-copper, center and the hemea-CuB center of cytochrome oxidase; proteins that contain multiple, multi-metal centers such as nitrogenase, hydrogenases, and carbon monoxide dehydrogenase. They have included the determination of ground-state structural details, but more importantly they have focused on catalytically important reactive intermediates that are refractory to other means of structure analysis. Particularly important here is work on high-valent states of peroxidases and non-heme diiron centers.

Brian Hoffman applied the Bruker Award funds to the purchase of his first cello, in futherance of a passion developed over the past few years of participating in the cello lessons of his daughter Alexandra. To date, he has received no offers from the Chicago Symphony Orchestra.

Peter Doan
Department of Chemistry and BMBCB
Northwestern University, Evanston, USA

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James S. Hyde, 1995 Zavoisky Awardee—

James S. Hyde (Medical College of Wisconsin, Milwaukee), the winner of the 1995 Zavoisky Award, needs no introduction to ESR spectroscopists. He has been a predominant figure in the instrumental and scientific developments in our field for more than 35 years! After a Ph.D. in Physics at MIT in 1959, Jim launched the first part of his famous career at Varian Associates, Instrument Division, as their leading researcher and developer of new instrumentation. By 1964 Jim, with Gus Maki, pioneered the first ENDOR experiments on free radicals in solution. Feher's great innovation of ENDOR had been confined to solid state systems, and major challenges had to be met to extend it to radicals in liquids. Also, in a key 1970 paper with Günther Rist, he showed how ENDOR in powders can succeed in providing orientational selectivity. The second great achievement of his Varian years was the development of ELDOR and its application to free radicals in solution in 1967–1968. It was my great pleasure to participate actively with Jim in this development. My experiences with Jim on visits to Varian in those years has led to a continuing friendship and source of inspiration. His final triumph in those years was his invention of saturation transfer spectroscopy, which made the study of ultra-slow motions by nitroxide spin labels accessible to the cw ESR spectroscopist.

The second phase of Jim's seminal contributions to ESR occurred (and continues) at the Medical College of Wisconsin, where he established what most of us in the field regard as the world's leading ESR Center, which has

inspired, aided, and rescued a whole generation of ESR spectroscopists. Aside from his many instrumental accomplishments and successful collaborations, let me mention his further development and perfection of saturation transfer and saturation recovery spectroscopies and his more recent developments of multi-quantum ESR, or cw ESR without field modulation. Of his many important biomedical applications of these methods, his studies of oxygen transport are clearly among the most creative and significant. Perhaps his most famous instrumental accomplishments of these years has been his development, with Wojciech Froncisz, of the loop gap resonator, which has greatly increased sensitivity in ESR to small samples, especially to those needed for biological studies.

It is a great pleasure for me to be able to write the Laudatio for Jim Hyde and I know I have the enthusiastic support of the whole ESR community when I wish him many more outstanding years of leadership in our field.

Jack H. Freed
Cornell University, Ithaca, USA

David Britt, Young Investigator 1995—

R. David Britt (U.C. Davis, USA) grew up in North Carolina in a family of peanut farmers. His early interest in science led him to obtain a B.S. degree in Physics from North Carolina State University in 1978, an M.A. in 1980 and a Ph.D. in 1988 in Physics at the University of California, Berkeley. After a further post-Doctoral year he became Assistant Professor in the Chemistry Department of the University of California at Davis and was promoted to Associate Professor in 1994. His first years in Berkeley were spent in the group of Prof. Paul Richards whose principle research is measuring the cosmic background radiation using far infra-red Fourier spectroscopic data acquired from high altitude balloon flights. It was during that time that David honed his skills as a machinist and cryogenist.

He joined my group knowing that he wanted to do magnetic resonance on a biological system. The major theme in our group is to understand the structure and function of the photosynthetic oxygen-evolving complex that oxidizes two water molecules to form molecular O₂ using the energy of four photons. This system provides the world's supply of oxygen. At the center of this complex is a cluster of four Mn atoms that act as the locus of charge accumulation.

Since the first observations of EPR in photosynthetic materials, the method has provided an enormous quantity and variety of information on the large number of one-electron carriers that result from photon absorption. To complement the X-ray absorption experiments we were performing to determine the structure and oxidation states of the tetra-Mn cluster, cw EPR measurements were used. David decided that he wished to extend the range of information attainable by performing time-domain EPR, e.g., electron spin echo and ESEEM spectroscopy.

He wrote a successful grant application to obtain the funds required to convert a direct detection spectrometer to an excellent pulsed EPR instrument. David's was the first

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pulsed instrument to employ a loop-gap resonator with a Gordon coupler that provides quick and easy sample change into the immersion He bath.

Using photosynthetic materials prepared by himself, he established N coordination to the Mn complex and has subsequently proven its origin to be a specific histidine in one protein unit. He also established that ammonia, a water mimic, and inhibitor of oxygen evolution, becomes bound to the Mn cluster. He also established histidine coordination to the Fe atoms in the Rieske Fe-S proteins.

Since joining the faculty at U.C. Davis, he has assembled a highly productive laboratory, has mentored several graduate students through their Ph.D.s, and become a prime exponent and user of pulsed ENDOR spectroscopy. He has applied these methods to further elucidate the Mn and ligand hyperfine parameters of the oxygen evolving complex as well as those from synthetic model complexes. His methods have also been used to resolve an important issue on the origin of another EPR signal in the photosynthetic apparatus. David has established successful collaborations with biochemists and molecular biologists who can engineer isotopically labeled amino acids into specific protein sites. Most recently he has proposed some mechanistic insights into water oxidation.

He has become a significant contributor to the fields of EPR and photosynthesis, and I anticipate that his influence will continue to expand.

Melvin Klein
Univ. California, Berkeley

Alexander Prokhorov, IES Fellow 1995—

Alexander Prokhorov (Inst. General Physics, Russian Academy Sciences, Moscow, Russia) was born on 11 July 1916 in Atherton (Australia), where his parents lived in emigration. His father, a Russian revolutionary, was sent in exile to Siberia for his revolutionary activity and then went to Australia. In 1923 the Prokhorov family returned to their Motherland Russia. In 1939 Alexander Prokhorov graduated from the Leningrad State University and became a postgraduate in the P.N. Lebedev Physical Institute of the USSR Academy of Sciences. In 1944-1950 he carried out investigations in the field of radio spectroscopy of gases, which resulted in the discovery of a new principle of enhancement and generation of electromagnetic vibrations.

This principle is based on usage of stimulated radiation of atoms and molecules. In 1953-1955, in co-authorship with N.G. Basov, he developed this principle, which started a new field of science and technique – quantum electronics. The theory of a molecular generator was developed and experimentally realized in 1954. A method of electromagnetic pumping, one of the most effective and universal methods to produce inversion of populations of a quantum state, was proposed in 1955. In 1953 Alexander Prokhorov extended his studies in the field of radio spectroscopy to the solid state and his attention turned to electron paramagnetic resonance in crystals. These investigations were fruitful and led to important results on spectra and relaxation of spin systems in crystals, which were an extremely valuable contribution to solid state physics and other fields. To name a few, the detailed studies of EPR in ruby resulted in creation of new quantum amplifiers in decimeter, centimeter and millimeter wavebands with extremely low noise. Usage of these amplifiers in radio astronomy enabled the obtaining of important results in studying space. The scientific interests of A.M. Prokhorov incorporate a wide range of problems of modern physics and other fields. For his outstanding scientific achievements he was awarded the Lenin Prize, the highest national award in the USSR (1959). As one of the founders of quantum electronics, he was awarded the Nobel Prize in Physics in 1964. He is also the winner of the USSR State Award for his studies in submillimeter spectroscopy. A.M. Prokhorov was awarded the Hero of Socialistic Labour (twice) and five Orders of Lenin, the highest national Order in the USSR. He is an Honorary member of many academies and scientific societies and an Honorary Doctor of many Universities. For a long period (1973-1991) he headed the Department of General Physics and Astronomy of the Academy of Sciences of the USSR. At present he is the Director of the Institute of General Physics of the Russian Academy of Sciences, the Advisor of the Presidium of the Russian Academy of Sciences, a member of the Presidential Council for Scientific Policy, the editor-in-chief of the Great Russian Encyclopedia, and President of the Academy of Engineering Sciences. To the best of knowledge of his colleagues Prokhorov's hobby is science.

K.M. Salikhov
Kazan Physical-Technical Institute
Russian Academy of Sciences, Kazan, Russia

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Professor Harden M. McConnell: 1997 IES Gold Medalist—

Harden McConnell (Stanford Univ.) is a physical chemist whose contributions to science fall into five distinct areas.

During the period 1955-1965, McConnell was active in both the theoretical and experimental applications of nuclear and electron magnetic resonance spectroscopy to chemical problems. The *McConnell equation* was introduced by him to describe how the NMR Bloch equations can be used to obtain chemical reaction rates from resonance spectra. However, his main objective in this period was to relate magnetic resonance spectra to molecular electronic structure. This work was particularly fruitful in leading to the *McConnell relation*. This has been used extensively to relate unpaired electron distributions in free radicals to proton nuclear hyperfine splittings in paramagnetic resonance spectra. The data so obtained provided the first convincing evidence for the utility of Hückel molecular orbital theory in describing pi-electrons in unsaturated organic molecules.

Between 1965 and 1975 McConnell introduced and developed the *spin label* technique. In this method a free radical molecule—usually a nitroxide free radical—is designed, synthesized, and introduced into a biological system so as to provide structural and dynamical information from magnetic resonance spectra. Discoveries made with this technique include the first measurements on the fluidity of the lipid bilayer in model and biological membranes, including lateral diffusion, phospholipid flip-flop and the fatty acid flexibility gradient of phospholipids.

McConnell has also used physical chemical approaches to problems in modern immunology. In 1984 McConnell's laboratory showed that T-helper lymphocytes can be activated by molecular complexes of antigenic peptides and class II molecules of the major histocompatibility complex reconstituted in lipid bilayer membranes, a model for a key event in self-nonspecific discrimination by the immune system. Work in his laboratory has also elucidated the kinetics of the reactions of antigenic peptides and class II proteins, and their relation to the activation of T-lymphocytes.

Since 1981 McConnell's laboratory has played a major role in understanding the remarkable superstructure phases observed in lipid monolayers at the air-water interface using

fluorescence microscopy. His laboratory discovered co-existing liquid phases in cholesterol-phosphatidylcholine mixtures and has accounted for these phases in terms of their thermodynamic, electrostatic, and hydrodynamic properties.

In 1983 McConnell founded Molecular Devices Corporation for the purpose of constructing biosensors. McConnell is a co-inventor of the light addressable potentiometric sensor, and the Cytosensor microphysiometer. The instrument with this name has been sold in significant numbers to most of the major pharmaceutical companies, as well as to biotech companies, and universities. In 1995 a Cytosensor was used to discover the function of a gene derived from brain tissue, and the product of this gene was later found to be a co-receptor for the AIDS virus.

McConnell is the author of more than four hundred scientific publications, most of which deal with the subjects listed above.

submitted by Arthur Schweiger
ETH Zentrum, Zürich, Switzerland



Jim Norris presents Harden McConnell (right) with Gold Medal citation.

Nominations Open for the Voevodsky Prize 1999

In memory of Academician V.V.Voevodsky and in connection with his 80th anniversary the Institute of Chemical Kinetics and Combustion of the Siberian Branch of Russian Academy of Sciences and the International Tomographic Center, established in 1996 the Voevodsky Prize. The Voevodsky Prize is recognized by the Groupement AMPÈRE, the International Society of Magnetic Resonance (ISMAR), the International EPR(ESR) Society, Committee of the European Federation of ESR groups, Novosibirsk State University.

The Voevodsky Prize and diploma are awarded to Russian and foreign scientists, in turn, for outstanding contributions to the investigation by using radiospectroscopic methods of mechanisms of chemical reactions, structure and properties of active intermediates, elementary reactions in photo- and radiation chemistry.

The Voevodsky prize has been awarded starting in 1997, once every two years (in the year when the Conference is dedicated to the memory of Academician V.V.Voevodsky). The first Voevodsky Prize was awarded in 1997 to Professor Anatoly Buchachenko (Institute of Chemical Physics, Moscow). Awarding of the Voevodsky prize is based on a competition. Candidates are nominated by scientific institutes or by scientists. The current Active Award Committee: V.I.Goldansky (Moscow), K.A.McLauchlan (Oxford), Yu.N.Molin (Novosibirsk), J.R.Norris (Chicago), R.Z.Sagdeev (Novosibirsk), and the Chairman

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Yu.D.Tsvetkov (Novosibirsk). The members of the Award Committee do not participate in the competition.

The Voevodsky prize (1000 USD in 1999) and diploma will be presented at the session of the Scientific Council of Institute of Chemical Kinetics and Combustion. An Awardee must participate in the session and deliver a lecture on his scientific work.

The Award Committee would welcome any nominations before the deadline, April 1, 1999. They should be accompanied by a brief summary of the achievements of the nominee, covering no more than two pages, and should be submitted to: Prof. Yu.D.Tsvetkov, Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Siberian Branch, 6300090, Novosibirsk-90, Institutskaya, 3, Russia; E-mail: tsvetkov@ns.kinetics.nsc.ru; Fax: 7-3832-34-23-50.

◆ IES AFFAIRS ◆
ANNOUNCEMENTS AND
REPORTS FROM THE INTERNATIONAL
EPR (ESR) SOCIETY

From the President—

The 1998 IES medals have been presented in two places, the annual EPR Symposium at the Rocky Mountain Conference in Denver and the Joint 29th AMPÈRE – 13th ISMAR international Conference on Magnetic Resonance and Related Phenomena, Berlin. IES Secretary John Pilbrow did the honors in Denver and we both presented awards in Berlin. For this year's winners see the front page and page 11 of this newsletter. The practice of making the award presentations at more than one international meeting will be continued, especially since as far as I know, everyone thought this is a good policy.

For the most part, the award process has gone smoothly, largely because of the wonderful cooperation that we had with Sandy and Gareth Eaton in Denver and Wolfgang Lubitz in Berlin. As I publicly stated in Berlin, we are most grateful to the organizers of these two meetings. Their patience was particularly noteworthy. I would also like to take this opportunity to invite suggestions for where next year's awards will be bestowed, particularly if you are organizing a meeting. Any suggestions can be forwarded either to John Pilbrow or to me.

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Since the beginning of the IES, the process of selecting award winners and selecting meeting sites at which to present the awardees to the public has been much too lengthy. The process this year was no exception. Encouraged and stimulated by our new Secretary, John Pilbrow, we will try a new procedure the coming year. Although most members of the IES have been supportive of these awards, some of you have suggested ways of enhancing the process. However, for any true improvement to occur, we definitely need the participation of as many members as possible. Therefore, I strongly encourage you to nominate people for the various medals and honors. For those whose favorite has not been honored by the IES yet, the most likely reason is that no one has put forth the case. Without nominations, all the new procedures in the world will not be sufficient to make the process work properly. So please note the deadlines and nominate your candidates.

As you know, a major purpose of the IES is to support new young EPR investigators. For evidence that the IES awards are of some value, I note that all except one of our former IES Young Investigator Awardees attended the Berlin conference in August.

As a final personal note, I am most pleased by all the efforts and new ideas of Secretary John Pilbrow. Please read his comments in this newsletter. I hope that this next year will see some changes made to the operation of the IES. For the most part, the changes will be minor and primarily represent reality instead of ideality in the yearly operating procedures of the IES. The IES is now old enough and with John's experience perhaps we are wise enough that we can see what is practical and what is not. Consequently, I am optimistic about the future of the IES

Sincerely, Jim Norris

From the Secretary—

I took over from Arthur Schweiger on 1 September of last year. In order to get properly under way I managed to visit Urbana and Milwaukee last November after the Spin Chemistry meeting in Jerusalem. That provided a good opportunity to meet with the Secretariat Staff in Urbana, Becky Gallivan and Martha Moore (who manages the data base) and to discuss the Newsletter with Linn Belford. The next day involved discussions with the IES Treasurer, Raman

Kalyanaraman, and the US Regional Treasurer, Chris Felix (who handles direct payment within US and internationally).

Just after Easter, my wife and I were able to stay overnight at the University of Chicago, and an Executive Meeting was scheduled for Tuesday April 14th. Present were Jim Norris (President), myself (Secretary), Chris Felix standing in for Raman Kalyanaraman, Linn Belford (Editor EPR Newsletter) and Becky Gallivan and Martha Moore from the Office. We spent about four hours going through the annual cycle of activities and generally familiarising ourselves with the operation of the IES.

Then recently during the AMPÈRE/ISMAR Congress in Berlin a further Executive Meeting was held, attended by the President (Jim Norris), Vice-President (Klaus Möbius), Secretary and, by invitation, the past Secretary, Arthur Schweiger. The Secretary had run through the Agenda the previous Saturday whilst visiting the Immediate Past President, Keith McLauchlan, in Oxford. Matters focussed on procedures for choosing winners of the various IES Awards. More details will be announced in a later EPR Newsletter.

I have found it of great value to have been able to make contact with other office bearers and the Secretariat staff face to face. I hope it will enable the Society to run smoothly for the benefit of members during my three year term as Secretary.

I want to thank everyone for their cooperation during the first year of my term. I would also like to thank Arthur Schweiger for some tutoring during his visit to Australia last December.

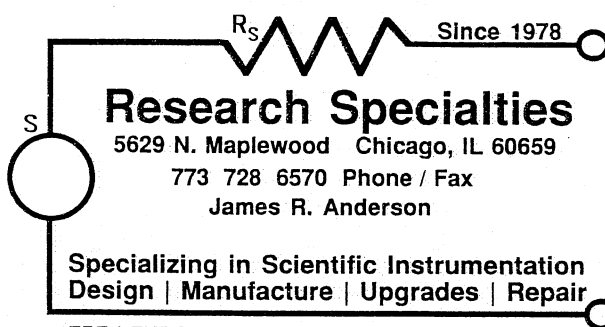
John Pilbrow
Secretary, International EPR Society

IES Awards —

Presentation of 1998 IES Awards

The Officers would like to thank Professors Gareth and Sandy Eaton for allowing the presentations of the Young Investigator Award to Alex Smirnov and the IES Fellowship to Charles Poole during the 21st International Symposium on EPR in Denver (July 26-30). We would also like to thank Professor Wolfgang Lubitz and his colleagues for making provision in the programme of the 29th AMPÈRE/13th Ismar Meeting in Berlin (August 2-7) for presentations of the Gold Medal to Arthur Schweiger, Silver Medal for Chemistry to Dick Fessenden, Young Investigator Award to Alex Smirnov (yes, Alex received his award twice!), and IES Fellowships to Karl Hausser and Charles Slichter.

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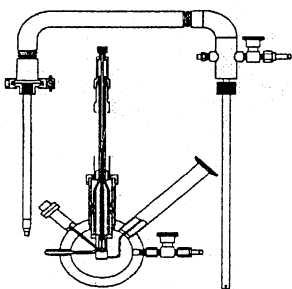
Previous IES Awards Winners

IES Gold Medal: 1992-George Feher; 1993-James Hyde; 1994-Jack Freed; 1995-Sam Weissman (Chemistry); 1996-Kev Salikhov (Physics & Instrumentation); 1997-Harden M. McConnell (Biology & Medicine); 1998-Arthur Schweiger (Chemistry). **IES Silver Medals/Biology/Medicine:** 1994-Hal Swartz; 1995-Lev Blumenfeld; 1996-Ron Mason; 1997-Anatole Vanin; 1998-Ed Janzen. **IES Silver Medals/Chemistry:** 1994-Keith McLauchlan; 1995-Clyde Hutchison; 1996-Klaus Möbius; 1997-Hanns Fischer; 1998-Richard W. Fessenden. **IES Silver Medals/Physics/Instrumentation:** 1994-Wojciech Froncisz; 1995-Jan Schmidt; 1996-Johann-Martin Spaeth; 1997-Roger Isaacson; 1998-William B. Mims. **Young Investigator Awards:** 1994-Devkumar Mustafi (Univ. Chicago); 1995-R. David Britt (Univ. California); 1996-Gunnar Jeschke (Univ. Bonn); 1997-Robert Bittl (Techn. Univ. Berlin); 1998-Alex Smirnov (Univ. Illinois). A listing of the Fellows of the Society appears on page 1.

Nominations Due Before the End of the Year.

From 1999 there is to be a new category of Silver Medal, specifically for Instrumentation, to recognise the fact that contributions to instrumentation belong to all discipline categories of the Silver Medal Awards. Thus the Silver Medal, formerly for Physics & Instrumentation, will now become two Silver Medals – for Physics/Materials Science and Instrumentation.

All nominations⁺ for 1999 Awards are to be sent directly to the President, International EPR Society, Prof. Jim Norris, Univ. Chicago, Dept. Chemistry (Searle 133), 5735 S. Ellis



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Ave., Chicago, IL 60637-1403 by the end of the year. Next year, nominations are due earlier—no later than November 30th, 1999.

We repeat here the Society's award policies: Awards are not restricted to IES members, but the committees may take membership into account when deciding on the award winners. Each year, three major awards, the IES Gold Medal, the Bruker Prize, and the Zavoisky Prize, are devoted to the recognition of outstanding achievements in EPR. By agreement between the British and Russian Groups and the IES, we co-operate in the award of the Bruker and Zavoisky Prizes and our Gold Medal Award each year. Each group is invited to make input into the selection of each, but the final choice is left to each group. The area of research interest rotates among the groups each year, with the three following loosely-interpreted categories: chemistry, physics and instrumentation, and biological sciences (including medicine). These categories are to be interpreted very liberally. The **Gold Medal** will stress contributions in Physics and Instrumentation for 1999.

Prof. Larry Berliner is the continuing Chair of the IES Gold Medal Award Committee.

Silver Medals: Four annually, *i.e.*, one each for outstanding EPR work in the general areas of Chemistry, Physics/Materials Science, Instrumentation, and Biology/Medicine.

Young Investigator Awards: One Young Investigator award each year; "young" means being under 35 on January 1 of the award year. Send nominations⁺ to Prof. James R. Norris, Jr. (E-mail to j-norris@uchicago.edu).

Fellows of the Society: The IES Fellowships recognize truly outstanding contributions and achievements in electron paramagnetic/spin resonance among distinguished scientists (hopefully, IES members) who are either retired or are close to retirement. As the highest international standards are to be applied to the recognition of those worthy of this distinction, their formal connection with the Society will enhance its own image. Send confidential nominations⁺ for the Committee's consideration by January 1st to Prof. James R. Norris, Jr., Univ. Chicago, Dept. Chemistry - Searle 133, 5735 S. Ellis Ave., Chicago, IL 60637 USA; ☎: 1-312-702-7864; FAX: 1-312-702-0805; E-mail: j_norris@uchicago.edu.

⁺Nominations must include an article on the nominee that may be used in the EPR Newsletter if the nominee is selected to receive an award.

THE COMPUTER CORNER

Edited by Keith P. Madden, Reef (Philip D., II) Morse, Graeme Hanson, Dave Duling & Richard Cammack

The EPR Computer Corner is a regular feature of the EPR Newsletter. It is managed and edited by:

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Dick Cammack	(richard.cammack@kcl.ac.uk)
Dave Duling	(sasdh@unx.sas.com)

Items for this column may be sent to any of the above authors. Submissions may be edited for publication.

Notre Dame Radiation Chemistry Data Center

by Keith Madden

There are many good chemistry sites available on the world wide web, and any brief overview has to reflect a rather specialized interest. The vast majority of chemical sites deal with stable chemical entities, as opposed to the free radicals and excited molecular states of interest to those working with transient intermediates. A serious issue concerning data on the web is the lack of standards of review of information presented -- the sites mentioned here contain authoritative material.

In the field of free radical chemistry, I have discovered a few sites that have made my research life easier; I'd like to share them with you. A good start for quantitative data on the thermodynamic and kinetic properties of free radicals, particularly in the gas phase, is the web sites of the National Institute for Standards and Technology (NIST). The NIST web site at <http://webbook.nist.gov> allows one to search for a chemical species on a formula, name, partial formula, CAS registry number, or molecular weight. My typical input is a formula search for a radical. The intended output from this site is thermochemical, thermophysical, and ion energetics data compiled by NIST under the Standard Reference Data Program. I generally use this site as a place to get a good CAS registry number for searching other sites, to get the correct IUPAC chemical nomenclature for a transient intermediate, and a view of the radical's structure.

With the name and chemical formula of the radical obtained from the NIST webbook, the Notre Dame Radiation Chemistry Data Center site can be searched for kinetic data for reactions induced photochemically and by radiation chemical methods. The URL is:

<http://allen.rad.nd.edu>.

The site contains rate constants for a wide variety of free radical reactions, and a compilation of one-electron reduction potentials. For the reactions of singlet oxygen, there is information on yields, and rates of both physical quenching and chemical reaction. A literature current awareness service, Recent Papers in Radiation Chemistry and Photochemistry, is also available here, offering in-depth coverage of the reactions of transient intermediates produced in condensed

media by the title modalities. Spin trapping is an excellent method for elucidating the identity of participants in free radical reactions, and the spin trapping database at the National Institute of Environmental Health Sciences makes identification of spin adducts manageable by providing a web-based query form to link measured hyperfine couplings to literature values of spin adduct parameters. Search capabilities are based on parent radical name, solvent composition, spin trap, and spin Hamiltonian parameter ranges. The URL for this database is:

<http://alfred.niehs.nih.gov/LMB/stdb/>.

EPR File Formats

by John Maher, University of Bristol
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The Computer Corner in Volume 8 Number 4 of the *EPR Newsletter* (Spring, 1997) contains some comments about EPR File Formats from Reef Morse, Graeme Hanson, Dave Duling and Richard Cammack, and the other two data formats, FLS from Scientific Software services, and the NIH LMB format implemented by Dave Duling. The note in the IES newsletter starts with the statement:

"There have been many discussions, in this column and elsewhere, regarding the possibility of having a file standard for exchange of EPR data. No such standard has emerged."

Well, perhaps the standard now needs to be the JCAMP-DX form, with some suitable filters to convert from one of the above three formats. Thus a colleague of mine in the University of the West Indies, Dr Robert Lancashire, and some of his computer science colleague have been working on the implementation of MIME types for viewing all forms of spectra over the Web. Ref:

<http://wwwchem.uwimona.edu.jm:1104/software/jcampdx.html> Robert is at : rjlanc@uwimona.edu.jm

Examples of JCAMP-DX EMR spectra can be see at:
<http://wwwchem.uwimona.edu.jm:1104/spectra/EPRIndex.html>

Paul May from here in Bristol has put a copy of the relevant zip file up:

<http://www.tlchm.bris.ac.uk/shared/npjcamp.zip>

(Win95/NT with Netscape only, unzip and place the dll into the Netscape plugins directory). Apparently the next version of Chime will have the JCAMP-DX plug-in already built into it.

Thus Robert and his colleagues have set up JCAMP filters for a number of types of spectroscopic data (IR, UV visible, mass spec, NMR). He has recently turned his



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attention to EMR. In particular a suitable filter for BES3T ↔ JCAMP would be very useful. It would be very helpful if progress is to be made on a common format for EMR, if the software people at Bruker could provide Robert and his colleagues in Jamaica with details of their code. This was done some years ago by Francisco Gent; thus I have 'Cisco's' C source code, and I corresponded with Francisco about the putative 'EMR database' at the time. The latter has been a gleam in the eye of various people for several years. The conversion routines seemed to work OK on our Bruker 300E's OS/9 system, but I admit they were not used much except for demonstration purposes. More up-to-date versions are needed.

The combination of the Web, suitable MIME types for viewing spectra (and making the data itself available where needed), makes provision of databases of spectra much closer to a reality.

To my mind it makes most sense for the "EMR community" to follow the route being used by other spectroscopists. In particular, JCAMP-DX is being used in the emerging CML (as part of XML) languages of the Web. See some of the discussions at the recent Oxford Chemistry Webmasters meeting:

<http://chemistry.rsc.org/rsc/chemwebm.htm>

In particular the work of Peter Murray Rust's group on the Virtual School of Molecular Sciences:

<http://www.vsms.nottingham.ac.uk/vsms/index.html>.

In addition the appearance of the new HTML 4 specification, (<http://www.w3.org/MarkUp/>) and of the provision for maths markup (<http://www.w3.org/Math/>) will make life much easier once they become accepted.

A further strand has appeared in recent interest among the W3 community in the methods for linking databases of information into the Web, particularly where large amounts of information are concerned. Finally, have a look at Robert Lancashire's 'Molecule of the Month' for September 1997, which was Alfred Werner's 'Hexol', and which contains some nice examples of both Chime molecular structure pictures and the use of the JCAMP-DX format for IR and UV/Vis spectra.

Direct URL:

<http://wwwchem.uwimona.edu.jm:1104/MOTM/hexol/hexol.html>
(MOTM URL:

<http://www.bris.ac.uk/Depts/Chemistry/MOTM/motm.htm>)

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Computer Package *cst*

C. Rudowicz

Department of Physics and Materials Science, City University, Hong Kong SAR; Fax: (852) 2788-7830; Email: apceslaw@cityu.edu.hk

The package *CST* [1] satisfies need for a user-friendly computer package for various general manipulations of the format of the experimental zero-field splitting parameters (ZFSP) as well as the crystal-field ones (CFP). The present (FORTRAN 77) version can handle ZFSP, CFP, and *g*-matrices of any symmetry. Its capabilities include: **CONVERSIONS: unit conversions** - between several units most often used for ZFSP (CFP) and **notation conversions** - between several major notations for ZFSP (CFP); **STANDARDIZATION** of orthorhombic, monoclinic and triclinic ZFSP (CFP); including the errors of the standardized parameters, and **TRANSFORMATIONS** of ZFSP (CFP) into an arbitrary axis system; including the rotation invariants and the errors of the transformed parameters. A separate *GTRANS* module for transformations of the Zeeman *g*-matrix is included. Detailed description and several examples of applications are provided in the Manual [2]; here a brief outline of the structure and capabilities of the *CST* package is presented.

The *extended Stevens (ES)* operators O_k^q [3] are adopted as the *reference* notation for ZFS Hamiltonian,

$$\tilde{H}_{ZFS} = \sum_{kq} B_k^q O_k^q(\tilde{S}_x, \tilde{S}_y, \tilde{S}_z) = \sum_{kq} f_k b_k^q O_k^q$$

with the 'scaling' factors: $f_k = 1/3, 1/60$ and $1/1260$ for $k = 2, 4$ and 6 , respectively. For orthorhombic symmetry \tilde{H}_{ZFS} can be standardized by limiting the ratio $\lambda' = B_2^2/B_2^0 = b_2^2/b_2^0$ to $(0,1)$. This is achieved by choosing, for the original $\{\lambda'\}$ in a given range, the transformation S_i as follows: $(-\infty, -3) S_6, (-3, -1) S_4, (-1, 0) S_3, (1, 3) S_2, (3, +\infty) S_5$. S_i ($i = 1$ to 6) are defined as: S_1 [original] (x,y,z) , S_2 $(x,z,-y)$, S_3 $(y,x,-z)$, S_4 (z,x,y) , S_5 (y,z,x) , S_6 $(z,y,-x)$. Three forms of monoclinic \tilde{H}_{ZFS} , differing by the choice of monoclinic direction C_2 , are dealt with: $C_2 \parallel z$ [with $k = 2, q = 0, \pm 2; k = 4, q = 0, \pm 2, \pm 4; k = 6, q = 0, \pm 2, \pm 4, \pm 6$]; $C_2 \parallel x$; $C_2 \parallel y$. Two standardization suboptions are provided for monoclinic ZFSP: (1) 'ORTHORHOMBIC', based only on the ratio $\{\lambda'\}$, and (2) 'MONOCLINIC', with the monoclinic B_2^2, B_2^0 or B_2^1 first reduced to zero by a suitable rotation α around the z -, x -, and y -axis, respectively. Transformation relations, $[B_k^q]^T \cdot [B_k^q]^T R_k$ for ES operators under a rotation $(\phi/Oz, \theta/Oy')$ are incorporated, and the norm N_k and the rotation invariants S_k are also calculated.

The package can run on a mainframe or PC computer. The input form: KEYBOARD or FILE, and the output form: SCREEN or FILE, are provided. The user selects options and/or suboptions from a MENU and controls flow of calculations according to prompts. The **MAIN MENU**

consists of six options: 1. Free Unit Conversion; 2. Unit Conversion; 3. Notation Conversion; 4. Standardization; 5. Transformation; Q. Exit. Two lower level menus: the **SYMMETRY MENU** followed by **RANK MENU** will be activated if one of the main options 2 - 5 is selected. The package can handle ZFSP (CFP) of arbitrary symmetry since it includes all possible point symmetry groups from CUBIC (O, T_d, O_h) to TRICLINIC (C_1, C_2). The following conversion factors are used to convert to the *standard unit* [10^{-4} cm^{-1}] a value U in a given unit: $8065.54077 * 10^4 * U$ [eV], $0.5035 * 10^{20} * U$ [erg], $g * 0.466856 * U$ [Gauss]; the *g*-factor must be provided, $6950.38605 * U$ [K], $0.33356 * U$ [MHz]. The **NOTATION MENU** enables conversions between major notations used for ZFSP (CFP). The following tensor-operator notations are included: 1. ES (B_k^q); 2. ES (b_k^q); 3. Normalized Stevens (NS); 4. Normalized combinations of spherical tensor operator (NCST); 5. Buckmaster and Smith & Thornley operators (BST); 6. Phase-modified BST operators (Ph.M.BST); 7. Koster & Statz and Buckmaster, Chatterjee & Shing (KS/BCS); as well as 8. **Conventional** notation for ZFSP (for definitions see [3]).

STANDARDIZATION MENU provides ZFS and CF **STANDARDIZATION**, each with three options: (i) **AUTOMATIC ST** - depending on the value of $\{\lambda'\}$, (ii) **ST TRANSFORMATION** - using a specified transformation S_i and (iii) **ST ERRORS**.

TRANSFORMATION module provides directly two options: ES and Wybourne (equivalent to BST) notation for input of ZFSP and CFP. "PHI" (ϕ - rotation about the original z axis) and "THETA" (θ - about the new y axis) must be provided. Input of ϕ and θ may be in the degrees or radians. The norm N_k and rotation invariants S_k are calculated automatically.

Menu driven structure and operating instructions displayed on screen during execution of each subprogram make usage of the package easy and convenient. The *CST* package facilitates interpretation and comparison of experimental data derived from various sources. The effort to convert ZFS and CF parameters expressed in different notations and formats can be substantially reduced by efficient usage of the package. Application of the package may also help to clarify confusion arising from inadvertent usage by some authors of identical symbols having sometimes different meanings; see [2, 3]. The package provides an efficient way for bringing various data available in the literature for a given paramagnetic ion and crystal system into a unified form.

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Hamiltonian and the Crystal field Hamiltonian, Research Report AP-97-12, Department of Physics and Materials Science, City University of Hong Kong (1997).

3. C. Rudowicz, *Magn. Reson. Rev.* 13 (1987) 1-89.

EPR SPECIALIST VIGNETTES

*Edited by
Arthur Schweiger*

ESR APPLICATIONS IN THE FIELD OF CULTURAL HERITAGE

by

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Introduction

The possibility of applying Electron Spin Resonance spectroscopy to problems which, being of predominantly artistic, historic or archaeological interest, are collectively grouped under the short heading of Cultural Heritage, is probably a rather unfamiliar topic for many researchers in the field. Among the few contributions reported so far, the most relevant and best known is, certainly, ESR dating, which has given essential support to our present knowledge of the origin and evolution of modern humans.¹ The method measures the

concentration of radiation-induced paramagnetic centres and operates in a time range where other dating techniques can not be applied or are unreliable.²

However, the capabilities of ESR are potentially much broader and refer to widely different materials and artifacts. Such expectation stems from the obvious observation that most diamagnetic materials, from glasses to wooden objects, to potteries, pigments, tissues, organic remains and others, contain measurable concentrations of paramagnetic impurities and are, therefore, amenable to ESR spectroscopy.

Such impurities and their spectroscopic details are more or less characteristic of the specific sample and may be used as probes for identification, provenance studies, detection of later modifications or forgeries, as well as for monitoring reassembling and restoration of fragments. More importantly the paramagnetic impurities often undergo time evolution or behave as active centres and catalysts for the onset of various chemical processes. This means that they can, in some way, trace the history of the artifact, define its conservation state on a physico-chemical basis and, sometimes, even suggest possible procedures for the restoration or, at least, for avoiding or slowing down further degradation.

In spite of the many possibilities, actual work in the field is very little. In the following the examples used to illustrate the points discussed above will be taken from our own work. They pertain to entirely different fields, namely the study of ancient and modern paper, and the characterization and provenance determination of marbles.

It is worth adding that this work is carried out in the framework of a general, long term program, called "Progetto

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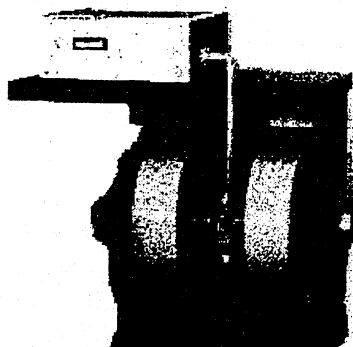
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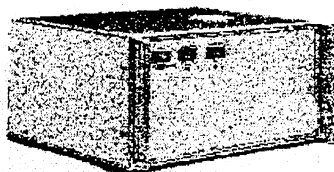
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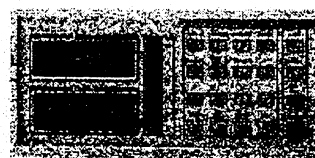
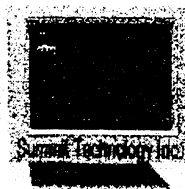
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**Model TC1
Temperature Controller**

Finalizzato Beni Culturali," launched this year in Italy by the National Research Council.

ESR Spectroscopy of Paper

Paper is a composite material whose main components are cellulose and water. In addition it may contain variable amounts of hemicellulose and lignin, plus a number of organic and inorganic additives and impurities. In the following the terms antique and modern paper will refer to samples manufactured before or after the mid-nineteenth century, when industrial production from wood-pulp was introduced. Before this date papermaking technology had remained unchanged for centuries and used linen, hemp or cotton rags to produce high-quality, lignin-free paper.

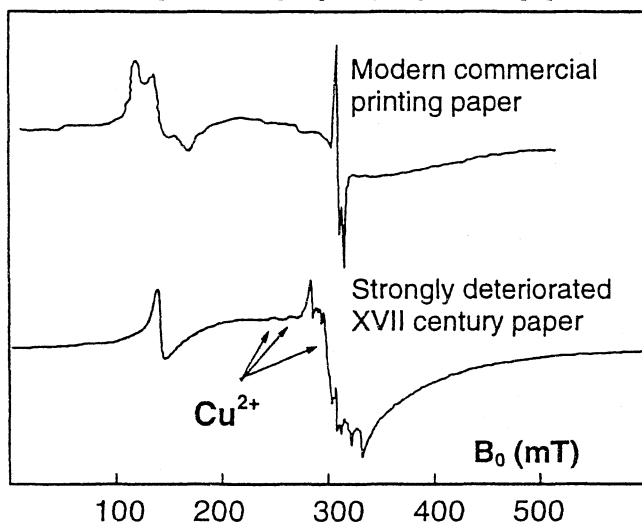


Figure 1. Two examples of the diverse ESR spectra exhibited by paper (X-band, 110K).

Samples of antique or modern paper, either well preserved or deteriorated, generally exhibit complex and widely different ESR spectra, where up to eleven different paramagnetic centres, including transition ions, organic free radicals and paramagnetic point defects, have been detected.^{3,4} Obviously, it must be realized that some of these centres are intrinsic impurities of the raw pulp, whereas others are introduced by the various chemicals used to modify and improve the properties of the final product. In this respect typical is the strong defect spectrum assigned to kaolin, which is commonly used as a whitening agent.

The sample spectra reported in Fig. 1 indicate that trivalent iron is the most common paramagnetic impurity in paper, with total concentration up to 500–700 ppm. Absorptions at characteristic values of g suggest that Fe^{3+} may be present in different symmetries, such as pseudo-octahedral ($g \approx 2.0$), axial ($g \approx 6.0$) and rhombic ($g \approx 4.3$). In addition extremely broad and intense signals detected in low-quality samples, are indicative of ferromagnetic impurities. Mn^{2+} and, occasionally, Cu^{2+} may also be present in paper, although at concentrations which never exceed 100 ppm and are, usually, much lower. Quantitative measurements have shown that the state of conservation of paper is strongly correlated with the presence and concentration of some metal ions in specific coordination geometries (Cu^{2+} , rhombic Fe^{3+}), whereas the presence of

other ions, or even the same ion in a different symmetry, seems to be irrelevant (Mn^{2+} , pseudo octahedral Fe^{3+}). In addition there are indications that the distribution of a transition metal between different, possible stereochemistries is an aging-dependent phenomenon. If this is true degradation may be defined as a two step process which can start only after that preliminary catalyst activation (i.e. transfer of the metal to the proper coordination site) has occurred.

While transition ions are commonly found both in antique and modern paper, the presence of organic free radicals is characteristic of the latter and is associated with its content of lignin, a complex, aromatically based polymer, known to undergo a number of photochemical processes. The formation of free radicals is considered to be the initial step in the auto-oxidation reaction sequence leading to paper yellowing; its inhibition, which might increase by several times the potential market for bleached wood-pulp paper, has long been pursued.

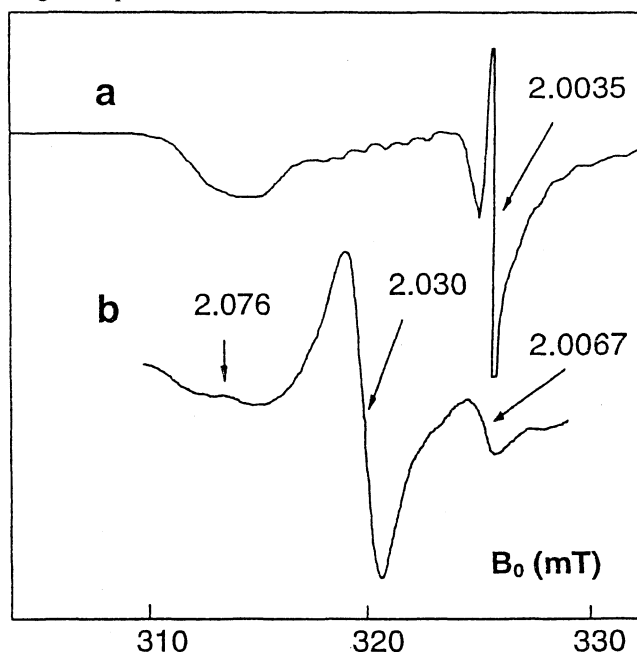


Figure 2. The region around $g=2.0$ for two different woodpulp samples. a shows signals due to copper, kaolin and carbon radicals. Signals in b are ascribed to O-centered radicals.

The preliminary results illustrated in Fig. 2 indicate that at least two different radicals, or groups of radicals, may be present in modern paper and are easily detected in aged samples or develop, with much higher intensity, upon UV irradiation of new ones.⁵ On the basis of their different g values and saturation behaviours we assume that they are, respectively, C- and O-centred radicals. Their thermal stability is also different in the sense that the oxy radicals decay much faster and rapidly reduce to a low, steady-state concentration. Although the reasons for the different behaviour of different wood-pulp papers are still unclear, the above results seem to follow the scheme of a classical autooxidation mechanism. The initially formed C-centered radicals might represent the initiation step of the reaction chain. In some cases they rapidly trap oxygen giving rise to

peroxy radicals, which further react in the so-called autooxidation propagation step. Fading of these latter indicates formation of non radical products and corresponds to the final or termination reaction step.

The above outline indicates that ESR may give some relevant clues, which refer, primarily, to the mechanism of paper degradation. However, for a deeper understanding of the overall process we have also carried out extensive, parallel NMR work.^{6,7} In this way it has been possible to follow in detail the aging process and the state of conservation of the samples has been estimated quantitatively. These results are based, essentially, on the increase of the fraction of amorphous cellulose and on the severe decrease of the amount of bound water induced by aging.

ESR Spectroscopy of Marbles

The characterization of marbles used in classical architecture and sculpture and, above all, the determination of the quarries of provenance is a problem of great archaeological relevance. As already pointed out it is essential for detecting later restorations, copies or forgeries. Beside that, and together with information from other sources, the determination of provenance contributes to a detailed picture of ancient trade, commercial routes and economic relationships between different countries.

Therefore solution of this problem has been attempted with various petrographical and physico-chemical methods, among which isotopic ratios, trace element analysis, and neutron activation of rare earths are the most common. The essential result is that a single technique capable of unequivocal origin identification does not exist and the problem must be dealt with by cross checking data from several different sources.

In this field the use of ESR spectroscopy is based, primarily, upon detection of the ubiquitous Mn^{2+} ion. However, additional and often essential information may be provided by the presence of other paramagnetic impurities, phases different from calcite, as well as line width and anisotropic data.

The first application of ESR to the marble problem dates back to the early 80's.⁸ Since then scattered reports have appeared, but the method has never gained wide popularity.^{9,10} This is partly due to the fact that generally accepted measuring procedures are not available and the results from different laboratories are not coherent and of little or no use to other research groups.

Recently we have started systematic work with the aim of assessing in detail advantages and drawbacks of the technique.^{11,12} In addition we are investigating the best suited experimental conditions for setting up acceptable standards for making ESR a current technique in marble characterization. Samples from various historic quarries are being used for setting up a starting database. Within each quarry the data dispersion is often high and the standard deviation correspondingly large. As a consequence, extensive superposition occurs and statistical assignment of unknown samples usually results in sizeable provenance probability values for several quarries. The results of Fig. 3 illustrate this point. The final uncertainty may be lowered by using data

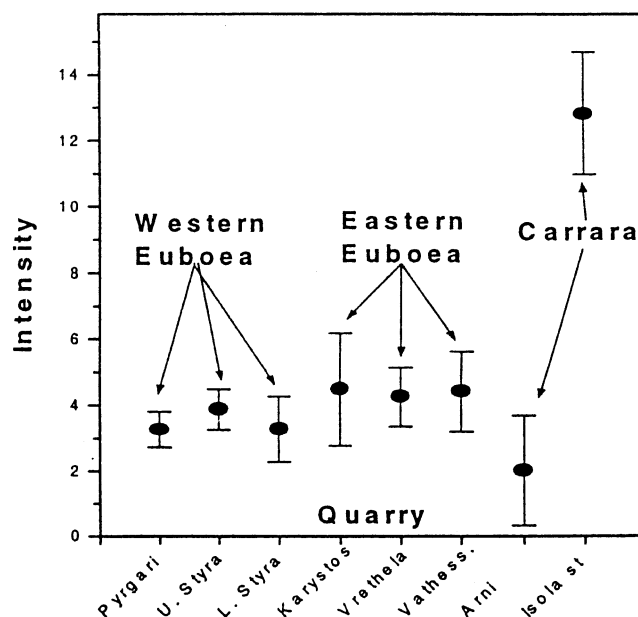


Figure 3. The ESR database for the "Cipollino Verde" marble. The most important, historically exploited quarries have been sampled. The average Mn^{2+} intensity is given, for each quarry, with its standard deviation.

from other techniques, but also taking advantage of other possible ESR provenance markers. One is the presence of the dolomite phase which gives rise to a Mn^{2+} spectrum, easily distinguishable from that of calcite, that can be detected with a sensitivity of a few percent. Another is the spectral line width, which shows variations up to 100% and considerable quarry dependence. According to a simple model the line width is expected to increase linearly with the spin concentration. An intrinsic value at zero concentration can be easily found and used, in some cases, as a further discriminating factor. The final point refers to the observation that the ESR spectrum of a piece of marble exhibits a residual anisotropy which is due to partial isoorientation of the microcrystals, a phenomenon also known as marble texture. This latter is obviously related to the exact formation conditions of the mineral and hence to the quarry of provenance, and might be used as a further marker.

Work on these last points is in progress and shows that the capabilities of ESR in marble characterization are far from being fully exploited.

Conclusions

The sample cases outlined above indicate that valuable information may be obtained by applying ESR spectroscopy to a number of problems in the field of Cultural Heritage. In spite of its selectivity, the technique may profitably be employed for characterizing several, widely differing materials, owing to the almost ubiquitous presence of trace paramagnetic impurities. It is worth noting that the above work is based, exclusively, on conventional, continuous wave ESR. Much more detailed information may, probably, be obtained by using more sophisticated paramagnetic resonance techniques. However, it must be realized that, in this field, a reasonable compromise between sophistication and the need for rapid and simple measurements is necessary.

Acknowledgments

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Building the Perfect Beast

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***ESR STUDIES OF PROTEINS CRYSTALLIZED
IN THIN WAFERS***

The Marshall Space Flight Center has an active program in materials and biotechnology science related to space payloads, and among their programs is developmental work on protein crystallization. For what little work I personally do with protein crystallization, I have always tended to use epitaxial methods, as described by Bernard Wunderlich in his classic text on macromolecular chemistry, but technical briefs from NASA's labs have provided some useful information. These notes are usually released in a general magazine *NASA Tech Briefs*, and one can request the more detailed report by filling out a bingo card.

A recent issue of *NASA Tech Briefs* contained three reports on protein crystallization methods. All were useful, but I found one that is particularly appropriate for ESR studies. One can put a drop of protein solution adjacent to a second drop of saline (or whatever one may wish to use to precipitate the protein) on a microscope slide. One then sandwiches the drops between a second microscope slide (there should be a predetermined gap between the slides), and

lets it sit for precipitation/crystallization. The crystals form as thin wafers on the surface of the slide. Precoating the slide and adjusting the gap leaves you with a lot of latitude for controlling crystallization conditions.

As for ESR, Wilmad Glass manufactures this flat-cellish sample holder for tissues. The tissue cell is basically a quartz plate (there is a well depression, but you can easily abrade this down some if necessary) with a cover plate, and so it is very nicely adapted to the crystallization method described above. Otherwise, one can spend a few minutes in a glassblower's shop and have some quartz plate fused to a pair of quartz rods and get pretty much the same thing.

The reports:

"Crystalizing Proteins in Thin Wafers" NASA Tech Brief MFS-31048

"Ring Method for Crystallization of Proteins" NASA Tech Brief MFS-31047

"Advanced Semicontainerless Crystallization of Proteins" NASA Tech Brief MFS-31046

***A DIELECTRIC SPHERE POWER LIMITER AND
SAMPLE RESONATOR***

There are two problems of pulsed EPR that may be ameliorated by a device that is described by Courton.¹ Typically, we apply high power microwave pulses to the sample in order to drive the spin dynamics that is necessary to detect an echo or FID, and this necessitates the implementation of some protection circuit for the receiver, whose function depends on the survival of semiconductor components (e.g. diodes). One can use a gas-filled TR tube (basically a spark gap) or a PIN diode limiter as a first defense, and then a PIN diode gating switch to isolate the receiver front end during the application of the rf pulses. One of the things you'll notice about the PIN limiter, however, is that it has a 'post-insult' recovery time. In other words, if you send in a pulse train, the diode takes a short period of time before it will pass a low-level signal. This may or may not be

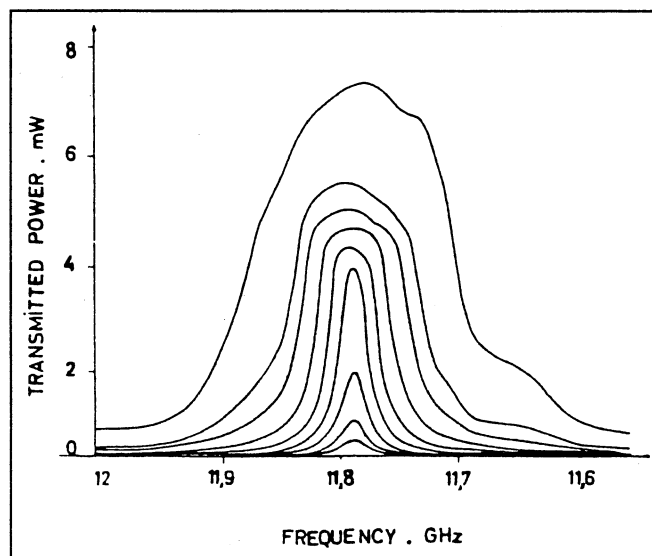


Figure 1..Power/frequency profile of dielectric sphere 'limiter'.

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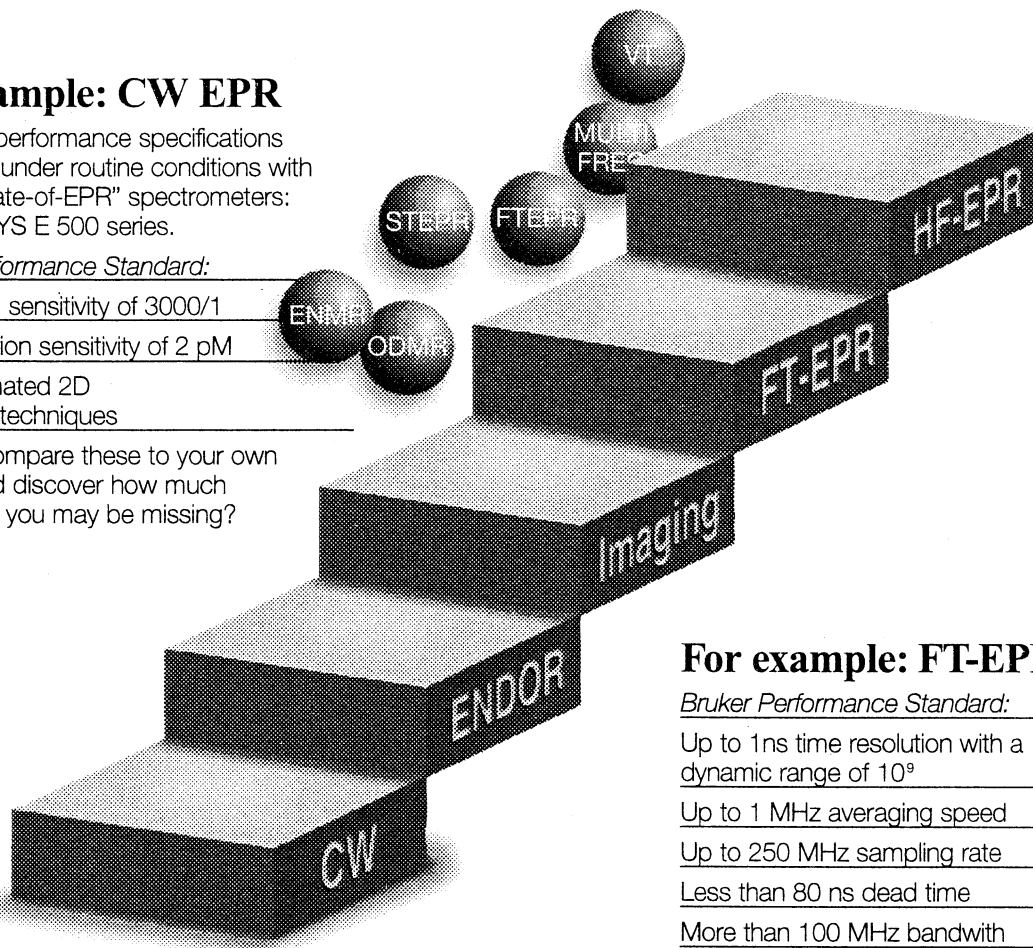
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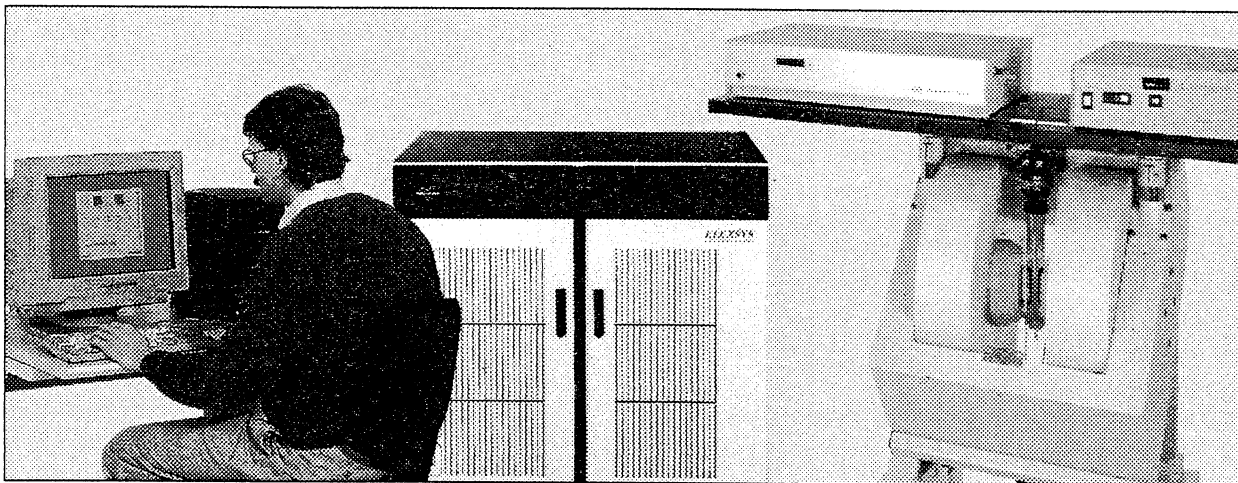
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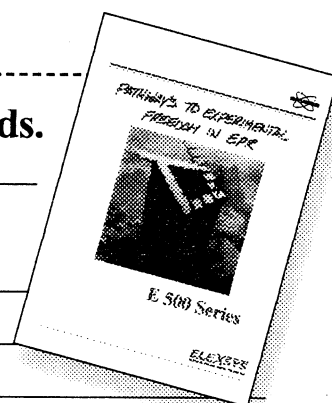
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a problem, depending on the quality of the limiter used, the pulse power level, and the timing of your pulse sequence. The easy way to mentally picture the process is to return to the TR tube. The high power rf pulse ionizes the gas molecules in the spark gap; after the pulse is gone, however, it takes a finite time period for those ions to clear the gap and allow the weak signal to get through.

Courton devised a low-level power limiter by using a dielectric (i.e. YIG) sphere in a section of waveguide. The sphere resides within a transmission-mode resonant cavity filter (the bandpass filter aspect is a convenient secondary feature), and it acts as a 'sample' in the sense that it is in resonance with the microwave field (you need to put a permanent magnet on this, like an isolator). Courton's power transmission plot for such a device is depicted in Figure 1.

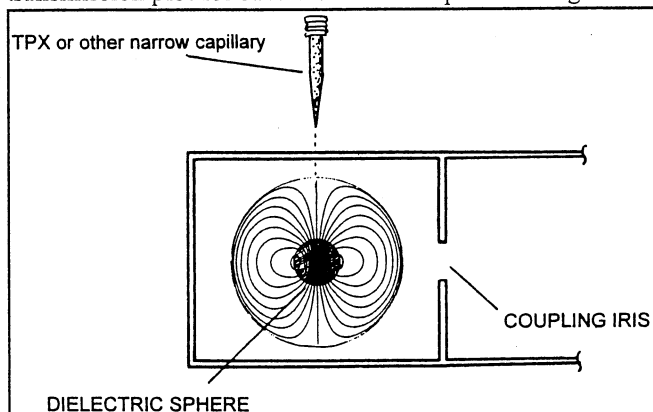


Figure 2: Mock-up of the limiter as sample resonator illustrating the field lines and direction of placement for a capillary sample holder.

I have also been toying with this design for use as a sample resonator. The Mims 'cavity', as you may recall, is basically a $\lambda/2$ bandpass filter into which a sample is poured. The problem with the Mims sample resonator is its incompatibility with standard use of quartz sample tubes or capillaries. On the other hand, this spherical dielectric resonator has well-defined field lines, and might be adapted for use as a low-Q bandpass filter-like resonator for pulsed EPR. Its use would be analogous to the hybrid loop-gap/cavity designs that couple together low- to high-Q structures. A diagram of one of my bench-top prototypes is illustrated in Figure 2; the 'trick' now is getting the sample and field axes aligned the way you want and dealing with spurious signals from the dielectric material.

Reference:

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TIPS & TECHNIQUES

NEW TRANSMISSION LINE RESONATORS FOR ELECTRON SPIN ECHO INSTRUMENTS

A. KOPTIOUG

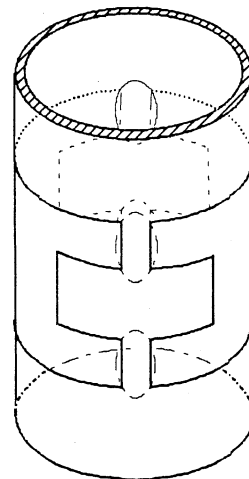
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Over the last years a lot of efforts have been made to develop new resonance structures for the EPR instruments. The main battlefield in the business still remains the Electron Spin-Echo technique. The quality factors of the corresponding ESE resonators are usually not explicitly high which allows experiments with the home-made structures. The main aim of the construction changes in the ESR resonance structure is to improve the signal-to-noise ratio at the output of the spectrometer for samples of small volume. Various technical problems related in particular to the requirements to have certain additional elements in the probe-like ENDOR coils or to have good optical access also contribute to the complexity of the design problem.

Commonly used resonators for ESE with the small working volume are the dielectric resonator [1], loop-gap resonator (LGR) [2], slotted tube resonator (STR) [3] and "Mims-type" strip line resonator (MSLR) [4] and its latest modifications [5]. Still all the above structures are not absolutely perfect. Dielectric resonators have very good parameters, but are not easily replicated in laboratory conditions. Basic problems of the traditional LGR, the structure most commonly used for ESE, have been mainly



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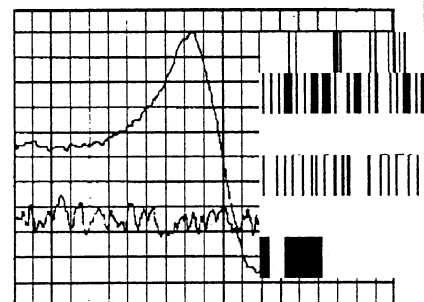
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The plot illustrated was taken with a Varian weak pitch sample in a TE102 cavity under the conditions specified in the Varian 5-line series unmodified (E102/E108 bridge) instruction manual. Signal to noise ratio represented is 248:1. A 2.6 conversion factor was used to convert raw noise to R-P noise. The weak pitch sample had a .683 multiplication factor. Without the multiplication factor, the signal to noise



overcome in so-called bridged LGR (BLGR) [6], which still leaves room for further improvements. Slotted tube resonators generally have poor electric and magnetic microwave field separation; Mims-type resonators have problems with the sample placement. And actually none of the above resonators allow for working frequency tuning in the desired range.

Searching for new solutions my attention has been attracted to the Alderman-Grant resonator [7,8] (AGR), a structure well studied with radio frequency applications in high resolution NMR and MRI. One of the versions of this resonator appeared to be transformable for use in the microwave region, which has been proven in design of structures operating in the C and S bands [9]. The Alderman-Grant resonator for radio frequency applications is usually manufactured of copper or aluminum foil with chip capacitors soldered into the structure. It is, in fact, a high-frequency version of the saddle coils constructed of wide foil strips. To work in the microwave region the AGR structure, dimensions have been scaled down, resulting in substantial decrease in the strip inductance, and chip capacitors were substituted by bridges like the ones used in the bridged LGR. The first structures were made of silver foil, but later models are silver-painted upon thin-wall quartz tubes and are electrochemically gold-plated. Figure 1 illustrates the design of the basic painted mw-AGR structure.

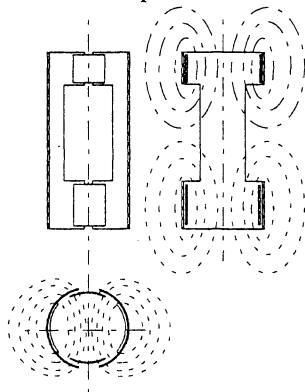


Figure 2

The described resonator has three main resonance frequencies corresponding to the AGR mode and two BLGR modes (Figure 2). BLGR resonances are due to the currents induced in the upper and lower belt rings and bridge capacitors and usually they have slightly different resonance frequencies (magnetic field structure for these modes is illustrated in the axial cross-section in the Figure). It

appeared to be easy to design the mw-AGR structure with all three resonance frequencies far apart from each other. This allows the excitation of the AGR mode without any interference with the BLGR ones: for the structures with the AGR resonances in the S and C bands the BLGR-type resonances were lying in the X band. Note here, that traditional formulae for the resonance frequency estimations of AGR [8] seem to be valid and give good estimates for the C- and S-band structures.

Preliminary experiments on the new resonator have been carried out with the home-built C/S band ESE spectrometer of the Department of Molecular Spectroscopy of the University of Nijmegen [10]. Working frequencies of the structures (AGR modes) were chosen to be within 2.5-6.5 GHz. Resonators of current design have the working area about 6 mm high (measured at the $0.7H_{\max}$ level); inner

diameter of the tube $d \approx 5.2$ mm. The achieved improvement of the S/N ratio compared to the home made LGR (made of bulk aluminum) with the same working volume is up to 30% for the selected structures at room temperature. The silver foil-based structures have quality factors about 500-600; the structures silver-painted on the quartz tube - about 200-300 before gold-plating and about 400-500 after plating.

A full cryogenic probe for the AGR structures has been designed, constructed and tested for temperatures down to 6 K [9].

Experiments have shown that AGR has:

- high frequency and coupling tuning stability (including small "acoustic" susceptibility);
- high filling factor and high loaded Q value;
- good microwave H - and E - field component decoupling;
- resonator with high microwave magnetic field homogeneity in the working area;
- multimodality of the mw- AGR structure that allows a single structure working in two frequency bands, for example in the C(S) and X- band;
- due to its construction, an advantageous structure for use in ENDOR probes;
- resonance structure and a whole probe that is axially symmetric with microwave magnetic field orthogonal to the symmetry axis, making it advantageous for the solenoidal magnets;
- with the common iron yoke magnets, ease of achieving the conditions both when B_1 is orthogonal and parallel to B_0 by just rotating the whole probe 90 degrees;
- large side windows of the AGR that could be advantageous for sample illumination.

Detailed investigations have shown that the mw-AGR has certain advantages over the LGR of traditional design and could be easily constructed in the laboratory. The idea of the resonator scaling from the radio frequency band on its own appeared to be very fruitful. For example, so-called Birdcage resonators (BCR), well-known in NMR and MRI [10], also work quite well in the microwave frequency region, being scaled as for the AGR. Figure 3 illustrates the design of the simplest painted mw-BCR (four-leg BCR structure aka double- AGR with the crossed fields).

These resonance structures appear to be very promising as they have extremely high microwave H -field homogeneity and also allow "quadrature" (frequency-degenerate crossed-field) operation.

Further development of the basic concept has led to the design of unique structures combining the advantages of the microwave AGR with a wide frequency tuning range (up to ± 30 -50% of the central frequency). Experimental structures installed in cryogenic probes allow continuous tuning and

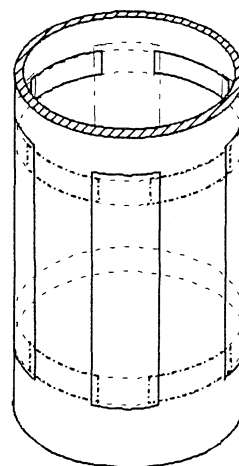


Figure 3

ESE signal detection in the range 3.5-6.5 GHz with roughly the same sensitivity as the LGR of the same volume. Work in this direction is now under way.

Acknowledgments

The trial experiments on the above resonators would be impossible without help from the Department of Molecular Spectroscopy and Technical Workshop of the University of Nijmegen and financial support from the NWO.

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BOOKS & PROCEEDINGS

Foundations of Modern EPR, G. R. Eaton, S. S. Eaton, and K. M. Salikhov, ed., World Scientific, 1998, 60 chapters, 800 pages, ISBN 981-02-3295-0, \$US86, UK£58. This volume includes personal descriptions of early experiments by pioneers who laid the foundations of the field, perspectives on the state of the art and glimpses of future opportunities. Available from the publisher (sales@wspc.com in US or sales@wspc.com.sg).

Spin Labeling: The Next Millennium (Editor: Lawrence J. Berliner), Biological Magnetic Resonance, Vol. 14 (1998), ISBN 0-306-45644-3. Price: US\$125.00, Published by Plenum Publishing Corporation, 233 Spring Street, New York, NY 10013-1378.

Contents:

Introduction: Reflections on the Beginning of the Spin Labeling Technique Lawrence J. Berliner, The Ohio State University, Columbus, Ohio.

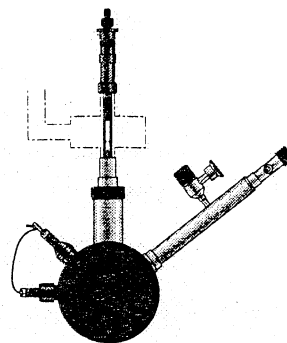
1. M.B. Sankarum and D. Marsh: Analysis of Spin Label Lineshapes with Novel Inhomogeneous Broadening from Different Component Widths. Application to

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2. D. Marsh, T. Pali, Laszlo Horvath: Progressive saturation and saturation transferred EPR for measuring exchange processes and proximity relations in membranes.
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6. Jimmy B. Feix and C. S. Klug: Site-Directed Spin Labeling of Membrane Proteins and Peptide-Membrane Interactions.
7. Robert S. Keyes and Albert M. Bobst: Spin-Labeled Nucleic Acids.
8. Marcus A. Hemminga and Ivon J. van den Dries: Spin Label Applications to Food Science.
9. Harold M. Swartz and Howard Halpern: EPR Studies of Living Animals and Related Model Systems (In-Vivo EPR).

Appendix - Corrections for Anisotropically Averaged Hyperfine Splittings and Order Parameters from Pseudo-Powder EPR Lineshapes. An Update for Slow-Motion Contributions of Lipid Spin-Label Spectra from Membranes.

PUBLIC TEST OF ESR SENSITIVITY

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April 13, 1998; updated July 9, 1998
for the EPR Newsletter

The comments in this note address the question of ultimate sensitivity for aqueous nitroxyl radicals within the context of the comparisons made at the Oxygen Club meeting. Reference within these notes is made to data posted on the Web on April 1, 1998, by Drs. Mason and Fann.

	E109	ESP300	ECS106	EMX, SHQ	FR30
S/N test1/test2	3.8	3.5	3.5	5.8	1.1
signal extrapolation proportional to \sqrt{P}	4	4	4	14	2

A table of data taken from the Mason and Fann report is presented at the start of these comments for the convenience of the reader.

April 14, 1998, Reef Morse sent us the following information about the tests JEOL ran in Japan after the "Public Test." These measurements were made on a research-grade spectrometer with a cylindrical resonator.

Test 1: Varian weak pitch, with extrapolation to 200 mW S/N = 1317

Test 2: Varian weak pitch with signal and noise at 4 mW S/N = 681

Test 3: 10^{-7} M tempol at same conditions as the Bruker test S/N = 68

1. Comparison of results from tests 1 and 2

Tests 1 and 2 were performed under similar conditions except that:

a) In test 1 noise was recorded at full microwave power and spectra were obtained at a power that did not significantly saturate the signal and extrapolated to full power to calculate S/N as if full power were used. (Notes: a) The extrapolation gives a "theoretical" S/N that could be achieved

spectrometer	Varian E-109	Bruker ESP300	Bruker ECS106	Bruker EMX	JEOL FR30
cavity	TE ₁₀₂	TE ₁₀₂	TE ₁₀₂	super-high Q	TE ₀₁₁
Test 1: weak pitch S/N	207	301	283	3389	303
Test 2: low-power S/N	54	87	82	580	281
Test 3: 10^{-7} M tempol S/N	34	39	31	121	12

Details of microwave power, modulation amplitude, gain, filter time constant, and other footnotes on the measurements are in the original Mason and Fann report.

if the signal did not saturate. b) Full power = 200 mW except for the FR30 for which full power = 16 mW).

b) In test 2 noise and signal were recorded at the same microwave power and S/N was recorded at that power.

For most EPR spectrometers the noise from the first stage detector dominates at lower powers and source noise makes increasing contributions at higher powers. If noise from the first stage detector dominated over the full range of powers, noise would be independent of incident power and S/N would be expected to go as \sqrt{P} . Thus comparison of the results from the two tests provides a measure of the significance of source noise at high power for each spectrometer.

The S/N ratios for tests 1 and 2 for the E109, ESP300, and ECS 106 are about what one would expect - the S/N does not go up quite as rapidly as \sqrt{P} because of the increased contribution of source noise at high power. For the SHQ resonator the larger discrepancy between the results predicted based on signal extrapolation, 14, and the observed ratio of calculated S/N, 5.8, is consistent with the expectation that there would be greater demodulation of source noise with the higher-Q resonator and therefore a greater contribution at high power from source noise. The fact that the S/N for the FR30 in test 1 was only marginally better than for test 2 suggests a serious contribution from source noise on this system also, possibly due to the high-Q TE₀₁₁ resonator.

The Bruker SHQ resonator gave impressive performance relative to the other resonators. It looks like this resonator deserves the kind of careful quantitative study that the Varian E-231 resonator has received for so many years.

2. EPR "Sensitivity" depends upon properties of the sample and on the information that is required from the spectra

In many analytical methods one can describe sensitivity simply in terms of minimum detectable concentrations. The problem is more complicated for EPR because of the wide range of line widths and large differences in power saturation between species of interest. The widely cited expressions for EPR sensitivity in terms of minimum number of detectable spins/gauss take account of line width differences by normalizing for spins per gauss line width. However, line width also impacts the modulation amplitude that can be used to record spectra as described in the following section. In addition one needs to take account of power saturation.

We propose that a distinction should be made between EPR spectrometer performance for two limiting conditions of data recording.

Case 1: Selection of microwave power, modulation amplitude, and time constant that provide undistorted line shapes. This mode of operation is crucial if one wishes to

obtain information concerning mobility of a spin-label attached to a protein, oximetry, or partially resolved hyperfine interactions, for example. Typically this would also require a S/N significantly greater than 1. This case might be called "minimum number of detectable spins with desired spectral information".

Case 2: Selection of microwave power, modulation amplitude, and time constant that provide the maximum signal amplitude, at the expense of lineshape information. This mode of operation might be selected, for example, in some spin trapping experiments, where one seeks to determine whether an EPR signal is present and one can obtain adequate information for identification of the species from observed hyperfine couplings even in the presence of lineshape distortions that come from power broadening or over-modulation. This case might be called "minimum number of detectable spins".

Unless these distinctions are squarely faced, the results of spectrometer intercomparison will not meet the desired goal of communicating between users and instrument designers the capabilities needed by spin trappers and spin labelers.

3. Selection of Parameters for Spectral Acquisition with maximum spectral information

Since phrases are sometimes used differently by different authors, we include some comments on the choice of microwave power and modulation amplitude and apply these criteria to spectra of nitroxyl radicals at room temperature.

a. Microwave Power

Some reports of EPR studies describe a signal as "saturated" when it no longer increases in amplitude with increase in incident microwave power. This is a point of extreme saturation, which distorts lineshapes and prevents quantitation of the data, although it improves S/N. The precise definition of saturation is given by the saturation factor, s , (see, for example (1) pp. 705ff and (2)):

$$s = \frac{1}{1 + B_1^2 \gamma^2 T_1 T_2}$$

This expression for s is in terms of the circularly polarized microwave magnetic field, which is the component that causes resonant transitions. In Poole's book (1) the expression is written in terms of the linearly polarized field, which has to be divided by 2, and since B_1 is squared there is a coefficient of $\frac{1}{4}$ in the related equations in (1).

The maximum microwave magnetic field, B_1 , at the sample in a critically-coupled TE_{102} X-band resonator is given by

$$B_1 = \alpha \sqrt{Q_L P}$$

Where Q_L is the loaded Q and P is the incident power in watts. For the Varian E-231 cavity, α is about 0.02 (3), and this is the value we will use in the following example. The value of α has to be calibrated for each resonator. To avoid misunderstanding, note that "loaded" here is a microwave engineering term meaning that the resonator is coupled to a transmission line. It does not mean loaded with a sample. Putting in a sample has a separate effect due to its dielectric constant and loss (4). When the resonator is critically coupled, the loaded Q is $\frac{1}{2}$ the unloaded Q . Since higher Q is "better" in most EPR measurements, vendors and researchers sometimes report the unloaded Q , which makes the resonator look twice as good. The loaded Q for a TE_{102} resonator containing a non-lossy sample such as weak pitch is about 3300. The incident power chosen for the standard weak pitch

measurement is 0.0125 W. These values result in $B_1 = 0.128$ G at the center of the cavity. If a different resonator is used, the incident power has to be adjusted to yield the same B_1 at the sample. If a resonator has a more uniform distribution of B_1 along the sample axis than does the TE_{102} it will inherently yield a better S/N for an extended non-lossy sample such as weak pitch, but it might require a smaller aqueous sample because of the larger interaction of the lossy solvent with the microwave field.

Let us consider some approximate values for nitroxyl radicals in order to guide the selection of spectroscopic parameters. A dilute nitroxyl radical in a de-oxygenated solvent at room temperature has $T_1 \approx T_2 \approx 0.5 \mu s$. The "Public Test" was conducted with air-saturated samples (near sea level), so we need an estimate of the relaxation times in aqueous solution saturated with air. Interpolation within the results summarized in (5) suggests that at room temperature collision with oxygen increases nitroxyl line widths by ca. 0.15 G, and that linewidths were relaxation-determined. Assuming that $T_1 \approx T_2 \approx 6.6 \times 10^{-8} / \Delta H_{pp}$, the relaxation times in the presence of air are 0.23 μs . This is consistent with the observation that it is difficult to measure T_1 directly by saturation-recovery in air-saturated samples. With these relaxation times and the B_1 estimate expression, we can estimate the degree of saturation for nitroxyl radicals for a range of incident microwave powers.

The calculations summarized in the table on the next page for room-temperature spectra display the extreme sensitivity of the saturation factor s to the relaxation times. Thus the numbers obtained in the following estimates of sensitivity are strongly dependent on relaxation times. Ideally, one would obtain spectra with $s = 1$, which would be called "unsaturated." This is never possible, but can be closely approached since the second term in the denominator can be kept very small relative to 1. It seems reasonable, for all but the most demanding measurements, to accept $s = 0.98$ as a definition of an "unsaturated" spectrum. The table below shows that this is achieved with ca. 0.2 mW incident power for a de-oxygenated nitroxyl and ca. 1 mW if the sample is air saturated. These calculations are consistent with our laboratory experience. (The effect of air is greater in air-saturated organic solvents, because of the higher solubility of oxygen in organics than in water.)

Another footnote to the table concerns the resonator Q . Early work showed that the best tradeoff for S/N with aqueous samples occurred when the sample was large enough that it reduced the Q by a factor of 2 (6). This occurred in a TE_{102} resonator with ca. 0.2 mm thick water sample in a flat cell. Reduction in Q becomes a reduction in B_1 at a given incident power, and hence a reduction in the saturation factor s . Consequently, if the Q is reduced by the aqueous sample, the power that results in the same degree of saturation is a factor of 2 greater than is presented in the table. The variable temperature quartz Dewar insert concentrates the microwave B_1 at the sample (4). So if the Dewar is present in the resonator, the actual saturation would be higher than is calculated in the table. Both of these effects can be significant, but we have not tried to include them in the following estimates of sensitivity.

b. Modulation Amplitude

Background information on the selection of modulation amplitude is given in ref. (1) pp. 398-413. The nitroxyl line shape can be approximated as Gaussian due to unresolved

hyperfine coupling, so figure 10-9 in (1) and Table 10-1 in (1) are applicable. The key message from the studies summarized by Poole (1) is that modulation amplitude much in excess of half of the line width distorts the spectrum significantly. It is useful to refer to the original paper by Smith (7). For a line that is substantially Gaussian, if the gain is kept constant while the modulation is increased beyond line width, the spectral amplitude goes through a maximum at a peak-to-peak modulation amplitude about 2 times the peak-to-peak width of the derivative EPR spectrum. With modulation about equal to line width there will be roughly a 20% reduction in spectral amplitude relative to that expected were there no modulation broadening. Approximately 15% reduction from the maximum amplitude occurs when the modulation amplitude is about 4 times the line width (note that in Smith's paper h_m is $\frac{1}{2}$ the p-p modulation). It would be good to actually measure this value for the nitroxyl radical. If one were attempting to record true line shapes, such as might be needed for identification of a spin-trapped radical, the modulation amplitude should be less than about 1/10 of the line width.

sample condition	incident power (mW)	B_1 (G)	saturation factors
RT, no O ₂	0.01	0.0036	0.999
	0.1	0.0115	0.99
	0.2	0.0162	0.98
	0.5	0.0257	0.95
	1	0.0363	0.91
	2	0.0514	0.83
	5	0.0812	0.66
	10	0.115	0.49
	12.5	0.128	0.44
	16	0.145	0.38
RT, air-saturated	0.1	0.0115	0.998
	0.2	0.0162	0.996
	0.5	0.0257	0.99
	1	0.0363	0.98
	2	0.0514	0.96
	5	0.0812	0.90
	10	0.115	0.82
	12.5	0.128	0.79
	16	0.145	0.74

The weak pitch S/N test is a formalized check of multiple aspects of spectrometer performance, as discussed in our article on Quality Assurance in EPR (8). The purposeful over-modulation of the weak pitch sample has validity to avoid effects on the measured S/N of small variations in the weak pitch line width.

4. Comments on conditions selected for Test 3. This was a test of minimum number of detectable spins

The 3.2 G modulation amplitude chosen to maximize the S/N on the Varian and Bruker systems is close to the value estimated from the data in reference (7), assuming a 1 G line width for the tempol signal. It is not clear why JEOL chose $\frac{1}{2}$ of this value. It would cause less line broadening, but is not consistent with the guidelines of achieving the best S/N,

unless there is a problem of noise due to eddy currents in the resonator at high modulation amplitude.

Presumably the extra signal observed in the Bruker super-high-Q resonator was dirt, and could be removed, so we will ignore this problem in the comparisons.

The microwave power chosen was surely strongly saturating in all cases except the 4 mW chosen by JEOL. Apparently the power selected by JEOL was limited by source noise.

The tradeoffs chosen regarding time constant, scan rate, and number of scans is interesting. If this was optimized for each spectrometer it potentially tells us something about the noise spectrum for the spectrometer. That, is, one would choose multiple scans with short time constant if (a) the low-frequency noise dominates, and (b) the data acquisition system averages high-frequency noise well by rapid sampling. Bruker and JEOL need to provide users with more information about their choices to be able to evaluate these results.

5. What do weak pitch results predict for nitroxyl radicals?

The Varian Century Series brochures in 1977 stated that "A signal-to-noise of 120:1 is considered equivalent to a sensitivity of 2.5×10^{10} ΔH spins." Recent Bruker brochures state "A Signal/Noise of 360:1 corresponds to a sensitivity of 0.8×10^{10} Spins/G." Neither source specifies the criterion for sensitivity. Older derivations set signal power equal to noise power in the calculation of minimum number of spins (see, chapter 14 in ref. (1)). Others use a criterion of S/N = 3.

To take the vendor-supplied numerical value of minimum detectable number of spins based on weak pitch and apply that to an aqueous sample of nitroxyl radical in a flat cell requires that we take multiple factors into consideration.

(1) The filling factor η for a flat cell will be different than for the cylindrical tube used for the weak pitch sample. Not only is the geometrical size different, but the aqueous sample concentrates microwaves due to the dielectric constant effect ("lens effect" or "sucking in" effect) (4).

(2) The resonator Q will be lower. Adjustment must be made for the ηQ product.

(3) One must divide by 3 to account for the three lines.

(4) The line width of the nitroxyl will be about 1 G, so the "per 1 G line width criterion" is reasonably applicable. For lines broader or narrower than 1 G adjustment must be made. There also are implications for modulation amplitude.

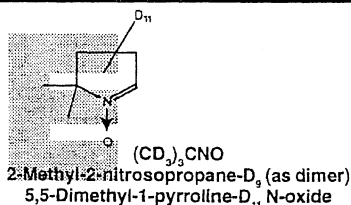
(Note: The ΔH in the sensitivity expression is defined in terms of "1-second integration time" in an old Varian document, but the data acquisition time constant has nothing to do with this width unless inappropriate scan time and time constant settings caused distortion of the line shape. The width is just a statement of spectral dispersion of the resonance. Since the height goes as width-squared, one would adjust the numerical sensitivity value for a line width that differed from 1 G.)

(5) The sensitivity specification based on the weak pitch sample assumes that the signal does not saturate at 200 mW. One needs to take account of the actual power saturation of the signal.

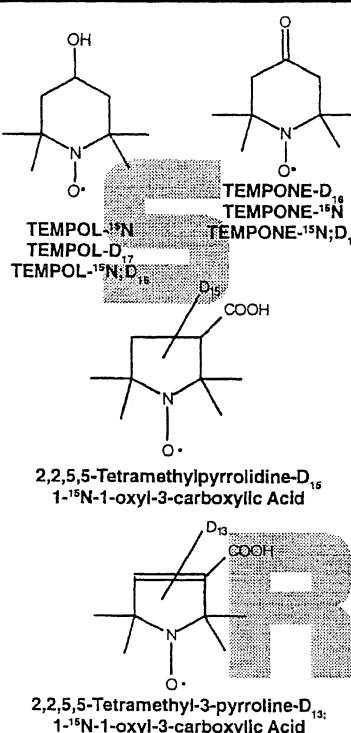
Based on the information presented above, if a nitroxyl radical had a line width of ca. 1 G, the EPR spectrum of an aqueous solution at room temperature would normally be recorded at ca. 1 mW incident power, with ca. 0.2 G modulation amplitude. Relative to the conditions for weak

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pitch this would reduce the spectral amplitude by $8/0.2 = 40$ (modulation effect is linear if there is no broadening) and $(200/1)^{1/2} = 14$ (signal scales as square root of power if there is no saturation), and 3 for the number of hyperfine lines, for an overall decrease of 1680. This factor of 1680 is missing from the preliminary report posted by Mason and Fann on 4/1/98.

Thus, if the weak pitch S/N specification of 360:1 for the modern Bruker spectrometer with a TE₁₀₂ cavity resonator corresponds to a sensitivity of 0.8×10^{10} spins, we would expect to be able to observe 1.3×10^{13} nitroxyl radicals. This is 2.2×10^{-11} moles. If we assume that about 50 μ L of solution in a flat cell contributes most of the signal, due to the distribution of B_1 and of the modulation field in a standard TE₁₀₂ resonator, we would expect to detect 0.4 μ M nitroxyl. In August 1986 we happened to measure 40 μ M tempol in 0.15 M aqueous KCl solution. A flat cell containing 48 μ L of solution was used in a Varian E-9 with an E-231 cavity. Our best

estimate was that $B_1 \approx 0.06$ G and modulation amplitude was 0.3 G. (Conditions were chosen to compare with a low-frequency spectrometer.) S/N was 177. We measured noise as the standard deviation using a least-squares computer routine. One would have to decrease the S/N by a factor of 2 to compare with manually measured peak-to-peak noise. Now, compare this result with the estimates made above: we have to divide by 1.65 to normalize for B_1 , and by 1.5 to normalize for modulation amplitude. Including the factor of 2 to compensate for our computer calculation of SD noise, we could find $S/N = 36$ for the conditions used in the estimates in the previous paragraph. Within the accuracy of these extrapolations, we would find a $S/N = 1$ for a 1 μ M solution under the conditions of the previous paragraph. Since the weak pitch S/N on this spectrometer is less than the

Bruker specification we actually come fairly close to the sensitivity implied by the weak pitch test.

Note that some of the assumptions in this analysis also point to ways to improve the experimental S/N for aqueous solutions. The TM cavity, for example, makes B_1 more uniform along the sample, so that a larger amount of solution yields signal (the filling factor is larger). One could also make the modulation coils such that they provided a more uniform field over the sample, thus providing significant B_m for more of the spins. The trade-off is that one would not be able to achieve the traditional 40 G peak-to-peak modulation amplitude, but that is not useful for most aqueous samples, and certainly not for nitroxyl radicals.

6. The next round of tests

There has been a suggestion that further comparisons be made. We suggest that the comparison for low concentration aqueous tempol solutions include tests for both

Case 1: Microwave power, modulation amplitude, and time constant selected to provide undistorted line shape information, and

Case 2: Microwave power, modulation amplitude, and time constant selected to provide the maximum signal amplitude, at the expense of line shape information.

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CONFERENCE REPORTS

V International Workshop Electron Magnetic Resonance of Disordered Systems and III International Seminar on Applied EPR, June 8-17, 1997, Sofia, Bulgaria

Following tradition, both biannual meetings were organized by the BULGARIAN EPR SOCIETY, in collaboration with Institute of Catalysis, Bulgarian Academy of Sciences and Department of Chemistry, Sofia University.

The EMARDIS workshop 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 through round-table discussions and lectures by top specialists and selected applicants.

The APPLIED EPR seminar topics were: Fundamental aspects of Quantitative EPR (standards, calibration, metrology and methodology of quantitative measurements, instrumentation - new methods, advanced techniques, automatization, etc.); EPR dosimetry (monitoring of high energy radiation, high energy radiation processing control in food preservation and sterilization, dating of archeological and geological samples, etc.); EPR in biology and medicine (clinical and biomedical studies); EPR in environmental control; EPR in petrol industry; EPR and fossil fuels; EPR in polymer chemistry, etc.

To facilitate personal scientific contacts and discussions, the number of participants was limited to about 30 for each event. Representatives from 16 countries (Austria, Belgium, Canada, France, Germany, Italy, Japan, Poland, Romania, Russia, Slovakia, Switzerland, The Netherlands, UK, USA and Bulgaria) attended. All participants were accommodated in one hotel, where the lectures were presented. The hotel is situated in the Vitosha mountains, about 15 km from downtown Sofia.

The scientific programme included lectures, posters, and round-table discussions. The following well-known experts delivered lectures at:

a. **EMARDIS**: •B.J. Gaffney, *Evaluation of Zero Field Splittings by Multi Frequency EMR*; •E.J. Reijerse *Concepts in High Frequency EPR: Applications to High Spin Systems*; •G. Grampp, *Application of Marcus-theory to Intramolecular Electron Transfer Reactions Within Organic Radical Anions*; •J. Ceulemans, *Structure-Reactivity Relationship in Reactions of Alkane Radical Cations. Study of the Proton Transfer from Alkane Radical Cations to Alkane Molecules in Gamma-irradiated Disordered CCl₃F/alkane Systems by ESR Spectroscopy at Cryogenic Temperatures*; •M. Zdravkova, *EPR*

Studies of X-irradiated Dithiophosphate Metal Complexes; •E. Giamello, *Generation, EPR Characterisation and Reactivity of Color Centers at the Surface of Ionic Oxides*; •C. Oliva, *O--Cu²⁺-O-(S=3/2) Formation in (CeO₂)_{0.75}(La₂CuO₄)_{0.25} Catalyst, During Reduction of NO by CO*; •H. Kurreck, *EPR Studies of Photoinduced Electron Transfer in Model Compounds of Photosynthesis*; •F. Lendzian, *Electronic Structure and Protein Interactions of Cofactors in Bacterial Photosynthesis as Studied by cw- and Pulsed EPR Techniques*; •R. Cammack, *Interaction of Metal Proteins in Cells with Nitrogen Oxide*; •A.J. Hoff, *Probing the Energy Landscape of Bacterial Photosynthetic Reaction Centers at Cryogenic Temperatures by ESEEM of Spin-polarised D+QA- Radical Pairs*; •S.K. Misra, *Electron Spin-lattice Relaxation in Amorphous Materials as Effected by Exchange Interactions, TLS Centers and Fractions*; •S.K. Hofman, *Electron Spin Relaxation of Cu(II) Ions in Diamagnetic Crystals*; •Y. Ohba, *A Study on Photoexcited Multiplets by Two-dimensional Nutation Spectroscopy*; •D. Gourier, *Bistable Magnetic Resonance of Conduction Electrons in Solids*; •M. Makinen, *ENDOR Determined Structure and Conformation of Small Molecules and Enzyme Reaction Intermediates in Solution*; •J. Telser, *EPR and ENDOR Studies of Native and Metal-substituted Fe-S Proteins Isolated from the Hyperthermophilic Archaeon Pyrococcus Furiosus*; •L.M. Antov, *Distant 31P and 195Pt and Local 31P ENDOR Studies of Powdered Samples of bis(O,O'-disubstituted-dithiophosphato)copper(II) Complexes Magnetically Diluted in the Corresponding Pd(II) and Pt(II) Host Lattices*; •H. Caldaradu, *Structural Aspects in Self-assembled Systems of Polyoxyethylene Surfactants, as Studied by Spin Probe Technique*; •J. Forrer, *Strongly Overcoupled Pulse EPR Resonators*.

b. **APPL-EPR**: •J. Raffi, *A Point about Electron Paramagnetic Resonance Detection of Irradiated Foodstuffs*; •W. Stachowicz, *Aspects of Detection the Irradiated Foods by EPR Spectroscopy*; •J.M. Dolo, *Evaluation of Some Parameters Which Influence the ESR Measurements Fading Study of Alanine Dosimetry*; •V. Gancheva, *New Generation of SS/EPR Dosemeters - Alanine/EPR Dosemeters*; •F. Callens, *EPR of Carbonate Derived Radicals: Applications in Dosimetry, Dating and Detection of Irradiated Food*; •L.J. Berliner, *In Vivo EPR in Living Systems*; •A. Jezierski, *EPR in the Environmental Control: Copper Complexes and Free Radicals in Soil and Municipal Solid Waste Compost*; •K. Dyrek, *EPR Study of the Mobility of Paramagnetic Species on the Surface and in the Bulk of Solids*; •A. Stasko, *EPR Investigations of C₆₀ Fullerene Anions*; •A.M. Wasserman, *EPR Spin Probe and Spin Label Study of Some Low Molecular and Polymer Micelles*; •N.D. Yordanov, *Studies on Some Non-linear Effects in the Quantitative EPR Spectrometry Due to the Commonly Used Cavities with TE₁₀₂ and TM₀₁₁ Modes*.

Poster Presentations:

a. **EMARDIS**: •M.A. Doicheva, B.G. Jeliaskova, *the Effect of Chloroalkane/alcohol Solvent Composition on the Properties of Copper(ii) Dithiocarbamate Mixed-ligand Complexes. EPR Study*; •M.A. Doicheva and B.G. Jeliaskova, *EPR Study on the Charge-transfer Photochemistry of the Bromide Mixed-ligand Dithiocarbamate Complex of Copper(II)*; •B.G. Jeliaskova, G.Ch. Sarova, S.N. Doneva, *EPR Study on the Thermal and Photochemical Reactions of Bis(8-quinolinolato)copper(II) and Bis(8-quinolinethiolato)copper(II) with Chloroalkanes*; •N.D. Yordanov, M. Michailov, P. O'Brien, *EPR and UV-VIS Study on Some Interactions of Bis(diethyl-diselenocarbamato)copper(II) in Solution*.

b. **APPL-EPR**: •J. Sadlo, P. Matthys, G. Vanhaelewyn, F. Callens, J. Michalik, W. Stachowicz, *EPR and ENDOR of CO₃₃-Radicals in Human Tooth Enamel Heated at 400°C*; •N.D. Yordanov, K. Rangelova, *Quantitative Spectrophotometric and EPR*

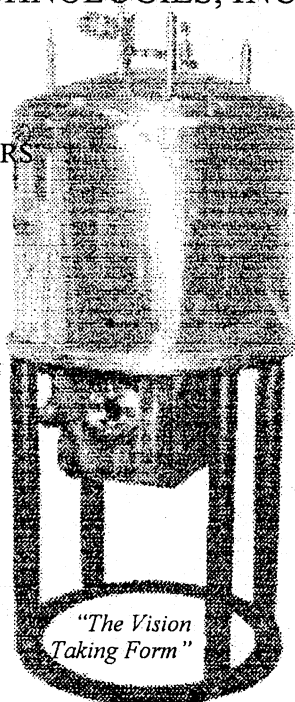
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Determination of the Free Radical 2,2,6,6-tetramethyl-4-hydroxypiperidine-1-oxyl; •N.D. Yordanov, V. Gancheva, M. Radicheva, B. Hristova, M. Guelev, O. Penchev, *Comparative Identification of Irradiated Herbs by the Methods of Electron Paramagnetic Resonance and Thermoluminescence*; •N.D. Yordanov, V. Gancheva, R. Tarandjiska, R. Velikova, L. Kulieva, B. Damyanova, S. Popov, *Simultaneous EPR and GC Studies on the Identification of Irradiated Meat*.

Two **Round Table Discussions**: "Trends on Increasing of the Resolution of EMR Spectra" (EMARDIS) and "Applications of EPR to Environmental Problems" (APPL-EPR) were organized. (The introductory remarks about them which were distributed among the participants are given separately).

Proceedings: Traditionally, EMARDIS/APPL-EPR meetings have had two kinds of Proceedings: one with short abstracts of all presentations which is available at the meeting and a second one containing the full text of all invited lectures as well as selections from the short original communications published within the year. This time the latter will be published in *Applied Magnetic Resonance*.

Social events included cocktails, farewell dinner in a traditional Bulgarian restaurant, and half-day sightseeing tours around Sofia (including a visit to the National Historical Museum) organized by participants. A one-day excursion to the Rila Monastery was organized in the gap between the two meetings.

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Sixth Annual Workshop: "Modern Development of Magnetic Resonance" 23-26 September 1997, Kazan, Tatarstan, Russia

The program of the Workshop was as follows:

V. E. Kataev (Zavoisky Physical-Technical Institute, Kazan, Russia) "Magnetic Properties of the Low Temperature Tetragonal Phase of RE Doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ " A. Schweiger (ETH, Zurich, Switzerland) "Two-Dimensional Pulse EPR Spectroscopy: Concepts and Strategies"

A. Hoff (Huygens Laboratory, Leiden, Holland) "Site-Specific Isotope Labelling as a Tool for Obtaining Structural Information with Multifrequency EPR and ESEEM" A.V. Klochov, S.P. Kurzin, I.R. Mukhamedshin, D.R. Nabiullin, V.V. Naletov, I.Kh. Salikhov, M.S. Tagirov, D.A. Tayurskii, R.Sh. Zhdanov (Kazan State University, Kazan, Russia), H. Suzuki (Kanazawa University, Kanazawa, Japan) "Magnetic Resonant and Non-Resonant Investigations of LiLnF_4 (Ln = Y, Tm) Powders"

M.V. Eremin (Kazan State University, Kazan, Russia), V.A. Ulanov, M.M. Zaripov (Zavoisky Physical-Technical Institute, Kazan, Russia) "Electronic Structure of Eightfold Coordinated Divalent Silver Complexes: Determination by Means of EPR"

C. Rudowicz (City University of Hong Kong, Hong Kong, China) "Applications of EPR from A to Z"

Yu. Shvachko (Institute of Metal Physics, Ekaterinburg, Russia), H.-H. Wang, J. M. Williams (Argonne Laboratory, Argonne, USA) "EPR-Probe Decoration: from Analysis of Superconducting Properties to ESR Imaging"

D. Schmid (Institut fuer Physik der kondensierten Materie, Duesseldorf, Germany) "Spatial Coherence in Optical Superradiance"

A.V. Il'yasov (Arbuzov Organical and Physical Chemistry Institute, Kazan, Russia) " ^{31}P -CIDNP in Chemical Reactions of Phosphorus-Organic Compounds Series at Different Magnetic Fields"

The Annual 1997 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professor Kamil A. Valiev (Inst. Physics & Technology, Russian Academy of Sciences, Moscow) on September 25 in a ceremony marking his outstanding contribution to the development of the theory of spin relaxation. The ceremony was chaired by the Chairman of the Award Committee, Professor K.M. Salikhov. Professor A. Schweiger announced the decision of the Zavoisky Award Committee. The presentation was made by Deputy Prime-Minister of the Republic of Tatarstan I.K. Khairullin. The Rector of the Kazan State University Professor Yu.G. Konoplev, the Chairman of the Presidium of the Kazan Scientific Centre of the Russian Academy of Sciences Professor A.I. Kononov, and the Principal Secretary of the Tatarstan Academy of Sciences Professor I.B. Khaibullin warmly congratulated the laureate. Professor S.V. Gaponov congratulated the laureate on behalf of the Department of General Physics and Astronomy of the Russian Academy of Sciences. Dr. V.G. Zhotikov announced the congratulation of the Ministry of Science and Technology of the Russian Federation. Professor A.A. Manenkov congratulated the laureate on behalf of the Scientific Council on magnetism and Commission on radiospectroscopy. Professor C. Rudowicz congratulated the laureate on behalf of the Asia-Pacific EPR/ESR Society. A Government telegram from the Minister of Science of the Russian Federation academician V.E. Fortov and letters of congratulations from Professor B. Maraviglia, President of the AMPÈRE Society, Professor J.R. Norris, President of the International EPR Society, Professor M. Goldman, President of ISMAR, Professor J. Stankovski, and Professor K. Möbius were handed to Professor Valiev.

During a stay in Kazan, the laureate visited places of historical and cultural interest in Kazan, and picturesque sites in the Mamadysh region.

The Organizing Committee owes special thanks to the NIOKR Fund of the Republic of Tatarstan, the Ministry of Science and Technology of the Russian Federation, the Russian Fund for Basic Research, the Administration of the Soviet District of Kazan and its Head A.A. Kamaleev, the firm "ICL" and its Deputy Director General V.V. D'yachkov, the firm "Abak" and its Director F.N. Markman, and the Head of the Administration of the Mamadysh region Dr. E.S. Gubaidullin and the Deputy Head of the Administration of the Mamadysh region Sh. N. Khasanov.

COMPANY PROFILE:**Toronto Research Chemicals, Inc.***Introduction*

Toronto Research Chemicals Inc. (TRC), a new sponsor of the International EPR Society, is a Canadian-owned private corporation specializing in the manufacture of complex organic chemicals for biomedical research. The company has been supplying biomedical research reagents and manufacturing services to a global client-base including major biotechnology corporations, pharmaceutical and diagnostics companies, manufacturers of specialty chemicals and hospitals, universities and research institutions for over 15 years.

Background

Toronto Research Chemicals Inc. (TRC) was established in 1982 as a service laboratory located at the University of Toronto. The main business activity was to supply Faculty of Medicine research staff with chemicals not available through existing commercial sources. Drawing from expertise in synthetic chemistry and a strong interest in biomedical research, TRC was established to service the unique needs of individual research scientists requiring specific chemicals for application in their work.

In July 1986, TRC secured new laboratories and manufacturing facilities in Toronto. Today, the company employs a staff of 18 people, and occupies a 15,000 sq. ft. facility for R&D and manufacturing. The company has developed a client-base of research scientists located around the world. With growing demand for new and innovative chemicals for various applications in biomedical research, TRC has also secured a number of manufacturing and custom synthesis contracts with large suppliers of research biochemicals. These relationships continue today and are a large part of TRC's ongoing success.

Capabilities and Focus

TRC has developed a broad base of proprietary knowledge and chemical manufacturing expertise. Technical strengths include carbohydrate chemistry, aromatic chemistry, organonitrogen, phosphorous and sulfur chemistry, as well as radioisotope and stable isotope labeling. The company currently manufactures more than 1500 organic chemicals for applications in biomedical research.

TRC is capable of doing complex chemistry on scales of up to 10 kg. For projects requiring a single manufacturing step, a much larger production volume can be achieved (up to 200 kg per year in some cases). Our equipment includes 50 L and 100 L all-glass reactors, 50 L and 100 L rotary evaporators, and a 20 L steel autoclave for pressure reactions and hydrogenation up to 600 psi. TRC also houses 3 pilot plants which will be equipped in the near future with reaction vessels in the 500 to 1200 L range. These plants will be used for the manufacture of complex pharmaceutical actives and intermediates on scales of up to 100 kg.

Toronto Research Chemicals' business focus is based primarily on customers' needs for new and innovative tools for biomedical research. By anticipating and responding to these needs, the company's goal is to provide a broad range

of high purity, low cost biomedical research chemicals. TRC is devoted to pursuing opportunities to develop new and innovative products for biomedical research. The company hopes to achieve this through partnership and collaboration with research scientists in both industry and academia and with those who share similar goals.

For more information about Toronto Research Chemicals Inc., and its products and services, please contact: Jason Savelli, Toronto Research Chemicals Inc., 2 Brisbane Road, North York, Ontario M3J 2J8, Canada; ☎: 1-416-665-9696, Fax: 1-416-665-4439; E-mail: torresch@interlog.com. Web site: www.trc-canada.com.

NOTICES OF MEETINGS

NOTICE: NOTICES AND UPDATES ABOUT SOME MEETINGS ARE NOT PRINTED IN THIS COLUMN IF THE INFORMATION ARRIVES TOO LATE OR IF SPACE IS LIMITED. BUT SUCH MEETINGS MAY BE ANNOUNCED ON THE EPR NEWSLETTER WEB SITE WITH LINKS TO DETAILED CONFERENCE INFORMATION WHERE POSSIBLE. CONTACT IERC@UIUC.EDU TO HAVE YOUR MEETING ADDED-

<http://ierc.scs.uiuc.edu/news.html>

32nd INTERNATIONAL MEETING, ESR GROUP, ROYAL SOCIETY of CHEMISTRY: ESR SPECTROSCOPY; RECENT ADVANCES and APPLICATIONS, University of York, UK, April 11-15, 1999.

Scientific Programme. The following have accepted invitations to give plenary lectures: R. L. Belford (Univ. Illinois), M. Ché (Univ. P. et M. Curie Paris), B.C. Gilbert (Univ. York), G.F. Pedulli (Univ. Bologna), J.M. Spaeth (Univ. Gesamthochschule Paderborn), J. Schmidt, the Bruker Lecturer (Univ. Leiden), A.J. Thomson (Univ. East Anglia), P. Tordo (Univ. Provence), J.C. Walton (Univ. St. Andrews), A. Watts (Univ. Oxford), B. Webster (Univ. Glasgow), and L. Yellowlees (Univ. Edinburgh). Further details can be obtained at the web site:

<http://www.cf.ac.uk/uwcc/chem/rowlandsec/conf.html>

ISMIRM 7th SCIENTIFIC MEETING and EXHIBITION, Philadelphia, PA, May 22-23, 1999.

The 1999 Scientific Meeting of the International Society for Magnetic Resonance in Medicine will combine traditional and new elements of interest to both basic scientists and clinicians to provide a program to appeal to all attendees.

Weekend Educational Courses will offer sessions on MR Imaging, spectroscopy and methodology.

The Plenary Lectures will begin the Scientific Meeting each day from Monday through Friday. Of particular interest is the Lauterbur Lecture at the opening session, which will be given by Prof. Erwin Hahn. The other Plenary Lecture topics include state of the art reviews of High versus Low Field MR Technology, Angiogenesis, Women's Health, Hemodynamic Responses to Neuronal Activity and MR in Pharmacologic Research.

The Oral Scientific Sessions, Poster Sessions and Clinical Focus Sessions will be constructed from proffered abstracts.

Special Courses include Morning Categorical Courses, Clinical Categorical Courses and Practical Courses. The three Morning Categorical Courses will address the topics of MRI of Sports Injuries, MR Angiography, and Clinical Applications of Spectroscopy. Clinical Categorical Courses will be offered on Cardiac Imaging, Hepatobiliary Imaging, GI Imaging, Neuroimaging, and Gynecological Imaging. Two practical

courses, "Hot Topics for Clinical Practice" and "MR Physics and Techniques for Clinicians," will be presented. Finally, a new symposium on Technology Assessment will round out the special education offerings.

Call for Papers: The Society invites submission of abstracts to be presented in oral and poster sessions; abstracts must contain new, previously unpublished material. The deadline for receipt of Abstracts in the ISMRM Office is January 12, 1999. Abstracts accepted for presentation will be printed in the proceedings of the meeting. Abstracts must be printed on official 1999 abstract forms. Detailed instructions are included on the forms. To receive abstract forms and instructions, please call, fax, or write to the International Society for Magnetic Resonance in Medicine, 2118 Milvia Street, Suite 201, Berkeley, California, 94704, USA. ☎: 1-510-841-1899; FAX: 1-510-841-2340; E-mail: info@ismrm.org.

41st ANNUAL ROCKY MOUNTAIN CONFERENCE on ANALYTICAL CHEMISTRY, Denver, Colorado, August 1-5, 1999, with 22nd INTERNATIONAL EPR SYMPOSIUM.

Sponsored by the Rocky Mountain Section of the Society for Applied Spectroscopy and the Colorado Section of the American Chemical Society. More information can be obtained at the web site for the meeting:

<http://www.rockychem.com/>

Check this web page for links to the EPR Symposium, or contact Prof. Sandra S. Eaton (seaton@du.edu) or Prof. Gareth Eaton (geaton@du.edu) for more details.

VI INTERNATIONAL SYMPOSIUM on MAGNETIC FIELD and SPIN EFFECTS in CHEMISTRY and RELATED PHENOMENA, August 21-26, 1999 Emmetten, Switzerland).

For information on the program, speakers, conference site, accommodations, costs and deadlines, please view the web site at:

<http://pciradic8.unizh.ch>

or contact Prof. Henning Paul; Physikalisch-Chemisches Institut; Univ. Zürich; Winterthurerstrasse 190; CH-8057 Zürich, SWITZERLAND; ☎: 41-1-6354422; Fax: +41-1-6356813; e-mail: hepaul@pci.unizh.ch

SPECIALIZED COLLOQUE AMPÈRE-99 on MOLECULAR DYNAMICS and PHASE TRANSITIONS in CONDENSED MATTER, Vilnius, Lithuania, September 18-23, 1999.

The Specialized Colloque AMPÈRE "Molecular Dynamics and Phase Transitions in Condensed Matter" will be organized by Vilnius University and Lithuanian Academy of Sciences, in accordance with the decision of the AMPÈRE Committee made at the meeting during the 28th Congress AMPÈRE (September 1-6, 1996, University of Kent at Canterbury, England).

Scientific Programme—The scientific program will include plenary invited lectures (highlighting the selected topics), oral and poster sessions. The final selection of the topics will be made from the following suggestions and according to the traditions of the AMPÈRE Conferences: •dynamical and structural aspects of various types of disorder in solids; •phase transitions and critical phenomena in partially disordered systems and glasses; •diffusion and relaxation in biological systems; •molecular dynamics in porous media; •structure and molecular dynamics in advanced materials.

Venue and Date—The Colloque AMPÈRE will take place at Vilnius University and Academy of Sciences (in the Centrum of Vilnius, Capital of Lithuania). It will start on Saturday, September

18, 1999 (registration, accommodation, welcome reception) and close on Thursday, September 23, 1999 around noon.

The WWW page of the Colloque opens the links to the home pages of Lithuania, Vilnius University, Lithuanian Academy of Sciences and etc.:

<http://www.vu.lt/menu/event1/AMPÈRE/index.htm>

For further information, or to receive the 2nd Circular (which will be mailed in December 1998), contact Prof. L. Kimtys, Chairman of the Organizing Committee, Faculty of Physics, Vilnius University, Universiteto Str. 3, 2734 Vilnius, LITHUANIA; ☎: 370-2-76-94-60; FAX: 370-2-76-44-55 or 370-2-22-35-63; E-mail: Liudvikas.Kimtys@ff.vu.lt

2nd ASIA-PACIFIC EPR/ESR SYMPOSIUM, Zhejiang University, Hangzhou, Peoples Republic of China October 30-November 3, 1999.

The 1st Asia-Pacific EPR/ESR Symposium was held at the City University of Hong Kong, January 20-24, 1997. The Asia-Pacific EPR/ESR Society will provide logistic support and coordination for organization of the future Symposia. The President of the Asia-Pacific EPR/ESR Society has recently conducted a search for an Asia-Pacific EPR/ESR group willing to host the next Symposium. After consultations with the potential hosts it has just been decided that the 2nd Asia-Pacific EPR/ESR Symposium will be held at Zhejiang University, Hangzhou, P.R. China, October 30-November 3, 1999. Prof. Yuanzhi Xu, the Chairman of the Local Organizing Committee (LOC), is the member of Magnetic Resonance Special Committee, Chinese Physical Society.

In the spirit of the 1st Symposium, the future Asia-Pacific EPR/ESR Symposia are aimed primarily at the Asia-Pacific countries but will be open to participants from all over the world. The 2nd Symposium (APS'99) targets all subareas of EPR/ESR. Contributions dealing with any aspects of recent developments in Theory, Methodology, Instrumentation, and Experimental Techniques are invited. The focus will be on recent applications of the EPR/ESR spectroscopy, e.g., conventional EPR/ESR, high-frequency and high-field EPR, ENDOR, ESEEM, MRI, ELDOR, CIDEP, ODMR, OPEPR. Four parallel topical sessions are planned: (1) Biology, Life and Medical Sciences, (2) Chemistry, Earth and Environmental Sciences, (3) Physics and Materials Science, (4) New Developments and Crossdisciplinary Areas.

Nominations (including self-nominations) are invited for up to eight invited speakers to deliver plenary lectures dealing with the most important current topics. Please provide a short abstract of the lecture and a brief CV of the potential speaker. Make the nominations immediately (preferably by E-mail or Fax) to the President of the Asia-Pacific EPR/ESR Society or the Chairman of the Local Organizing Committee. A selection committee will announce its decisions by the end of June 1998.

The host city, Hangzhou, is a beautiful location, especially in autumn. A famous idiom in China is: "We have Su & Hang in the Earth as well as Paradise in the sky." It means that Suzhou & Hangzhou are as beautiful as Paradise. You can directly fly from Singapore or Hong Kong to Hangzhou, and it can also be easily reached via Shanghai. From Shanghai to Hangzhou it is only 180 km, and it takes about 2.5 hours by train or by car on highway.

The Second Announcement and Call for Papers will be circulated in December, 1998. If your name is not on the list of the 1st Asia-Pacific EPR/ESR Symposium participants, please provide us with your name and full address as soon as possible.

For more information contact: Prof. Yuanzhi XU, Chairman, LOC, The 2nd Asia-Pacific EPR/ESR Symposium (AP

EPR/ESRS'99), Department of Chemistry, Zhejiang University, Hangzhou 310027, P. R. China ☎: 86-571-7984095/86-571-7951352; Fax: 86-571-7984095/86-571-7951895; E-mail: xyz@public.hz.zj.cn or Prof. Czeslaw Rudowicz, The President, The Asia-Pacific EPR/ESR Society, Department of Physics and Materials Science, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong SAR, P.R. China; ☎: 852-2788-7787 Fax: 852-2788-7830; E-mail: apsepr@cityu.edu.hk.

POSITIONS AVAILABLE

POSITIONS AVAILABLE at the EPR CENTER for VIABLE BIOLOGICAL SYSTEMS at DARTMOUTH MEDICAL SCHOOL

We have immediate openings for several positions. The positions, depending on the qualifications of the individual and their skills, could range in duration from two years (absolute minimum) to as long as we have funding for the EPR Center and other research grants. The rank for the positions will be Research Associate (equivalent to post-doctoral) or Research Assistant Professor and will depend on the background and experience of the applicants. The positions will be fully supported by existing external grants and the applicants will be expected to devote their full efforts to the research activities whose funding provides their support. While obtaining independent additional external support will be encouraged, it is not a requirement. The areas of expertise that are needed include:

1. Scientific Lab Manager for the EPR Center to both help manage the projects and to work with visitors who use the Center. This person needs to have excellent skills in management of a scientific laboratory and a high level of competence in EPR spectroscopy. Skills and knowledge in working with biological systems and in free radicals are very desirable.

2. EPR spectroscopist with particular expertise in free radicals, both stable and reactive (including spin trapping). This position requires experience and knowledge in the technique of spin trapping and also in free radical chemistry. Experience in working with biological systems also would be very desirable.

3. Cell Biologist, to work on studies to elucidate the mechanism for the occurrence of gradients of oxygen between the extracellular and intracellular compartments. This position requires a high level of skill and experience in working with mammalian cells and maintaining them under physiological conditions during the studies. Prior experience in EPR spectroscopy would be helpful but is not a requirement.

4. EPR Instrumentalist to be involved with the development of and improvement of instrumentation in the EPR center, with particular emphasis on in vivo EPR. This position requires prior extensive experience in the construction of new EPR equipment. A strong background in engineering would be very desirable.

All positions require a relevant PhD or the equivalent. Dartmouth Medical School is an equal opportunity/affirmative action employer. Minorities and women are encouraged to apply.

Applications and three letters of recommendation should be sent directly to Harold M. Swartz, either by mail or by e-mail: Harold M. Swartz, MD, PhD; Dartmouth Medical School; 7785 Vail, Room 702; Hanover, NH 03755; Fax: 603-650-1717; E-mail: harold.swartz@dartmouth.edu.

POST-DOCTORAL POSITION AVAILABLE at NIEHS

A post-doctoral position (less than five years of post doctoral experience) in a biological ESR group is available October 1, 1999 with a salary of \$26,500 or more depending on experience. Health insurance is included at no extra cost. Experience in immunology, cell biology, and/or electron spin resonance is necessary. Please send *curriculum vitae* to Dr. Ronald P. Mason, NIEHS/NIH, P.O. Box 12233, Research Triangle Park, NC 27709 or e-mail mason4@niehs.nih.gov.

POST-DOCTORAL POSITION at LEIDEN UNIVERSITY DEPARTMENT of BIOPHYSICS

Applications are invited for an EU-TMR funded post-doctoral research assistantship, tenable for a period of 36 months, to work with Prof. A.J. Hoff and Dr. P. Gast. The research project involves the study of the fundamental mechanism of solar energy conversion in photosynthesis with advanced electron paramagnetic resonance (EPR) techniques. The work will be carried out in the Dept. of Biophysics, where in a stimulating, multidisciplinary environment teams of (bio)physicists, chemists and biologists closely collaborate in studies involving sophisticated optical, magnetic resonance and molecular biology techniques. Applicants with experience in cw and pulsed EPR techniques will be particularly welcome.

Salary will be NLG 4806 per month. Applicant must be a citizen of one of the EU or associated countries, excluding The Netherlands. The post is available immediately.

Further information may be obtained from Prof. A.J. Hoff (hoff@biophys.leidenuniv.nl) or Dr. Peter Gast (gast@biophys.leidenuniv.nl) or at the web site: <http://www.biophys.leidenuniv.nl/home.html>. Applications, together with a curriculum vitae and the names of two referees should be sent to Prof. A.J. Hoff, Biophysics Department, Huygens Laboratory, PO Box 9504, 2300 RA Leiden, The Netherlands.

EQUIPMENT & SUPPLIES EXCHANGE

AVAILABLE: ISOTOPE-CONTAINING SPIN PROBES

A wide assortment of special ^{15}N - and/or ^2H -containing spin probes is available at moderate prices. For a catalog and price list of available compounds, contact Prof. Igor' Grigor'ev, Inst. of Organic Chemistry, Novosibirsk 630090 Russia; E-mail: maxx@nioch.nsc.ru. In the US, contact Sergei Dikanov, E-mail: sdikano@binghamton.edu.

WANTED: MICROWAVE BRIDGE

One X-band microwave bridge for old type of Bruker spectrometer (Model 420). The purpose is to put a spectrometer in operation at the Physics Department, University of Khartoum, Sudan. Contact: Anders Lund, Linköping University, Department of Physics & Measurement Technology, Linköping S-58183 Linköping, Sweden, Fax: 46-13-137568, E-mail ald@ifm.liu.se.

FOR SALE - NMR MAGNETOMETER

Sentec Model 1001, including 3 standard probes covering the range of 1 to 10 kG. In good working order, this 1981 model (uses NIM bin!) includes 7-digit display, 0.01 Gauss resolution, accuracy: 10⁻⁶ relative, 10⁻⁵ absolute, has automatic peak search feature, BCD output, etc. Can be bought with or without NIM bin and CRT display. Make an offer! Prof. E. J. Knystautas, Physics Dept., Univ. Laval, Quebec City (Quebec) G1K 7P4; ☎: 1-418-656-5569, FAX: 1-418-656-2040, E-mail: ejknyst@phy.ulaval.ca

WANTED: USED VARIAN SPECTROMETER

Searching for used Varian EPR Spectrometer and/or parts: E-4 or E104 Spectrometer and/or Spectrometer modules, Field Controller as top priorities. Non-working units OK, the only hard to solve problem is a water-leaking magnet. Cash payment or parts/equipment exchange. I'll directly pick up the system if in Europe, and arrange for shipment elsewhere. Contact Vanni Piccinotti, Magnetic Resonances, Via del Berignolo 5, 50141 Firenze, Italy; ☎/FAX: 39-55-434841; E-mail: vpmnr@ats.it; web: <http://www.webspace.it/vpmnr>.

WANTED: VARIAN MICROWAVE BRIDGE

One Varian X-band microwave bridge — Varian Model E-102. Contact: Lon B. Knight, Jr., Furman University, Department of Chemistry, Greenville, SC 29613, USA; ☎: 1-864-294-3372; FAX: 1-864-294-3559; E-mail: knight_lon@furman.edu.

JEOL TE2000 SPECTROMETER

JEOL has a TE2000 EPR spectrometer in stock in Boston that it is willing to let go at a substantial discount. For further information, contact Robert DiPasquale at dipas@jeol.com.

AVAILABLE: VARIAN COMPONENTS and MAINTENANCE

Varian VT components available for sale at symbolic prices: Cavity quartz dewars, transfer dewars, heat exchangers, heater-sensors. Maintenance problems on your good old Varian EPR Spectrometer? With over 20 years experience, maybe I can help you! Professional service, spare parts, modifications, upgrading. Available at interesting rates all over Europe and overseas! Contact Vanni Piccinotti Magnetic Resonances, Via del Berignolo 5, 50141 Firenze, Italy; ☎(VOICE/FAX): 39-55-434841; E-mail: vpmnr@ats.it; or visit the website:

<http://www.webspace.it/vpmnr>

FOR SALE: VARIAN

Resonance Instruments has available:

- 1) replacement Klystrons for Varian EPR Bridges (at reduced prices)
- 2) VARIAN V4500-41A low/high power microwave bridge with new klystron—excellent condition

For more information on these units contact Clarence Arnou, President, Resonance Instruments. ☎: 1-847-583-1000; FAX: 1-847-583-1021; E-mail: rii@wwa.com.

NEED HELP in DESIGN and CONSTRUCTION of EPR ELECTRONICS?

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 KHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a

conversion kit to convert Varian field control units to voltage-controlled scan operation. A 6 digit 1 ppm frequency counter is available in X-, C-, S- or L-band or Megahertz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the University of Denver. Contact Richard W. Quine, ☎: 1-303-871-2419; E-mail: rquine@du.edu.

AVAILABLE: TWO IBM 9000 COMPUTERS

We have two IBM 9000 computers that were used to control our IBM (Bruker) EPR spectrometer, including the double floppy disk drive and a hard disk, to give away. They were still working well when we switched them off about two years ago. For information, contact: Eicke Weber, Materials Science Division, Berkeley Lab, and Dept. Materials Science and Mineral Engineering, Univ. California, 587 Evans Hall, Berkeley, CA 94720, USA; ☎: 1-510-642-0205; FAX: 510-642-2069. The E-mail address is: weber@garnet.berkeley.edu; the web site is:

<http://www.mse.berkeley.edu/faculty/weber/weber.html>

AVAILABLE: USED VARIAN EPR EQUIPMENT:

1) Two Varian E-3's are in the process of being refurbished. I expect to have them ready in early spring of 1999. They will meet factory specifications and will come complete with a one year warranty. The units may also include some upgrades.

2) Varian ENDOR accessory, with Varian ENDOR cavity.

3) Varian TM cavity with flat cell holders and flat cells.

4) Varian E-257 variable temperature controller with heater sensor and insert holder.

5) Varian E-272B field/frequency lock accessory.

Call or fax for details, James R. Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL, 60659, USA; ☎/FAX: 1-773-728-6570.

FOR SALE: VARIAN SYSTEM

1) Varian EPR Spectrometer E-12, 12 inch magnet, operational frequencies 9 and 12 GHz, in very good condition for sale. Optionally also as parts (magnet, cavities, micro wave bridge separately).

2) Test Equipment for sale: Brand New SpectraNova EPR spectrometer, test equipment from the manufacturer is for sale at reduced price. (Technical details may be seen on [www. http://members.eunet.at/dr-kondor](http://members.eunet.at/dr-kondor)). For more information contact please dr. L. Kondor, fax + 43 1 877 8446, tel + 43 1 877 0553, E-mail: dr-kondor@eunet.at

WANTED: X-BAND BRIDGE

We want a used X-band EPR microwave bridge of any type, especially with solid oscillator microwave source. Must be available at a low price. Please contact Wu Ke, Inst. of Radiation Medicine, 27 Taiping Rd., Beijing 100850, People's Republic of China; FAX: 86-01-68214653; E-mail: wangs@med1.bmi.ac.cn.

ERRATUM—

Our sincerest apologies to Professor Erwin Hahn. The Hahn that has been listed in recent issues of the *EPR Newsletter* as a Fellow of the IES but with a different first name is indeed Erwin.

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All these Centers are Research Resources sponsored by the National Institutes of Health. They cooperate to facilitate research involving EPR and related techniques. Prospective users may contact the staff at any of the Centers.

Please direct your communications about the EPR Newsletter or prospective material for publication to Becky Gallivan in the Editorial Office at the IERC address above or by e-mail: ierc@uiuc.edu; FAX: 1-217-333-8868.