EPR NEWSLETTER

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National Biomedical ESR Center, Prof. James S. Hyde, Director. Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226, USA. ☎: 414-266-4000. FAX: 414-266-4007. E-Mail: felix@mis.mcw.edu

Biotechnology Resource in Pulsed EPR Spectroscopy, Prof. Jack Peisach, Director. Albert Einstein College of Medicine, Department of Molecular Pharmacology, 1300 Morris Park Avenue, Bronx, New York 10461, USA. ☎: 212-430-2175. FAX: 212-829-8705. E-mail: peisach@aecom.yu.edu

Illinois EPR Research Center (IERC), Prof. R. Linn Belford, Director; Prof. Harold M. Swartz, Co-Director; Prof. Robert B. Clarkson, Associate Director; Prof. Peter G. Debrunner, Co-Principal Investigator; other senior staff: Prof. Mark J. Nilges, Dr. Alex Smirnov, Laboratory Manager, and Dr. Tadeusz Walczak. University of Illinois at Urbana, 190 MSB, 506 South Mathews, Urbana, IL, 61801, USA. ☎: 217-244-1186. FAX: 217-333-8868. E-mail: ierc@uiucvmd.bitnet; r-belford@uiuc.edu; or belford@rlb6000.scs.uiuc.edu. (IERC also operates a satellite site for EPR *in vivo* at Dartmouth University in Hanover, New Hampshire; ☎: 603-650-1955; FAX 1935. E-mail: harold.swartz@dartmouth.edu)

These Centers, which were described in our first issue (Volume 1, #1), cooperate to facilitate research requiring EPR-related techniques. Prospective collaborative or service users may contact the staff at any of the Centers.

IN THIS ISSUE

HOW TO REACH US — To communicate about the EPR Newsletter or submit material, contact R. Linn Belford, Editor or Becky Gallivan, Editorial Assistant, at IERC (address above).

IES MEMBER JANICE DeGRAY WINS WALTER J. JOHNSON PRIZE — A

prestigious award has been won by a member of the International EPR(ESR) Society. Dr. Janice DeGray, postdoctoral fellow in the Free Radical Metabolites Workgroup of the Laboratory of Molecular Biophysics, National Institute of Environmental Health Sciences (NIH), shared the 1993 Walter J. Johnson Prize awarded by the Editorial Board of the Archives of Biochemistry and Biophysics. This award is based on the outstanding quality of a paper authored by a recent Ph.D. and published in the Archives of Biochemistry and Biophysics during the previous three years. Dr. DeGray's prize-winning article, entitled "Reduction of Paraquat and related Bipyridylium Compounds to Free Radical Metabolites by Rat Hepatocytes" (Arch. Biochem. Biophys. 289: 145-152, 1991), was co-authored by Dr. R.N. Ramakrishna Rao and Dr. Ronald P. Mason. The study demonstrated that paraquat and related herbicides are metabolized to free radicals by liver cells. These free radicals are ultimately responsible for the many deaths resulting from accidental poisonings by these chemicals. The prize, which includes a cash award, is being presented to Dr. DeGray during an all-expenses-paid trip to the American Society of Biochemistry and Molecular Biology/American Chemical Society Joint Meeting in San Diego, CA on June 1, 1993.

From the Editor

Each year there are four issues of the EPR Newsletter, which go to press in Spring, Summer, Fall, and Winter. I am pleased that interesting contributions and news items have been coming in, but it's up to you, the members of the Society, to keep them coming. I know that a lot of you who have never sent in material have interesting items to contribute, and I would like to hear from you. If you notice announcements of pertinent meetings, books, conference proceedings, or the like, please inform us. You cannot safely assume that they have come to our attention! Please help us spot such material and inform us just as soon as possible to enable us to publish dated material in a timely fashion.

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I have enjoyed working with the first officers of our Society. All of them have given useful feedback about the Newsletter; Hal Swartz and the Eatons (Gareth and Sandy) have provided particularly frequent and effective advice and good counsel. While I expect that they will continue to do so after their terms as IES officers have expired, I also look forward to working with the new Society officers. The incoming officers may help us give the EPR Newsletter an even more truly international flavor.

Linn Belford

✦ *IES AFFAIRS* ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR SOCIETY

PRESIDENT'S REPORT

This is my last message as president of the Society. It has been a challenging, interesting, and often exciting opportunity to participate in the development of our field and to interact with so many excellent researchers in the course of the development and operation of the Society, but I must confess that I also am looking forward to having more time to devote to other responsibilities! I can do this with considerable confidence that the Society will continue to grow and develop, because the new officers are absolutely outstanding both in their scientific reputations and their capabilities to run the Society, and the Council of the Society provides a continuing source of very high level support and advice for the officers. My role in the Society will not end completely, of course, both because of my continuing commitment to its development and my official role as an officer (the immediate past-president).

As I reflect back on the progress of the Society, I find that its development has probably exceeded the most optimistic projections of those involved in its establishment. We now have more than 1,000 members, a very active and productive quarterly newsletter, and a membership that has responded very positively to many initiatives of the Society. I think that the efforts of the Society to provide support for two important groups: young investigators and colleagues from countries with limited support for scientists, have been especially important and productive. We also have developed very productive relationships with many corporate members, which has added greatly to the scholarly and financial development of the Society.

This progress has occurred because of a real need for the Society and the considerable efforts of a large number of individuals. There have been far too many members who have made important contributions for me to attempt to name them all, but I would like to draw particular attention to the contributions by two of the outgoing officers, Sandy Eaton and Gareth Eaton. Their efforts, which began at the very onset of the idea to establish the Society, have continued and grown with the Society and we could not possibly have reached the state where we find the Society without the tremendous amount of time and energy that they have devoted to the Society. I tried to interest them in staying on as officers but they, too, seem to have reached the point where, while their support for the Society remain undiminished, they need to refocus their efforts on their other professional activities. I also would like to express my special gratitude to Becky Gallivan who has provided the Society with an unswerving loyalty and effectiveness in dealing with the many details, small and large, which have allowed us to succeed, and to Linn Belford who has so successfully shepherded the newsletter through its development to its present state.

In the long run, of course, the only reason for having the Society and the only firm basis for its success is the membership. I hope that all of you will continue and expand your interest and activities in the Society. The new officers, no matter how capable and energetic, cannot succeed without you.

Thank you very much for the opportunity to participate in the development of the Society.

Hal Swartz

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NOTICE: ELECTION OF OFFICERS; 1993 DUES:

Ballots for election of officers were mailed to all members of the International EPR(ESR) Society the week of May 4, 1993. The ballots are to be returned to the IERC at the University of Illinois by May 31, 1993. To save on postage costs, 1993 dues notices were sent to members at the same time. Dues payments may also be sent to the IERC and we will forward to the appropriate regional treasurer. Chris Felix, National Biomedical ESR Center, Milwaukee, WI is now the regional treasurer for the USA.

EPR CONFERENCE TRAVEL GRANTS FOR STUDENTS - CALL FOR APPLICATIONS:

The International EPR Society provides grants to students (including postdoctoral student members of the Society) to help defray expenses of long-distance travel to present EPR-related work at an appropriate conference (see "Notices of Meetings" in each Newsletter). A student may apply for an award of up to $250(US) in a brief (1-2 page) letter with (1) some information about him/herself, (2) reasons for wishing to attend and present work at the particular meeting specified, and (3) the endorsement of the student's research advisor. The Awards Committee makes all decisions and announces results to all applicants. *Send applications to Prof. L. J. Berliner, co-Chair, IES Awards Committee, Dept. of Chemistry, The Ohio State University, 120 West 18th Ave., Columbus, OH 43210-1173, USA. ☎: 614-292-0134; E-Mail: berliner@livers.mps.ohio-state.edu*

"APPLIED MAGNETIC RESONANCE" – **SPECIAL OFFER FOR IES MEMBERS:** (*Repeated announcement*). By arrangement with the publisher, members of the International EPR(ESR) Society may subscribe to the journal "*APPLIED MAGNETIC RESONANCE*" (K.M. Salikhov, Ed.) for a very small fraction of the public subscription cost. For example, in the USA the IES members' rate is $92 (plus postage). Orders and inquiries must go directly to Springer-Verlag Wien, Sachsenplatz 4-6, A-1200 Wien, AUSTRIA. FAX: 43-222-330-24-26. Payment may be made by check or standard credit card.

NOMINATIONS FOR IES AWARDS INVITED

If you would like to propose one or more names for any of the following IES awards, please send your suggestion(s), or preferably full nomination(s), to the appropriate Disciplinary Awards Subcommittee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow; George Feher; & Jan Stankowski. *For Chemistry* - Bruce Gilbert, Chair; J. Sohma; Jim Bolton; & Kev Salikhov. *For Biology/Medicine* - Larry Berliner, Chair; Marjeta Sentjurc; Hideo Utsumi; & Tadeusz Sarna).

Gold Medal: The Gold Medal, recognizing benchmark contributions to EPR spectroscopy as a whole; one award per year (first 2 winners: George Feher and Jim Hyde);

Silver Medals: Three Silver Medals each year, one each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine;

Young Investigator Awards: Three Young Investigator awards each year, in the same fields as the Silver Medals; "young" is defined as less than 7 years since the Ph.D. degree.

TRAVEL SUPPORT TO MEETINGS IN EASTERN EUROPEAN COUNTRIES: The Society currently has a system of small grants to facilitate travel to EPR-related meetings within those Eastern European countries which recently suffered calamitous declines in research funds. As described in more detail in previous Newsletters, all scientists, junior and senior, in Eastern Europe are eligible to apply for these hard currency

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grants of $10 to $25 each to enable travel to meetings in these countries. IES funds for this are administered by a committee chaired by Yakov Lebedev (Institute of Chemical Physics, Russian Academy of Sciences, Kosygin Str.4, 117977 Moscow V-334, Russia). Write directly to him providing details on the meeting to be attended and the amount of hard currency required for the travel expenses. This program is strictly temporary.

LETTER TO THE EDITOR

Sir:

This letter relates to our discussions of the acronyms EPR, ESR, and EMR and the confusion generated by the use of different nomenclature for the same thing and the same acronyms for different things. It is fun to see the references that sometimes result from a literature search keying on these acronyms. A search of physics literature last year turned up a paper [A. Hájek and J. Bub, *Foundations of Physics* **22**, 313 (1992)] entitled simply "EPR"! But it has nothing to do with electron paramagnetic resonance. The first sentence of the paper is "The 1935 paper 'Can quantum-mechanical description of physical reality be considered complete?' by Einstein, Podolsky, and Rosen—usually referred to as 'EPR'—is widely regarded as a landmark in the philosophy of quantum mechanics." Not quite the EPR I was seeking! In another search I found "Timing in EPR Correlation" [O. C. de Beauregard, *Foundations of Physics Letters*, **5**, 489 (1992)] - where EPR has the same meaning.

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THE COMPUTER CORNER

Edited by Philip D. Morse II and Keith P. Madden

The *Computer Corner* is a regular column in the EPR Newsletter. It is dedicated to all computer-related aspects of EPR spectroscopy. We are always interested in receiving articles, comments, tips, and the like for this column. Please send submit your contributions to Reef Morse at Illinois State University (E-mail: reef@xenon.che.ilstu.edu) or Keith Madden at Notre Dame University (E-mail: keith.p.madden.1@nd.edu).

In the last EPR Newsletter, we gave instruction on how to use ftp to obtain software by way of the Internet Keith Madden reviewed a suite of programs written by Dave Duling at NIEHS. We continue the task of providing space for various authors and companies to describe their recent software materials from some of the major suppliers of EPR software and hardware.

This month we present information on two lines of commercial software - one from Bruker Instruments and another from Scientific Software Services. We also provide a description of user-supported software supplied by John Weil.

The letters and comments this month seem to get at the heart of several issues in the EPR community: what constitutes good use of simulation software (especially that written by other people) and whether or not commercial vendors should supply source code with their software. There are certainly a number of pros and cons in these issues. We invite your comments.

Commercial Software - The BRUKER EPR Software Library:

Bruker currently offers software for data acquisition and processing on the Bruker EPR spectrometer as well as software for remote data processing on IBM compatible computers.

1. *Software for Bruker EPR Spectrometers*

The main task of the spectrometer computer is the real-time control of experiments. The multi-tasking OS-9 operating system also allows spectrum processing while acquiring data. The following software is available to assist you with your EPR needs:

1.1 *Bruker ESP Software*

Since the debut of the ESP 300 EPR spectrometer, Bruker spectrometers have been delivered with the ESP software. The ESP program was developed to:

- *Acquire Data.* A large variety of EPR experiments

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can be performed under complete computer control. With the aid of automation routines and computer controlled spectrometer accessories, such arduous tasks as temperature variation and single crystal studies can be fully automated.

- *Manipulate Data.* Many of the standard operations such as spectral additions and subtractions, peak-picking, integration, and differentiation are available. The software also supports more advanced operations such as FFT's, smoothing and resolution enhancement filters, and interactive spectral titration capabilities.

- *Plot Results.* You can produce standard spectral plots, stack plots, and plots with magnified regions. The software supports many Hewlett-Packard plotters and LaserJet printers.

1.2 *Enhancements*

Enhancements of the Bruker ESP Software are possible by the addition of user-modules. These are subroutines, which can be called from a program menu and which have access to all spectra currently in the ESP program. Bruker distributes ready-to-use modules for some common applications, like LPSD (linear prediction by singular value decomposition), BCF (baseline cosine fitting), multiexponential fitting, etc. (cf. Bruker price list or consult your Bruker representative).

Modules also can be easily written by users themselves. They can be added at any time. No program recompilation or linking is required due to the modular design of the ESP software and the architecture of the computer's operating system, OS-9.

A user-module accesses a spectrum as a data structure containing measured data, parameter data, etc. It has access to all these values, i.e. it can calculate its results with a complete knowledge of experimental parameters and resulting data. If required, a user-module may even access multiple spectra.

The implementation of user-modules is greatly simplified by a complete, documented source code package on floppy, available from Bruker. It contains all structure definitions required to write a module, plus an easy-to-understand example using these structures. Contact your Bruker representative for more information about this package.

1.3 *Simulation Software*

The ESP software includes a small complimentary simulation program, EPRCalc, for solution spectra, which is capable of simulating many simple spectra. For example, the >1000 line spectra in one of Wang's recent papers (H. Q. Wang et al., Magn. Res. In Chemistry 30 p150 ff (1992)) have been simulated with this program. However, the growing need of EPR scientists for more complex simulations has lead to the development of BRUKER's Simfonia package. This is an advanced simulation package for solution and powder spectra which combines an intuitive and simple graphical user interface with virtually unlimited multinuclear simulation capabilities. A few highlights are:

- Automatic accounting of isotopic abundances for solution simulations.
- Solution simulations using up to third order perturbation theory, powder simulations up to second order.
- Anisotropic linewidths for powder systems.

Simfonia employs a fast time domain simulation with subsequent Fourier transformation to the frequency domain for the solution simulations. Besides a considerable reduction in simulation time, this method allows the inclusion of instrument responses due to time-constants and modulation amplitude. Therefore, Simfonia can also be used as a pedagogical tool. Contact your BRUKER representative for more information about this package.

2. *Software for IBM Compatibles*

Bruker has offered a PC based software package called WIN-EPR for a few years now. Recently, WIN-EPR 2D, which performs many sophisticated manipulations on two dimensional data sets, has been released. These programs offer the user the following advantages:

- They provide off-line presentation and processing, thus freeing the spectrometer for acquisition tasks. This feature is particularly useful for "departmental" spectrometers.
- Many people are familiar with the MS-Windows user interface. This makes learning the program's many

operations and features simple and intuitive. Additionally, the graphical user interface of MS Windows eases the difficulty of performing complicated interactive tasks

- The extensive graphical and numerical capabilities of today's state-of-the-art PC's permit spectral representations and data processing methods that complement the ESP software features.

As for all other products, contact your BRUKER representative for more information about this package. If you do not know your representative, contact one of BRUKER's Main offices:

For the USA:
Dr. Art Heiss
Bruker Instruments Inc. / EPR
Manning Park, Billerica, MA 01821, USA

For Europe:
Dr. Dieter Schmalbein
BRUKER ANALYTISCHE MESSTECHNIK GMBH
Silberstreisen, D-7512 Rheinstetten
GERMANY

For Switzerland and the Near and Far East:
Dr. Francisco Jent
SPECTROSPIN AG
Industriestrasse 26
CH-8117 Faellanden
SWITZERLAND

Commercial Software - Scientific Software Services' ImageWare (IW):

IW is a program developed primary for the purpose of CW EPR imaging, providing flexible and convenient user-interactive analysis of experimental data on a personal computer (386 or 486 IBM compatible). The program is capable of processing two types of experimental data at the same time - one and two dimensional arrays with flexible sizes. Two dimensional arrays can be handled in both ways - as a projection set (a sequence of EPR spectra recorded at different magnetic gradient orientations) or as truly 2-D objects (a two dimensional map of density of paramagnetic centers). Various algorithms are implemented in the program including image reconstruction from projections, deconvolution using filtered Fourier Transform and maximum entropy algorithms, non-linear baseline correction, non-linear image smoothing and many others. The program also permits simulation of EPR imaging data and distribution (density) functions including noise simulation and can also act as a very powerful extension of EW for data manipulation purposes.

The program features automatic saving and loading of the data set every time when the user starts or terminates the program (to save time for the users). Also, the program keeps tracking most of parameters (or defaults) which are used in its operations. The defaults, provided by the Scientific Software Services, can be modified by the user and then saved so that the user is encouraged to create and use his/her own configuration of the program.

Scientific Software Services offers a complete CW EPR imaging package that also includes a data acquisition program designed for 2D EPR imaging collection and data acquisition boards. Spectral data is stored as a single file of data arrays whose length is dependent on the number of projections and the size of the array taken at each projection. Some simple data manipulation can be done in the data acquisition program. IW uses the stored data as the input for image reconstruction and its more advanced data manipulation and visualization routines including 1- and 2-D spectrum editor.

As usual, IW comes complete with an operations manual and all source code.

Please feel free to ask the Scientific Software Services about custom-modified version of the Imaging package for your experimental needs. For more information and a free demonstration copy of the ImageWare contact Scientific Software Services at:

Scientific Software Services
305 E. Locust
Bloomington, IL 61701, USA
☎: 309-829-9257

Non-commercial software - Computer program

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EPR.FOR:

Program EPR.FOR can use spin-hamiltonian parameters to simulate spectra using selected line shapes, and is capable of fitting spin-hamiltonian parameters to experimental spectral line-position data. The program was written primarily to achieve complete generality and flexibility in handling magnetic-resonance spectra of single crystals, powders and non-viscous liquids. The program sets up a very general spin Hamiltonian which includes parameters up to 6th order in spins S and/or I. The program operates at four categories of complexity:

1. energy-level calculation,
2. spectrum simulation,
3. comparison with observed line-position and intensities,
4. spin-hamiltonian parameter optimization.

Category 2 includes simulation of liquid, single-crystal and powder spectra from EPR (field-swept and frequency-swept), ENDOR and ESEEM [but not (yet) ESEEM intensity calculations] experiments. Hyperfine effects for (at present) ten nuclei can be handled quantitatively. Categories 3 and 4 accept experimental data from EPR, ENDOR and ESEEM experiments. The program can be used for NMR analysis as well, although the method of input is not currently optimized for this type of experiment.

The program is written in standard FORTRAN 77 and currently runs on four types of computers: a VAX running VMS operating system, a Bruker spectrometer M68000 running OS9, a DEC Station 5000 running ULTRIX and an Intel 486DX33 running OS/2. The software will run on any platform which runs FORTRAN 77. Graphical output is in several formats for use in graphics packages such as Bruker's ESP spectrometer software, program WIN-EPR(C) for Windows 3.x from Bruker, CA Cricket-Graph(C) for Windows 3.x, as well as any graphics package which can read in an ASCII x-y data file.

Future plans for enhancement include: the use of fast fourier transform to speed up the graphics part of the spectral simulation, automatic fitting of spectral line-shape parameters (including powders), automatic archiving of spin-hamiltonian parameters for easy access and a data-base utility to maintain the archive (we currently have a data base of hundreds of sets of spin-hamiltonian parameters and plan thus to automate its use), as well as simulation of dynamic effects.

The EPR.FOR program comes on a distribution diskette containing source code and utilities, along with a printed user's manual complete with theoretical discussions of all calculations performed by the program as well as many input and output examples to facilitate using the program. The example files are included on the distribution diskette.

For information please contact :

Prof. John A. Weil, Department of Chemistry
University of Saskatchewan, Saskatoon, SK
S7N 0W0, Canada
E-mail: Weil@sask.usask.ca ☎: 306-966-4688

A Contribution from David Duling, NIEHS:

I'm not sure this applies, but it is interesting nonetheless. There is a little freebie monthly magazine called "Personal Engineering" which is focused on many of the same things you and I discussed regarding data acquisition, Windows, etc.... and other things. It actually has a lot of info. They can be reached at:

Personal Engineering, Reader Service Dept.
Box 430, Rye, NH 03870-0430, USA
☎: 603-427-1377 Circulation: 603-427-1427
Fax. 603-427-1388.
Email: "duling@postoffice.niehs.nih.gov"

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A Contribution from David Collinson, The University, Manchester:

Software for simulation of powder EPR spectra.

The use of computers in the analysis of EPR spectra is now widespread due largely to the easy access to computers, their increasing power and decreasing cost, and their associated graphical capabilities. As the problems tackled by scientists using EPR spectroscopy have become more complex there has been a concomitant need for accurate simulation procedures to analyze the spectra obtained. Many different programs have been written for simulation of EPR spectra. Which one to choose? If we consider only the simulation of continuous-wave spectra of anisotropic species, 48 programs are cited on the database managed by Richard Cammack at King's College, London. (This database is now accessible by Anonymous FTP at the IERC; see last Newsletter.) Some of these programs are written for specific applications, others are more general. We have discussed some of the different philosophies behind some of the simulation programs in the recent book "Electron Paramagnetic Resonance of d Transition Metal Compounds" by F. Mabbs and D. Collison (Elsevier). Different strategies used in these programs range from:

- perturbation to matrix diagonalization methods and combinations of these;
- symmetry limitations from isotropic or axial through to triclinic;
- inclusion of a variety of terms in the spin-Hamiltonian.

In general, software has been developed by the gradual extension and refinement of a basic program. That has certainly been the case in our own laboratory. Program development usually takes place with one or more of the following aims in mind:

- to speed up the simulation procedure;
- to generalize the procedure in order to account for new situations and chemical systems;
- to make the program more portable for implementation on other computer platforms.

As a software package becomes more sophisticated and applicable to more situations, it tends to become more difficult to use. It may become either very general, but impractically time-consuming, or it may be applicable only to a restricted range of systems. In addition it may become less easy for anyone other than the original programmer to modify, amend or add to the computer code. Therefore we offer: A note of caution to users of imported programs.

It is unwise to use a simulation program as a "black box". This can lead to artefacts in the simulated spectrum. Be aware of the theoretical background to the program. For example:

- if it is based on perturbation expressions, are those expressions strictly applicable to the problem being studied?
- what are the natures of the linewidth and lineshape parameters?
- how is the transition probability calculated?
- how does one use the parameters needed for simulation in addition to the spin-Hamiltonian and instrumental parameters, such as 'incremental angles', or where $S > 1/2$, various field-dependent parameters.

When examining for the first time a set of spin-Hamiltonian parameters that are unlike any that used previously, it is often useful to examine the component parts of the calculation. This is especially true when powder spectra are being simulated. If there is any doubt about the validity or authenticity of the final simulated spectrum it is advisable to experiment with the program at first to investigate energy level variation with magnetic field, energy level differences, transition probabilities and single-orientation spectra.

To writers of new software

Detailed documentation of both the underlying theory and the operation of the software should be provided by the programmer. A range of data files, covering all aspects of the use of a particular program should also accompany the source code.

The intelligent maintenance of software databases and other sources is of great importance in this respect. The developments in electronic mail should enhance the use of software within the EPR community. A dialogue between programmer and user can be readily set up by

email and information and advice exchanged with ease. Whilst a collaboration as extensive in scope as that of the Genome Project is unlikely within the magnetic resonance community world-wide, it may be to the benefit of the discipline of EPR that, at least for the utilization of software, we do not remain parochial. Indeed, an exchange of information about software, combined with a directory of email addresses of EPR laboratories throughout the world would serve our community well.

David Collison, Chemistry Department
The University, Manchester, M13 9PL, UK
(email: mbdisdc@uk.ac.mcc.cms)

(Editors note: in the US, use an email address of mbdisdc@cms.mcc.ac.uk).
☎: 44-61-275-4660-4653 Fax: 44-61-275-4598

(Editors' note: Scientific Software Services provides original source code with their data acquisition and simulation software.)

A Contribution From Reef Morse:

There has been a need for an accessible EPR spectral database for years. The IERC is beginning to meet this need by providing an ftp server. Now what is needed is the actual database itself. What should such a database contain? Should it contain the actual spectral data itself? Should we limit ourself to certain formats or should we write software to allow interconversion between a number of formats? Should we have a keyed relational database for doing searches and should this database be separate from the spectral data itself? What are the important keys for doing searches. And finally, who will pay for and maintain such a database? Should selected members of the EPR community apply for agency funding? Should this be undertaken by the Society?

We need answers to these questions from you. There is probably no one "good" way to set up this database although there are examples from other spectral communities from which we can draw. We should begin this task and we need your advice. Please send thoughts, comments, ideas, and suggestions to reef@xenon.che.ilstu.edu.

A list of available software may be obtained directly by electronic mail. Dr. Frank Auteri has installed the database on an anonymous FTP server at the Illinois EPR Research Center (IERC), so that it can be downloaded directly. Users: Note that it occupies 90 kilobytes of space. We give access instructions modified from those in the last issue of the EPR Newsletter.

Here is how to access the database:

From your Internet site or any network service which supports ftp, do the following (don't enter the quotes):
1) Type **"ftp rlb6000.scs.uiuc.edu"** (or, if that doesn't work, **"ftp 128.174.90.135"**).
2) At the user prompt, enter **"anonymous"**
3) For the password, enter your full E-mail address (for example, auteri@rlb6000.scs.uiuc.edu)
4) Now you should be logged in. If this is your first time logging in, you should first download the information file as follows: **"get README.EPR"** (Do use the capital letters).
Next, you should **"get eprsftwr.txt"**
5) Type **"quit"** to end session. The two files now should be downloaded to your system. Read the README.EPR file first. If you have trouble, send E-mail to auteri@rlb6000.scs.uiuc.edu or phone Frank Auteri at 217-333-3776. Send Frank the following if you wish to get onto the IERC E-mail list: Name, full E-Mail address (also TCP/IP address if known), alternate E-Mail address (also TCP/IP address if known), Mailing Address and Phone.

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TIPS & TECHNIQUES

COUPLER GEOMETRY AND SPECTROMETER DEADTIME VARIATIONS

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For most EPR applications, coupling between the transmission line and the resonant cavity is achieved by a circular aperture in a common wall. This aperture constitutes a reactive element of the microwave circuit whose properties are geometry-dependent. When employed as a variable impedance matching device, the aperture is outfitted with a geometrically varying element and is called an iris.

Optimal performance of a pulsed EPR spectrometer is dependent upon the deadtime of the resonant structure, which is typically a measure of the cavity ringdown time. Minimization of the cavity ringdown requires a low Q-factor, which is somewhat dependent upon the coupling arrangement. The most common technique is to overcouple the cavity using an aperture that is enlarged relative to those used to critically couple cavities for cw operation (diameters of ≥8 mm vs. 6 mm at X-band). The variable element is typically a dielectric plug, the so-called Gordon Coupler [1].

In one of its experimental configurations our spectrometer employs a reflection cavity detection scheme, and I find that the deadtime measured at the receiver is longer (and "uglier") than the ringdown directly observed when I put a probe within the cavity. This initial observation was made by replacing our normal cavity with test bench cavities that are each fitted with a probe at some location along the walls (you might consider these things shorted slotted lines); the experiment was repeated and verified with the normal cavity by inserting a probe in place of the sample. Since our transmission (Mims-style) cavities do not behave this way I suspect that the coupler might in some way be interfering with the performance. Reflections of multiple shock waves in mechanical systems cause aberrant behavior in contrast to single shock waves [2]; since overcoupling results in a mismatch and hence some reflection from the coupler, it seems plausible that perhaps there might be an electromagnetic analogue applicable to this circuit.

As it turns out, the deadtime waveform at the receiver can be improved (meaning reduced) and matched to cavity ringdown by altering the geometry of the aperture. My test system consisted of a cylindrical TE_{111} cavity that was coupled to magnetic modes via a centrally-located aperture in the end wall (Figure 1). The cavity choice was based on its inherently high suppression of spurious modes due to its small size. The remainder of the test bench components are modular circuit elements. The iris is fabricated from brass sheet stock of varying thicknesses; a gasket of matching thickness centers the iris. The tapered inserts of the Gordon Coupler are also removable. This feature allows us to test for optimized geometry while designing for various applications. A detailed report of my findings is in preparation, but for practical purposes I found that the best deadtime performance was achieved by opening the aperture along the waveguide's H-plane, that is, capacitative. A catalog of the best performing irides is illustrated in Figure 2; however, it should be borne in mind that these iride geometries will vary with the cavity used and the size/shape of dielectric plug.

1. Gordon, J.P. *Rev. Sci. Instrum.*, **32**, 658 (1961).
2. Ben-dor, G. *Shock Wave Reflection Phenomena.* Springer-Verlag, Berlin 1992.

Addendum:

In the last issue of the Newsletter a brief description of VXI omitted some source material for further

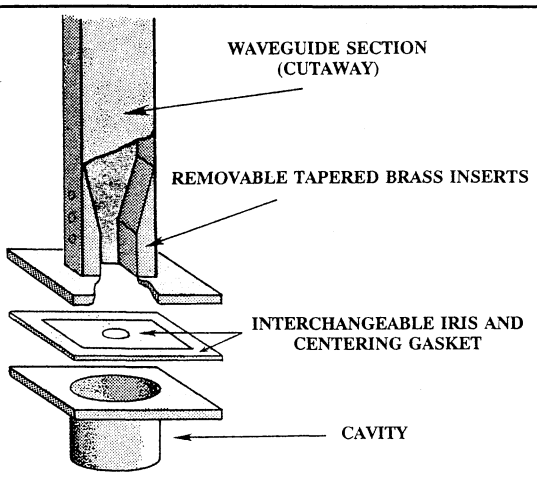

Figure 1: Test bench apparatus for prototyping Gordon coupler transitions. All parts are modular and fabricated from brass. Conducting surfaces are polished. Not shown is a second waveguide assembly used for asymmetric transitions.

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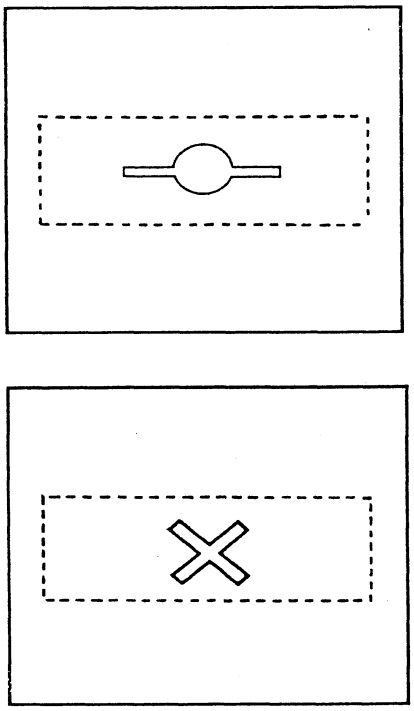

FIGURE 2: Coupling apertures that provide a reduced instrument deadtime with the Gordon Coupler arrangement illustrated in Figure 1. The dashed line indicates the orientation relative to the WR-90 waveguide. No changes in tuning properties could be discerned during the testing procedure.

information on VXI based instrumentation. Interested readers may wish to take note of a recent article in *Computers in Physics* entitled 'Catching the Right Bus I: An Overview of Architectures for Instrument Systems' [3]. It is the first of a series of articles devoted to hardware and laboratory applications in this relatively new APS journal. A good source of additional reading material is supplied in a short bibliography.

3. Matey, J.R.; Stein, P. Computers in Physics, 7, 130 (1993).

Lastly, this same issue of *Computers in Physics* features an article that discusses the numerical computation of angular momentum coefficients that should be of interest to those who write EPR simulation programs [4].

4. Shriner, J.F.; Thompson, W.J. Computers in Physics, 7, 144 (1993).

MISCELLANEOUS TIPS FOR EPR USERS

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In over 20 years of working with EPR instruments, and in my current business (Research Specialties) specializing in repairing and upgrading EPR spectrometers, I have learned many things which would be helpful to users. Here are a few such items:

(a) Protecting the cavity – Parafilm makes a quick cover to exclude contamination from the microwave cavity even with accessories mounted, such as flat cell holders. Parafilm is nonparamagnetic and leaves no sticky residue, as tape does.

(b) Handling the hall probe – The Varian hall probe is very fragile. The case can crack when trying to remove it from the pole face of the magnet and it is very sensitive to shock when unmounted. The internal wires connected to the hall effect element are just a few thousandths of an inch in diameter and can easily disconnect from the element. Be careful! Repair is possible, but very difficult. Suitable replacements are available; it's only a matter of money.

(c) Adjusting the iris – When tuning the iris adjustment screw on various microwave cavities, keeping its penetration into the waveguide to a minimum will eliminate additional dielectric loss from the plastic screw. Such losses will degrade sensitivity slightly, especially on non bias-arm machines. If penetration is deep a second tuning position can usually be found. If the iris tuning screw is loose, be careful at high powers to prevent detector diode damage on non-protected units. Better yet, replace the screw.

(d) Working on Bruker power supplies –

i. Bruker console power supplies have bridge rectifier assemblies with a spot-welded tab that sometimes fracture if mechanically stressed while working on the unit.

ii. Bruker magnet power supplies in some cases have intermittent interlocks that are attributable to modules with improperly inserted leads that fail to be clamped by the terminal screw, i.e. look for loose wires.

(e) Working with Bruker Q-band dewar – Bruker Q-band dewar/cavity plastic support buttons (12 mm dia.) attached to the magnet coils are glued onto the painted

surface, allowing the possibility of breaking off with the dewar installed. Spilled cryogenic fluids may hasten the possibility. Additional supports are warranted to eliminate the expensive consequence of support failure.

(f) Caution in water-cooling Varian units – Watch out for condensation on the Varian units if running cold tap water as this can short out the klystron as well as the magnet power supply pass bank. Using temperature regulated distilled/deionized water is best, since it minimizes long term leakage currents between the magnet power supply and the magnet cooling plates (most noticeable on older-style pass-bank-only power supplies), which hasten the corrosion of the magnet cooling plates, possibly to the point where they leak. A less desirable preventive method for the leakage current can be in the form of a bias voltage introduced to counteract this current.

FROM EPR CENTERS

FROM the NATIONAL BIOMEDICAL CENTER FOR SPIN TRAPPING AND FREE RADICALS:

The National Biomedical Center for Spin Trapping and Free Radicals is located within the Free Radical Biology and Aging Research Program (formerly Molecular Toxicology Research Program) of the Oklahoma Medical Research Foundation. Director: Edward G. Janzen, Ph.D. *Inquiries should be directed to Audrey Winkles, OMRF, 825 NE 13th Street, Oklahoma City, OK, 73104, USA;* ☎: *405-271-7570, FAX: 405-271-3980.*

This Center is hosting the 4th International Symposium on Spin Trapping and Organic EPR Spectroscopy with applications in Chemistry, Biology and Medicine on October 25-28, 1993 at the Oklahoma Medical Research Foundation in Oklahoma City, Oklahoma (see meeting Notices section below; a registration form was included in the previous issue of the EPR Newsletter).

FROM the NATIONAL BIOMEDICAL ESR CENTER in Milwaukee:

TRAINING AWARDS — As described more extensively in a previous issue (EPR Newsletter, v.3#4, Winter, 1991, p. 10), some $500 awards are available to pre- and post-doctoral young investigators to help expenses for 2-week visits to this Center during 1993. The purposes are to provide training in modern EPR methods and to permit the investigators to use the unique facilities of the Center in their on-going research. The faculty and staff of the Center have expertise in the three main areas of EPR research: free radicals, spin labels and transition metals. To apply, send a letter and one-page research plan; student applications should be accompanied by a letter from the graduate faculty advisor. Address applications to Dr. Ching-San Lai, National Biomedical ESR Center, Medical College of Wisconsin, 8701 Watertown Plank Road, Milwaukee, WI 53226, USA; ☎: 414-266-4051.

FROM the ILLINOIS EPR RESEARCH CENTER (IERC) in Urbana:

TRAINING AWARDS — To inquire about the possibility of a graduate or postdoctoral student traineeship (similar to those offered by the Milwaukee center; see above), contact Becky Gallivan, Univ. of Illinois, 190MSB/MC-714, 506 South Mathews Ave., Urbana, IL 61801, USA; ☎: 217-244-1186; FAX: 217-333-8868.

FROM the BIOTECHNOLOGY RESOURCE FOR PULSED EPR SPECTROSCOPY at the Einstein College of Medicine in New York:

A new edition of this Resource's directory of pulsed EPR spectrometers is in preparation. To inquire about it or

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about use of the Resource for collaborative or service research projects, contact Prof. Jack Peisach, Director of the Biotechnology Resource for Pulsed EPR Spectroscopy, Albert Einstein College of Medicine, Department of Molecular Pharmacology, 1300 Morris Park Avenue, Bronx, New York 10461, USA. ☎: 212-430-2175. FAX: 212-829-8705. E-mail: peisach@aecom.yu.edu

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FROM LIVERS (Laboratory for In-Vivo Electron Spin Resonance Spectroscopy) at the Ohio State University, Columbus, Ohio, USA:

This Laboratory, although not an official NIH ESR Center, is an NIH Research Resource Development, which may eventually attain full-fledged Center (Research Resource) status. Our laboratories are always open to collaborators, especially NIH grantees. The previous issue of the EPR Newsletter contains more information about LIVERS. The laboratory's principal investigator is Dr. Lawrence J. Berliner; the associate director is Dr. Janusz Koscielniak, engineer.
☎ Lab: 614- 292-4178 or 292-9432; ☎ Office: 292-0134 (LJB) or 292-6161 (secretary). FAX: 614 292-1532.
E-mail addresses:
janusz@livers.mps.ohio-state.edu,
jkosciel@magnus.acs.ohio-state.edu, or
berliner@livers.mps.ohio-state.edu,
lberline@magnus.acs.ohio-state.edu.

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CONFERENCE REPORT

Gareth and Sandra Eaton
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Denver, CO 80208

An NIH-sponsored Workshop on the Future of EPR was held in Denver, Colorado, August 7, 1992, following the 15th International EPR Symposium. It was attended by about 65 scientists from many countries.

In addition to the well-known review series in magnetic resonance, five recent books provide summaries of individual topics in EPR (1-5). More detailed discussions and references are in an extensive report of the Workshop (6).

There emerged from the previous (1987) Workshop a statement that the EPR field, as it was then, needed the very best sensitivity and signal-to-noise (S/N) that one could get in the standard X-band region of the spectrum. This was a high priority. Also important, was to exploit the information that could come from broadband EPR. Researchers wanted a frequency range of 60 Mhz to greater than 250 GHz, but suggested that 1-18 GHz would be a nice goal for the commercial instruments that would end up in all of the laboratories. As a short term matter the goal was narrowed to 3-15 GHz. It was also recognized that the tradeoffs required two types of EPR bridges: one type for continuous wave (CW) and saturation recovery (SR), and a second type for electron-spin-echo (ESE) and Fourier transform (FT) EPR.

I. Research Advances

EPR is becoming multi-frequency, multi-dimensional, multi-resonance; it is non-linear, time-domain; many of the experiments in research laboratories now are being done with home built resonators designed specifically for the purpose; often experiments are being done in gradient fields for imaging or in vivo. These changes are becoming necessary because of the many applications for EPR.

The advances in EPR during the past five years have been phenomenal. For many scientists an introduction to EPR was via one of the texts that implies that EPR is obtaining a CW field-swept scan to reveal the hyperfine splitting of an organic radical, or to characterize the formation of a copper complex. The present and future reality is starkly different.

Professor Arthur Schweiger described the new ways of studying electron spins accessible through pulsed EPR techniques, many of which have been developed recently in his laboratory (7, 8). Pulsed EPR is undergoing extraordinary rapid development. instrumental capabilities and new pulse techniques make it possible to reduce the measurement times, to increase sensitivity, to improve resolution, and to simplify complicated spectra.

A totally new branch of EPR, multiquantum EPR (MQEPR), has been developed by James S. Hyde and his colleagues, so now we should categorize EPR in three modes: CW, pulse, and multiquantum. Activities in other fields influence EPR also. For example, there has been a rebirth of spin labeling (a technique which

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had become thought of as "the old stuff") due to combinations of loop gap resonators (LGRs) and site-directed mutagenesis.

Pulsed EPR

Today almost all topic areas of EPR spectroscopy are, or will soon be, affected by various pulse methods. Techniques of particular importance include time-resolved EPR spectroscopy, methods for measuring relaxation times, techniques for studying molecular motions, methods for the indirect detection of nuclear transition frequencies, electron-nuclear double resonance, and EPR imaging. Recent examples from the Schweiger lab include FID-Detected Hole Burning, and Fourier-Transform Hyperfine Spectroscopy. In FID-detected hole-burning, a transient spectral hole burnt into an inhomogeneously broadened EPR line by means of a selective microwave pulse is shifted or broadened by various types of perturbations (radio-frequency field, B_0-field jump, electric field, sample rotation, etc.), and is subsequently recorded in a single experiment via an FID following a nonselective microwave pulse. The FID-detected hole-burning experiment can be applied to any EPR spectrum with inhomogeneously broadened lines, provided the relaxation times are sufficiently long. Many of the well-known ESE pulse sequences have an analogous FID-detected hole-burning sequence that is often superior to the ESE experiment. Fourier-transform hyperfine spectroscopy is based on the FID-detected hole-burning approach. In the spectrum obtained each group of equivalent nuclei is represented by one peak at the hyperfine frequency, independent of the nuclear spin quantum number.

FT EPR

The modern era in FT EPR, including initial realization of 2D FT EPR starts in about 1986. Professor Jack H. Freed revealed that there has been a great deal of progress in FT EPR in the past few years in the following areas: motionally narrowed FT EPR and 2D ELDOR spectra, including studies of diffusion in liquid crystals and model membranes; viscous fluids and powders - These experiments are more challenging but they yield more microscopic details about motion. Applicable techniques include 2D ESE, 2D FT, SECSY, and 2D ELDOR. These techniques are also useful for structural studies via nuclear modulation.

2D FT EPR imaging with pulsed field gradients - spatially resolved 2D FT EPR.

For example, the good S/N that is achievable in FT EPR was illustrated with a 0.75 mM sample of perdeuterated tempone in 16 microliters of a smectic liquid crystal. The effective decay rate of the FID following a microwave pulse for this sample is 200 ns. This is T_2*, which includes both homogeneous and inhomogeneous broadening. With pulse widths of 5.5 ns and time resolution of 5 ns, some 40,000 FIDs can be averaged in 6 s. The FID can be observed for more than 10 times the T_2*. In addition to the possibilities for enhanced S/N, FT EPR can also be applied to the study of transient species. One can measure radicals with submicrosecond lifetimes, generated for example by a laser pulse, by recording the single pulse FID and performing Fourier transforms.

With 2D FT EPR one can obtain nuclear spin flip rates, Heisenberg exchange rates, and from them molecular rotational and translational diffusion coefficients. All of these are measured simultaneously on the same sample, so there is no problem with comparisons due to sample preparation or sample conditions. And they are obtained quickly.

Pseudomodulation

Pseudomodulation is the convolution of a sinusoidally modulated delta function with the digitized data. When one uses pseudomodulation one gets the derivative effect of the modulation simultaneous with filtering, with a distortion that is about the same as would be caused by the field modulation itself. The use of pseudomodulation to provide more features in the spectrum that can be parameterized, combined with dispersion mode STEPR in the new Hyde Q-band system, make possible major advances in the use of STEPR.

Multiquantum EPR

Multiquantum EPR (MQEPR) is an exciting new opportunity. There are two general thrusts in MQEPR: as a practical alternative to magnetic field modulation for improved system stability, and as a way to obtain information on relaxation rates. Magnetic field modulation is a severe technical problem for the design of EPR resonators. For the future one should consider multiquantum EPR as a practical alternative to magnetic field modulation. One could pseudomodulate to get the familiar first derivative display. Indeed, multiquantum EPR (MQEPR) is proposed for many types of experiments, such as high pressure, or low temperature, where it is technically difficult to get modulation to the sample. It looks especially promising for Q-band

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because operation of Q-band EPR systems at liquid He temperature is very difficult with 100 KHz magnetic field modulation.

The microwave bridge for MQEPR uses two sources locked a specific frequency apart. Irradiation with two microwave frequencies is equivalent to irradiating with a single frequency that has been sinusoidally modulated. Non-linear response of the spin system can result in intermodulation sidebands, which can be detected. The outputs are the multiquantum transitions, which can be combined in various ways to get useful displays.

EPR Resonator Design

The most significant innovation in resonator design in recent years is the introduction of the EPR loop-gap resonator (LGR) by Hyde and coworkers, and the development of related structures for different types of pulsed EPR experiments, including pulsed ENDOR, and magnetic field jumps. In addition to lumped-circuit resonators of the LGR type, increasingly dielectric resonators are finding application in EPR.

In Vivo EPR and EPR Imaging

Exciting *in vivo* EPR is being done in many laboratories around the world. Some years ago it appeared that *in vivo* EPR imaging was not going to be feasible, but in his lecture Professor Harold M. Swartz demonstrated that *in vivo* EPR and *in vivo* EPR imaging are now providing important new information. The scope of current *in vivo* EPR encompasses:

* low frequency, low resolution, EPR imaging *in vivo*
* high resolution microscopic imaging *in vitro*
* *in vivo* spectroscopy, with and without spatial localization

High resolution microscopic imaging of biological systems is difficult to do at frequencies below 9 GHz. However, important information can be obtained from *in vivo* imaging even if the resolution is low. The key is to keep in mind the biological goals of the measurement. A useful perspective on *in vivo* EPR is that imaging and high resolution spectroscopy are different ends of a continuum of multidimensional spectroscopy. For a particular problem one optimizes a tradeoff between spatial resolution and spectral resolution.

Increasingly, the information one can expect to get from *in vivo* EPR is the full spectrum that one can get from non-*in vivo* EPR of model systems. In addition, one gets information that is pertinent to complex tissues. This includes:

* oximetry
* distribution of MRI contrast agents
* distribution of spin-labeled drugs
* redox metabolism
* detecting reactive intermediates via spin trapping
* biophysical measurements such as fluidity, similar to those used for *in vitro* systems
* pharmacokinetics, using the paramagnetic species as the tracer
* redox metabolism, using metabolism of nitroxides as the parameter
* oximetry, emphasizing repeated non-invasive measurements in tissues
* viability of cells
* temperature and distribution of temperature

Ultimately, one should expect to be able to obtain EPR spectra on almost all except the trunk of a human being, if one works at 250 MHz. However, in experiments reported to date the EPR spectra obtained have been from paramagnetic species added to the organism, from spin-trapped radicals, or from melanin.

Q-Band EPR

Recently there has been a major advance in Q-band (35 GHz) EPR technology in the laboratory of Professor James S. Hyde. The contributing advances were each first developed for or demonstrated at a lower EPR frequency, but now they jointly revolutionize Q-band EPR. The key contributors are low-noise microwave sources, loop-gap resonators, low-noise GaAsFET microwave preamplifiers, and pseudomodulation for resolution enhancement. When taking advantage of modern low-noise GaAsFET microwave amplifiers, overall system improvement requires also decreasing the phase noise of the oscillator. The improved Q-band spectrometer incorporates two essential components - a GaAsFET preamplifier and a Gunn diode source. It can now be predicted that one should be able to achieve equivalent S/N in STEPR experiments at X-band and Q-band.

Spectrometer Frequency

In addition to the advances at Q-band (35 GHz) described by Hyde, there was a strong emphasis at the Workshop on the advantages of EPR spectroscopy at frequencies other than X-band. This included Professor Howard Halpern's EPR imaging spectrometer at 250 MHz, and Professor Jack Freed's 250 GHz EPR spectrometer.

Professors Jack Freed and Linn Belford pointed out

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that high frequency EPR yields:

* ***Higher g-factor resolution*** - One can read the three nitroxyl g-values directly from the spectrum at 250 GHz. Even for the nearly free electrons trapped in solids the g-tensors can be measured.

* ***Greater sensitivity to dynamics*** - One can measure picosecond motions, since the sensitivity of line widths to motion is about a thousand times greater at 250 GHz than at 9 GHz.

* ***Transition metal spectra with large zero-field splittings (ZFS)*** - For example, a Mn(II) complex with a ZFS of 5800 G can be analyzed in terms of second-order perturbation theory.

There are benefits to high-field high-frequency that come principally from having the high frequency, and other benefits that come from having the very high magnetic fields. One advantage of high frequency is that one can cover large ZFSs. One expects extensive applications to important problems in metalloproteins. The high sensitivity expected at high frequency suggests the possibility of studying very small samples. One benefit of high field EPR is that the importance of the Zeeman term relative to the ZFS terms in the Hamiltonian increases at high field. The more nearly first-order spectra at high field increases the chance of interpretation of the spectra.

Signal to Noise

Underlying much of the discussion at the Workshop was a concern that there is a very serious S/N problem in EPR. In the biomedical area one of the key priorities is improved S/N. Concerns with the quality and availability of klystron sources at X- and Q-band, and the strong push to frequencies away from X-band, focus EPR instrumentation development on the phase noise of microwave sources.

Software

In modern EPR, one must pay as much attention to the quality of the software as to the hardware. Increasingly scientists see that software is a central and crucial part of EPR spectroscopy. Color graphics displays can help visualization of the information content of the EPR data, but can also deflect attention from the computational artifacts. The field needs a series of well-posed problems against which new software can be tested. For example, in the field of image analysis there are standard problems such as the Shepp-Logan head phantom, against which each new algorithm is tested. It used to be that when a lab needed software, someone just went home and wrote it at night, but now software needs are too sophisticated for this approach.

There are some thorny issues about software. For example, even if you can write it in a night, it will take a week to document it in such a way that someone can use it. There is a lesson in commercial spread-sheet software. Sometimes it is better to force an application into some documented and supported commercial software rather than writing your own special-purpose software. It is difficult to make excellent general-purpose software. Maybe the emphasis should be on subroutine libraries, and easily modified software.

The new EPR spectrometers and experimental methodologies described at the Symposium and Workshop will provide enormous amounts of information (or at least raw data that somehow must become information). Relative to slow-scan CW EPR, the new EPR technologies produce data at such a prodigious rate that data storage and subsequent manipulation becomes a larger problem than EPR labs have had to deal with in the past. Although trivial by comparison with data generation rates in other fields of science (e.g., MRI, particle physics, or the space program), the amounts of data require qualitatively different computational approaches than are available in most EPR labs. Some labs already approach this problem by using data compression techniques, which can make the data storage requirements modest. For example, Jack Freed's FT EPR can produce a few 1 MB spectra per hour of spectrometer operation. Huge amounts of data are transferred to a supercomputer for the most substantive analyses. Linear predictive methods can be used to reduce the volume of data for storage. Another approach is to recognize that the result of an experiment may be a series of Fourier coefficients, and these are what one would store, not all of the raw data. Others might be uncomfortable with the irreversible interim interpretation imposed on the data by these approaches.

Now that EPR has a standard (Bruker BES^{3}T) for storage and transfer of EPR data we need to consider how to present the data for visualization. This is a major problem. Specialized software is needed for visualization of the multidimensional information that now can be generated so quickly, in order that it be communicated to human beings. The solutions in other areas of science, where the visualization problem is

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analogous, are large software packages which are expensive because of the development effort to create them. A key issue is whether the EPR community will be able to support the effort needed to develop this software. More than 90% of the EPR spectrometers are delivered to universities or government institutes. In contrast, 80-90% of the customers for NMR spectrometers are in industry. In the NMR field a professional software package can be sold to industry for a substantial amount of money, because industry can see the cost savings in terms of time saved by the software.

Dissemination of Modern Techniques

A colleague once commented with regard to a lecture presentation of exciting new techniques, "another experiment I cannot do." Engineers are not available in all labs to implement new techniques. Of the new CW EPR techniques that have been developed, the most generally applied, because it can be implemented on largely standard spectrometers, is STEPR. Possibly a double-quantum EPR experiment using double sideband/suppressed carrier techniques could be implemented with a simple accessory to existing CW EPR spectrometers. Where local expertise is available, pulsed EPR spectrometers are being built. Commercial pulsed spectrometers are available, but have not become common yet.

II. The Funding Agency Perspective

Dr. John Beisler, Division of Research Grants, NIH, presented a perspective on funding for research involving EPR, based on the information in the CRISP data base at NIH and on his observations and perspective as Executive Secretary of the Biophysical Chemistry Study Section at NIH.

In FY87 there were 327 EPR-related awards totalling $45.8M. EPR was a primary thrust of 16% of these awards. In FY92 there were 415 such awards, totalling $57.3M. For comparison, in FY92 there were 1,762 NMR grants, and NMR was the primary thrust of 20% of these. In FY92 General Medical Sciences funded 43% of EPR-related awards. There is a lot of opportunity for applications of EPR in some of the other Institutes. About three EPR spectrometers are funded each year by NIH.

Dr. Beisler asked various other people at NIH and members of study sections (past and present) about some of the questions asked for this Workshop. Some of the impressions and opinions offered were:

1. NMR and EPR proposals fare about equally well.
2. The perception is that the real richness of EPR applications to lipid or membrane research has been mined. There is a low opinion of EPR in lipid research.
3. EPR proposals need to emphasize what information on a particular problem EPR can give that other techniques such as NMR, fluorescence, X-ray, etc., cannot.
4. For greater success, put EPR in the broader context of other spectroscopies. How does it complement the information available from other spectroscopies? For structural biochemistry, for example, what does EPR reveal about distances, angles, etc.
5. Remember to speak to the reviewers rather than making assumptions that they have a background in EPR.
6. The advantages EPR has relative to NMR are small sample size and high sensitivity relative to NMR.
7. In the context of discussion about new hardware development, it is well to keep in mind that one can often get very reasonable data from a 15-year-old Varian spectrometer. Elegant solutions to problems

can often be done with very simple instruments.

III. The Vendor Perspective

At the close of the Workshop the community sought the response of instrument and software vendors to the challenges and opportunities presented.

As a manufacturer, Bruker finds Q-band unprofitable but has decided not to discontinue it! The Bruker Q-band system has switched from klystrons, which are no longer available, to Gunn oscillators, and the sensitivity is about the same. With the new helium FlexLine cryostat, which is also used by the L-, S-, and pulsed X-band systems, the Q-band system can operate to 1.8 K, with magnetic field modulation from 1.5 KHz to 100 KHz without problem. Bruker continues to offer a diverse range of microwave bridges for many specific applications. The high output 2-8 GHz Multi-Frequency Bridge should meet the needs of many researchers.

Over the seven year period, 1985-1992, 37% of the EPR spectrometers produced by Bruker were delivered in the US, 19.4% in Germany, 6.5% in Japan, 4.4% England, in terms of dollars, not number of spectrometers. In the past 12 months the situation has changed, and 59% of EPR sales (in dollars) have been to Europe, 20% to Japan, and only 10% to the US. This may change in the near future.

Since EPR is a very low volume market, Bruker has to be very careful in selecting the areas in which to invest development effort and capital. In the recent past they have put this effort into developing the most advanced spectrometers that are possible in a commercial market, culminating in the ESP380E. About 40 of these have been sold so far. Bruker has the impression that the ESP380E is ahead of the users - people cannot exploit the capabilities of the ESP380E. There is a need for more institutes around the world to teach people how to use non-stationary EPR techniques and to provide service to people to help them start using these techniques. Before Bruker can invest in making these spectrometers even more complicated, with capabilities such as pulsed ENDOR, multifrequency pulsed EPR, and pulsed EPR imaging, there has to be more use of the existing capabilities of the spectrometer. Then, Bruker can consider the commercial implementation of these new techniques.

Up to now Bruker has not charged for EPR Software - it was delivered as part of the spectrometer. Now there is evident need for much more professional, sophisticated, and diversified software, and Bruker anticipates having to hire more programmers and hence to have to charge for the software.

Bruker has tried very hard to listen to what the researchers and other customers say they want in an EPR instrument. In the past everyone wanted the best spectrometer possible, and the specifications of the spectrometer were very important. Recently, this has changed in a few markets, especially in the US. In the US people seem to want the lowest price spectrometer, and the specifications usually are a minor consideration. In Europe price/performance is the most important consideration. In Japan, however, performance is most important. Bruker has to decide whether to develop two types of spectrometers, one with the highest possible performance and sophistication for part of the market, and another spectrometer at the lowest possible price. During the Workshop scientists have expressed desire to have spectrometers with higher performance and to have hardware and software from the manufacturer. But the part of the market not represented at the Workshop may require Bruker to put its development effort not into spectrometers for advanced techniques but into spectrometers at lower prices.

Bruker will continue to improve the FT spectrometers. Pulsed ENDOR will come on the market next year. They will experiment with imaging techniques. At the moment there are no plans to go into high-field EPR, because they cannot foresee a market in this area.

JEOL will be involved in the development and marketing of EPR spectrometers for a long time, and hopes to be more involved in conferences like this by next year, and possibly add a bit to what is being discussed.

Micro-Now has been involved in EPR instrumentation for over 25 years, mostly with accessories. They built an L-band spectrometer and a Q-band spectrometer about 20-25 years ago. In the last five years they have put more effort into building EPR spectrometers. They have built four types of spectrometers - for teaching, for dosimetry, a more complete system in modular form, and a new spectrometer, demonstrated at the Symposium this year. This new spectrometer incorporates a magnet built in Russia, uses a Gunn source, and is very portable. Their effort will generally be in the direction of spectrometers such as this new one, which essentially address the part

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of the market that once was served by the Varian E-4.

IV. Summary Perspective

Pulsed, Fourier transform, non-linear CW, imaging, and *in vivo* techniques are increasingly important. Resonators are being designed to fit the needs of the experiment, rather than fitting the experimental design to the resonator (or deciding not to do the experiment). Very low (e.g. 250 MHz) and very high (e.g. 250 GHz) frequency EPR have expanded our view of spins. Multiple pulse techniques are bringing to EPR powerful insights analogous to those that are becoming commonplace in NMR. Imaging and *in vivo* techniques are letting us see EPR spectra at each location in space, permitting us to perform, for example, oximetry in living animals. EPR without magnetic field modulation opens new vistas, in saturation recovery EPR, fast-response EPR, and multiple-quantum EPR.

One can hope that some time not too far in the future at another workshop the focus will have changed to the now largely unexplored regions of EPR spectroscopy: 4D, multiquantum, multifrequency, etc. What will be possible when we can see EPR spectra of brain tissue, *in vivo*, localized in a living animal, using all of the advanced EPR techniques we learned about at the Symposium and Workshop. This is where EPR is really going to be able to solve problems. The future has some exciting possibilities. Almost nothing that was reported in the 1992 Workshop could have been done even a few years ago.

The goals set in 1987 were ambitiously forward-looking. With all of the exciting new developments in EPR, instrumentation and software are still way behind the needs of researchers. In fact we haven't come very far in five years toward the goals set in 1987. This statement, which is true with respect to the full scope of the demonstrated possibilities of EPR, is not meant to in any way detract from the almost revolutionary advances made by instrument vendors in the past five years. The Bruker ESP380E has capabilities for pulsed X-band EPR that users have not yet learned to exploit. The Micro-Now 8400 bench-top size EPR makes it possible to expand the applications (and importantly the instruction) of CW X-band EPR into labs that previously could not afford a spectrometer. The Bruker EMS104 is the first spectrometer built for quantitative EPR, a severely under-exploited area. The software becoming available is of a sophistication well beyond anything even dreamed of a few years ago. The hopes for extracting information from spectra in the near future are bright. At the time of the 1987 Workshop it was a valid point of view to declare that the "new" spectrometers of the day were not enough of an improvement over existing spectrometers to justify replacement of a functioning old spectrometer. Now, in 1993, these new instrumentation and software capabilities change the situation entirely.

Acknowledgment

In this paper Gareth R. Eaton and Sandra S.Eaton serve as reporters/reviewers of the information (some of it unpublished) and opinions presented at the Workshop. Special acknowledgment is due to those who presented State-of-the-Art Lectures at the Workshop - Professors Jack H. Freed, James S. Hyde, Arthur Schweiger and Harold M. Swartz. Important contributions during and in some cases after the Workshop were made by Linn Belford, Harvey Buckmaster, Howard Halpern, Arthur Heiss, Roger Isaacson, Melvin Klein, Ron Mason, Philip Morse and Ralph Weber.

Partial support of the Workshop was provided by NIH grant GM46669. Support of the preceding 15th International EPR Symposium by Bruker Instruments, Inc., Medical Advances, Inc., Norell, Inc., Wilmad Glass Inc., Scientific Software Services, and Micro-Now Instruments Inc. also contributed to the success of the Workshop.

V. References

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BOOKS and PROCEEDINGS

The following book is available from World Scientific Publishing:

NEW APPLICATIONS OF ELECTRON SPIN RESONANCE, Dating, Dosimetry and Microscopy, by Motoji Ikeya (Osaka University). This is the first book covering an interdisciplinary field between microwave spectroscopy of electron spin resonance (ESR) and chronology science or radiation dosimetry. The main object is to determine the elapsed time with ESR from forensic medicine to the age and radiation dose in earth and space science. This book is written primarily for earth scientists as well as for archaeologists and for physicists and chemists interested in new application of the method. This book can serve as an undergraduate and graduate school textbook on applications of ESR or electron paramagnetic resonance (EPR) to geological and archaeological dating radiation dosimetry and microscopic magnetic resonance imaging (MRI). Introduction to ESR(EPR) and chronology science and principle of ESR dating and dosimetry are described with applications to actual problems according to materials. Contents: Clock of Elapsed Time: The Place of ESR Dating; Introduction: What is ESR?; ESR Dating and Dosimetry: Principles and Procedures; Assessment of Radiation Dose Rate; Carbonate ($CaCo_3$): Cave Deposits; Aragonite ($CaCo_3$): Shells and Corals in Marine Geology; Sulfates and Other Carbonates: Evaporates; and others. Readership: Students, researchers in geochronology, geology, archaeology, magnetic resonance and radiation dosimetry. 480 pp (approx), Pub. date Spring 1993, order 981-02-1199-6 US$78/£49; 981-02-1200-3(pbk) US$38/£24.

To order the above book, contact one of the following: **World Scientific Publishing Co., Inc.**, 1060 Main Street, River Edge, NJ 07661, USA ☎: 201-487-9655; Toll-free: 800-227-7562; FAX: 201-487-9656, **World Scientific Publishing Co.**, 73 Lynton Mead, Totteridge, London, N208DH, ENGLAND ☎: 44-81-446-2461; FAX: 44-81-446-3356, **World Scientific Publishing Co. Pte. Ltd.**, Farrer Road, P.O. Box 128, SINGAPORE 9128, Cable: "COSPUB"; Tlx: RS 28561WSPC; ☎: 65-382-5663; FAX: 65-382-5919, or **World Scientific Publishing Co. Pte. Ltd.**, 4911, 9th Floor, High Point IV, 45 Palace Road, Bangalore 560 001, INDIA Tlx: 0845-2900 PCO IN; FAX: 91-812-34-4593.

BIOLOGICAL MAGNETIC RESONANCE, Edited by Lawrence J. Berliner, Ohio State University, and Jacques Reuben, Hercules Incorporated Research Center, Wilmington, DE. Corrections from Winter 93 Newsletter: New Volumes through #13 (not #14); Vol #8 Spin Labeling (not Labelling)- Theory and Application. The following recent volumes are in print and will soon be available:

Volume 13, EMR of Paramagnetic Molecules. Contents: Simulation of the EMR Spectra of High-Spin Iron in Proteins (B.J. Gaffney, H.J. Silverstone); Mössbauer Spectroscopy of Iron Proteins (P.J. Debrunner); Multifrequency ESR of Copper: Biophysical Applications (R. Basosi, W.E. Antholine, J.S. Hyde); Metalloenzyme active site structure and function by multifrequency CW and pulsed electron nuclear double resonance (ENDOR) (B. Hoffman); ENDOR of randomly oriented mononuclear metalloproteins: towards structural determinations of the prosthetic groups (J. Hütterman); High Field EPR and ENDOR on Bioorganic Systems (K. Möbius); Pulsed ENDOR and Multiple Resonance Spectroscopy in Proteins and Enzymes (H. Thomann, M. Bernado); Transient EPR of Spin-Labeled Proteins (D.D. Thomas, M.Ostap, C.L. Berger, S.M. Lewis, P.G. Fajer, J.E. Mahaney); Artifactual spin trapping in biological model systems: facts and artifacts (A. Tomasi, A. Iannone).

Volume 12, NMR of Paramagnetic Molecules. Contents: NMR Methodology for Paramagnetic Proteins (G.N. LaMar, J.S. de Ropp); Nuclear Relaxation in

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Paramagnetic Metalloproteins (L. Banci); Paramagnetic Relaxation of Water Protons (C.C. Lester, R. Bryant); Proton NMR Spectroscopy of Model Hemes (F.A. Walker, U. Simonis); Proton NMR Studies of Selected Paramagnetic Heme Proteins (J. D. Satterlee, S. Alam, Q. Yi, J.E. Erman, I. Constantinidis, D.J. Russell, S. J. Moench); Heteronuclear Magnetic Resonance: Applications to Biological and Related Paramagnetic Molecules (J. Mispelter, M. Momenteau, J.M. Lhoste); NMR of Polymetallic Systems in Proteins (C. Luchinat, S. Ciurli).

Volume 11, *In Vivo* Spectroscopy. Contents: Localization in Clinical NMR Spectroscopy (L. Bolinger, R.E. Lenkinski); Off-Resonance Rotating Frame Spin-Lattice Relaxation: Theory, and *In Vivo* MRS and MRI Applications (T. Schleich, G.H. Caines, J.M. Rydzewski); NMR Methods in Studies of Brain Ischemia (L.H. Chang, T.L. James); Shift-Reagent-Aided ^{23}Na NMR Spectroscopy in Cellular, Tissue and Whole-Organ Systems (S.K. Miller, G.A. Elgavish); *In Vivo* ^{19}F NMR (B.S. Selinsky, A.T. Burt); *In Vivo* ^{2}H NMR Studies of Cellular Metabolism (R.E. London).

Volume 10, Carbohydrates and Nucleic Acids, focuses on *Carbohydrates and Nucleic Acids.* In an extensive chapter, Kamerling and Vliegenthart use oligosaccharide-alditols released from mucin-type O-glycoproteins to illustrate the power of proton NMR spectroscopy in the determination of carbohydrate structure. Wemmer gives a detailed coverage of the arsenal of modern NMR methods now available for structural studies of nucleic acids. **Contents:** High-Resolution ^{1}H-Nuclear Magnetic Resonance Spectroscopy of Oligosaccharide-Alditols Released from Mucin-Type O-Glycoproteins (J.P. Kamerling, J.F.G. Vliegenhart); NMR Studies of Nucleic Acids and Their Complexes (D.E. Wemmer).

Series Volumes 1-9 also available. Contact **Plenum Publishing Corporation,** 233 Spring Street, New York, NY 10013-1578. United Kingdom: 88/90 Middlesex Street, London E1 7EZ, ENGLAND.

PREVIEW: "ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY. THEORY AND EXAMPLES," John A. Weil§ and James R. Bolton†, with John E. Wertz‡. To be published by John Wiley & Sons (NY), 1993. This is the long-awaited new edition of the famous Wertz/Bolton text (McGraw-Hill 1972), thoroughly revised and updated by Professor John A. Weil in consultation with the original authors. The book is now (late April) in the page-proofs stage, and should appear in early autumn.

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OUTLINE

Chapter 1. BASIC PRINCIPLES OF ELECTRON PARAMAGNETIC RESONANCE. Introduction; Historical Perspective; A Simple EPR Spectrometer; Scope of the EPR Technique; Energy Flow in Paramagnetic Systems; Quantization of Angular Momenta; Relation between Magnetic Moments and Angular Momenta; Magnetic Field Quantities and Units; Magnetic Dipolar Moments; Magnetic Energies and States; Interaction of Magnetic Dipoles with Electromagnetic Radiation; Characteristics of the Spin Systems; The g Factor; Characteristics of Dipolar Interactions; References/Notes/Further Reading/Problems.

Chapter 2. MAGNETIC INTERACTIONS BETWEEN PARTICLES. Introduction; Theoretical Considerations of the Hyperfine Interaction; Angular-momentum and Energy Operators; Spin Operators and Hamiltonians; Electronic and Nuclear Zeeman Interactions; Spin Hamiltonian Including Isotropic Hyperfine Interaction; Energy Levels of a System with One Unpaired Electron and One Nucleus with I = 1/2; Energy Levels of a System with S = 1/2 and I = 1; Signs of Isotropic Hyperfine Coupling Constants; Dipolar Interactions between Electrons; References/Notes/Further Reading/Problems.

Chapter 3. ISOTROPIC HYPERFINE EFFECTS IN EPR SPECTRA. Introduction; Hyperfine Splitting from Protons; Single Set of Equivalent Protons; Multiple Sets of Equivalent Protons; Hyperfine Splittings from Other Nuclei with I = 1/2; Hyperfine Splittings from Nuclei with I >1/2; Useful Rules for the Interpretation of EPR Spectra; Higher-order Contributions to Hyperfine Splittings; Other Problems Encountered in EPR Spectra of Free Radicals; References/Notes/Further Reading/Problems.

Chapter 4. g-ANISOTROPY IN SOLIDS. Introduction; Systems with High Local Symmetry; Systems with Rhombic Local Symmetry; Construction of the g Matrix; Symmetry-related Sites; EPR Line Intensities; Randomly Oriented Solids; Spin-orbit Coupling and the Λ Matrix; References/Notes/Further Reading/Problems.

Chapter 5. HYPERFINE ANISOTROPY IN SOLIDS. Introduction; Origin of the Anisotropic Part of the Hyperfine Interaction; Determination and Interpretation of the Hyperfine Matrix; The Anisotropic Breit-Rabi Case; The Case of Dominant Electron Zeeman Energy; General Case; The Case of $B \ll B_{hf}$; The Case of $B \gg B_{hf}$; Combined g and

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Hyperfine Anisotropy; Multiple Hyperfine Matrices; Systems with I>1/2; Hyperfine Powder Line Shapes; References/Notes/Further Reading/Problems.

Chapter 6. SYSTEMS WITH MORE THAN ONE UNPAIRED ELECTRON. Introduction; Spin Hamiltonian for Two Interacting Electrons; Electron Exchange Interaction; Electron-electron Dipole Interaction; Systems with S = 1; Spin Energies and Eigenfunctions; "$\Delta M_s = \pm 2$" Transitions; Randomly Oriented Systems; Photoexcited Triplet-state Entities; Thermally Accessible Triplet Entities; Ground-state Triplet Entities; Carbenes and Nitrenes; Dianions of Symmetric Aromatic Hydrocarbons; Inorganic Triplet Species; Biradicals; Systems with S > 1; High-spin and High-field Energy Terms; The Spin Hamiltonian - a Summing Up; References/Notes/Further Reading/Problems.

Chapter 7. PARAMAGNETIC SPECIES IN THE GAS PHASE. Introduction; Monatomic Gas-phase Species; Diatomic Gas-phase Species; Triatomic and Polyatomic Molecules; Laser Electron Paramagnetic Resonance; Other Techniques; References/Notes/Further Reading/Problems.

Chapter 8. TRANSITION-GROUP IONS. Introduction; The Electronic Ground States of d-Electron Species; The EPR Parameters of d-Electron Species; Tanabe-Sugano Diagrams and Energy-level Crossings; Covalency Effects; An f-Electron System; References/Notes/Further Reading/Problems.

Chapter 9. THE INTERPRETATION OF EPR PARAMETERS. Introduction; π-Type Organic Radicals; Anions and Cations of Benzene and Some of its Derivatives; Anions and Cations of Polyacenes; g Factors of π-Radicals; Origin of Proton Hyperfine Splittings; Sign of the Proton Hyperfine Splitting Constant; Methyl-proton Hyperfine Splittings and Hyperconjugation; Hyperfine Splitting from Nuclei Other than Protons; One-dimensional Chain Paramagnets; σ-Type Organic Radicals; Triplet States and Biradicals; Inorganic Radicals; Electrically Conducting Systems; Metals; Metals in Ammonia and Amine Solutions; Semiconductors; Techniques for Structural Estimates from EPR Data; The Newman Superposition Model; The Pseudo-cube Method; Distances from Parameter D; Eatons' Interspin-distance Formula; Summary; References/Notes/ /Further Reading/Problems; Appendix 9A. Hückel Molecular-orbital Calculations; HMO References; HMO Problems;

Chapter 10. RELAXATION TIMES, LINEWIDTHS AND KINETIC PHENOMENA. Introduction; Spin Relaxation - A General Model; Spin Temperature and Boltzmann Distribution; Spin Dynamics; Mechanisms for τ_1; Spin Relaxation - Bloch Model; Magnetization in a Static Magnetic Field; Addition of an Oscillating Magnetic Field; Rotating Frame; Steady-state Solutions of the Bloch Equations; Linewidths; Homogeneous Broadening; Inhomogeneous Broadening; Dynamic Lineshape Effects; Generalized Bloch Equations; Other Theoretical Models; Examples of Line-broadening Mechanisms; Electron-Spin Exchange; Electron Transfer; Proton Transfer; Fluxional Motion; Linewidth Variation - Dynamic Hyperfine Contributions; Single Nucleus; Multiple Nuclei; Molecular Tumbling Effects; Dipolar Effects; Spin-rotational Interaction; General Example; Saturation-transfer EPR; Time Dependence of the EPR Signal Amplitude; Concentration Changes; Chemically Induced Dynamic Electron Polarization; Summary; References/Notes/Further Reading/Problems.

Chapter 11. TIME-DEPENDENT EXCITATION OF SPINS. Introduction; The Idealized $\beta 1$ Switch-on; The Single $\beta 1$ Pulse; Fourier-transform EPR and FID Analysis; Multiple Pulses; Electron Spin-echo Envelope Modulation; Advanced Techniques; References/Notes/Further Reading/Problems.

Chapter 12. DOUBLE-RESONANCE TECHNIQUES. Introduction; A Continuous-wave ENDOR Experiment; Energy Levels and ENDOR Transitions; Relaxation Processes in Steady-state ENDOR; An ENDOR Example: The F Center in the Alkali Halides; ENDOR in Liquid Solutions; Pulsed ENDOR Experiments; ENDOR in Powders and Non-oriented Solids; Electron-electron Double Resonance; Optically Detected Magnetic Resonance; Fluorescence-detected Magnetic Resonance; References/Notes/Further Reading/Problems.

Chapter 13. OTHER EPR TOPICS - REFERENCES

Appendix A. MATHEMATICAL OPERATIONS. Complex Numbers; Operator Algebra; Properties of Operators; Eigenvalues and Eigenfunctions; Determinants; Vectors: Scalar, Vector and Outer Products; Matrices; Addition and Subtraction of Matrices; Multiplication of Matrices; Special Matrices and Matrix Properties; Dirac Notation for Eigenfunctions and Matrix Elements; Diagonalization of Matrices; Perturbation Theory; Dirac Delta Function; References/Notes/Further Reading/Problems.

Appendix B. QUANTUM MECHANICS OF ANGULAR MOMENTUM. Introduction; Angular-momentum Operators; Commutation Relations for General Angular-momentum Operators; Eigenvalues of J^2 and J_z; Angular-momentum Matrices; Addition of Angular Momenta; Notation for Atomic and Molecular States; Angular Momentum and Degeneracy of States; Time Dependence; Summary; References/Notes/Further Reading/Problems.

Appendix C. THE HYDROGEN ATOM AND AN RH_2 RADICAL. Free Hydrogen Atom; Spin Hamiltonian; The Spin of Eigenfunctions and Energy Matrix; Exact Solution for the Energy Eigenvalues; Energy Eigenstates and Allowed Transitions; Resonant Frequencies in Constant Magnetic Field; Resonant Magnetic Fields at Constant Excitation Frequency; Calculation of the Spin Energy Levels by Perturbation Theory; RH_2 Radical; Spin Hamiltonian and Energy Levels; EPR transitions; References/Notes/Further Reading/Problems.

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Appendix D. INSTRUMENTATION AND TECHNICAL PERFORMANCE. CW EPR Spectrometers; Magnet System; Radiation Source; Microwave Transmission; Coupling of the Source to the Resonator; Resonator System; Field-modulation System; Coupling of the Resonator to the Detector; Detection System; Pulsed EPR Spectrometers; Computer Interfacing with EPR Spectrometers; Techniques for Temperature Variation and Control; References/Notes/Further Reading/Problems.

Appendix E. EXPERIMENTAL CONSIDERATIONS. Line Shapes and Intensities; Lineshapes; Signal Intensities and Spin Concentrations; Sensitivity and Resolution; Optimum Sensitivity; Modulation Amplitude; Modulation Frequency; Microwave Power Level; Temperature; Q Factor of the Resonator; Microwave Frequency; Concentration of Paramagnetic Centers; Measurement of g Factors and Hyperfine Splittings; Measurement of Relaxation Times; Techniques for Generation of Paramagnetic Species; References/Notes/Further Reading/Problems.

Appendix F. BIBLIOGRAPHY -- EPR-Related Books and Selected Chapters therein.

Appendix G. FUNDAMENTAL CONSTANTS, CONVERSION FACTORS AND KEY DATA. Fundamental Constants; Useful Conversion Factors; Selected Free Atom/Ion One-electron Spin-orbit Coupling Parameters ζ_{nl}; Properties of Selected Nuclides/Atoms.

ELECTRON SPIN ECHO ENVELOPE MODULATION (ESEEM) SPECTROSCOPY, S.A. Dikanov and Y.D. Tsvetkov, (Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk).

Contents: Principles of ESE and ESEEM, ESEEM Spectroscopy in Orientationally Disordered Systems, Applications of ESEEM Spectroscopy, APPENDIX: List of Books and Reviews on ESEEM Spectroscopy. The Catalog number is No. 4224; the domestic price for this title is $159.95 and the foreign market price is $192.00. Orders may be sent to:

CRC Press, Inc., 2000 Corporate Blvd., NW, Boca Raton, FL 33431, USA ☎: 407-994-0555; FAX: 407-997-7249 or 407-997-0949.

NOTICES OF MEETINGS

SIXTEENTH INTERNATIONAL EPR SYMPOSIUM at the 35th Annual Rocky Mountain Conference, Denver, CO, USA, July 25-29, 1993. To be held at the Hyatt Hotel in Denver. Prof. James S. Hyde will receive the Gold Medal of the International EPR Society. A technical Session in his honor is being arranged by Professors Wayne Hubbell and David Thomas. Papers and posters applying and extending Prof. Hyde's innovations are particularly solicited. There also will be general sessions as well as a special session on electrically-detected magnetic resonance arranged by Dr. James Stathis, IBM Watson Research Center. A PC-type computer will be available in the poster area for software demonstrations. For more information, contact Profs. Gareth R. Eaton or Sandra S. Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208, USA. ☎: 303-871-2980 or 303-871-3102; FAX: 303-871-2254; E-mail: seaton@ducair.bitnet.

TWELFTH ANNUAL SCIENTIFIC MEETING AND EXHIBITION, THE SOCIETY OF MAGNETIC RESONANCE IN MEDICINE, New York, New York, USA, August 14-20, 1993. The Society invites submission of Abstracts to be presented in oral and poster sessions at the Twelfth Annual Meeting. Abstracts must contain new, previously unpublished material. There will be no Works-in-Progress this year. The deadline for receipt of Abstracts in the SMRM Business Office is April 27, 1993. Abstracts accepted for presentation will be printed in the *Proceedings of the Society of Magnetic Resonance in Medicine* (formerly titled *SMRM Books of Abstracts*).

For meeting information, contact the Society of Magnetic Resonance in Medicine, 1918 University Avenue, Suite 3C, Berkeley, CA 94704, USA ☎: 510-841-1899; FAX: 510-841-2340.

SECOND FAR EASTERN CONFERENCE ON MEDICAL AND BIOLOGICAL ENGINEERING 1993, Beijing, CHINA, August 15-17, 1993. The purpose of this meeting is to exchange information and encourage cooperative development of medical and biological engineering in the Far East and the other parts of the world. The theme of this conference is to look at high level science and technology, especially to accelerate the progress of medical and biological engineering and to promote medical care. For more information, contact Secretariat of 2nd FECMBE, c/o Chinese Society for Biomedical Engineering, 5 Dong Dan San Tiao, Beijing 100005, China.

THIRD NATIONAL CONVENTION OF THE ITALIAN ELECTRON SPIN RESONANCE GROUP (GIRSE), Alghero, September 24-27, 1993. The conference will focus primarily on brief oral communications. In keeping with GIRSE conference tradition, space will be allocated for work on the development and applications of EPR spectroscopy in diverse national research sectors. There will be oral presentations and posters. To be held at the hotel Corte Rosada on the bay of Porto Conte. Thematic sessions:

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Inorganic spectroscopy, Solid state and interfaces, Biological and medical applications, Methodologies of instrumentation and data treatment, Free radicals, Reaction mechanisms and kinetics in solution.

Organizing Committee: E. Alberico, M. Branca, A. Dessi', G. Micera, D. Sanna.

Secretaries for Meeting: Prof. M. Branca and Prof. G. Micera, Dipartmento di Chimica, Università di Sassari, Via Vienna2, 07100 Sassari; ☎: 079/229555-229541-229487; FAX: 079/229559-212069; decnet:mvchss::girse; Bitnet: girse@mychss.cineca.it

Registration forms due May 31, 1993. Contact: Segretaria del Terzo Convegno GIRSE, Dipartimento di Chimica, Via Vienna 2, 07100 SASSARI, ITALY.

WORKSHOP ON IN VIVO EPR AND EPR STUDIES OF VIABLE BIOLOGICAL SYSTEMS, at the Dartmouth Medical School, Hanover, New Hampshire, USA, October 17-21, 1993. Sponsored by the Illinois EPR Research Center (IERC) and held at the IERC Dartmouth site. The dates are set to coordinate with (immediately precede) the 4th International Symposium on Spin Trapping and Organic EPR Spectroscopy with Applications in Chemistry, Biology and Medicine. This meeting is aimed at bringing together members of all of the laboratories that are directly and indirectly applying EPR to viable biological systems, with a special emphasis on In Vivo EPR.

The format will stress discussion and sharing of information, in order to facilitate progress in this field. Attendance will be limited in order to achieve the goals of the workshop. **Those planning to attend are encouraged to send in a registration form (see p. 27 of the previous issue of the Newsletter) as soon as possible.** Housing is limited as the meeting is at the peak time for viewing autumn colors.

Correspondence on the meeting should be addressed to: Harold M. Swartz, M.D., Ph.D., Dartmouth Medical School, HB-7250, Strasenburgh 308, Hanover, NH 03755-3863, USA. Phone No: 603/650-1754; Fax No: 603/650-1935; E-Mail: Harold.Swartz@Dartmouth.Edu

4TH INTERNATIONAL SYMPOSIUM ON SPIN TRAPPING AND ORGANIC EPR SPECTROSCOPY WITH APPLICATIONS IN CHEMISTRY, BIOLOGY AND MEDICINE, Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma, USA, October 25-28, 1993 (Monday to Thursday). Note that the name and dates of this symposium were changed since the announcement in the Summer '92 issue of the EPR Newsletter. It will immediately follow the IERC (Dartmouth) Workshop on In Vivo EPR and EPR Studies of Viable Biological Systems.

For this meeting, spin trapping is defined as any radical addition reaction (trapping) which produces an addition product (adduct) with the radical group attached. The structure of the adduct can be determined by any means, e.g. EPR, MS, NMR, etc. Hydrogen atom abstraction reactions are not considered spin trapping.

The organizing committee is as follows: Edward G. Janzen, Host; Keisuke Makino and Toshikazu Yoshikawa, Honorary Members; Coit M. DuBose, Robert A. Floyd, Yashige Kotake, Paul B. McCay, J. Lee Poyer, Lester A. Reinke and Mrs. Audrey Winkles, Secretary. This symposium will include oral and poster presentations. Abstracts are invited. Arrival and registration is planned for Sunday, October 24 with talks and posters, Monday through Thursday, October 25-28.

Suggested topics are:

- Kinetics and Rates of Spin Trapping
- Kinetics and Rates of Spin Adduct Decay
- EPR Spectroscopy of Spin Adducts
- Mass Spectrometry of Spin Adducts
- Synthesis of Spin Traps and Spin Adducts
- Biological Chemistry and Metabolism of Spin Traps
- Biological Chemistry and Metabolism of Spin Adducts
- Spin Trapping and Drug Toxicity
- Beneficial Effects of Spin Traps
- Pharmacology of Spin Traps and Spin Adducts
- Spin Trapping in CCl_4 Metabolism
- Spin Trapping in Phagocytosis
- Spin Trapping in Ischemia/Reperfusion
- Radical Trapping by Salicylate
- Nucleic Acids/DNA Radical Adducts
- EPR Spectroscopy of Organic and Organometallic Radicals
- Radical Reactions with Quinones
- Tocopheroxyl, Ascorbyl and "Paraquat" Radicals
- Other Topics

For your convenience, a registration form is printed on p. 27 of the previous issue of the Newsletter.

Contact: Free Radical Biology and Aging Research Program, Oklahoma Medical Research Foundation, 825 N.E. 13th St., Oklahoma City, OK 73104 USA. ☎: 405-271-7570; FAX: 405-271-3980.

FIRST ANNUAL MEETING OF THE OXYGEN SOCIETY, Omni Hotel, Charleston, SC, USA, November 12-16, 1993: OXYGEN SOCIETY EPR SESSION, ***EPR(ESR) CENTERS: WHAT THEY CAN DO FOR YOU,*** Noon Monday Nov. 15, Gary R. Buettner (Organizer), **Program:** The National Biomedical EPR Center, Dr. B. Kalyanaraman, Wisconsin Medical College, Milwaukee, WI; The National Biomedical Center for Spin Trapping and Free Radicals, Dr. Edward Janzen, Oklahoma Medical Research Foundation, Oklahoma City, OK; The Illinois EPR Research Center and the Dartmouth Satellite, Dr. R. Linn Belford, University of Illinois, Urbana, IL, and Dr. Harold Swartz, Dartmouth; An EPR Laboratory as a Core Facility at The University of Iowa,

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Dr. Garry Buettner, ESR Facility, The University of Iowa, Iowa City, IA. For O_2 Meeting information, Contact: Dr. Kelvin J.A. Davies, Chair, Dept. of Biochem. & Mol. Biol., Albany Medical College, Albany, NY 12208-3479, USA. ☎: 518-262-5315 (FAX 5689)

INTERNATIONAL CONFERENCE on BIORADICALS DETECTED by ESR SPECTROSCOPY, Institute for Life Support Technology, Yamagata, Japan, June 12-16, 1994. The organizers are Hitoshi Kamada, Yamagata Technopolis Foundation (YTF), president, and Hiroaki Ohya-Nishiguchi (YTF), general secretary.

The conference will treat an aspect of life-support technology with special attention to ESR spectroscopy including new technology and technology transfer, ESR imaging, spin trapping and labeling, metalloproteins, medical applications, antioxidants and food sciences, and characterization of bio-materials. The conference program will include opening lecture, plenary lectures, session lectures, invited reports, original research contributions, and poster session.

YTF is now organizing a world-wide research center for investigating bioradicals based on ESR spectroscopy, *Institute for Life Support Technology (LIST)*. The research center will be opened in April, 1993. Thus the conference has yet another meaning--namely, celebrating inauguration of the kernel of its researches on bioradicals.

The organizing committee will try to do their best in involving you in the warm and friendly atmosphere of Yamagata, offering the nature and natural foods most famous in Japan, *the other side of Japan.*

Scientific scope of the Conference: The conference will treat all aspects on bioradicals with special attention to ESR spectroscopy, including the following sessions: 1) New technology and technology transfer; 2) ESR imaging; 3) Spin trapping; 4) Spin labels and oximetry; 5) Metal complexes and metallo proteins; 6) Biomedical applications; 7) Antioxidants and food sciences; 8) Tissues, cells and biomaterials; 9) Others.

The Organizing Committee consists of: H. Kamada (YTF), *Chairman*; H.Ohya-Nishiguchi (YTF)*, *General Secretary*; M. Hiramatsu (YTF), *Secretary*; T. Akatsuka (Yamagata Univ.); N. Hirota (Kyoto Univ.)*; M. Inoue (Osaka City Univ.)*; Y. Ikegami (Tohoku Univ.); M. Iwaizumi (Tohoku Univ.); K. Kuwata (Osaka Univ.); A. Mori (Okayama Univ.); H. Nakazawa (Tokai Univ.)*; E. Niki (Univ. of Tokyo); T. Ogata (Yamagata Univ.); K. Ohno (Univ. Industrial Technology)*; H. Sakurai (Kyoto Pharm. Univ.)*; T. Shiga (Osaka Univ.), J. Sohma (Kanagawa Univ.)*, H. Utsumi (Showa Univ.)*; T. Watanabe (Tokyo Univ. Marine Science)*; T. Yoshikawa (Kyoto Pref. Univ. of Medicine). (*program committee)

The International Advisory Board consists of E.G. Janzen (USA), E. Niki (Japan), L. Packer (USA), H.M. Swartz (USA), M.C.R. Symons (UK).

For more information please contact Dr. Midori Hiramatsu, Institute for Life Support Technology, Yamagata Technopolis Foundation, 683 Kurumanomae, Numagi, Yamagata 990, Japan, 81-236-44-8088; FAX: 81-236-44-9640.

THIRTEENTH ANNUAL SCIENTIFIC MEETING AND EXHIBITION OF THE SOCIETY OF MAGNETIC RESONANCE IN MEDICINE, San Francisco, CA, August 6-12, 1994, at the San Francisco Hilton.

XXVII CONGRESS AMPÈRE ON MAGNETIC RESONANCE, Kazan, Russia, August 22-29, 1994. The scientific program will include plenary lectures, symposia, and poster sessions covering the latest achievements in current research, and new developments, trends, and applications in the field of magnetic resonance.

Special attention will be given to the following subjects:

- EPR, NMR and NQR Microimaging and Material Science
- Glasses, Liquid Crystals, Polymers
- Low Dimensional Systems
- Magnetic Resonance in Very High Fields
- Magnetic Resonance of Intermediates
- Modern Developments in Solid State NMR
- Multiple Resonance and Multi-Dimensional Spectroscopy
- New Materials (High - Tc, Cn, etc.)
- New Methods and Techniques
- Non-Equilibrium Processes and Non-Linear Phenomena
- Phase Transitions
- Spin Dynamics at Ultra Low Temperatures
- Spin Polarization Phenomena
- Systems with Orbital Degeneracy
- Time Domain EPR.

The official language at the Congress is English. Young scientists and students are strongly encouraged to participate. Special student rates, i.e., significantly reduced registration and accommodation fees are available. The Congress will take place in the Cultural Centre of Kazan State University founded 1804), which has modern and well-equipped facilities for scientific meetings.

At the Congress, the 1994 Zavoisky Award will be presented, previously awarded to Dr. W. Mims and Prof. B. Bleaney.

Organizing Committee: Prof. Kev M. Salikhov, Chairman and Dr. Nail M. Suleimanov, Scientific Secretary.

Program Committee: Prof. V.A. Atsarkin (Moscow), Prof. E. Hahn (Berkeley), Prof. B.I. Kochelaev (Kazan), Prof. E.T. Lippmaa (Tallinn), Prof. Yu. N. Molin (Novosibirsk), Prof. I.V. Ovtchinnikov (Kazan), Prof. K. M. Salikhov

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(Kazan), Prof. D. Stehlik (Berlin), Prof. M.A. Teplov (Kazan).

Executive Committee: I.A. Aksenov, V.A. Khramov, R.B. Malikova, A.K. Salikhova, E.A. Turiyansky.

Please send your notice of intent to participate to arrive as soon as possible. Send your name, address, phone, FAX, and E-mail to Zavoisky Physical-Technical Institute, Sibirsky trakt 10/7, Kazan, 420029, Tatarstan, Russian Federation. ☎: (8432) 760503; FAX: (8432)765075; TELEX 224 864 PTB SU: E-mail: vitali@adonis.ias.msk.su.

Organizers are thankful to our magnetic resonance colleagues from the Free University of Berlin for support and encouragement.

NOTICE

The Walter J. Johnson Prize for the Encouragement of Postdoctoral Research was established by the Board of Directors of Harcourt Brace Jovanovich, Inc., to be awarded to a deserving individual or individuals having recently completed doctoral studies in the life sciences. The award was established in recognition of Mr. Walter J. Johnson (founder of Academic Press, a division of Harcourt Brace Jovanovich), who has engaged in a lifelong dedication to excellence in scientific publishing. The editorial administrators of three Academic Press journals have been vested with the authority to select the recipients of the Walter J. Johnson Annual Prize: *Archives of Biochemistry and Biophysics*, Experimental Cell Research, and *Journal of Molecular Biology*. A $10,000 prize is awarded every three years. The following guidelines apply:

(1) The nomination should be based on the quality of a paper published in *Archives of Biochemistry and Biophysics* during the preceding three years. The nominee must be the first-listed author. (2) The nominee should have received a Ph.D. or M.D. no more than five years prior to the publication date of the article. (3) The Prize may be awarded to one nominee or divided among several. (4) Nominations should be made in writing to the Chairman of the Editorial Committee by a member of the Editorial Board of *Archives of Biochemistry and Biophysics*. (5) Selection is made by a Committee of Executive Editors of *Archives of Biochemistry and Biophysics* .

For further information, contact Academic Press, Inc., Editorial Office: Third Floor, 1250 Sixth Avenue, San Diego, CA 92101, USA; ☎:619-230-1840; FAX: 619-699-6859; Email: acadpres@sds.sdsc.edu.

POSITIONS OPEN

POSTDOCTORAL FELLOWSHIP. One position available in projects using EPR spectroscopy in viable biological systems *in vitro* and *in vivo*. Required: background in EPR spectroscopy and/or working with viable cells and animals. Contact:

U.S. Army Medical Research Institute
of Chemical Defense
ATTN: SGRD-UV-YY/Dr. Carmen M. Arroyo
Aberdeen Proving Ground, MD 21010 USA
☎: 410-671-3691; FAX: 410-676-7045

SITUATION WANTED

Ph.D. student finishing his thesis in September 1993 on the EPR study of intermediates in electrochemical reactions seeks a postdoctoral position in an EPR laboratory.

Peter Rapta
Dept. of Physical Chemistry
Slovak Technical University
CS-812 37 Bratislava, CZECHOSLOVAKIA

EQUIPMENT & SUPPLIES EXCHANGE

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Mr. C. Arnow
Micro-Now Instrument Co.
☎: 708-677-4700; FAX: 708-677-0394.

WANTED: HALL PROBE.

Varian E-4 magnet Hall Probe - P/N - 908742 - 05 as well as E-112 magnet Hall Probe - P/N - 929279 - 02 B are required urgently.

If available, please contact or send it to
Prof. P.T. Manoharan
RSIC, IIT, Madras - 600 036, INDIA.

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AVAILABLE: VARIAN V 4500 MODULES.

Modules for the Varian V4502 EPR spectrometer are available from G. R. or S. S. Eaton at the University of Denver. E-Mail: geaton@ducair.bitnet.

AVAILABLE: BOXCAR AVERAGER

An inexpensive boxcar averager designed for use in ESE spectrometers is available from the University of Denver. At slow repetition rates it gives about two orders of magnitude better S/N than the well-known PAR 162/164 boxcar. Contact Richard Quine at the University of Denver, Denver, CO 80208 USA ☎: 303-871-2419.

AVAILABLE: VARIAN 620L BOARDS.

A full set of boards for the Varian 620L computer is available.

Contact Sandra or Gareth Eaton
University of Denver. E-mail: seaton@ducair.bitnet.

WANTED TO BUY: USED EPR SPECTROMETER.

A unit such as a Varian E-4 or E-9 would be ok. Electromagnet (or cavity) not necessary.

If you know of such a unit that might be available, please contact Mark Rubinstein at the Naval Research Laboratory, Washington, DC 20375, USA
☎: 202-747-4207.

TEMPO DERIVATIVES FREE!

We have small amounts — 50 to 200 mg each — of unique derivatives of TEMPO to give away: 4-nitro-, 4,4-dinitro-, 4-chlor-4-nitro-, 4-brom-4-nitro-, 4-iod-4-nitro-, 4-hydroxy-4-butyl-, 4-hydroxy-4-hexyl-. Also, there are some amounts of corresponding nonoxidized amino compounds containing the 4-nitro group. Contact :

Anatol E. Myshkin,
N.N. Semenov Institute of Chemical Physics
of the Russian Academy of Sciences,
Kosygin str., 4, 117977
Moscow V-334, RUSSIA

OFFERED: VARIAN FIELD SCAN CONTROLLER CARDS

Any Varian magnetic field controller can be modified to permit control of the magnetic field by a computer. A fully documented printed circuit card and controller modifications is available from the University of Denver.

Contact: Richard Quine ☎: 303-871-2419.

AVAILABLE: STANDARD Li-LiF SAMPLES

Samples of extremely pure Li-in-LiF crystals containing small spherical or variously shaped "massive" metal particles of Li are stable markers of intensity and other EPR characteristics (up to 600C). Samples with either small or large particles are available. These samples, which were described in the EPR Newsletter (vol. 4, No. 2, Summer, 1992, p. 8), can be used in a variety of EPR and NMR investigation — for example, for standards, analysis of magnetic fields, or education. The crystals are being made available to interested colleagues at a pro-forma price of US$ 650-700 per kit (2 types of samples for various measurements), with package and marking by agreement.

For additional technical information, the contact is:
Dr. F.G. Chercasov, Kazan, Phys-Techn. Institut
420029 Kazan Sibirsky tract, 10/7
Tatarstan (Russian Federation) ☎: (8432) 39-30-87.

The administrative contacts are:
In Moscow: Dr. G.A. Denisenko, Institute of Crystallography, Leninsky pr., 59 Moscow 117333 RU; ☎: 7-095-135 6420; FAX: 7-095-135 1011. In Kazan: Dr. F. Gubin, 420020 Kazan Volodarskogo, 1-60, Tatarstan (Russian Federation). ☎: 8432-39-3087, telex: 224864 ptb su

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MESSAGE TO IES MEMBERS IN THE FORMER SOVIET UNION

Ballots mailed in the week of May 4 to members in the former Soviet Union and addressed to the USSR are being returned to us without explanation. We regret the delay and are attempting to determine where and why the mail is being stopped. In the meanwhile, we are readdressing all such returned ballots to the individual republics (i.e., Russia, Ukraine, etc.) and are remailing them.

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This publication is the official newsletter of the INTERNATIONAL EPR(ESR) SOCIETY. It is supported by the Society, by corporate and other donors, and by three national Centers for EPR/ESR spectroscopy in the USA. These Centers are sponsored by the Division of Research Resources, U.S. National Institutes of Health:

National Biomedical ESR Center, Prof. James S. Hyde, Director. Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226, USA. ☎: 414-266-4000. FAX: 414-266-4007. E-Mail: cfelix@mis.mcw.edu

Biotechnology Resource in Pulsed EPR Spectroscopy, Prof. Jack Peisach, Director. Albert Einstein College of Medicine, Department of Molecular Pharmacology, 1300 Morris Park Avenue, Bronx, New York 10461, USA. ☎: 718-430-2175. FAX: 718-829-8705. E-mail: peisach@aecom.yu.edu

Illinois EPR Research Center (IERC), Prof. R. Linn Belford,* Director; Prof. Harold M. Swartz,† Co-Director; Prof. Robert B. Clarkson,* Assoc. Director; Prof. Peter G. Debrunner,* Co-Principal Investigator; other senior staff: Prof. Mark J. Nilges,* Dr. Alex Smirnov,* Laboratory Manager and Dr. Tadeusz Walczak.†
*University of Illinois at Urbana, 190 MSB, 506 South Mathews, Urbana, IL, 61801, USA. ☎: 217-244-1186. FAX: 217-333-8868. E-mail: ierc@uiucvmd.bitnet; r-belford@uiuc.edu; or belford@rlb6000.scs.uiuc.edu. (IERC also operates a satellite site for EPR *in vivo* at
†Dartmouth University in Hanover, New Hampshire; ☎: 603-650-1955; FAX 1935. E-mail: harold.swartz@dartmouth.edu)

These Centers, described in our first issue (Volume 1, #1), cooperate to facilitate research involving EPR. Prospective users may contact the staff at any of the Centers.

IN THIS ISSUE

HOW TO REACH US — To communicate about the EPR Newsletter or submit material, contact R. Linn Belford, Editor or Becky Gallivan, Editorial Assistant, at IERC (address above).

HAL SWARTZ IS AWARDED SMRM'S SILVER MEDAL

— We are pleased to learn that Harold M. Swartz, immediate past president of the International EPR Society, has been honored by a sister society. During the 12th annual meeting of the Society for Magnetic Resonance in Medicine, held in New York August 14-20, 1993, Hal received that Society's Silver Medal, recognizing his outstanding work in promoting, organizing, and serving as the only EPR member of the first Board of Trustees and as Secretary of the SMRM. During the years of this diligent service, Hal was Professor at the University of Illinois at Urbana/Champaign. He is now Professor at the Dartmouth University Medical School. Since Hal had to be absent from the meeting, Dr. Seymour Koenig accepted the award on his behalf.

JIM HYDE ACCEPTS IES GOLD MEDAL

— On July 26, 1993 during the annual EPR Symposium in Denver, Colorado, USA, Professor James S. Hyde of the Medical College of Wisconsin, Milwaukee, WI, USA, was presented with the International EPR(ESR) Society's second annual Gold Medal. The citation was presented by Hal Swartz, immediate past president of IES, and was followed by an award address by Dr. Hyde on the subject of "Multiquantum EPR". Much of this year's Denver meeting directly or indirectly was a tribute to Jim's extraordinary influence on developments in EPR over the years, and it included a gala awards banquet featuring anecdotes and stories about him by several of his many friends and colleagues, past and present.

From the Editor

In this issue (Appendix) are 3700 entries from our databases, with addresses and other information on both IES members and nonmembers on our distribution lists. *This list is published solely as a service to the Members of the International EPR(ESR) Society. It is copyrighted and may not be used for commercial purposes without explicit permission from the Editor of the EPR Newsletter.* We know that there are some errors, omissions, and outdated and incomplete information in

this list. Please inform us of any that you spot! We hope you find this listing to be useful. If our mail indicates that it is, we will print updated lists from time to time.

Again, I remind you that the EPR Newsletter is worth putting out only so long as you, the readers, keep furnishing interesting material - articles, notices, letters, advertisements, etc. Send us your contributions, please. When you notice announcements of pertinent meetings, books, conference proceedings, or the like, please inform us. Please help us spot such material and inform us just as soon as possible to enable us to publish dated material in a timely fashion.

Linn Belford

✦ *IES AFFAIRS* ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR SOCIETY

THE END OF THE BEGINNING

A few short years ago a bunch of enthusiasts within the U.S. decided to establish the International EPR (ESR) Society. Although, from the very start, they envisaged it as a truly international one, the majority of the initial officers were from the USA, and all of the complex work of setting up the Society was done in the USA. This formative stage of the Society was the most crucial of all, and EPR scientists the world over are indebted to our American colleagues for what they have accomplished. Although we probably should not pick out individuals from amongst all those who have contributed, we really should acknowledge the outstanding parts played by Hal Swartz, and by Sandra and Gareth Eaton, whose efforts and tact have not only set the Society in being, but have also accomplished its acceptance as a major scientific body in a very short period of time.

The first officers of the Society were very aware of a possible geographical divide, accentuated by the fact that there already existed EPR societies in Europe, at the time in the U.K. and in Italy. Since that time similar societies have been created in the Netherlands, in France and in Poland, whilst, also, our Russian friends have had unprecedented access to the West. Curiously, there existed no North American equivalent, and when the International Society was created in the U.S.A. it was seen from Europe, to some extent, as trying to replace its existing societies in importance. Hal Swartz has performed great feats of persuasion to overcome this perception, and to convince scientists that the International Society exists to encourage EPR (ESR) spectroscopy wherever it is performed. With the background of a rapidly changing Europe, this task has yet to be fully accomplished, and the new Officers see the need to continue this work as one of their priorities. There will be the second Pan-European conference involving all the societies in that continent in Paris next year, and we shall be represented at it (as we were at the first) to persuade them gently to become more outward-looking. As the Chairman of that meeting is our old friend Klaus Möbius (the most international of men), this is unlikely to be a hard task. Wherever and whenever a meeting is held we need to keep ourselves informed about the latest developments in our field, to encourage emerging nations and their scientists to present their work, and to facilitate international co-operation at all levels, ranging from full research projects, to sharing software and to sharing technical tips. This Newsletter has already provided an unprecedented opportunity for these latter objectives, and all of us feel less isolated as a result.

It happens that all the new Officers are European, although we are delighted that Hal Swartz will remain amongst our number as the past President; his advice is likely to be needed regularly, and it will be given freely. We have, therefore, rather the inverse of what has gone before, and we must be careful to protect the interests of our North American colleagues, although during our period of office we should be in an excellent position to increase the co-operation with our sister societies. The Society will continue to support the Denver Meeting each year, as the major and regular U.S. meeting; this

will be our highest priority. We should like to encourage, too, our distinguished Canadian colleagues to arrange a meeting themselves. In Europe our support will have to be given to the international, rather than national meetings, simply because our resources are finite. This should allow all the countries which have EPR societies to benefit in turn, as the Pan-European meeting rotates between them (assuming we are permitted to become closely allied to these meetings). The possibility also exists of providing support for Groupement Ampère, I.U.P.A.C., I.S.M.A.R. and other major international meetings with an EPR content. But the world is larger than Europe and the U.S., and we shall hope to help with supporting EPR meetings in other continents too.

This Society will prosper only if the Officers remain open to your comment, and we shall welcome your suggestions on any aspect of our operations. We shall not be able to support all that we are asked to, or should like to, but decisions will be made by the international committee adhering to the principles laid down here. We shall welcome any suggestions for how EPR scientists can help each other, and we shall try always to be positive and responsive.

Finally, in taking control of the Society for our period of office, we should thank all of those who have not yet been mentioned here but whose work is essential to its continuance. Their names regularly appear in this Newsletter, the effectiveness of which is entirely due to Linn Belford and Becky Gallivan, and they have given much of their time to setting up the Society and for helping it to run. We are extremely grateful to them and hope that we can count on their further help. We thank, too, our industrial sponsors whose support has been, and will continue to be, crucial to our existence. They deserve the support of all of us when new equipment or software is being sought.

If we can be as successful as our predecessors in furthering the interests of EPR (ESR) scientists we shall feel that in three years' time a job has been well done.

Keith McLauchlan, President
Karl Hausser, Vice President
Arthur Schweiger, Secretary
David Greenslade, Treasurer

ATTENTION, PLEASE. YOUR 1993 DUES ARE URGENTLY NEEDED

If you have not sent your 1993 Dues payments please do so now. If you have misplaced your dues notice, just send your payment to one of the addresses listed on the enclosed IES registration form (end of this issue); indicate any changes that should be made to our information about you (Appendix of this issue).

IES TRAVEL AWARDS

Awarded for June, 1993

To attend SUMMER SCHOOL ON ACIDITY AND BASICITY OF SOLIDS, June 13-23, 1993 in Nice, NATO International. *Svetlana Filimonova*, Russian Academy of Sciences, Novosibirsk, Russia.

To attend INTERNATIONAL SCHOOL ON ESR DOSIMETRY, June 2-11, 1993, Elba Intl. Physics Center, Italy. *Eli Olaus Hole*, University of Oslo, Oslo, Norway.

To attend 5TH CHIANTI WORKSHOP, May 30-June 3, 1993, *Malsorzata Jelen*, Inst. Molecular Biology, Krakow, Poland. *Teresa J. T. Pinheiro*, University of Oxford, Oxford, United Kingdom.

Awarded for August, 1993

To attend SMRM MEETING, New York, August, 1993. *Fuminori Goda*, Dartmouth-Hitchcock Medical Center, Hanover, New Hampshire, USA.

Awarded for October, 1993

To attend WORKSHOP ON *IN VIVO* EPR AND EPR STUDIES OF VIABLE BIOLOGICAL SYSTEMS, October 18-22, 1992, Dartmouth, New Hampshire, USA. *Valentina Quaresima*, University L'Aquila Collemaggio, L'Aquila, Italy. *Mark Symms*, University of Surrey, Guildford, England. *Antelava Alexander*, Tbilisi State Medical University, Republic of Georgia. *Sharashenidze Zurab*, Institute of Sanitation and Hygiene, Republic of

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Georgia. *Papava Manana*, Central Scientific Laboratory of TSMU, Republic of Georgia. *Janusz Koscielniak*, The Ohio State University, Columbus, Ohio, USA. *Jelka Svetek*, Inst Jozef Stefan, Slovenija.

To attend 4TH INTERNATIONAL SYMPOSIUM ON SPIN TRAPPING & ORGANIC EPR SPECTROSCOPY WITH APPLICATIONS IN CHEMISTRY, BIOLOGY AND MEDICINE, Oklahoma City, Oklahoma, USA, October 25-28, 1993. *Dinorah Barasch*, Hebrew University, Jerusalem, Israel.

EPR CONFERENCE TRAVEL GRANTS FOR STUDENTS - CALL FOR APPLICATIONS: The International EPR Society provides grants to students (including postdoctoral student members of the Society) to help defray expenses of long-distance travel to present EPR-related work at an appropriate conference (see "Notices of Meetings" in each Newsletter). Examples of some recent awards are given in the preceding item. A student may apply for an award of up to $250(US) in a brief (1-2 page) letter with (1) some information about him/herself, (2) reasons for wishing to attend and present work at the particular meeting specified, and (3) the endorsement of the student's research advisor. The Awards Committee makes all decisions and announces results to all applicants.

Please send all applications to
Prof. L. J. Berliner, co-Chair
IES Awards Committee
Dept. of Chemistry
The Ohio State University
120 West 18th Ave.
Columbus, OH 43210-1173, USA.
☎: *614-292-0134*
E-Mail: berliner@livers.mps.ohio-state.edu

IES AWARD NOMINATIONS INVITED

If you would like to propose one or more names for any of the following IES awards, please send your suggestion(s), or preferably full nomination(s), to the appropriate Disciplinary Awards Subcommittee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow; George Feher; & Jan Stankowski. *For Chemistry* - Bruce Gilbert, Chair; J. Sohma; Jim Bolton; & Kev Salikhov. *For Biology/Medicine* - Larry Berliner, Chair; Marjeta Sentjurc; Hideo Utsumi; & Tadeusz Sarna).

Gold Medal: The Gold Medal, recognizing benchmark contributions to EPR spectroscopy as a whole; one award per year (first 2 winners: George Feher and Jim Hyde);

Silver Medals: Three Silver Medals each year, one each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine;

Young Investigator Awards: Three Young Investigator awards each year, in the same fields as the Silver Medals; "young" is defined as less than 7 years since the Ph.D. degree.

TRAVEL SUPPORT TO MEETINGS IN EASTERN EUROPEAN COUNTRIES: The Society currently has a system of small grants to facilitate travel to EPR-related meetings within those Eastern European countries which recently suffered calamitous declines in research funds. As described in more detail in previous Newsletters, all scientists, junior and senior, in Eastern Europe are eligible to apply for these hard-currency grants of $10 to $25 each to enable travel to meetings in these countries. IES funds for this are administered by a committee chaired by Yakov Lebedev (Institute of Chemical Physics, Russian Academy of Sciences, Kosygin Str.4, 117977 Moscow V-334, Russia). Write directly to him providing details of the meeting to be attended and the amount of hard currency required for the travel expenses. This program is strictly temporary.

MINUTES OF IES MEETING

Minutes of the Meeting of the International EPR Society Held on July 26, 1993, in Denver, CO, USA:

During the 16th International EPR Symposium in

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Denver, a meeting of the International EPR Society was held on July 26, 1993, from 16:30 to 17:15. The meeting was chaired by Professor Harold M. Swartz, President of the Society.

Professor Swartz reported the results of the recent election, which accomplishes an orderly democratic transition to a new set of officers effective August 1, 1993: Professor Keith McLaughlan, President, Professor Karl Hausser, Vice President, Dr. Arthur Schweiger, Secretary, and Dr. David Greenslade, Treasurer. The founding officers were thanked for their service to the Society. That the new officers are from Europe (England, Germany, and Switzerland) was purposeful, emphasizing the international scope of the Society. It is hoped that in due course there will be officers from other countries, including Pacific rim nations. The use of regional treasurers has been effective in dealing with the problems of currency exchange. For this reason, dues from members in the USA (who constitute ca. 40% of the total membership) will be paid to Regional Treasurer Dr. Christopher Felix, at the National Biomedical ESR Center in Milwaukee.

The meeting of the Society followed a symposium honoring Professor James S. Hyde, Gold Medal Awardee for 1993. Professor Swartz noted the high standard set by the first two Gold Medal Awards (Professor Feher received the 1992 award), and stated that the next Gold Medal Award, and the new Silver Medals and Young Investigator Awards will be selected and announced by the new officers. Nominations for these awards are solicited from all members.

Membership of the Society has increased to 1091 scientists in 51 countries, of whom 390 are from soft-currency countries. Accommodating the financial problems of members from soft-currency countries by keeping the dues payments within the respective countries, while continuing to provide the newsletter, travel grants, etc., as previously announced, is one of the major financial commitments of the Society.

Professor Sandra Eaton, Treasurer, provided a snapshot of the finances of the Society (see separate report). Although the report for 1/1/93-7/24/93 shows an excess of expenditures over income, this is due in part to timing of corporate contributions, and to the fact that significant portions of the dues paid to regional treasurers or to the incoming Treasurer were not aggregated with the dues received in Denver in this report. Overall, the Society has a solid financial base from which to increase its support of travel to meetings for young investigators and to continue the high-quality Newsletter. Bruker was especially thanked for the large contribution of mailing the Newsletter, which does not show up in the contribution/expense ledger of the Society.

The report of the Workshop on the Future of EPR, held in Denver in 1993, has been prepared for publication. (A summary was in the Spring 1993 Newsletter.) A version of this report will be sent by the Society to representatives of funding agencies. Names of people to whom to send it, in the US or in other countries, were requested.

Professor Swartz reminded people that the Society continues to adhere to the policy of not having a separate annual meeting. Instead, it endorses existing meetings with a large EPR program, such as the Denver meeting, and the meetings in England and Italy. Travel awards can be made to attend meetings endorsed by the Society. In 1995 the Society will cooperate with the International Society for Magnetic Resonance (ISMAR) to enhance the EPR program at the ISMAR meeting in Australia. This is an attempt to establish a long-term cooperation between the Society and ISMAR.

In the year 1994 will be the 50th anniversary of the discovery of EPR by Zavoiskii in Kazan. There will be a joint celebration in Kazan and in Denver in August 1994, planned cooperatively by Dr. Kev Salikhov and by the Eatons, recognizing that travel to or from the former Soviet Union will not be feasible for very many people. The President and Past-President of the Society will participate in this celebration. All who can are urged to do so. Some funds have been raised to partially subsidize some special events at the Denver meeting, including participation by Dr. Kev Salikhov. Suggestions for EPR pioneers to invite to the meeting were requested. Other 1994 EPR meetings worldwide are urged to include celebration of the 50th anniversary of the discovery of EPR.

Professor Rudowicz reported on the status of the EPR Database project. Unfortunately, there was only

about 8% response to the 900 questionnaires he sent out, so it is hard to tell what the needs of the whole membership are for the database. Should effort be directed toward setting up an EPR database? Should there be a committee on nomenclature to reach agreement on conventions for reporting systems with S>1/2 to facilitate retrieving information from the database? A poster at the EPR Symposium provided details, and a report will be submitted to the Society in the coming months. Greater support from the membership is needed to justify the effort involved, and there should be a committee to oversee the implementation. Each year there is discussion of need (see Fall 1992 Newsletter), but the effort still lacks clear direction, and feedback from members is needed.

There being no new business (and a strong desire to attend the reception in the scientific exhibit area), Professor Swartz stated that he greatly enjoyed his term of office and thanked the members for their support in setting up the Society.

Submitted August 1, 1993
Gareth R. Eaton, ex-Secretary
Denver, Colorado, USA

EPR Society Treasurer's Report for the Period 1/1/92 to 12/30/92. (This report includes information from the mid-year report submitted 7/31/92.)

I. Income

A. Membership Dues	$10,357.82
B. Corporate Support received	3,650.00

(JEOL, Medical Advances, Norell, Oxford Instruments, Scientific Software, Sumitomo Special Metals, Wilmad Glass. In addition, note that Bruker has assisted with mailing costs for the EPR Newsletter; these are very substantial costs which are not included in the $3650 reported here.)

C. Interest on Bank Account	321.31
Total Income =	$14,329.13

II. Expenses

A. Postage for Treasurer's Office	30.40
B. Expenses at University of Illinois for EPR Newsletter and Society records	6319.38
C. IRS filings	159.91
D. Awards	1500.00
Total Expenses =	$8009.69

Account balances

On January 1, 1992:	$11,969.52
On December 30, 1992:	$18,288.96

Submitted August 1, 1993
Sandra S. Eaton, ex-Treasurer
Denver, Colorado, USA

EPR Society Treasurer's Mid-year Report for the Period January 1 to July 23, 1993. (This does not include payments or expenses recorded by Chris Felix or David Greenslade since June 1, 1993.)

I. Income

A. Membership Dues	$3352.00
B. Corporate Support received	1100.00

(GMW Associates, Micro-Now. In addition, Bruker has assisted with substantial mailing costs for the EPR Newsletter; these are not included in the $1100 reported here.)

C. Interest on Bank Account	208.20
Total Income =	$4660.20

II. Expenses

A. Expenses at University of Illinois for EPR Newsletter and Society records	$4874.88
B. IRS report	5.00
C. Awards	2200.00
Total Expenses =	$7079.88

Account Balances

On January 1, 1993:	$18,288.96
On July 23, 1993:	$15,869.28

Submitted August 1, 1993
Sandra S. Eaton, ex-Treasurer

DUTCH EPR DISCUSSION GROUP MEETS; RENAMED BENELUX EPR DISCUSSION GROUP; IS AFFILIATED WITH IES

On May 18, the Dutch EPR discussion group held its first 1-day meeting in Nijmegen. It was decided to join with Belgium and Luxembourg and change its name to The Benelux EPR Discussion Group. The aims of the Benelux EPR Discussion Group are to stimulate contacts between EPR users in the Benelux and to serve as a subsidiary of the IES. It also provides the possibility to transfer the yearly fees for the IES at lower costs. Membership costs (including the IES Dues) are:

Full Member Dfl *50* *Postdoctoral Member* Dfl *20*
Associate Member Dfl *50* *Student Member* Dfl *10*
Emeritus Member Dfl *20*

Anyone who is interested in joining the Benelux EPR Discussion Group should contact

Peter Gast
Huygens Lab/POB 9504/2300 RA
Leiden/Netherlands;
Bitnet: GAST@RULHL1.LEIDENUNIV.NL;
FAX: 31-71-275819

THE COMPUTER CORNER

Edited by Philip D. Morse II and Keith P. Madden

This column is a regular feature of the EPR Newsletter, covering all computer aspects of EPR. We solicit comments, suggestions, tips and questions from our readers. Please send contributions to either Keith Madden (e-mail: keith.p.madden.1@nd.edu) or Reef Morse (e-mail: reef@xenon.che.ilstu.edu).

First of all, a notice to the people who wished to download a copy of David Duling's EPR package (discussed in the winter 1992 issue of Computer Corner), but had some problems gaining network access. The program suite has been moved to a UNIX-based server to improve access for ftp users. The new host name is zebra.niehs.nih.gov, with an IP address of 157.98.8.243. The EPR files are in directory /pub/pc/epr. E-mail questions concerning the package can be addressed to duling@niehs.nih.gov or duling@niehs.bitnet.

This month we will extend our consideration of on-line resources to a literature current-awareness service of interest to the EPR community run by the Notre Dame Radiation Chemistry Data Center. and will report on the use of a Microsoft Windows-based graphics server to facilitate the writing of EPR software. Finally, we'll look at some of the mail we have received.

Information Services Offered by the Notre Dame Radiation Chemistry Data Center.

In the winter 1992 issue of EPR Newsletter we discussed the availability of ESR/EPR software on-line with emphasis on data acquisition and analysis. This issue we'll discuss an on-line information service of interest to the EPR community, the on-line service of the Radiation Chemistry Data Center (RCDC), located at the Notre Dame Radiation Laboratory, and supported jointly by the US DOE and NIST. The mission of the center is to compile and distribute critically evaluated data on processes initiated by light or ionizing radiation. Both functions are accomplished on-line in the databases maintained by RCDC. These include the RATES database, giving rate constants for free radical reactions in aqueous solution, the triplet-triplet

absorption database, containing the spectral parameters for excited species in condensed-phase media, and the bibliographic database, the source for the Biweekly List of Papers on Radiation Chemistry and Photochemistry, which is available by subscription. The bibliographic database is of particular interest to EPR spectroscopists, since the literature is scanned for articles using the EPR technique for radiation-produced radicals. The database contains bibliographic information from 1965 to the present, and is updated biweekly. The on-line database is hosted on a DEC Micro VAX II, and is available on Internet; subscribers to the Biweekly List may use the on-line service without charge. In order to use the RCDC databases, one should apply to the RCDC for a password (see address below). The conversation with the RCDC host is menu driven. First, one must select the database to use -bibliographic, rates, or triplets. For the bibliographic database, one can then enter the appropriate terms for the literature search. This can be done by author's name, keyword, or any Boolean combination thereof. A User Guide containing directions for the search, logon information, and a thesaurus of keywords is available from the data center. The result of the search can be displayed on the screen, and captured into a file by the Telnet program.

An example search is reproduced below.

Username:
Password:

Welcome to VAX/VMS version V5.5-1 on node RCDVAX

Last interactive login on Friday, 9-APR-1993 15:52

Last non-interactive login on Sunday, 4-APR-1993 17:53

Welcome to RCDC online.The Radiation Chemistry Data Center is operated within the Notre Dame Radiation Laboratory under contract with the U.S.Department of Energy and supported jointly by the Office of Basic Energy Sciences of the U.S. Dept. of Energy and the Office of Standard Reference Data of the National Institute of Standards and Technology

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Search: (1)Bibliographic (2)Triplets (3)Rates (0)Quit
DataBase: 1

Radiation Chemistry Data Center Bibliographic File, RCDCbib

Last updated 9-APR-1993

Select papers by author or keyword from the RCDC bibliographic database.

1Author 2Keyword 3Combine 4Display 5Save/Search 6 Exit 7 Print 8 Memo 9 Year Help ?

Select next operation: 1

AUTHOR NAME: 1 Gordy, W.
FILE 1 CONTAINS 27 PAPERS

Select next operation: 4

Display file number: 1

Display N papers, N = 4

80R048
Electron spin resonance of ^17@O-labeled protein-peroxide
radicals: Zein and edestin.
Dimmey, L.J.; Gordy, W.
Proc. Natl. Acad. Sci. USA 77(1): 343-6 (1980)
CHAB 92: 123658c

755339
Nuclear coupling of ^33@S and the nature of free radicals in irradiated crystals of cysteine hydrochloride and N-acetyl methionine. Hadley, J.H.,Jr.; Gordy, W.
Proc. Natl. Acad. Sci. U.S.A. 72(9): 3486-90 (1975)
CHAB 84: 31403x

755296
Free radicals formed by exposure of pyrimidine solids to sodium atoms: An electron spin resonance study.
Johnson, G.A.; Gordy, W.
Proc. Natl. Acad. Sci. U.S.A. 72(3): 974-8 (1975)
CHAB 83: 130845d

745386
Nuclear coupling of ^33@S and the nature of free radicals in irradiated crystals of cystine dihydrochloride.
Hadley, J.H.,Jr.; Gordy, W.
Proc. Natl. Acad. Sci. U.S.A. 71(8): 3106-10 (1974)
CHAB 81: 162031k

Display N papers, N =

Select next operation: 6

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Search: (1)Bibliographic (2)Triplets (3)Rates (0)Quit
DataBase: 0
SEARCH logged out at 12-APR-1993 15:10:48.55

The bibliographic database search program permits use of Boolean expressions to narrow a search; that is, a search can be performed to obtain the set of publications from a specific author, involving a specific chemical intermediate, from a certain time period. The search would involve an author search (menu option 1) to generate solution set one, and a keyword search (menu option 2) using a name (e.g. alkyl radicals) to generate solution set two. These two sets would be combined (menu option 3) using a logical AND operation to give solution set three. Solution set three would then be subjected to the year filter (menu option 9) to give the desired search result. Further details on the mechanics of an RCDC database search are available in the RCDC publication "User Guide to the RCDC Databases", which can be obtained at a cost of $20.00(U.S.). In addition to the on-line service, the RATES database has been updated, revised and implemented for use on IBM-PC-compatible computers. The database is called NDRL / NIST Solution Kinetics database, and is available on diskette as NIST Standard Reference Database 40; the cost is $190.00(U.S.). For more information on these information services, please write to the following address:

Dr. Alberta Ross, Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556, USA.
☎: 219-631-6527.

A Contribution from Keith Madden — A Graphics Server for EPR Programs

Although there are a large number of EPR data acquisition and analysis packages available both commercially and as freeware, a special circumstance might dictate writing one's own data acquisition/analysis software. For example, analysis of kinetic EPR data frequently necessitates solving the Bloch equations, modified specifically to model the chemical kinetics of the radical and non-radical species present in the reaction mixture. One can then simulate the EPR spectrum, with the lines perhaps in enhanced absorption / emission due to chemically induced spin polarization. Or one can consider the temporal evolution of a single EPR line. One major difficulty in writing one's own program is that EPR is a very visually oriented technique -- we want to see spectra and kinetic curves. Unfortunately, writing graphical computer programs is usually a challenge on several levels. First, graphics programs at their lowest level, are extremely hardware specific. We have written a series of graphics-based packages for our studies, porting the software in turn to DEC VT55s, DEC VT100s, TEK 4014s, TEK 4105s, and finally the PC compatible platform (CGA only!). The addition of such niceties as mouse-driven graphics cursors with screen readout is sufficiently time-consuming that the advantage in data analysis is perhaps more than balanced by the prospect of writing the code for the feature. The addition of graphics support in popular PC-based compilers from Borland, Zortec, and Microsoft alleviates some of the pain involved in graphics programming, but still sophisticated functionality requires much more than minimal programming effort.

When last confronted by the prospect of rewriting our EPR package again, I decided to see whether third-party programs could solve my problems. Under DOS, GraphiC by Scientific Endeavors Corporation (Kingston, TN) provided a series of C language subroutines that I could include in my code to develop my graphics environment. This package, I believe, offers an optimal solution for spectrum and kinetics display in the DOS mode. But the graphics code must be built into the program source, and linked into the binary executable at link time; therefore, each program needs explicit reference to the GraphiC subroutines in its source. I was looking for an easier solution. At the suggestion of our systems manager, Marc Cozzi, I purchased a copy of Origin, by MicroCal Software, Inc. (Northampton, MA), and started rewriting my code to execute in the Microsoft windows environment.

On the surface, Origin resembles a legion of other Microsoft-Windows-based programs for producing plots from spreadsheet or database data. But of specific interest was the incorporation of DDE, dynamic data exchange, a feature of the Microsoft windows environment. Windows can provide a messaging service between a user's client application requiring graphics services and a server application, such as Origin, which listens for such messages, provides the service, and then sends a report of the result back to

the user's application. By graphics service, I mean drawing and scaling plots, using a mouse-driven cursor to measure the x and y coordinates of absorption peaks, or even performing non-linear least-squares fitting to a Lorentzian, Gaussian, or user-defined function. The specifics of starting a DDE conversation between a client application and Origin are included in the Origin advanced technical information package available at nominal cost directly from MicroCal. The package includes a disk with sample source code for DDE.

Although there are a number of subtleties involved with DDE programming, essentially the DDE protocol (1) allows a program to identify applications running in the windows environment that offer various services, (2) allows a program to establish a data conversion with one or more suitable server applications, (3) defines the data structure of the memory space used to pass data between the client and server, (4) coordinates the use of this shared memory between the two applications, (5) provides a channel for the client to send commands for execution on the server, and (6) terminates the conversation in an orderly manner at the request of either partner. The code sample provided with Origin is complete enough that anyone with some windows programming experience should be able to add functional DDE code. (Make sure your copy of Petzold's Programming Windows is close by!).

The resulting program combination accomplishes my needs for interactive spectral/kinetic EPR data display. The hardware-dependence problem is eliminated by allowing Windows to provide the display resources. Printing and storage of the EPR data is also handled effortlessly by the Origin server, saving the time that would have been required to develop the code for these functions. Origin provided exactly what I needed -- a package to do all the hard graphics programming, so I could spend the time on the magnetic resonance specific code. I recommend it highly.

A Contribution from David Close.

Kudos for the new Computer Corner in the EPR Newsletter. I find the information presented to be very useful. I have a suggestion that I would like to see discussed in this column concerning source code. First to illustrate the problem. I have obtained two new programs recently for manipulation of ESR data. They are SUMSPC92 from the National Biomedical ESR Center and Dave Duling's EPR.EXE program. Both programs have all sorts of bells and whistles and work just fine with data supplied or internally generated. However the real purpose of any such program is for use on "local data", and this presents all sorts of problems. Since there is no agreed-upon standard format, "local data" must be reformatted. That's no problem for the EPR.EXE program since it accepts an ASCII string for ESR data.

The SUMSPC92 program, however, requires a complicated set of headings at the end of the data string. These appear to be in a tight FORTRAN format, so every space and line is critical. It took some time for me to make my own data readable by this program. I could have saved a lot of time if the source code had been available. Then I could have just looked up the various READ statements and made the appropriate changes. Getting a new program to accept "local data" is only part of the problem, however. No matter how fancy a new program is, one is always going to find "bugs", or places where changes need to be made to suit the local environment. These changes can only be made if source code is available.

Consider, for example, the problem of double integration of spectra to obtain the number of spins in a sample. The program SUMSPC92 has elegant baseline correction and integration subroutines. When I was all done with this procedure, I had the proper "step curve" on the screen. However, the program scales this curve to fit the screen and no information seems to be available to relate this curve to the spin concentration. Since the integration was properly performed, one should be able to extract this information from the program if the source code were available. Therefore, I hope that future discussions of a standard ESR data format by the EPR Society will include the need for making source code available to users.

David Close
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(e-mail: R29CLOSE@ETSU.BITNET)

In the next issue of the EPR Newsletter, we will discuss mail list servers, and the possibility of setting up a list server to discuss issues such as source code availability, data file formats, and spectral database characteristics. Please keep your contributions coming in!

EPR NEWSLETTER

Publication of the International EPR(ESR) Society

Volume 5, Number 2 Page 11 Summer, 1993

TIPS & TECHNIQUES

MISCELLANEOUS TIPS FOR EPR USERS

James R. Anderson
Research Specialties
5629 N. Maplewood
Chicago, IL 60659, USA
(312-728-6570 Phone/Fax)

* Liquid helium users may want to evaluate how the boil-off gas from their dewars or cryostats is vented, so as to avoid flooding the microwave bridge with helium gas and possibly exposing the klystron, with its associated vacuum, to the diffusing properties of helium. This exposure over time might prematurely degrade the klystron's vacuum. According to Varian, the single largest failure mode of a klystron is due to the device becoming gassy and is usually due to internal out-gassing. It would be hard to rule out long term external diffusion of helium gas as a contributing factor. This tiny molecule readily diffuses through otherwise vacuum-tight materials and ionizes at low pressure. If the venting of the gas is difficult to control, a purge tube might be added to the bridge of the klystron shield assembly. Supplying a continuous flow of helium-free air at a small positive pressure will help minimize the chance of He gas entering the klystron compartment. The source of air might be an oil-less pump placed near the floor away from the system.

* Cryogenic users should cover the Hall probe assembly with a suitable shield if liquid nitrogen is spilled or splashed routinely while filling dewars. The epoxy case of the Hall probe may fracture from the low temperatures. Wide insulated tape covering the Hall probe may be all that is necessary.

* Most EPR users who work at cryogenic temperatures know that bubbling He gas above the cavity's active region in a liquid nitrogen dewar reduces boiling of the liquid nitrogen. This eliminates a source of noise on weak samples. (Are there any other kind?) This, however, does cause the vacuum of the dewar to degrade, thereby requiring more helium gas to be used. The helium usage will eventually require the pump-out of the vacuum jacket in two or three months. One should dedicate one dewar for this type of use or obtain a dewar with a vacuum pump-out valve.

(Note: Mr. Anderson has over 20 years experience in EPR instrumentation. He is arranging for his business, Research Specialties, to become a new corporate member of the International EPR(ESR) Society. Research Specialties provides EPR services that range from routine troubleshooting and repair to system upgrades, supplying of critical replacement parts, and fabrication of specialized application modules as well as cavity rebuilding and replacement.)

EPR NEWSLETTER

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CONFERENCE REPORTS

The Polish-American Workshop on EPR Spectroscopy & Imaging in Biology & Medicine: This workshop, organized by the Polish Biophysical Society and supported by the State Committee for Scientific Research in Warsaw, was held on November 30 through December 5, 1992, at the Jagiellonian University, Krakow, Poland. The meeting gathered about 50 participants, mainly from Poland. The following topics were addressed:

In vivo EPR spectroscopy (Swartz, USA), *In vivo* EPR spectroscopy and imaging of free radicals in the heart (Zweier, USA), Photoreactivity of retinal pigments (Sarna, Pol.), Metal-binding properties of neuromelanins (Korytowski, Pol), EPR criteria of tumor-host interactions (Plonka, Kaminska, Lukiewicz, Pol.), Evaluation of implant-recipient interaction by EPR spectroscopy (P. & B. Plonka, Lukiewicz, Pol.), Using very low-frequency EPR to define bulk characteristics of pharmacologic compartments of specific tissues in vivo (Halpern, USA), Whole-body S-band *in vivo* ESR studies on bioreduction of nitroxides in new-born mice (Cleszka, Elas, Wojcik, Dubis, Pajak, Lukiewicz, Pol.), Site-directed spin labelling studies on protein structure and dynamics (Hubbell, USA), ESR measurements in the presence of external electric fields (Froncisz, Pol.), Measurements of the concentration of oxygen under biologically pertinent conditions (Swartz, USA), Spin-label oximetry in dense cell suspension: problems in closed- and open-chamber methods (Ligeza, Swartz, Subczynski, Pol.-USA), Changes in the redox properties of normal and neoplasic cells during cell cycle (Panz, Pol), Bacterial mutant strains unable to reduce nitroxides (Lukiewicz, Nealson, Saffarini, Pol-USA).

The main purpose of the Workshop was to summarize the results of collaborative research done so far by the participating scientists, and to discuss its future, as well as to consider new joint projects.

The papers presented during the Workshop will be published as a special EPR issue February 17, 1993, of Current Topics in Biophysics. The readers of the EPR Newsletter interested in purchasing this particular issue may contact Mrs. M. Elas, Jagiellonian University, Laboratory of Radiospectroscopy of Cancer, Institute of Molecular Biology, Al. Micklewicza 3, Krakow 31-120, Poland, phone 48-12-341-422, fax 48-12-336-907, E4-mail: UBELAS@PLKR CY11.BITNET. A very significant promotional reduction in price of this special EPR issue will be offered to all Members of the International EPR (ESR) Society.

S. J. Lukiewicz

The 3rd International Workshop on "Electron Magnetic Resonance of Disordered Systems" and 1st International Expert Meeting on "Quantitative EPR Spectrometry": The 3rd International Workshop on "Electron Magnetic Resonance of Disordered Systems" (EMARDIS-93) was held June 7-14, 1993 in Bojana (near Sofia), Bulgaria. Traditionally, EMARDIS meetings are directed to the most recent developments of Electron Magnetic Resonance (EPR, ENDOR, ESE) in the theory, instrumentation and qualitative applied studies. In contrast to the successful development in these topics demonstrated in the previous EMARDIS meetings, a lot of symptoms suggested that Quantitative EPR spectrometry is not as highly developed. Because of this, and having in mind the international experiment of quantitative EPR measurements performed in the period 1991-1992, the organizers of the EMARDIS decided to extend it with the 1st International Expert Meeting on Quantitative EPR Spectrometry.

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EMARDIS-93: The EMARDIS meeting was held June 7 -11, 1993. The attendance of the meeting was drawn from 12 countries (from America, Asia, Australia, Europe): Australia, Belgium, Canada, Germany, Italy, Japan, Netherlands, Poland, Switzerland, Ukraina, USA and Bulgaria. Two kinds of presentations were accepted - oral (45 min main lectures, 20 min short communications) and poster presentations of recent results. The following distinguished specialists delivered main lectures: R.L. Belford - Multi-Frequency EMR of disordered systems; J. van den Brink - Inversion of the triplet Y-lines of the reaction center of RPS. Viridis revisited: A time-resolved EPR study of RCs in single crystals and in solid solution; A. Colligiani - ESR and ENDOR experiments using a disc-shaped resonator working in the whispering-gallery mode; G. Gochev - A Program for simulation of powder-type EPR and ENDOR spectra; M. Iwaizumi - Orientation of imidazol- type ligands in copper complexes and ESEEM; H. Kurreck - Fate of the photoexcited electron in the primary processes of photosynthesis: Synthesis and EPR studies of novel covalently linked porphyrin quinones; P. Moens - EPR study of carbonate-derived and ozonide radicals in carbonated apatites synthesized from aqueous solutions; Y. Ohba - Observation of broad-band EPR spectra of transient free radicals by FT-EPR; J. Pilbrow - EPR spectroscopy of poorly characterized systems - a historical and current view; J. Stankowski - Nature of paramagnetic centers in fullerenes; J. A. Weil - EPR of iron centers in silicon dioxide; M. Zdravkova - "ENDOR Crystallography" - current practical applications. In addition, a discussion on the "Future of EPR" (based on the report by the Eatons in the previous EPR Newsletter) was led by John A. Weil, R. Linn Belford, and Robert B. Clarkson.

Q-EPR: The 1st International Expert Meeting on Q-EPR Spectrometry meeting (held immediately after EMARDIS - June 11 - 14, 1993 Bojana, Bulgaria) as a first step in this field was planned to be attended by selected top specialists with the main goal of discussing the present state and to make conclusions for the future of this important area of EPR spectroscopy via main lectures and posters as well as round-table and informal discussions. The attendance of that meeting was from Canada, Japan, Poland, Russia, Switzerland, USA and Bulgaria. The following main lectures were presented: R. B. Clarkson - Characteristics of a carbon-based standard for EPR spectroscopy; K. Dyrek - Spin dosimetry in catalysis research; V. Nagy - Quantitative EPR: Some of the most difficult problems; J. A. Weil - Multi-purpose program EPR.FOR; N. D. Yordanov - Quantitative EPR spectrometry -"State of the art". A Round-Table Discussion on Perspectives of Q-EPR spectrometry was organized. The main topics discussed are given separately. Following EMARDIS practice, the day and early-evening times were intensive working hours whereas late evening was reserved for impromptu discussions on the individual level, sometimes accompanied and aided by Bulgarian wine-tasting.

Both meetings began with a cocktail party and finished with a farewell dinner. The social programme for the EMARDIS participants included visiting one of the most famous and attractive of the national historical places in Bulgaria - Rila Monastery. Those attending Q-EPR visited some of the most attractive places in Sofia (historical museum with gold treasures, several old (built during 6-8 centuries) churches (St. George, St. Petka, basilica St. Sofia), and of course Alexander Nevski Cathedral with the famous icon exhibition in the basement. In addition, Bojana (situated on Vitosha mountain, 10 km. from Sofia) is a famous place in Bulgaria known for its many historical monuments, the most important among them being the Bojana Church situated within walking distance from the meeting site. It was built during the 11th-13th centuries and its frescoes (wall icons) are considered as an evidence for the beginning of the Renaissance era in that time and in this region of the world. Some EMARDIS participants were treated to a special viewing of this church, which is under restoration.

The organizers plan to publish all lectures presented at the EMARDIS-93 and Q-EPR meetings in full text by the end of the year. The next EMARDIS meeting is planned to be organized at the beginning of June 1995. For information on the Proceedings or details on the next meeting, please write to the convener.

Nicola D. Yordanov

EPR NEWSLETTER

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BOOKS and PROCEEDINGS

PREVIEW: "HANDBOOK OF ELECTRON SPIN RESONANCE," Edited by Charles P. Poole, Jr. and Horatio A. Farach. This book is scheduled for release mid-September, 1993. To order, call toll-free 800-488-BOOK in the USA (in Vermont, 802-878-0315; FAX, 802-878-1102) or write AIP Press, c/o AIDC, 64 Depot Road, Colchester, VT 05466, USA.

Fifty years of steady growth in the field of electron paramagnetic resonance (EPR, also ESR or EMR) have produced an extensive body of theoretical and experimental research. While vital data from its various subfields have been reviewed in numerous books and journals, the field has lacked an overall reference that presents, tabulates, and correlates these accumulated data. The Handbook of Electron Spin Resonance aims to fill this gap in the literature by bringing together wide-ranging data from diverse disciplines within EPR and integrates the data into a comprehensive and definitive resource. The book offers reviews of major theories, methods, and instrumentation written by leading authorities in the field. Following an overview of the EPR field, the book goes on to cover critical topics such as: the use of computer techniques in making EPR measurements and in processing the obtained data; the nature of relaxation in diluted solids, liquids, and concentrated systems; comprehensive data tabulation of exchange effects, temperature dependence, and motional aspects of various relaxation phenomena. A comprehensive survey of the ENDOR literature for radicals in liquids, liquid crystals, single crystals, polycrystalline solids, and biological materials also is included.

OUTLINE

Chapter 1. DATA SOURCES; C. P. Poole, Jr. and H. A. Farach. (Introduction; Extent of the Literature; Textbooks and Monographs; Literature Reviews; Data Tabulations; Societies and Conferences; Conventions and Notation; Physical Constants and Conversion Factors).

Chapter 2. COMPUTER TECHNIQUES; Burkhard Kirste. (Spectrometer Control and Data Sampling; Data Processing and Analysis; Spectrum Simulation; Line-Shape Analysis; Hamiltonian Fitting; Literature Searches).

Chapter 3. RELAXATION: BACKGROUND AND THEORY; Ivano Bertini, Giacomo Martin, and Claudio Lucinat. (Introduction; Relaxation Time Constants; Bloch Equations; Chemical Exchange, Relaxation in Diluted Solids, Relaxation in Liquids, Concentrated Systems; Experimental Techniques).

Chapter 4. RELAXATION DATA TABULATION; Ivano Bertini, Giacomo Martin, and Claudio Lucinat. (Introduction; Transition Metal Ions in Solids; Solvated Electrons and Inorganic Radicals; Organic Radicals; Motional Effects; Exchange).

Chapter 5. ENDOR, BACKGROUND AND THEORY; Lowell Kispert. (Introduction: Fundamentals of Magnetic Resonance; ENDOR Fundamentals; ENDOR in Liquid Phase; Solid-State ENDOR; Pulsed ENDOR).

Chapter 6. ENDOR DATA TABULATIONS; Janina Goslar, Lidia Piekara-Sady, and Lowell D. Kispert. (Introduction; Liquid Phase: ^{1}H and ^{2}H, ^{13}C, ^{14}N and ^{15}N, ^{19}F, ^{31}P, Alkali Nuclei, ^{27}Al, ^{203}Tl and ^{205}Tl, ^{117}Sn and ^{119}Sn, ^{29}Si, and ^{25}Mg Data; Organic Radicals in Crystals and Solutions; Radicals in Matrices; Triplet Radicals; Radicals in Biological Systems; Inorganic Radicals and Ions; Defects and Complexes on Surfaces; Impurity Centers in Semiconductor Host Crystals; Spin Centers in Silicon; Paramagnetic Centers in Cubic Host Crystals; Perovskite-Type Materials; Fossil Fuels, Derivatives, and Related Products; Index of Materials).

Other volumes are planned. The object of the present handbook is to provide a convenient source of information on EPR. In some subfields this information is intended to be reasonably comprehensive so that other sources need not be consulted, except perhaps original articles for more details. Examples of these are the relaxation and the electron-nuclear double resonance (ENDOR) articles which, in addition to the computer-techniques article, appear in the present volume. In other subfields the coverage will be representative only because comprehensive data tabulations already exist which are far too long to be duplicated here. Examples of this case are the transition-metal ion and the free radical chapters which will appear in the next volume. The very new subfields of EPR imaging, Fourier-transform EPR, two-dimensional EPR, and high-field EPR do not yet have an extensive literature, and the object of these review chapters will be to describe each technique, explain what can be learned from it, and list results available to date.

NOTICES OF MEETINGS

WORKSHOP ON IN VIVO EPR AND EPR STUDIES OF VIABLE BIOLOGICAL SYSTEMS, at the Dartmouth Medical School, Hanover, New Hampshire, USA, October 17-21, 1993. This meeting, sponsored by the Illinois EPR Research Center (IERC) and held at the IERC Dartmouth site, brings together members of all of the laboratories that are directly and indirectly applying EPR to viable biological

systems, with a special emphasis on In Vivo EPR. Information on this meeting was published in previous EPR Newsletters. Correspondence should be addressed to: Harold M. Swartz, M.D., Ph.D., Dartmouth Medical School, HB-7250, Strasenburgh 308, Hanover, NH 03755-3863, USA.
☎: 603/650-1754; FAX: 603/650-1935;
E-Mail: Harold.Swartz@Dartmouth.Edu

4TH INTERNATIONAL SYMPOSIUM ON SPIN TRAPPING AND ORGANIC EPR SPECTROSCOPY WITH APPLICATIONS IN CHEMISTRY, BIOLOGY AND MEDICINE, Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma, USA, October 25-28, 1993 (Monday to Thursday). Information on this meeting was published in previous EPR Newsletters. It immediately follows the IERC (Dartmouth) Workshop on In Vivo EPR and EPR Studies of Viable Biological Systems. Contact: Free Radical Biology and Aging Research Program, Oklahoma Medical Research Foundation, 825 N.E. 13th St., Oklahoma City, OK 73104 USA.
☎: 405-271-7570; FAX: 405-271-3980.

FIRST ANNUAL MEETING OF THE OXYGEN SOCIETY, Omni Hotel, Charleston, SC, USA, November 12-16, 1993: OXYGEN SOCIETY EPR SESSION, *EPR(ESR) CENTERS: WHAT THEY CAN DO FOR YOU,* Noon Monday Nov. 15, Gary R. Buettner (Organizer), **Program:** The National Biomedical EPR Center, Dr. B. Kalyanaraman, Wisconsin Medical College, Milwaukee, WI; The National Biomedical Center for Spin Trapping and Free Radicals, Dr. Edward Janzen, Oklahoma Medical Research Foundation, Oklahoma City, OK; The Illinois EPR Research Center and the Dartmouth Satellite, Dr. R. Linn Belford, University of Illinois, Urbana, IL, and Dr. Harold Swartz, Dartmouth; An EPR Laboratory as a Core Facility at The University of Iowa, Dr. Garry Buettner, ESR Facility, The University of Iowa, Iowa City, IA. For O_2 Meeting information, Contact: Dr. Kelvin J.A. Davies, Chair, Dept. of Biochem. & Mol. Biol., Albany Medical College, Albany, NY 12208-3479, USA. ☎: 518-262-5315 (FAX 5689)

STABLE ISOTOPE APPLICATIONS IN BIO-MOLECULAR STRUCTURE AND MECHANISMS, March 27-31, 1994, Santa Fe, New Mexico.. A meeting to bring together producers and users of stable-isotope-labeled compounds to assess current and future needs. Invited speakers will discuss applications of stable isotopes to the study of RNA, DNA, peptides, and proteins. Recent advances in scattering and spectroscopy techniques as well as synthesis and production of labeled compounds will be highlighted. Organizing Committee: Jill Trewhella, Chairperson, Donald Ott, Louis A. (Pete) Silks, Mary Ann D. Martinez, Jean Stark, all of Los Alamos National Lab. Program Committee: Nicholas A. Matwiyoff, Univ. of New Mexico, Chairperson, Gerald T. Babcock, Michigan State Univ., Timothy Cross, Florida State Univ., Roger A. Jones, Rutgers Univ., John Markley, Univ. of Wisconsin-Madison, Arthur Pardi, Univ. of Colorado, Clifford J. Unkefer, Los Alamos National Lab. Meeting to be held at Eldorado Hotel. For more information write to: Stable Isotope Applications Conference, Protocol Office, MS P366, Los Alamos National Laboratory, Los Alamos, NM 87545.

INTERNATIONAL CONFERENCE on BIORADICALS DETECTED by ESR SPECTROSCOPY, Institute for Life Support Technology, Yamagata, Japan, June 12-16, 1994. The organizers are Hitoshi Kamada, Yamagata Technopolis Foundation (YTF), president, and Hiroaki Ohya-Nishiguchi (YTF), general secretary.

The conference will treat an aspect of life-support technology with special attention to ESR spectroscopy including new technology and technology transfer, ESR imaging, spin trapping and labeling, metalloproteins, medical applications, antioxidants and food sciences, and characterization of bio-materials. The conference program will include opening lecture, plenary lectures, session lectures, invited reports, original research contributions, and poster session.

YTF is now organizing a world-wide research center for investigating bioradicals based on ESR spectroscopy, *Institute for Life Support Technology (LIST).* The research center was opened in April, 1993. Thus the conference has

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yet another meaning--namely, celebrating inauguration of the kernel of its researches on bioradicals.

The organizing committee will try to do their best in involving you in the warm and friendly atmosphere of Yamagata, offering the nature and natural foods most famous in Japan, *the other side of Japan.*

Scientific scope of the Conference: The conference will treat all aspects on bioradicals with special attention to ESR spectroscopy, including the following sessions: 1) New technology and technology transfer; 2) ESR imaging; 3) Spin trapping; 4) Spin labels and oximetry; 5) Metal complexes and metallo proteins; 6) Biomedical applications; 7) Antioxidants and food sciences; 8) Tissues, cells and biomaterials; 9) Others.

The Organizing Committee consists of: H. Kamada (YTF), *Chairman*; H.Ohya-Nishiguchi (YTF)*, *General Secretary*; M. Hiramatsu (YTF), *Secretary*; T. Akatsuka (Yamagata Univ.); N. Hirota (Kyoto Univ.)*; M. Inoue (Osaka City Univ.)*; Y. Ikegami (Tohoku Univ.); M. Iwaizumi (Tohoku Univ.); K. Kuwata (Osaka Univ.); A. Mori (Okayama Univ.); H. Nakazawa (Tokai Univ.)*; E. Niki (Univ. of Tokyo); T. Ogata (Yamagata Univ.); K. Ohno (Univ. Industrial Technology)*; H. Sakurai (Kyoto Pharm. Univ.)*; T. Shiga (Osaka Univ.), J. Sohma (Kanagawa Univ.)*, H. Utsumi (Showa Univ.)*; T. Watanabe (Tokyo Univ. Marine Science)*; T. Yoshikawa (Kyoto Pref. Univ. of Medicine). (*program committee)

The International Advisory Board consists of E.G. Janzen (USA), E. Niki (Japan), L. Packer (USA), H.M. Swartz (USA), M.C.R. Symons (UK).

For more information please contact Dr. Midori Hiramatsu, Institute for Life Support Technology, Yamagata Technopolis Foundation, 683 Kurumanomae, Numagi, Yamagata 990, Japan, 81-236-44-8088; FAX: 81-236-44-9640.

SEVENTEENTH INTERNATIONAL EPR SYMPOSIUM at the 36th Annual Rocky Mountain Conference, Denver, CO, USA, July 31-August 4, 1994. To be held at the Hyatt Hotel in Denver. A joint celebration of the 50th anniversary of the discovery of EPR by Zavoisky in Kazan is planned cooperatively by Dr. Kev Salikhov at Kazan and by Profs. Sandra and Gareth Eaton at Denver. For information, contact Profs. Gareth R. Eaton or Sandra S. Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208, USA. ☎: 303-871-2980 or 303-871-3102; FAX: 303-871-2254; E-mail: seaton@ducair.bitnet.

THIRTEENTH ANNUAL SCIENTIFIC MEETING AND EXHIBITION OF THE SOCIETY OF MAGNETIC RESONANCE IN MEDICINE, San Francisco, CA, August 6-12, 1994, at the San Francisco Hilton.

XXVII CONGRESS AMPERE ON MAGNETIC RESONANCE, Kazan, Russia, August 22-29, 1994. The scientific program will include plenary lectures, symposia, and poster sessions covering the latest achievements in current research, and new developments, trends, and applications in the field of magnetic resonance.

Special attention will be given to the following subjects:

- EPR, NMR and NQR Microimaging and Material Science
- Glasses, Liquid Crystals, Polymers
- Low Dimensional Systems
- Magnetic Resonance in Very High Fields
- Magnetic Resonance of Intermediates
- Modern Developments in Solid State NMR
- Multiple Resonance and Multi-Dimensional Spectroscopy
- New Materials (High - Tc, Cn, etc.)
- New Methods and Techniques
- Non-Equilibrium Processes and Non-Linear Phenomena
- Phase Transitions
- Spin Dynamics at Ultra Low Temperatures
- Spin Polarization Phenomena
- Systems with Orbital Degeneracy
- Time Domain EPR.

The official language at the Congress is English. Young scientists and students are strongly encouraged to participate. Special student rates, i.e., significantly reduced registration and accommodation fees are available. The Congress will take place in the Cultural Centre of Kazan State University founded 1804), which has modern and well-equipped facilities for scientific meetings.

At the Congress, the 1994 Zavoisky Award will be presented, previously awarded to Dr. W. Mims and Prof. B. Bleaney.

Organizing Committee: Prof. Kev M. Salikhov, Chairman and Dr. Nail M. Suleimanov, Scientific Secretary.

Program Committee: Prof. V.A. Atsarkin (Moscow), Prof. E. Hahn (Berkeley), Prof. B.I. Kochelaev (Kazan), Prof. E.T. Lippmaa (Tallinn), Prof. Yu. N. Molin (Novosibirsk), Prof. I.V. Ovtchinnikov (Kazan), Prof. K. M. Salikhov (Kazan), Prof. D. Stehlik (Berlin), Prof. M.A. Teplov (Kazan).

Executive Committee: I.A. Aksenov, V.A. Khramov, R.B. Malikova, A.K. Salikhova, E.A. Turiyansky.

Please send your notice of intent to participate to arrive as soon as possible. Send your name, address, phone, FAX, and E-mail to Zavoisky Physical-Technical Institute, Sibirsky trakt 10/7, Kazan, 420029, Tatarstan, Russian Federation. ☎: (8432) 760503; FAX: (8432)765075; TELEX 224 864 PTB SU: E-mail: vitali@adonis.ias.msk.su.

Organizers are thankful to our magnetic resonance colleagues from the Free University of Berlin for support and encouragement.

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Publication of the International EPR(ESR) Society

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POSITION WANTED

EPR and NMR Spectroscopist Seeks an Academic or Industrial Position.

Biophysicist-solid state physicist, Ph. D. '87, research/teaching experience. Now research worker/teacher at Department of Physical Chemistry, Faculty of Chemical Technology, Slovak Technical University. Research experience: A) liquid- and solid-state EPR spectroscopy of biological, organic and inorganic materials (Bruker 200D SRC NMR Spectrometer with Aspect 2000 Computer). Special research experience: membrane biophysics, drugs-membrane interaction, spin-label EPR spectroscopy (International Training Course, Hungarian Academy of Sciences, Szeged, Hungary). Also sol-gel or glass solid-state EPR spectroscopy; transitio-metal spin labels. B) liquid- and solid-state NMR spectroscopy of biological, organic, and inorganic materials (Varian 300 MHz VXR spectrometer). Special research experience: 1D, 2D, and pseudo-3D multinuclear NMR spectroscopy of bioploymers, using Varian Unity 500 MHz spectrometer (postdoctoral fellowship at McGill University, Pulp and Paper Research Center, Montreal, Canada). Also sol-gel or glass multinuclear NMR spectroscopy. Wanted: faculty or research post, or opportunity to teach basic principles of resonance spectroscopy or biophysics.

Please contact:

Dr. Milan Mazur
Department of Physical Chemistry
Faculty of Chemical Technology
Slovak Technical University
Radlinskeho 9,
CS-812 37 Bratislava, SLOVAKIA
FAX: 42-7-493-198

POSITION OPEN

POSTDOCTORAL FELLOWSHIP. One position available in projects using EPR spectroscopy in viable biological systems *in vitro* and *in vivo*. Required: background in EPR spectroscopy and/or working with viable cells and animals. Please contact:

U.S. Army Medical Research Institute
of Chemical Defense
ATTN: SGRD-UV-YY/Dr. Carmen M. Arroyo
Aberdeen Proving Ground, MD 21010 USA
☎: 410-671-3691; FAX: 410-676-7045

EQUIPMENT & SUPPLIES EXCHANGE

AVAILABLE: GUNN OSCILLATOR REPLACEMENT FOR E4 KLYSTRON

Micro-Now has 150 mw Gunn Oscillator replacement. To inquire, contact:
Mr. C. Arnow
Micro-Now Instrument Co.
☎: 708-677-4700; FAX: 708-677-0394.

WANTED: HALL EFFECT SENSOR

We are seeking a Hall effect sensor for the Varian V-4500 EPR (V-2100 B power supply). Please contact: Eliane Wajnberg, Centro Brasileiro de Pesquisas Fisicas, R Xavier Sigaud 150, 22290-180 Rio de Janeiro Brazil. E-mail: ElianeW@brlncc.bitnet.

WANTED: HALL PROBE.

Varian E-4 magnet Hall Probe - P/N - 908742 - 05 as well as E-112 magnet Hall Probe - P/N - 929279 - 02 B are required urgently.

If available, please contact or send it to Prof. P.T. Manoharan, RSIC, IIT, Madras - 600 036, INDIA.

AVAILABLE: VARIAN V 4500 MODULES.

Modules for the Varian V4502 EPR spectrometer are available from G. R. or S. S. Eaton at the University of Denver. E-Mail: geaton@ducair.bitnet.

AVAILABLE: BOXCAR AVERAGER

An inexpensive boxcar averager designed for use in ESE spectrometers is available from the University of Denver. At slow repetition rates it gives about two orders of magnitude better S/N than the well-known PAR 162/164 boxcar. Contact Richard Quine at the University of Denver, Denver, CO 80208 USA
☎: 303-871-2419.

OFFERED: DESIGN AND CONSTRUCTION OF EPR ELECTRONICS

The University of Denver is able to provide design and construction services for EPR related electronics such as low noise signal pre-amps, timing systems for pulsed EPR

or complete microwave bridges. Contact: Richard Quine, phone: 303-871-2419. E-mail: rquine@diana.cair.du.edu

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WANTED TO BUY: USED EPR SPECTROMETER.

A unit such as a Varian E-4 or E-9 would be ok. Electromagnet (or cavity) not necessary. If you know of a unit that might be available, please contact Mark Rubinstein, Naval Research Laboratory, Washington, DC, 20375, USA; ☎: 202-747-4207.

DIODES FOR VARIAN. Varian E-101 & E-102 Dispersion-style microwave bridge users.

I have arranged for a custom order of replacement microwave diodes using Varian's specifications and vendor part number. (pill style case). If you would like to participate and make this order possible please contact Research Specialties regarding your interest. Each dispersion bridge uses two microwave diodes. Fortunately the diodes don't fail often because of the diode protection circuitry. However, failures have occurred with replacements being difficult to obtain.

The price would be $125. US each plus a $25. US handling fee per order. (A large order may lower the price). Since this is a custom order, there would be no returns possible. The suitability of the diode for this purpose is based on Varian's prior usage of this vendor part number for this item. A purchase order would be required. The order date is to be November 1, 1993.

If interested, contact me now at the address below:

Jim Anderson
Research Specialties
5629 N. Maplewood
Chicago, IL 60659, USA
312-728-6570 Phone & Fax

TEMPO DERIVATIVES FREE!

We have small amounts — 50 to 200 mg each — of unique derivatives of TEMPO to give away: 4-nitro-, 4,4-dinitro-, 4-chlor-4-nitro-, 4-brom-4-nitro-, 4-iod-4-nitro-, 4-hydroxy-4-butyl-, 4-hydroxy-4-hexyl-. Also, there are some amounts of corresponding nonoxidized amino compounds containing the 4-nitro group. Contact :

Anatol E. Myshkin,
N.N. Semenov Institute of Chemical Physics
of the Russian Academy of Sciences,
Kosygin str., 4, 117977
Moscow V-334, RUSSIA

OFFERED: FIELD SCAN CONTROLLER CARDS FOR VARIAN FIELD CONTROLLERS

Any Varian magnetic field controller can be modified to permit control of the magnetic field by a computer. An improved scan card design with better documentation at a lower price is now available from the University of Denver.

Contact: Richard Quine ☎: 303-871-2419. e-mail: rquine@diana.cair.du.edu

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AVAILABLE: STANDARD Li-LiF SAMPLES

Samples of extremely pure Li-in-LiF crystals containing small spherical or variously shaped "massive" metal particles of Li are stable markers of intensity and other EPR characteristics (up to 600C). Samples with either small or large particles are available. These samples, which were described in the EPR Newsletter (vol. 4, No. 2, Summer, 1992, p. 8), can be used in a variety of EPR and NMR investigation — for example, for standards, analysis of magnetic fields, or education. The crystals are being made available to interested colleagues at a pro-forma price of US$ 650-700 per kit (2 types of samples for various measurements), with package and marking by agreement.

For additional technical information, the contact is:

Dr. F.G. Chercasov, Kazan, Phys-Techn. Institut
420029 Kazan Sibirsky tract, 10/7
Tatarstan (Russian Federation) ☎: (8432) 39-30-87.

The administrative contacts are:

In Moscow:
Dr. G.A. Denisenko, Institute of Crystallography, Leninsky pr., 59 Moscow 117333 RU.
☎: 7-095-135 6420; FAX: 7-095-135 1011.

In Kazan:
Dr. F. Gubin, 420020 Kazan Volodarskogo, 1-60, Tatarstan (Russian Federation).
☎: 8432-39-3087, telex: 224864 ptb su

CORRECTION

The new e-mail address for Dr. Valery V. Khramtsov, Russian Academy of Sciences, Inst. Chemical Kinetics & Combustion, Novosibirsk 630090, Russia, is: KHRAMTS@KINETICS.NSK.SU.

EPR NEWSLETTER

Volume 5, Number 3 Page 1 Fall, 1993

This publication is the official newsletter of the INTERNATIONAL EPR(ESR) SOCIETY. It is supported by the Society, by corporate and other donors, and by three national Centers for EPR/ESR spectroscopy in the USA. These Centers are sponsored by the Division of Research Resources, U.S. National Institutes of Health:

National Biomedical ESR Center, Prof. James S. Hyde, Director. Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226, USA. ☎: 414-266-4000. FAX: 414-266-4007. E-Mail: cfelix@mis.mcw.edu

Biotechnology Resource in Pulsed EPR Spectroscopy, Prof. Jack Peisach, Director. Albert Einstein College of Medicine, Department of Molecular Pharmacology, 1300 Morris Park Avenue, Bronx, New York 10461, USA. ☎: 718-430-2175. FAX: 718-829-8705. E-mail: peisach@aecom.yu.edu

Illinois EPR Research Center (IERC), Prof. R. Linn Belford,* Director; Prof. Harold M. Swartz,† Co-Director; Prof. Robert B. Clarkson,* Assoc. Director; Prof. Peter G. Debrunner,* Co-Principal Investigator; other senior staff: Prof. Mark J. Nilges,* Dr. Alex Smirnov,* Laboratory Manager and Dr. Tadeusz Walczak.†
*University of Illinois at Urbana, 190 MSB, 506 South Mathews, Urbana, IL, 61801, USA. ☎: 217-244-1186. FAX: 217-333-8868. E-mail: ierc@uiucvmd.bitnet; r-belford@uiuc.edu; or belford@rlb6000.scs.uiuc.edu. (IERC also operates a satellite site for EPR *in vivo* at †Dartmouth University in Hanover, New Hampshire; ☎: 603-650-1955; FAX 1935. E-mail: harold.swartz@dartmouth.edu)

These Centers, described in our first issue (Volume 1, #1), cooperate to facilitate research involving EPR. Prospective users may contact the staff at any of the Centers.

IN THIS ISSUE

HOW TO REACH US — To communicate about the EPR Newsletter or submit material, contact R. Linn Belford, Editor or Becky Gallivan, Editorial Assistant, at IERC (address above).

INTERNATIONAL EPR(ESR) SOCIETY 1993-94 GOLD & SILVER MEDAL AWARDS:

We have received news that recipients for senior IES awards have been selected. The following awards will be presented at the Denver and/or Kazan meetings in the summer of 1994. The winners were selected for their outstanding scientific contributions in electronic magnetic resonance spectroscopy and their sustained outstanding efforts in demonstrating to the international scientific community the power and value of EPR (ESR) methods:

GOLD MEDAL WINNER-- PROFESSOR JACK FREED, Cornell University, Ithaca, NY, USA.

SILVER MEDAL WINNER IN CHEMISTRY-- PROFESSOR KEITH A. MCLAUCHLAN, Oxford University, Oxford, UK.

SILVER MEDAL WINNER IN PHYSICS/INSTRUMENTATION-- PROFESSOR WOJCIECH FRONCISZ, Jagiellonian University, Krakow, POLAND, and National Biomedical ESR Center, Medical College of Wisconsin, Milwaukee, WI, USA.

SILVER MEDAL WINNER IN BIOLOGY/MEDICINE-- PROFESSOR HAROLD M. SWARTZ, Dartmouth-Hitchcock Medical Center, Hanover, NH, USA.

ARTHUR SCHWEIGER IS AWARDED BOTH THE BRUKER PRIZE AND THE ZAVOISKY AWARD –

I. THE 1994 BRUKER PRIZE

The 1994 Bruker Prize of the ESR Discussion Group has been awarded to Professor Arthur Schweiger of ETH, Zurich, for his work on the development of new ESR techniques, particularly pulsed ESR Spectroscopy. The award lecture will be delivered at the group's meeting at Cardiff, UK, in the week beginning March 20, 1994.

II. THE 1993 ZAVOISKY AWARD

The Annual 1993 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Prof. Arthur Schweiger on September 30 in a ceremony marking his outstanding contributions to the development of pulsed EPR spectroscopy. The award consists of a Diploma, a Medal and one thousand US dollars. In the morning, a reception for Prof. Schweiger and his wife was held by the Prime Minister of the Tatarstan Republic, M.G. Sabirov. The Award Ceremony that afternoon was attended by over 300 people, including scientists from over a dozen countries. Among them were the scientists who had participated in the preceding workshop, Prof. Yu.N. Molin (Novosibirsk), a member of the Zavoisky Award Committee, and Prof. A.A. Manenkov (Moscow). The ceremony was chaired by Deputy Prime-Minister of the Tatarstan Republic, I.K. Khairullin. The Chairman of the Zavoisky Award Committee, Prof. K.M. Salikhov, announced the decision. The President of the Tatarstan Academy of Sciences, M.Kh. Khasanov, made the presentation. Prof. J. Stankowski (Poznan), a member of the Ampère Committee, warmly congratulated the laureate on behalf of the President of the Ampère Society, Prof. R. Blinc. The Rector of Kazan University, Prof. Yu.G. Konoplev, added his congratulations. Letters of congratulations from Prof. A. Pines, the President of the International Society of Magnetic Resonance, and Bruker and Varian firms were presented to Prof. Schweiger. Prof. Schweiger gave a lecture entitled "Concepts for the Measurement of Hyperfine Structure in EPR Spectroscopy". A concert by the string orchestra of the Kazan State University preceded and followed the ceremony. After a meeting with journalists, the guests visited the Museum of History of Kazan State University. A choral concert followed to mark the event, which concluded with a gala banquet in honor of Prof. Schweiger and his outstanding contributions to EPR. During a stay in Kazan the laureate and his wife visited the School of Arts for Children and the museum of the Tatar poet Gabdulla Tukaiin at the suburban place "Tukai-Kyrlai".

From the Editor

Again, I remind you that the EPR Newsletter is worth putting out only so long as you, the readers, keep furnishing interesting material - articles, notices, letters, advertisements, etc. Send us your contributions, please. A special plea: When you notice announcements of pertinent meetings, books, conference proceedings, or the like, please inform us. You should not assume that we shall, in some other way, receive or notice these announcements soon enough for timely listing in the Newsletter. Please help us spot such material and inform us just as soon as possible to enable us to publish dated material in a timely fashion.

It is a pleasure to welcome two new corporate member-supporters to the Society — Research Specialties (Chicago; see p. 14) and Resonance Technologies, Inc. (W. Franklin, NH; see displays starting in the next issue).

Linn Belford

✦ *IES AFFAIRS* ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR SOCIETY

From the President — OBSERVATIONS ON MEMBERSHIP

Quite the most remarkable feature of the Summer edition of this Newsletter was the membership list of the Society. By any standards of international societies the list is a long one, and I have already received comment from the envious secretaries of others, and requests that they might be allowed access to our database of members. Where I have perceived this to be contributing to the advance of our society, and to the advantage of our members, I have allowed this. Our policy is, however, to restrict commercial access only to those companies who support us. What the Society is able to offer them is an uniquely targeted list of potential customers, and advertising in our Newsletter must be the most cost-effective way for contacting them which exists. Our industrial support comes overridingly from manufacturers of equipment with EPR application, and we should like to widen this to include companies which could be thought of to have essential interests in the health and welfare of EPR(ESR).

These might include those with general free radical, transition metal chemistry, etc. interests and therefore most of the chemical, oil and pharmaceutical companies. What we have to offer them, besides support of an area of science becoming more essential to some of their research and development projects, is immediate contact with experts and trained scientists, and a highly efficient means for advertising for specialised staff. If consultancy is needed in any area, e.g. of transition metal, free radical chemistry or free radical biology and medicine, we could offer to name experts from amongst our membership who might be approached. We believe that this is a service to industry which we should provide world-wide, and for which we should charge a modest retainer. If any members have contacts through which these thoughts could be pursued, we hope that they will make suggestions to the President. In a Society as numerous as ours these contacts should exist, but they are not necessarily vested in our committee, which needs your help.

One look at the list of members, and of the information provided in it, reminds us that the database is large and growing. This has recently caused us to have to commit more of our revenue to maintaining it, and to helping in the publishing of this Newsletter. This is an inevitable stage in the life of a successful Society, and we should rejoice in it. The flip side is, of course, that our resources are limited and this necessity will have knock-on effects elsewhere. We should be grateful if everyone remembers to pay their subscriptions promptly when they are due, and temporarily, we hope, we are suspending our policy of providing limited travel funds to our members. The position here should be clear by the time of the next Newsletter.

Our membership is growing healthily but there are still appreciable numbers of practising EPR(ESR) scientists who are not members of the Society. We hope everyone will encourage them to join. Many are in the ranks of other, more local, societies which provide for the immediate needs of their members, and we have no wish to appear rivals for their membership. Rather we hope that they will belong to both, and there are already some societies which charge a joint subscription which includes that for us besides that of the local one; we hope this practice will become more general. It is a great pleasure for us all, here, to record the setting up of the new German Society, under the Chairmanship of Dieter Beckert. Our Society offers something different and extra to the others, mainly through the Newsletter: an unique international forum whose major objects are to facilitate research collaboration, to provide contacts for post-doctoral work, to provide the means for mutual help of all sorts and to provide lists of names to *bona fide* conference organisers. We regard one of our functions to be the advertising of relevant conferences, wherever they occur.

One final matter on membership. We should like to hear whether there would be support for widening our range of interests to include subjects closely related to our own, such as spin chemistry, stimulated nuclear polarization, CIDNP, ODMR, RYDMR, magnetic field effects in chemistry and biology (MFE), etc. These are growing areas and appear to lack any central body similar to this.

When sitting down to write this, I had intended it to be about our policy on conferences, Society awards, etc. etc. Oh well, next time!

Keith McLauchlan, President

AWARDS COMMITTEE

At the time of the election of new officers of the Society, Larry Berliner, Chair for the Awards Committee since the inception of the Society, asked that someone else take over this responsibility. At the present time Keith McLauchlan, President, will Chair the Committee on Awards. The Society takes this opportunity to thank Larry for his work in the past few years and while we regret his decision, one can well appreciate it is now time to shift the responsibility. Communications to the Committee should go to:

Keith McLauchlan, Oxford University
Physical Chemistry Laboratory
South Parks Road
OX1 302 Oxford UK
FAX:4-865-275410; E-mail:kamcl@physchem.ox.ac.uk

IES AWARD NOMINATIONS INVITED

To propose names for any of the following IES awards, please send your suggestion(s), or preferably full nomination(s), to the appropriate Disciplinary Awards Subcommittee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow; George Feher; & Jan Stankowski. *For Chemistry* - Bruce Gilbert, Chair; J. Sohma; Jim Bolton; & Kev Salikhov. *For Biology/Medicine* - Larry Berliner, Chair; Marjeta Sentjurc; Hideo Utsumi; & Tadeusz Sarna).

Gold Medal: One Gold Medal per year, recognizing benchmark contributions to EPR spectroscopy as a whole;

Silver Medals: Silver Medals each year, one each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine;

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Young Investigator Awards:

Three Young (less than seven years since the Ph.D. degree) Investigator awards each year, in the same fields as the Silver Medals.

CALL FOR NOMINATIONS FOR THE FOURTH ZAVOISKY AWARD

The 4th Zavoisky Award will be presented at the 27th Congress Ampère on Magnetic Resonance to be held August 21-28, 1994 in Kazan where E.K. Zavoisky demonstrated EPR in 1944. There will be two Awardees in 1994 to mark the 50th anniversary of EPR. This prestigious award, given to recognize an outstanding contribution to the development of EPR, is presented by the Kazan Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, Kazan State University, the Tatarstan Academy of Sciences, the Tatarstan Republic, the Ampère Society, the International EPR Society, and Springer-Verlag Wien-New York. The award-winners' lectures will be published in the journal "Applied Magnetic Resonance". Nominations are sought from the International EPR community. A brief (1-2 page) presentation of the applicant is expected. The final decision is made by the Award Selection Committee, which comprises these well-known experts in EPR: B. Bleaney (Oxford), K.H. Hausser (Heidelberg), C.A. Hutchison, Jr. (Chicago), Yu.N. Molin (Novosibirsk), A. Schweiger (Zurich) and the Chairman, K.M. Salikhov (Kazan). Submit nominations to Dr. Laila V. Mosina, Executive Secretary of the Zavoisky Award Committee, Kazan Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, Sibirsky trakt, 10/7, Kazan, 420029 Russian Federation. The deadline for submission of nominations is March 1, 1994.

GRANT OPPORTUNITIES FOR USA AND NON-USA SCHOLARS

IREX has grants available for citizens or permanent residents of the USA for Advanced Research Programs, Language and Developmental Programs and Short-term Travel Grants for use in the following geographic regions: Central & Eastern Europe, Eurasia, Mongolia. Grants also are available for Advanced Research Programs in the USA for scholars from Eurasia, Central and Eastern Europe, the Baltics, and Mongolia. Contact:

International Research & Exchanges Board (IREX)
1616 H Street, NW
Washington, DC 20006
☎: 202-628-8118; FAX: 202-628-8189
E-mail: irex@gwuvm.gwuedu

GERMAN ESR GROUP FORMED

This group is part of the Fachgruppe "Magnetische Resonanzspektroskopie" of the Gesellschaft Deutscher Chemiker (GDCh) and was founded October 1st, 1993 in Friedrichroda at their 15th Discussion Meeting. Dr. Dieter Beckert (Leipzig) was elected as chairman and Prof. Harry Kurreck (Berlin) and Prof. Gerd Kothe (Stuttgart) as Vice Chairmen. The new ESR group has applied for membership in the European ESR Society. For information, contact:

Dieter Beckert.
☎: 49-341-2352317; FAX: 49-341-2352630
e-mail: beckert@mpgag.uni-leipzig.d400.de

THE COMPUTER CORNER

Edited by
Philip D. Morse II and Keith P. Madden

This column is a regular feature of the EPR Newsletter and covers all computer aspects of EPR. We solicit comments, suggestions, tips, and questions from our readers. Please send contributions to Reef Morse (E-mail: reef@xenon.che.ilstu.edu), Keith Madden (E-mail: keith.p.madden.1@nd.edu) or Dick Cammack (E-mail: udbc033@hazel.cc.kcl.ac.uk).

EPR List Server

Many times we have EPR-related questions to which we don't have the answer but have the vague feeling that "someone out there" does know the answer. The problem is that there has been no way to ask such questions of the general EPR community.

This problem has now been solved. Reef Morse has established a list server on the main VAX computer at Illinois State University, Department of Chemistry.

Computer list servers act in the following way. If you are a subscriber to the list (and we'll explain below how to subscribe), you can "post" messages to the list, and these messages go out to all other subscribers. Anyone receiving these postings can respond to them, ignore them, or forward them on to colleagues who may be able to help. Answers can be posted back to the list (so that everyone will receive a copy) or can be posted back to the individual.

In a sense, the list server acts as a forum for EPR-related topics. In our initial tests of the list, we have processed letters asking for information about graphics programs for presenting EPR data, comments about a

generalized EPR data acquisition package, and questions about how to use the list. Because our initial test of the list involved a small number of people, the traffic was not very heavy (one or two posting every few days), but we anticipate considerable growth now that we have made the list open to the public. We will keep you informed on topics of interest and use of the list in subsequent newsletters.

What is a "list"?

A computerized list is a list of electronic mail addresses. When someone on this list sends an E-mail letter to the list address, it is automatically sent to everyone else on the list.

What is the purpose of the EPR list?

The purpose of the EPR list is to foster communications about EPR-related topics. Newsletters and the like are excellent examples of communication devices, but their communication is one-way (the editors and publishers send out material to the readers) and slow (the EPR newsletter is published 4 times a year). Frequently we have questions to which we need immediate answers, but don't know who to ask. A computerized list server solves the problem of speed and dissemination by posting communications to every member of the list as soon as the communication is received.

How is this list set up?

The EPR list is set up with two electronic mail addresses. One is the address of the list administrator. This address is: epr-list-request@xenon.che.ilstu.edu (please DO include the hyphens). As shows below, you can get information from this address about who is currently subscribing to the list, the status of your postings, and other administrative details. The list itself has an E-mail address of epr-list@xenon.che.ilstu.edu, and this is the list to which mail is posted.

How do I get on the list?

You can get on the list by sending the single word SUBSCRIBE to the list administrator at epr-list-request@xenon.che.ilstu.edu and you will be automatically placed on the list. You will receive a response from the list processor, usually within one or two minutes. A copy of the response to Reef Morse's SUBSCRIBE request is shown below:

From: MX mailing list processor <mxserver@xenon.che.ilstu.edu>
To: reef@xenon.Che.Ilstu.Edu
Subject: Subscription to mailing list epr-list

You have been added to mailing list epr-list@xenon.che.ilstu.edu.
Further administrative requests regarding this list should be sent to

Internet: epr-list-Request@xenon.che.ilstu.edu

The following commands can be handled automatically by epr-list-Request@xenon.che.ilstu.edu:

SIGNOFF	- to remove yourself from the list
REVIEW	- to get a list of subscribers
QUERY	- to get the status of your entry on the list
SET NOMAIL	- to remain on the list but not receive mail
SET MAIL	- to reverse the NOMAIL setting
SET CONCEAL	- to conceal yourself from REVIEW listings
SET NOCONCEAL	- to reverse the CONCEAL setting
SET NOREPRO	- to prevent the list from sending you your own postings
SET REPRO	- to reverse the NOREPRO setting
LIST	- to get a list of mailing lists available on this

host
HELP - to receive a help file
QUIT - to terminate processing (skipping signature, etc.)

The syntax of these commands for use with the LISTSERV emulator is:

SIGNOFF epr-list
REVIEW epr-list
QUERY epr-list
SET epr-list [NO]MAIL
SET epr-list [NO]CONCEAL
SET epr-list [NO]REPRO
LIST
HELP
QUIT

(This message was generated automatically.)

Notice that you can obtain information about the subscribers to the list using the REVIEW command. You can also hide yourself from REVIEW requests (so that others will not receive your E-mail address). The REPRO command allows you to receive your own messages (default). The NOREPRO command disables this facility so that you do not receive copies of the messages you send to the list. You can remain on the list but not receive mail. Finally, you can sign off from the list. All these commands should be sent to the address

epr-list-request@xenon.che.ilstu.edu.

How do I send messages to the list?

Messages to the list are sent to the address epr-list@xenon.che.ilstu.edu and will be posted to the other subscribers on the list immediately. As the list is set up now, you will also receive a copy of your posting. This confirms that your posting has been sent out.

Is the list moderated?

Currently no one is moderating the list. Thus, whatever you post to the list goes out to everyone who subscribes to the list.

Is access to the list limited?

Currently there is no limitation on who may subscribe to the list.

What are appropriate topics for the list?

Any topic of interest to the EPR community is appropriate. Example of such topics could be: requests for information about samples, formats for exchange of EPR data, information about spectrometer construction and repair, sample preparation, requests for post-doctoral or other staff positions, and the like.

Mistakes and errors:

The major error seems to be mistaking the administrator address and the list address. Administrative requests like SUBSCRIBE should be sent to epr-list-request@xenon.che.ilstu.edu, whereas actual E-mail posting should go to epr-list@xenon.che.ilstu.edu. If you accidently send E-mail to the administrator address, you'll get a message back that the administrator doesn't know what you want, and your message will not be sent out. Likewise, if you send administrative requests to the list address, the administrative request will not be carried out.

Cost to subscribe: none.

Comments and questions:

If you have any questions or comments regarding this list, send them directly to Reef Morse: reef@xenon.che.ilstu.edu. He is the person responsible for setting up and maintaining this list.

Finally...

Please feel free to subscribe to and use this list. A list is only as useful as its subscribers want it to be.

TIPS & TECHNIQUES

WINDING COILS FOR THE BRUKER ENDOR CAVITY

Chris Bender
Biotechnology Resource for Pulsed EPR
Albert Einstein College of Medicine
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Bronx, NY 10461 USA

Success at ENDOR spectroscopy is largely dependent upon the interaction between the rf structure and the resonant microwave field, especially the electric field

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component. In general, one wants the geometric lines of the rf structure perpendicular to the microwave electric field lines, and in the TM cavity of Biehl[1] (and now offered commercially by Bruker) the rf structure takes the form of a coil whose cylindrical axis is oriented coincident with the cavity's. The principal advantage of this design is that it is compact (10 mm o.d.) and is capable of generating a larger rf field than other designs (e.g. parallel posts in TE cavities), for a given current.

I tend to adjust my coil-winding strategy to the nature of the experiment. The useable volume for loading a TM cavity extends along the entire cylindrical axis, and one wants to use all this space for solution samples in capillaries. In this case, my ENDOR coil extends the entire length of the cavity with the helix pitch originating directly from the brass collars that are used for electrical contact (Figure 1A).

I compromise cavity filling factor with samples in a flow dewar. Since I usually perform replicate experiments at different temperatures, I prefer small sample sizes (~1 cm axial length) in order to minimize gradients. The sample is therefore centered in the cavity, and the coil is likewise compacted (2 cm length) and centered (Figure 1B). I find that positioning the axial leads opposite one another causes the least perturbation of the cavity field. Centering the sample requires some care with the Oxford ESR9 cryostat because the helium delivery jet is close to the tube bottom with the standard 'hourglass' holder and will encroach into the cavity; at Michigan State I had slightly longer hourglass holders made (one can also flip over the commercial hourglass, which has one side longer, but the jacketed flow region around the sample is consequently made smaller).

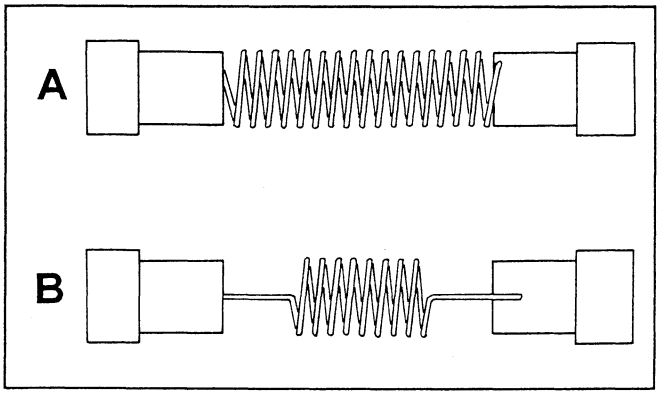

Figure 1: Silver wire coils for ENDOR. A) Coil for samples extending through axial length of cavity; B) coil for reduced sample size (flow dewar).

Coils are either cemented onto a dewar insert or made free-standing.[2] The choice is a matter of personal preference; the principal advantage of the latter is that one does not have to commit a dewar to a given coil. In both cases I use a template to make the coil before putting it on the dewar.

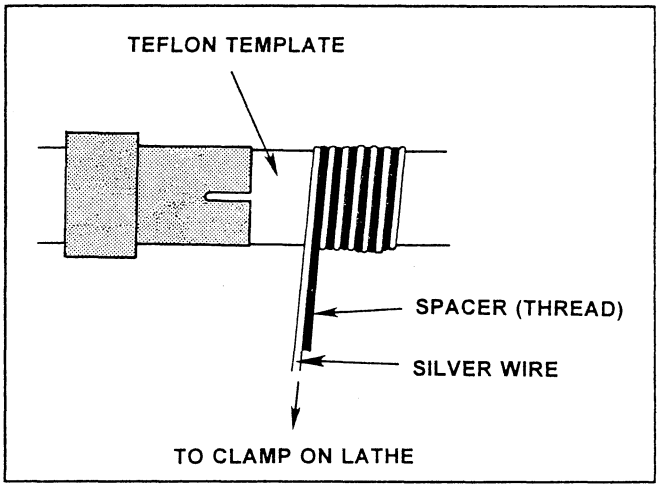

Figure 2: Procedure for hand-winding coils; thread is the winding spacer.

The Oxford dewar insert is symmetric around the cylindrical axis and its (and coil's) position can be easily optimized by rotation. My preference is to own a couple of dewar inserts and use fixed (cemented) coils. The fixed coils are wound and soldered on a template and then transferred to the dewar. I use a template because I

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do not want to bend the wire, tighten it to get the right dimensions, nor solder it to the collars while on the dewar. In making the transfer to the quartz, I tack one end piece with cyanoacrylate cement, then coax the remainder of the coil into position and likewise cement the opposite end. Cyanoacrylate comes in several viscosities that dry at varying rates (available from Aldrich). Be sure that the brass collars precisely fit the dewar and are uniformly cemented, or mechanical stress from the cavity's contacts will crack the dewar. If you choose to also make your own dewars, likewise be sure to buy precision wall quartz tubing, for the same reason. Lastly, to get the coils off, I use dichloromethane or nitromethane.

Once it is cemented in place, the coil is bound with teflon tape in order to hold it tight and reduce the possibility of microphonics.[3] One can use teflon heat shrink, but I tend to avoid the latter because inevitably one will have to remove the coil, with concomitant risks associated with cutting the tube while on the dewar.

As suggested by Hurst et al.[2] in their manuscript describing the free-standing coil design, a teflon rod serves as a template on which one winds and solders the wire. However, I use a 0.25" (10 mm o.d.) brass rod as a template core in order to keep it straight. The template is fashioned from teflon tube pushed over the brass, and the piece is turned on a lathe to size (10 mm o.d.).[4]

At Michigan State I would mount the template onto the spindle of the lathe (used here only as a stage for winding - the template is not permitted to rotate) and wind the coil by hand keeping one end of the wire clamped on one of the lathe's tool mounts. I used the radio hobbyists' trick of thread as a spacer for the wire. Nylon fishing line also worked well and comes in various diameters. The above method allowed me to wind a coil of a given axial length, and with both ends clamped, I would bind the wire (after removing the spacer) with teflon tape before making the axial leads. For a 4-cm coil (entire length of cavity), I would just solder the ends directly onto the brass collars.

Once the coil is bound, the clamped ends can be cut without recoil and the axial leads fashioned from the exposed wire. I used a fork-shaped soldering tool to bend the wire into the proper angle before soldering my leads. With both ends soldered and the spacer removed, the heat shrink can be applied. See refs. 2 and 4 for procedural details.

I have used the above method for several years although it is as tedious as rigging a model ship. On a given day you are either in the right mood or you are not. I have recently been playing with a jig design for winding springs that I found in a textbook on technique for experimental physics, and a few adaptations have resulted in a useful coil-winding device. The device is illustrated in Figure 3. The pitch of the coil is set by threads on the rotating mandrel/template, and the axial leads are set by

the collars (one of which is fixed). In the diagram, two positions are shown to provide some idea of how the jig works. The upper portion of the diagram illustrates the approximate starting positions of mandrel, spacers, and brass collars. The wire is fed through the leftmost support and spacers, then soldered to the rightmost brass collar. The template is turned using a crank on the right (not shown), and the direction of travel is counterclockwise and towards the right. The lower portion of the figure illustrates the position of the components after two turns.

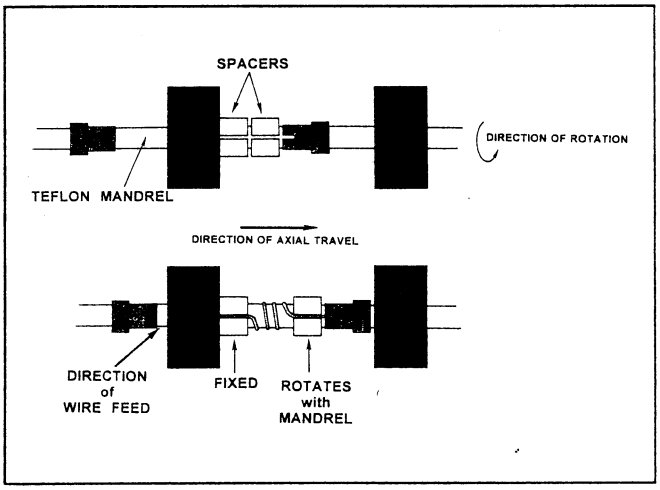

Figure 3: Functional schematic of coil winding jig.

Tension is maintained on the wire by two rollers (not shown).[5] The mandrel is turned until the leftmost brass collar hits the stationary spacer. At this point the slot in the collar should be aligned with the axial wire lead. The support (dark rectangle) has an access hole that permits soldering of the wire to the leftmost brass collar. Once soldered, the support and spacers are removed, freeing the mandrel for application of the heat-shrink tubing.

Lastly, a few words on impedance matching and whether it is really necessary. On an open test fixture, all the coils I have ever made with silver wire have an impedance (@15 MHz) in the range of 8-12 Ω, and this value changes linearly with frequency in the manner

characteristic for an inductor. If you set up a transmission line circuit containing an inductor of 10 Ω and a terminal load of 50 Ω, the total impedance can be approximated by the simplified expression $Z_{TOTAL}=Z_{COIL}+Z_{LOAD}$, and it follows that the match to the 50 Ω output of the amp is pretty good (one can, in principle, use a pair of 1:4 broadband transformers to isolate the coil). Most commercial amps can tolerate mismatch, so that the worst possible scenario in such a case is inefficient power delivery to the coil.

When the coil is in the cavity, however, there is a parasitic capacitance set up between the coil and cavity walls of about 100 pf, and this changes the Z_o vs. frequency profile.[6] As previously described in a note,[6] this circuit consisting of inductance and parasitic capacitance goes into resonance at about 30 MHz and may be a cause of baseline artifacts often observed in this region.[7] A matching network that removes the resonance condition is described in the note,[6] and a more comprehensive review[4] gives details of other impedance-matching strategies.

ACKNOWLEDGEMENT

I am grateful to Martin Baumgarten and Hans van Willigen, both of whom have provided me with valuable tips in the art of coil winding.

REFERENCES AND NOTES:

1. Biehl, R.; Lubitz, K.; Möbius, K.; Plato, M. J. Chem. Phys., **66**, 2074 (1977).
2. Hurst, G.; Kraft, K.; Schultz, R.; Kreilick, R. J. Magn. Reson., **49**, 159 (1982).
3. Microphonic noise can arise from vibrations that cause changes in capacitances as the distance between opposing plates varies. With ENDOR coils, the capacitance usually associated with microphonics is between the coil turns and is ordinarily a problem only at high powers (>200 W).
4. Bender, C.J.; Aisen, P. *Continuous Wave ENDOR Spectroscopy* in Methods of Enzymology, Vol. 227, p.190 (1993).
5. If the coil is longer than the cavity and extends out of it, a more simple lateral feed can be used for the wire.
6. Bender, C.J.; Babcock, G.T. Rev. Sci. Instrum., **63**, 3523 (1992).
7. Another source of the 30 MHz baseline glitch seems to be attributable to band-switching in the rf synthesizer (see Clarkson, R.B.; Belford, R.L.; Reiner, C., *Rev. Sci. Instrum.*, **61**, 3356 (1990)). One can distinguish between the two glitches (circuit resonance vs. synthesizer switching) by inserting a frequency doubler between the synthesizer and amp. One can then test the system at 30 MHz while the synthesizer is still operating well within the band.

Note: Failure of the potentiometers that regulate beam voltage and current seems to be a problem common to Space Microwave Model 6000 Traveling Wave Tube Amplifiers. These are the Bourne 2k Ω potentiometers that are adjustable from the front panel of the drawer in which the traveling wave tube is housed. Ordinarily, their failure occurs after 300-500 hours of service, and is often manifest as a dramatic loss of linearity in the potentiometer and/or instability in the beam parameters. The former, although benign, becomes problematic if one wants to optimize the tube's performance after changing the operating microwave frequency. I have found that the solution to this problem is had by replacing the standard Bourne components with their military spec. counterparts; so far, we have gone nearly four years without a failure (>5000 hrs. of service). The failure, incidently, is not inherent to Bourne components; I have executed many a Clarostat and other makes of potentiometer in this drawer.

MISCELLANEOUS TIPS FOR ESR USERS

James R. Anderson, Research Specialties
5629 N. Maplewood, Chicago, IL 60659, USA
(312-728-6570 Phone/Fax)

*Xenon/mercury-vapor cs-UV light sources and Xenon flash lamps usually have a high-voltage starter circuit that radiates large RF pulses that will cause either degradation or extreme damage to the EPR system. The typical open wiring for the lamp and the numerous leads associated with the EPR act as antennas to transmit and inject this large pulse into the EPR unit. It is easiest to stop this radiation at the source. Several solutions are available, depending upon how frequent your usage of this source is.

1. Twist the lamp DC power-connection leads two or more turns per foot to reduce radiated fields. (This fix is simple but effective in reduction of radiated fields.)

2. Shield the resulting twisted cable with copper braid grounded to the lamp power supply, using metal covers for the lead connectors.

3. Move the starter circuit into the lamp housing using a suitable extension to the housing and filter the DC power leads.

NOTE: Item #1 is the minimum approach to this problem. Items #1 & 2 together offer better protection

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and item #3 is needed for continuous users. Do not allow usage to continue without at least doing item #1. Pulsed lasers can also cause problems.

*Surge protectors (MOVs) for three-phase and single-phase power are available for installation on your electrical service to help guard the entire EPR system from electrical transients due to electrical storms and in-house electrical disturbances. Additional transient protection can be obtained with the use of Faraday shielded isolation transformers, in addition to the surge protectors. The transformers also help reduce ground loops, which are a source of instability to the EPR system. As more auxiliary instruments are added to the EPR system, ground-loop problems can surface.

*Varian E-4 users can monitor microwave diode degradation by observing the mode sweep height at a specific microwave power and a specific frequency. The microwave frequency should be off the cavity resonance. This method can show changes from the previous run, and is quite sensitive to diode changes. Powers of 28-30 db down keep the display on the screen and yield a sufficient mode-sweep height. Obviously this is quicker than running a signal-to-noise test and is particularly useful when multiple users are involved.

*On Varian systems that have an instrument malfunction, a quick method of checking the main power supply is to see if the recorder pen-position control on the 100-kHz receiver controls the pen. This observation checks the plus and minus 20-volt supplies for functionality.

[Note: Mr. Anderson's business, Research Specialties, is a new corporate member of the International EPR(ESR) Society.]

CONFERENCE REPORT

"MODERN DEVELOPMENT OF EPR: MULTIFREQUENCY EPR," TATARSTAN REPUBLIC, SEPTEMBER 28-29, 1993. The program of the Workshop, which preceded the Zavoisky Award ceremonies (see p. 2) was as follows: A. Schweiger (Zurich), "Pulsed EPR: Methods and Instrumentation"; A.V. Il'yasov (Kazan), "EPR and ENDOR Studies of Nitrogen Containing Free Radicals"; J. Stankowski (Poznan), "EPR in Fullerenes"; V. Shlenkin, D. Fushman, N. Vylegzhanina, L. Jagodina, V. Fedotov (Kazan), "Molecular Motion of Spin-Labeled Lysozyme in Solution Studied by Use of Electron Spin Relaxation"; S.K. Hoffmann (Poznan), "High Pressure Effects in Intermolecular Interactions Studies by Single Crystal EPR"; Ya.S. Lebedev (Moscow), "The Very High Frequency EPR in Relaxation Studies"; H. Cho (Richland), "Pulsed EPR: Ideas from NMR"; V.A. Atsarkin, G. Vasneva, A. Bush (Moscow) "EPR and Electron Spin-Lattice Relaxation of Paramagnetic Centres of HTSC".

NOTICES OF MEETINGS

27th ANNUAL INTERNATIONAL MEETING OF THE ELECTRON SPIN RESONANCE GROUP, ROYAL SOCIETY OF CHEMISTRY, "ELECTRON SPIN RESONANCE OF INORGANIC RADICALS AND METAL IONS IN INORGANIC AND BIOLOGICAL SYSTEMS," The University of Wales, Cardiff, March 21-25, 1994. The 27th meeting of the ESR Group of the Royal Society of Chemistry, London will celebrate 26 consecutive years of International meetings on the topic of Electron Spin Resonance Spectroscopy. The meeting will be held at The University of Wales, Cardiff during the period 21st - 25th March 1994. The Conference opens with dinner on the Monday evening and closes after lunch on the Friday morning. The organizers are pleased to extend a cordial invitation to all persons interested in ESR spectroscopy in chemistry, physics and biology to attend. Accommodation will be in individual rooms in Aberdare Hall of Residence. The lectures will take place in the School of Chemistry and Applied Chemistry, a few minutes' walk away.

Registration forms will be sent out in November to all who have indicated an interest in the Conference. The deadline for registration and submission of posters will be 10th January 1994. For information & registration forms, contact Mrs. J. Taylor, School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK.

Scientific Programme, plenary lectures: V. Beltran, University of Mexico, Title to be announced; L.C. Brunel, CNRS, Grenoble, *Recent Developments in High Field CW ESR: Applications in Chemistry and Biology;* M. Brustolon, University of Padua, *Molecular Dynamics of Radicals in Single Crystals: ESR, ENDOR and ESE Studies;* P. Day, The Royal Institution, London, *Magnetic States in Molecular Conductors;* J. Hütterman, Universität des Saarlandes, *ENDOR on Mononuclear Metalloproteins: Structure Determination of the Prosthetic Group from Randomly Oriented Specimen;* N. Kernevez, Centre d'Etudes Nucléaires de Grenoble, *Weak Field ESR and Dynamic Nuclear Polarization on Free Radicals: Application to Magnetometry and Oxymetry;* L. Kevan, University of Houston, *Applications of Electron Spin Echo Modulation Spectroscopy to Transition*

Metal Ions in Molecular Sieves; L.B. Knight, Jr., Furman University, *ESR Studies of Small Radical Cations in Neon Matrices Generated by Laser Vaporization and X-irradiation;* P. Lay, University of Sydney, *EPR Characterisation of the Cr(V) Intermediates in the Cr(VI/V) Oxidations of Organic Substrates and in Cr Induced Cancers;* D. Lowe, University of Sussex, *ENDOR of Metalloproteins;* P.H. Rieger, Brown University, *Non-Coincident g and Hyperfine Matrix Principal Axes: A New Twist in ESR Powder Spectra;* A. Schweiger, University of Zürich, *The Bruker Lecture, Title to be Announced;* K. Wieghardt, Ruhr-Universität Bochum, *Exchange and Double Exchange Phenomena in Polynuclear Transition Metal Compounds.* Also, it is intended to hold a session on the demonstration of software, written by users. The Committee of the ESR Group of the Royal Society of Chemistry: Prof. A.G. Davies, FRS (Chairman), Dr. C.C. Rowlands (Secretary), Prof. R. Cammack, Dr. D. Lowe, Dr. D. Collison, Dr. B. Tabner, Dr. M. Davies, Prof. A.J. Thomson, FRS, and Dr. R.A. Jackson.

STABLE ISOTOPE APPLICATIONS IN BIO-MOLECULAR STRUCTURE AND MECHANISMS, March 27-31, 1994, Santa Fe, New Mexico.. A meeting to bring together producers and users of stable-isotope-labeled compounds to assess current and future needs. Invited speakers will discuss applications of stable isotopes to the study of RNA, DNA, peptides, and proteins. Recent advances in scattering and spectroscopy techniques as well as synthesis and production of labeled compounds will be highlighted. *Organizing Committee*: Jill Trewhella, Chairperson, Donald Ott, Louis A. (Pete) Silks, Mary Ann D. Martinez, Jean Stark, all of Los Alamos National Lab. *Program Committee*: Nicholas A. Matwiyoff, Univ. of New Mexico, Chairperson, Gerald T. Babcock, Michigan State Univ., Timothy Cross, Florida State Univ., Roger A. Jones, Rutgers Univ., John Markley, Univ. of Wisconsin-Madison, Arthur Pardi, Univ. of Colorado, Clifford J. Unkefer, Los Alamos National Lab. Meeting place - Eldorado Hotel. For information, write to: Stable Isotope Applications Conference, Protocol Office, MS P366, Los Alamos National Lab., Los Alamos, NM 87545.

INTERNATIONAL CONFERENCE on BIORADICALS DETECTED by ESR SPECTROSCOPY, Institute for Life Support Technology, Yamagata, Japan, June 12-16, 1994. The organizers are Hitoshi Kamada, Yamagata Technopolis Foundation (YTF), president, and Hiroaki Ohya-Nishiguchi (YTF), general secretary.

The conference will treat an aspect of life-support technology with special attention to ESR spectroscopy including new technology, technology transfer, ESR imaging, spin trapping and labeling, metalloproteins, medical applications, antioxidants and food sciences, and characterization of bio-materials. The conference program will include opening lecture, plenary lectures, session lectures, invited reports, original research contributions, and poster session. YTF is now organizing a world-wide research center for investigating bioradicals based on ESR spectroscopy, *Institute for Life Support Technology (LIST)*. The research center was opened in April, 1993. Thus the conference has yet another meaning--namely, celebrating inauguration of the kernel of its researches on bioradicals.

The organizing committee will try to do their best in involving you in the warm and friendly atmosphere of Yamagata, offering the nature and natural foods most famous in Japan, *the other side of Japan.*

Scientific scope of the Conference: The conference will treat all aspects on bioradicals with special attention to ESR spectroscopy, including the following sessions: 1) New technology and technology transfer; 2) ESR imaging; 3) Spin trapping; 4) Spin labels and oximetry; 5) Metal complexes and metallo proteins; 6) Biomedical applications; 7) Antioxidants and food sciences; 8) Tissues, cells and biomaterials; 9) Others.

The Organizing Committee consists of: H. Kamada (YTF), *Chairman*; H.Ohya-Nishiguchi (YTF)*, *General Secretary*; M. Hiramatsu (YTF), *Secretary*; T. Akatsuka (Yamagata Univ.); N. Hirota (Kyoto Univ.)*; M. Inoue (Osaka City Univ.)*; Y. Ikegami (Tohoku Univ.); M. Iwaizumi (Tohoku Univ.); K. Kuwata (Osaka Univ.); A. Mori (Okayama Univ.); H. Nakazawa (Tokai Univ.)*; E. Niki (Univ. of Tokyo); T. Ogata (Yamagata Univ.); K. Ohno (Univ. Industrial Technology)*; H. Sakurai (Kyoto Pharm. Univ.)*; T. Shiga (Osaka Univ.), J. Sohma (Kanagawa Univ.)*, H. Utsumi (Showa Univ.)*; T. Watanabe (Tokyo Univ. Marine Science)*; T. Yoshikawa (Kyoto Pref. Univ. of Medicine). (**program committee*)

The International Advisory Board is E.G. Janzen (USA), E. Niki (Japan), L. Packer (USA), H.M. Swartz (USA), M.C.R. Symons (UK). For information, contact Dr. Midori

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Hiramatsu, Institute for Life Support Technology, Yamagata Technopolis Foundation, 683 Kurumanomae, Numagi, Yamagata 990, Japan, 81-236-44-8088; FAX: 81-236-44-9640.

SEVENTEENTH INTERNATIONAL EPR SYMPOSIUM at the 36th Annual Rocky Mountain Conference, Denver, CO, USA, July 31-August 4, 1994. To be held at the Hyatt Hotel and cover all aspects of EPR spectroscopy. As 1994 is the 50th anniversary of Zavoisky's discovery of EPR in Kazan, we plan a special celebration in cooperation with the Zavoisky Institute. Representatives from the Zavoisky Institute at Kazan are expected to participate in the Denver conference. In addtion to our traditional sessions on new EPR techniques and applications, there will be talks by early workers in the field and a celebratory banquet at the Denver Phipps Conference Center. The deadline for abstracts is April 5, 1994. If you have not yet received a meeting notice, contact Profs. Gareth R. Eaton or Sandra S. Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208, USA. ☎: 303-871-2980 or 303-871-3102; FAX: 303-871-2254; E-mail: seaton@ducair.bitnet.

THIRTEENTH ANNUAL SCIENTIFIC MEETING AND EXHIBITION OF THE SOCIETY OF MAGNETIC RESONANCE IN MEDICINE, San Francisco, CA, August 6-12, 1994, at the San Francisco Hilton.

XXVII CONGRESS AMPERE ON MAGNETIC RESONANCE, Kazan, Russia, August 22-29, 1994. The scientific program will include plenary lectures, symposia, and poster sessions covering the latest achievements in current research, and new developments, trends, and applications in the field of magnetic resonance.

Special attention will be given to the following subjects:

- EPR, NMR and NQR Microimaging and Material Science
- Glasses, Liquid Crystals, Polymers
- Low Dimensional Systems
- Magnetic Resonance in Very High Fields
- Magnetic Resonance of Intermediates
- Modern Developments in Solid State NMR
- Multiple Resonance and Multi-Dimensional Spectroscopy
- New Materials (High - Tc, Cn, etc.)
- New Methods and Techniques
- Non-Equilibrium Processes and Non-Linear Phenomena
- Phase Transitions
- Spin Dynamics at Ultra Low Temperatures
- Spin Polarization Phenomena
- Systems with Orbital Degeneracy
- Time Domain EPR.

The official language at the Congress is English. Young scientists and students are strongly encouraged to participate. Students will pay significantly reduced registration and accommodation fees. The Congress will take place in the Cultural Centre of Kazan State University (founded 1804); it has modern, well-equipped facilities for scientific meetings.

At the Congress, the 1994 Zavoisky Award will be presented, previously awarded to Dr. W. Mims and Prof. B. Bleaney.

Organizing Committee: Prof. Kev M. Salikhov, Chairman and Dr. Nail M. Suleimanov, Scientific Secretary. ***Program Committee:*** Prof. V.A. Atsarkin (Moscow), Prof. E. Hahn (Berkeley), Prof. B.I. Kochelaev (Kazan), Prof. E.T. Lippmaa (Tallinn), Prof. Yu. N. Molin (Novosibirsk), Prof. I.V. Ovtchinnikov (Kazan), Prof. K. M. Salikhov (Kazan), Prof. D. Stehlik (Berlin), Prof. M.A. Teplov (Kazan). ***Executive Committee:*** I.A. Aksenov, V.A. Khramov, R.B. Malikova, A.K. Salikhova, E.A. Turiyansky.

Please send your notice of intent to participate to arrive as soon as possible. Send your name, address, phone, FAX, and E-mail to Zavoisky Physical-Technical Institute, Sibirsky trakt 10/7, Kazan, 420029, Tatarstan, Russian Federation. ☎: 84-

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32-760503; FAX: 84-32-765075; TELEX 224 864 PTB SU: E-mail: vitali@adonis.ias.msk.su. The organizers are thankful to our magnetic resonance colleagues from the Free University of Berlin for support and encouragement.

EUROPEAN ESR MEETING ON RECENT ADVANCES AND APPLICATIONS TO ORGANIC AND BIOORGANIC MATERIALS, Paris, September 5-9, 1994. Organized by the European Federation of ESR Groups presently consisting of: ESR Group of the Royal Society of Chemistry (UK), Gruppo Italiano di Resonanza di Spin Elettronico (I), Nederlandese EPR Discussie Groep (NL), Polish ESR Group (PL), Bulgarian ESR Group (Bul), and Groupe d'Application de la Résonance Paramagnétique Electronique (F). Chairman: Klaus Möbius, Berlin, Germany. The European Symposium will be held at the Ministére de l'Enseignement Supérior et de la Recherche (Ministry of Universities and Research) "Carré des Sciences," 1 rue Descartes - PARIS 5éme (in the center of Paris, 2 minutes walk from la Sorbonne, le Quartier Latin, le Panthéon...). The accommodations will be in hotels in the city and can be chosen from a number of hotels of various categories. A limited number of individual rooms in the Cité Universitaire de Paris, 19 Boulevard Jourdan, close to the Parc de Montsouris, will be available. The French Scientific and Organizing Secretary: Dr. Bernard Catoire, GARPE, c/o ITF - Lyon, B.P. 60, F-69132 ECULLY, FRANCE. ☎: 78-33-34-55; FAX: 78-43-39-66. A first circular will be distributed at the beginning of 1994.

EMARDIS-95, Sofia, Bulgaria, June, 1995. For information, contact: N. D. Yordanov (Convener) or M. Zdravkova (Sci. Secretary), Institute of Kinetics and Catalysis, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria; ☎: 3592-724-917 or 713-2546 (Yordanov) or 713-3917 (Zdravkova); FAX: 3592-756-116 or 720-038; telex 22729 echban; E-mail: banchem@bgearn. A preliminary announcement will be distributed in February 1994.

POSITION WANTED

EPR and NMR Spectroscopist Seeks an Academic or Industrial Position. Biophysicist-solid state physicist, Ph.D. '87, research/teaching experience. Now research worker/teacher at Department of Physical Chemistry, Faculty of Chemical Technology, Slovak Technical University. Research experience: A) liquid- and solid-state EPR spectroscopy of biological, organic and inorganic materials (Bruker 200D SRC NMR Spectrometer with Aspect 2000 Computer). Special research experience: membrane biophysics, drugs-membrane interaction, spin-label EPR spectroscopy (International Training Course, Hungarian Academy of Sciences, Szeged, Hungary). Also sol-gel or glass solid-state EPR spectroscopy; transition-metal spin labels. B) liquid- and solid-state NMR spectroscopy of biological, organic, and inorganic materials (Varian 300 MHz VXR spectrometer). Special research experience: 1D, 2D, and pseudo-3D multinuclear NMR spectroscopy of bioploymers, using Varian Unity 500 MHz spectrometer (postdoctoral fellowship at McGill University, Pulp and Paper Research Center, Montreal, Canada). Also sol-gel or glass multinuclear NMR spectroscopy. Wanted: faculty or research post, or opportunity to teach basic principles of resonance spectroscopy or biophysics.

Please contact:

Dr. Milan Mazur, Department of Physical Chemistry
Faculty of Chemical Technology
Slovak Technical University
Radlinskeho 9, CS-812 37 Bratislava, SLOVAKIA
FAX: 42-7-493-198

POSITION OPEN

POSTDOCTORAL RESEARCH POSITION available beginning immediately to study the structure and function of the iron storage protein ferritin using EPR, ENDOR, ESEEM and Mossbauer spectroscopies and other biophysical techniques. Opportunities to be involved in instrument development. Minimum qualifications: Ph.D. in chemistry, biochemistry or biophysics; experience in magnetic resonance desirable.

Send resume (noncitizens must include current visa status) and 3 letters of recommendation to:

Prof. N. Dennis Chasteen
Department of Chemistry, Parson's Hall
University of New Hampshire
Durham, NH 03824, USA

(UNH is an AA/EEO Employer.)

EQUIPMENT & SUPPLIES EXCHANGE

LAB RENOVATION SALE

Bruker Aspect 2000 Computer; Bruker 10" Magnet, moveable pole pieces; Nicolet 1280 Computer. Prices Negotiable. Contact: Brian Hoffman, Department of Chemistry, Northwestern University, ☎: 708-491-3104; FAX: 708-491-7713; e-mail: bmh@nwu.edu.

WANTED: HALL EFFECT SENSOR

We are seeking a Hall effect sensor for the Varian V-4500 EPR (V-2100 B power supply). Please contact: Eliane Wajnberg, Centro Brasileiro de Pesquisas Fisicas, R Xavier Sigaud 150, 22290-180 Rio de Janeiro Brazil. E-mail: ElianeW@brlncc.bitnet.

WANTED: HALL PROBE

We urgently need a Varian E-4 magnet Hall Probe - P/N - 908742-05 and an E-112 magnet Hall Probe - P/N - 929279-02B. If available, please contact or send to Prof. P.T. Manoharan, RSIC, IIT, Madras - 600 036, INDIA.

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AVAILABLE: VARIAN V 4500 MODULES.

Modules for the Varian V4502 EPR spectrometer are available from G. R. or S. S. Eaton at the University of Denver. E-Mail: geaton@ducair.bitnet.

AVAILABLE: BOXCAR AVERAGER

An inexpensive boxcar averager designed for use in ESE spectrometers is available from the University of Denver. At slow repetition rates it gives about two orders of magnitude better S/N than the well-known PAR 162/164 boxcar. Contact Richard Quine at the University of Denver, Denver, CO 80208 USA ☎: 303-871-2419.

OFFERED: HELP IN THE DESIGN AND CONSTRUCTION OF EPR ELECTRONICS

The University of Denver is able to provide design and construction services for EPR-related electronics such as low noise signal pre-amplifiers, timing systems for pulsed EPR, or complete microwave bridges. Contact: Richard Quine, ☎: 303-871-2419. E-mail: rquine@diana.cair.du.edu

WANTED TO BUY: USED EPR SPECTROMETER

A unit such as a Varian E-4 or E-9 would be ok. Electromagnet (or cavity) not necessary. If you know of a unit that might be available, please contact Mark Rubinstein, Naval Research Laboratory, Washington, DC, 20375, USA; ☎: 202-747-4207.

OFFERED: FIELD SCAN CONTROLLER CARDS FOR VARIAN FIELD CONTROLLERS

Any Varian magnetic field controller can be modified to permit control of the magnetic field by a computer. An improved scan card design with better documentation at a lower cost is now available from the University of Denver. Contact: Richard Quine, ☎: 303-871-2419. e-mail: rquine@diana.cair.du.edu

ADDITIONS AND CORRECTIONS

CORRECTED & NEW ENTRIES FOR THE PREVIOUSLY-PUBLISHED ADDRESS DIRECTORY (VOL. 5, #2):

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EPR NEWSLETTER

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Editor: R. Linn Belford, Urbana, IL (address below).
Assistant Editor, Becky Gallivan, Urbana, IL (address below).
This publication is the official newsletter of the INTERNATIONAL EPR(ESR) SOCIETY. It is supported by the Society, by corporate and other donors, and by three national EPR/ESR centers in the USA:

National Biomedical ESR Center, Prof. James S. Hyde, Director. Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226, USA. ☎: 414-266-4000. FAX: 414-266-4007. E-Mail: cfelix@mis.mcw.edu

Biotechnology Resource in Pulsed EPR Spectroscopy, Prof. Jack Peisach, Director. Albert Einstein College of Medicine, Dept. of Molecular Pharmacology, 1300 Morris Park Avenue, Bronx, New York 10461, USA. ☎: 718-430-2175. FAX: 718-829-8705. E-mail: peisach@aecom.yu.edu

Illinois EPR Research Center (IERC), Prof. R. Linn Belford,* Director; Prof. Harold M. Swartz,† Co-Director; Prof. Robert B. Clarkson,* Assoc. Director; Prof. Peter G. Debrunner,* Co-Principal Investigator; other senior staff: Prof. Mark J. Nilges,* Dr. Alex Smirnov,* Laboratory Manager at Urbana, Dr. Tadeusz Walczak,† and Dr. Jim Liu,† Laboratory Manager. at Dartmouth
*University of Illinois at Urbana, 190 MSB, 506 South Mathews, Urbana, IL, 61801, USA. ☎: 217-244-1186. FAX: 217-333-8868.. E-mail: ierc@uiucvmd.bitnet or rlbelford@uiuc.edu
†IERC also operates a satellite site for EPR *in vivo* at †Dartmouth University, Hanover, New Hampshire; ☎: 603-650-1955; FAX: 603-650-1935. E-mail: harold.swartz@dartmouth.edu

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

IN THIS ISSUE

Please direct communications about the EPR Newsletter or prospective material for publication to the Editorial Office at the IERC address above.

FROM THE EDITOR

Spring is on the way. It's hard to believe that a year has passed since our last public issue of the EPR Newsletter, and even harder to realize that it has been half a century since Zavoisky in Kazan discovered electronic magnetic resonance. HAPPY GOLDEN ANNIVERSARY, EPR (or ESR, EMR, or whatever you prefer to call it)! Several celebrations are in the works; some of them are described in this issue.

The past year has been an interesting one for the EPR Newsletter and the Society. We have welcomed a whole new set of IES officers - Keith McLauchlan, President (Oxford), Karl Hausser, Vice President (Heidelberg), David Greenslade, Treasurer (Colchester), and Arthur Schweiger, Secretary (Zürich); we have announced several important awards and published for the IES members our full directory of EPR scientists. Reminder: The EPR Newsletter depends heavily upon you, the readers, to furnish interesting material - articles, notices, letters, advertisements, etc. Please send your contributions. When you notice announcements of pertinent meetings, books, conference proceedings, or the like, please inform us, as we may not otherwise receive or notice these announcements soon enough for timely listing in the Newsletter.

Nonmembers: please join us in IES. It's easy (see pp. 30-31), inexpensive, informative for you, and encourages support of high-quality EPR-related activities. In the last issue, I welcomed two new corporate affiliate-supporters to the International EPR(ESR) Society, and I am pleased now to welcome two more - OMRF Spin Trap Source and the American Institute of Physics. Although our current industrial supporters are based in several countries, well over half of them are US concerns. While we are glad to have more corporate affiliates from the US, our readership (and the IES membership) is broadly distributed over this planet. We hope for better geographical balance in the future and specially invite more companies of Europe, Asia, and other continents to join the Society as corporate members.

R. Linn Belford

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✦ IES AFFAIRS ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR SOCIETY

From the President —

A NEW YEAR

On behalf of all of the Committee of the IES, I should like to take this opportunity of wishing all our members a very happy, prosperous and research-successful New Year. It is a particularly significant year for us, since it marks the 50th anniversary of the discovery of EPR. Why this observation of electron resonance rather than the later observation of NMR was not recognised with a Nobel Prize remains unclear. Despite the advances in modern medicine, it appears unlikely that many of your present Committee will be around to celebrate either the 50th anniversary of the founding of this society or, slightly later, the centenary of the discovery itself, and so we intend to make the most of the celebrations this year! Notably, these will take place at two meetings, in Kazan (where it all started) and Denver. The Society will be officially represented at both, but we urge as many as are able to attend these meetings and to help ensure that they are appropriately memorable.

The start of a new year is a traditional time for taking stock and thinking about the future. With a comparatively new committee, of brief reign, it is particularly important to take a critical look at the Society and to see how it might be further improved. Our attitude is that it exists to provide services and recognition to its members, and to heighten the perception of EPR/ESR in the general scientific community. Our predecessors accomplished a great deal, but there is always room for progress. One particular area we are paying attention to is that of conferences. When the IES was set up, it was wisely decided that it should not run its own meetings, since there were so many scientific meetings, even involving magnetic resonance, already in existence. Rather, it was decided to give the support of the Society to conferences which would occur anyway. This has led to our support of a forthcoming ISMAR meeting in Australia next year, and to the Kazan AMPÉRE meeting. Nevertheless, these are piecemeal arrangements, and we now feel that for our Society to thrive we should meet every year at a conference which is identified with us. Only in this way shall we be able to preserve our corporate identity and enlarge our influence. The principle of non-proliferation still applies, however, and so we are negotiating with our friends in other societies in the hope that they might allow us to become involved as full partners in their regular meetings. One attractive scenario is to make formal arrangements with societies which meet in three-year cycles (e.g. ISMAR and the European group of ESR Societies) and which hold meetings in different years, so as to provide two of the meetings every three years, and to make the Denver meeting our conference in the third. It would clearly be impossible to tie up with every society with resonance interests, and this is why two international societies have been named. It would be anticipated that the IES would be strongly represented on each organising committee, and this would allow more of our membership to play an active role in Society matters.

We should like to hear the reactions of our Members to these thoughts, either through the pages of the Newsletter, or by direct correspondence to the President.

We hope you find the Newsletter provides unique and essential information, but it needs more input from you. Anyone with helpful hints, crazy problems you know the answers to, problems you have come across and seem insuperable, etc, etc, please let us know about them. In the normal world, after all, a problem shared is a problem halved. We cannot guarantee you that, but at least another few thousand scientists will be baffled too!

Keith McLauchlan, President of IES
Oxford University
Oxford, United Kingdom

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LETTER TO THE PRESIDENT:

Dear Sir:

With full assent and appreciation I read your contribution "The End of the Beginning" in the EPR Newsletter, Vol. 5, No. 2 (Summer 1993). I want to join you in thanking your predecessors for all the effort they have put into the benefit of the International EPR(ESR) Society. At the same time I want to congratulate the "new" officers team, Keith McLauchlan, Karl Hausser, Arthur Schweiger, and David Greenslade, for having been elected by the EPR community. I wish you success and satisfaction in your work for the years to come. Very likely, these years will bring more and more restrictions also to fundamental science in consequence of the world-wide political and economical turmoil. Nevertheless, I am optimistic that the International EPR Society will continue to prosper thanks to the dedication of its officers and members.

I was particularly touched by your comments about the relation between the International EPR Society (IES) and the various European EPR groups and their Federation. Explicitly, I want to take this opportunity to renew the understanding among the participants of the first Pan-European EPR conference in Padova (1991) who approved the formation of a European Federation that should not become a competitor of the IES, but should rather keep a close working relationship with the IES and should be "regarded as a complementary institution with the goal of addressing the specific problems presently pressing the scientific communities in Eastern and Western Europe" (see EPR Newsletter, Vol. 3, No. 4 (Winter 1991), p. 15).

In accordance with this spirit I cordially invite European and Non-European EPR scientists to participate in the second "European EPR Meeting on Recent Advances and Applications to Organic and Bioorganic Materials" in Paris, September 5-9, 1994 (see Notices of Meetings) I am strongly supporting the idea of international cooperation between Non-European (US, Canadian, Japanese, Israeli, ...) and European EPR communities and I would be very glad about a strong participation of scientists from the US and other Non-European countries in the Paris symposium. I am looking forward to seeing you in Paris!

Best Regards,
Klaus Möbius
(Chairman of the Steering Committee of a European Federation of EPR Groups and of the Organizing Committee of the Pan-European EPR meeting in Paris, 1994)

AWARDS COMMITTEE To propose names for any of the following IES awards, please send your suggestion(s), or preferably full nomination(s), to the appropriate Disciplinary Awards Subcommittee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow; George Feher; & Jan Stankowski. *For Chemistry* - Bruce Gilbert, Chair; J. Sohma; Jim Bolton; & Kev Salikhov. *For Biology/Medicine* - Larry Berliner, Chair; Marjeta Sentjurc; Hideo Utsumi; & Tadeusz Sarna).

Gold Medal: One Gold Medal per year, recognizing benchmark contributions to EPR spectroscopy as a whole;

Silver Medals: Silver Medals each year, one each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine;

Young Investigator Awards: Three Young (less than seven years since the Ph.D. degree) Investigator awards each year, in the same fields as the Silver Medals.

IES Awards Committee Chair: Keith McLauchlan, Oxford University, Physical Chemistry Laboratory, South Parks Road, OX1 3Q2 Oxford, UK FAX: 4-865-275410; E-mail: kamcl@physchem.ox.ac.uk.

LETTER TO THE EDITOR

Dear Sir:

In the course of preparing a review article on detection and quantification of nitric oxide, I felt obliged to explain why I use the term "electron magnetic resonance (EMR)" rather than the more commonly used "EPR" or "ESR". I know that I am not alone in this, although I am certainly in the minority! Below is an early paragraph from this manuscript; I would appreciate feedback on it:

"Many paramagnetic molecules can be quantified and

characterized by the magnetic resonance technique known either as electron paramagnetic resonance (EPR) or electron spin resonance (ESR) spectroscopy and this technique has the ability to detect NO at very low concentrations. Historically the name ESR has been used in studies of molecules with an unpaired electron located on C, O, N or S (free radicals), while the name EPR has been used in studies of transition metal complexes with unpaired electron(s) located primarily in d orbitals. Both terms have been used in studies involving NO because this "free radical" is often trapped and stabilized as a nitrosylated paramagnetic metal complex. By analogy to nuclear magnetic resonance (NMR) spectroscopy, which is based on properties of the nuclear magnetic moment, electron magnetic resonance (EMR) spectroscopy has been introduced as an inclusive and unifying name for this technique and is used throughout this review."

Dean Wilcox, Dartmouth University
(Dean.E.Wilcox@dartmouth.edu)

INFORMATION FROM EPR CENTERS

FROM UNIVERSITY OF SURREY DEPT. OF CHEMISTRY: Professor Les Sutcliffe and Dr. Duncan Gillies have interests in EPR and NMR. Their research group currrently includes two postdocs (Mark R. Symms and Xiaoping Wu) and two graduate students (Stefan Luff and Melanie Britton).

NMR is used generally and for the study of model lubricants at high pressures. EPR is used to study molecular motion in these liquids and in surfactant solutions and in model foods. For spin probes we use conventional nitroxides, some novel aromatic nitroxides and some sulfur-nitrogen radicals we discovered. We have a program directed towards the synthesis of radicals with specific chemical properties and having high stability and narrow EPR lines. We are also developing radiofrequency EPR spectroscopy and imaging.

Other members of the Centre are Dr. Peter McDonald and his research group who are working on NMR imaging of materials. There are others using a NMR body scanner for medical research.

For more information, contact: Prof. Les H. Sutcliffe, University of Surrey, Department of Chemistry, Guildford, GU2 5XH SURREY UK; ☎: 44-0483-509586; FAX: 44-0483-300803 E-mail: chs11s@uk.ac.surrey.

FROM THE RUSSIAN ACADEMY OF SCIENCE, YEKATERINBURG, RUSSIA: We have ESR-230 and ESR-231 X-band spectrometers made in DDR (former Eastern Germany) and an ER-200 Bruker. The spectrometers are equipped with Q-band block, Nitrogen temperature controller 77-550 K, Oxford helium flow controller 3.5-300 K, ESR-tomograph. Two spectrometers are combined with IBM PC/AT equipped with home-made software. The personnel are: Yurii N. Shvachko, Dr. (SOLID, SUPERC, COAL); Alaxander A. Romanyukha, Dr. (FERR, SOLID, RAD, SUPERC); Nikolai A. Viglin, Dr. (FERR, SOLID, INSTR); Alexander A. Koshta, postgraduate student (SOLID, COAL); Eugene A. Ignatyev, student (RAD).

For information, contact: Yurii N. Shvachko, Russian Academy of Science, Inst. Met. Phys., Kovalevskaya Str 18, GSP 170, 620219 Yekaterinburg, RUSSIA; ☎: 7-343-2-444-482; FAX: 7-343-2-445-244; e-mail: either elph@ifm.e-burg.su or ifmUE@imm.e-burg.su.

FROM THE BIOTECHNOLOGY RESOURCE FOR PULSED EPR SPECTROSCOPY, BRONX, NEW YORK: The Biotechnology Resource for Pulsed EPR Spectroscopy was established in 1985 and is located at the Albert Einstein College of Medicine in the Bronx. It is supported under the NIH Division of Research Resources,

and the Principal Investigator is Jack Peisach.

1. SERVICES AVAILABLE

A) INSTRUMENTATION

The centerpiece of the Resource is a pulsed EPR spectrometer that operates at frequencies 6-18 GHz in three bands. Operation at a given band is facilitated by interchangeable electron tubes (klystron source and high power pulsed traveling wave tube; Space Microwave 6000 modulator). Low power microwave pulses are generated using a two channel circuit that permits independent control of pulse width and amplitude. The minimum pulse width using a single switch is 15ns (delivering a maximum of 25W); for special applications we can configure switches sequentially to provide shorter pulse widths. Pulse timing is provided by three Berkeley Nucleonic programmable generators (leading and falling edge to 1ns); a PAR delay generator (four additional leading edges to 1ns) can also be incorporated into the spectrometer logic configuration. Timing pulses are fed to custom modules that define and control a given experiment. Detection is homodyne and the transient signal is captured using a custom-built boxcar integrator with an aperture of 16ns.

Two- and three-pulse electron spin echo modulation spectral studies are routinely performed on this instrument. More complicated pulse sequences can also be implemented. Other experimental capabilities include measurement of the Linear Electric Field Effect, echo-detected EPR, and electron spin echo detected ENDOR. Computer programs that support the data processing for each of these applications are provided on a PDP-11 connected to the spectrometer. Advanced analysis (e.g. spectral simulations) is performed on a lab MicroVAX II or DECstation.

The pulsed spectrometer operates with a liquid helium immersion dewar (approximately 10-14 hrs. on a single fill); typical operating temperature ranges span 1.3 to 4.2K. Other temperatures (e.g. liquid argon, 20K) can be arranged in advance, subject to availability from our gas supplier. The spectrometer can be configured to operate with commercial cavities and flow cryostat; standard operating procedure entails the use of either a Mims-type transmission cavity or rectangular TE cavity outfitted with either a loop-gap or stripline resonator (Britt/Klein design). Specialized cavities include a rectangular TE for single crystal studies as well as axially shortened TM_{110} and dielectric TE_{011} cavities, all of which are compatible with the immersion dewar. Samples are accepted either in precision bore 3.8mm o.d. tubes (we will supply) or free form.

The pulsed spectrometer is housed in a specialized instrument laboratory with capability for engineering. A second biochemical preparatory lab houses a Varian E-112 X-band EPR spectrometer for standard analyses. This spectrometer is augmented with accessories, including: flow helium cryostat and nitrogen dewars, coldfinger dewars, NMR gaussmeter, high intensity uv/vis sources for photochemical studies, a TE_{102} rectangular cavity, and TE_{011} cylindrical cavity for single crystal work. A Bruker ER200 with an ESP300 upgrade is available in an affiliated laboratory (P. Aisen) and can be used for cw-ENDOR studies. This spectrometer is outfitted with an Oxford Instruments ESR900 series cryostat for operating temperatures as low as 1.3K.

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The laboratory also features a UV/vis spectrophotometer, high vacuum lines with accessories for synthesis and preparatory work, atomic absorption spectrometer, centrifuge (including access to departmental preparative ultracentrifuges), photochemical synthesis apparatus (samples size 5 ml to 300 ml), Fast Performance Liquid Chromatograph, and electrophoresis (disk/slab) apparatus.

B) ENGINEERING CAPABILITY

The pulsed EPR laboratory is equipped with test equipment for design and development. These include rf/microwave power and frequency meters, a Tek spectrum analyzer plug-in (8-40 GHz), waveguide and coax components for prototyping, HP 65000 series digital oscilloscope and logic analyzer, rf/microwave sweepers, NIM and VXI prototyping modules.

A machine shop is on the college premises for routine milling and lathe work. Specialized prototyping is handled by outside subcontractors, including glass/quartz fabrication, ceramic work, and electroforming of critical cavity/waveguide components.

C) USER INTERACTION

The Resource provides services such as in-house training and consultation. Experimental collaboration on specific projects is handled by mutual arrangement: we can provide lab space and instrumentation access (with staff support, if desired) for visiting researchers, or, alternatively, provide a spectroscopy service via submitted samples (shipping dewars are available for use). Engineering service for constructing spectrometer components is provided, subject to limitations in our expertise (call for info). Housing for visitors is available at a college-run apartment house across the street. The facility is a 15-20 min. taxi ride from LaGuardia Airport; an express bus service runs to midtown Manhattan on a 20 min schedule from 6AM to 11PM.

2. EXPERIMENTAL CAPABILITY AND EMPHASIS

Electron spin echo and ENDOR spectroscopies are effective at resolving weak hyperfine coupling interactions that are often obscured in powder averaged EPR spectra. Our principal area of specialization is the application of electron spin echo and ENDOR to study of the hyperfine interactions of ligands to paramagnetic metal ions in proteins. The spectra yield electron-nuclear coupling parameters that can be used to identify ligands and determine spatial distributions of the ligand nuclei and/or unpaired spin density with respect to the metal center.

The unique features of our spectrometer enable us to thoroughly examine the hyperfine interactions of a metal coordination sphere. The extended operating frequency range permits one to track the magnetic field dependence of a spectroscopic transition and therefore unambiguously assign nuclear transitions on the basis of their Larmor frequency shifts. Broadband operation also permits us to exploit the condition of 'exact cancellation' for a wide distribution of hyperfine interactions. Exact cancellation denotes a condition when the nuclear Larmor energy cancels the hyperfine interaction term of the hamiltonian and leaves behind only the quadrupole term. The much simplified resultant spectra are less ambiguous to interpret and therefore more informative with regard to correlation with structure and function of the metal coordination sphere.

The Linear Electric Field Effect is a measure of the EPR spectrum g-shift in a Stark field. Applications using the pulsed spectrometer (echo detected) are more sensitive

than the direct measurement of the shifted EPR spectrum. The resultant data are indicative of coordination site symmetry and charge delocalization. With adequate analysis the data can be used to assign g-tensor orientation.

Electron spin echo ENDOR capability extends the range of hyperfine interactions that are observable using the pulsed spectrometer by removing the high frequency limitation of the fourier transform. The technique is also advantageous in that it is effective in resolving weakly coupled hyperfine interactions that constitute the often unresolvable matrix line in powder ENDOR.

Much of our work focuses on the study of ligand binding to metals in protein (and models thereof). Although much of this emphasis has been on Cu(II) and Fe(III) (heme) proteins, we now have active programs devoted to Co(II) substituted metalloproteins and

cofactors. We are also studying ligand binding and symmetry properties (LEFE) of mixed valence species. Along with our expertise with metalloproteins, we have considerable experience with free radical systems and are open to collaborative work in this area of EPR research. In recent years we have conducted several studies using spin labels or traps for collaborators in the NY metropolitan area. Preliminary FID data have been collected on the pulsed spectrometer; however, we currently limit our radical studies to cw-EPR or ENDOR.

3. INQUIRIES SHOULD BE DIRECTED TO:
Jack Peisach or Chris Bender (718-430-2175)
Albert Einstein College of Medicine
1300 Morris Park Avenue, Bronx, NY 10461 USA

FROM THE NATIONAL BIOMEDICAL ELECTRON SPIN RESONANCE CENTER, MILWAUKEE, WISCONSIN: The National Biomedical Electron Spin Resonance (ESR) Center was established in April 1976 at the Medical College of Wisconsin in Milwaukee, Wisconsin by a grant from what is now the Biomedical Research Technology Program, National Center for Research Resources of the National Institutes of Health.

Staff: Dr. James S. Hyde serves as Principle Investigator and Director of the Center. Eight ESR spectroscopists are available for collaborative research, system instruction, and discussion. There are also an electronics shop, machine shop, and other support services including organic synthesis and a tissue culture facility.

Equipment: Two Varian E-109 ESR spectrometers, ELDOR (Varian E-9 ESR spectrometer with E-800 frequency-swept ELDOR accessory); two multifrequency ESR spectrometers with bridges at 0.5-1, 1-2, 2-4, 4-8, 9, 19, and 35 GHz; time-domain ESR (saturation-recovery measurements of relaxation times) at 2-4, 9, and 19 GHz; and an IBM Instruments, Inc., ER 200 D ESR spectrometer system. There are numerous loop-gap resonators for special experiments. Magnetometers and frequency counters are available for precise field and frequency measurements (including 35 GHz).

Special Features: Extensive cryogenic equipment including liquid-helium apparatus for all available microwave frequencies (Q-, K-band limited to ~20 K) at the present time; online computers for data acquisition and spectral simulation; Tektronix workstation; Hewlett Packard 735 workstation with high-frequency structure simulator (HFSS) and microwave design software (MDS); copper vapor laser (MetaLaser Technologies, 1051); vacuum line; photochemical facilities include Xe and Hg lamps and monochromator; Update Instruments stopped-flow ESR apparatus; Perkin-Elmer 320 UV-VIS spectrophotometer; Sorvall RC5B superspeed refrigerated centrifuge; Beckman Model 167 HPLC; Hewlett Packard series 1050 HPLC; Cahn balance (microgram sensitivity); and other routine chemical and biological laboratory equipment are available. Also available are microwave test equipment including two Hewlett Packard Network Analyzers model 8566 (to 24 GHz) and model HP 3577A (5 Hz to 200 MHz), two Hewlett Packard Spectrum Analyzers (models 8596E and 8566B), extensive electronic equipment and machine shop.

Capabilities: The ESR Center staff has broad experience in the use of nitroxide radical spin labels to measure translational and rotational diffusion in biological systems, with particular emphasis on measurement of rotational correlation times in the range of 10^{-3} to 10^{-7} s and on measurement of slow-translational diffusion constants (10^{-6} to 10^{-9} cm^2/s). These are characteristic values for components of biological membranes. Several spin-probe methods have been developed and are available for measuring oxygen concentrations and diffusion in cells and other complex systems. Identification and characterization of transient and stable free radicals is accomplished in various ways, using the several types of ESR equipment available in the Center, including multifrequency ESR and electron-nuclear double-resonance (ENDOR) spectroscopy. It is often possible to identify paramagnetic metal ions and determine the symmetry of the crystal field, the charge, and the ligation. $^{63}Cu^{2+}$ is being used as an extrinsic probe of the structure of metal-binding sites, primarily using the multifrequency ESR capability. Recent

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studies focus on "blue" copper sites in proteins and on mixed-valence [Cu(1.5)...Cu(1.5)], S=1/2 centers in nitrous oxide reductase and cytochrome *c* oxidase. Study of relaxation processes by means of which paramagnetic centers are maintained in thermal equilibrium with their environment is possible, using the pulse (saturation recovery) ESR spectrometer with multifrequency capability.

Areas of Current Research: Physical studies of nitroxide radical spin labels; measurement of spin label T_1's; diffusion processes in synthetic and biological membranes; measurement of oxygen concentrations in synthetic membranes and oxygen uptake in cellular systems; spin-label studies of fibronectin; peptide-membrane interactions; site-directed spin labeling of membrane proteins; ESR characterization of immobilized free radicals; phototoxicity in pigmented tissues; oxidation mechanisms and toxicity of catecholamines; spin trapping and spin stabilization of carbon-centered, sulfur-centered, and oxygen-centered free radicals; photochemistry and photophysics of merocyanine dyes; ESR assays for nitric oxide; free radicals in cardiac surgery, free radical mechanism of oxidation of low-density lipoproteins, radical production during merocyanine-mediated photoactivation; spin-labeled oximetry in photodynamic therapy; copper ligation and charge of copper proteins and copper-containing chemotherapeutic and radiosensitive drugs; multifrequency ESR and saturation-recovery ESR of mixed-valence binuclear copper centers; and characterization of higher order effects occurring in transition-metal spectra measured with lower-frequency microwaves. Under development is a general purpose ESR spectrometer for multiquantum experiments.

Users: Visitors and collaborators to the Center cover the complete spectrum of ESR experience from established spectroscopists who need only to be given a box of chart paper and a pen that works to scientists who may never have seen an ESR spectrometer before. Scientists with a great deal of ESR experience usually need to only contact the Center and reserve spectrometer time. Other scientists wishing to use the Center should submit a letter giving a short proposal of what they want to do at the Center. Also, we encourage people, if possible, to come to the Center and give an informal seminar about their research in order to discuss with personnel at the Center ways in which ESR spectroscopy might be beneficial.

A limited number of young scientists are invited each year to spend two weeks at the Center to obtain experimental knowledge of advanced or specialized ESR techniques. There is limited financial support of up to $500 for these training visits.

Whom to Contact: The person to contact about using the Center or obtaining more information is:
Christopher C. Felix, Ph.D., Scientific Administrator
National Biomedical ESR Center
Medical College of Wisconsin
8701 Watertown Plank Road,
Milwaukee, WI 53226 USA
☎: 1-414-266-4008 (June 94: 1-414-456-4000)
Fax: 1-414-266-4007 (June 94: 1-414-456-4007)
E-mail: cfelix@mis.mcw.edu

COMPANY PROFILES

(Corporate affiliates of the International EPR Society are invited to provide profiles of their companies or other descriptive material about the nature of their organizations, products, and services for the information of the Newsletter readers.)

I. OXFORD INSTRUMENTS Ltd.

Since our foundation in 1959, Oxford Instruments has been at the forefront of the application of cryogenics and superconductivity to a wide, and ever increasing, range of techniques. The Research Instruments business concentrates on the needs of researchers in the physical sciences. Areas of involvement include high energy and nuclear physics, condensed matter physics, materials characterisation, microscopy and general spectroscopy in physics, chemistry, and biophysics. The following paragraphs summarise our current activities in the EPR field.

The value of cooling samples to cryogenic temperatures for spin resonance measurements is well known. Enhanced

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signals, sharper lines and the ability to study interactions and phase transitions only present at low temperatures are a few examples. Our commitment to support the EPR community is demonstrated by the continuing development of our cryostats. Currently three cryostats are available which cover the temperature range from 1.9 to 500K and are suitable for operation in L, S, X, and Q band spectrometers. Standard variations of these products include optical windows for both optically induced and optically detected EPR. The ongoing development programs for these cryostats aim to address the needs of our customers in the future.

High frequency measurements are an important experimental technique for increasing the sensitivity and resolution of EPR signals and for samples with very large zero field splittings. For excitation frequencies above 50GHz it is impractical to use electromagnets. On the other hand superconducting magnets can readily achieve the fields required. To facilitate high field EPR measurements Oxford instruments has developed the Teslatron H range of high homogeneity superconducting magnet systems. Field strengths from 7 to 18 Tesla with bore sizes up to 98mm are available with integral variable temperature inserts for temperature operation from 1.5 to 300K. The Teslatron concept is the incorporation of support electronics and software for the magnet resulting in an easy to use temperature and magnetic field environment allowing the user to concentrate on the experiment rather than the equipment.

We recognise that pushing the limits of scientific understanding sometimes requires novel experimental instrumentation. To support innovative research Oxford Instruments' technical specialists are available for consultation to help in designing equipment for specific applications.

Oxford Instruments is an international organisation with offices in England, USA, France, Germany and Japan and agents in many other countries. For more information please contact your local representative. Oxford Instruments, Ltd., Eynsham, Oxford OX81TL, UK; ☎ 44-865-822-855; FAX: 44-865-881-567; or Oxford Instruments North America, Inc., Concord, MA, 01742, USA; ☎: 1-508-369-9933; FAX: 1-508-369-6616.

II. RESONANCE TECHNOLOGIES, Inc.

Product & Application Profiles

Dr. Ray C. Perkins, Jr., Founder & President

The extraordinary effectiveness of very-high-field, electron paramagnetic resonance (VHF EPR) has been proven. Thanks to the efforts of a handful of laboratories around the world, employment of frequencies above 90GHz and corresponding field strengths above 3.3 Tesla has demonstrated dramatic improvements in both resolution and detectability. A new door has been opened in EPR spectroscopy with Res-Tech's HMF Series of spectrometers in the commercial vanguard.

For some classes of unpaired electrons, VHF EPR is effectively a new spectroscopy. The resolution of overlapping peaks, suppression of "forbidden transitions," full g-matrix expression, radiation quanta greater than zero-field splittings and point-sensitivity improvement by nearly three orders of magnitude combine to produce truly stunning results. Below are noted a few of the application's areas in which the viability of VHF EPR has been shown. Before proceeding, it is appropriate to highlight the design philosophy of the HMF Series.

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HMF SERIES DESIGN PHILOSOPHY. We rely on two primary resources: 1) the researchers[1] who have performed the work already and 2) industry experts in each of the technologies represented in the HMF. The former resource insures that we create a design known to work while the latter insures that components and subassemblies reflect state-of-the-art technologies. The resulting composite design is flexible, expandable, modular, easily adapted to special needs and, therefore, well positioned for growth. Key subassemblies/components include precision-swept, superconducting magnets; millimeter-wave or μwave bridge assemblies; high-performance personal computers; and a range of resonator designs. Overall system integration assures accessibility and ease-of-use while "virtual instrument" programming improves the slope of the learning curve.

The HMF is currently available with frequencies in the range of 94-250 GHz with corresponding magnetic field strengths of 3.36 to 9.4 Tesla[2]. We have also taken care to insure that low-frequency EPR - e.g., S-, X-, and Q-bands - may be supported on the HMF platform. Lastly, bridge design and data acquisition methods anticipate the needs of pulsed VHF EPR Spectroscopy.

FREE RADICALS. VHF EPR Spectroscopy appears to be the technique of choice for free radical work. Multiple radicals formed by irradiation or thermal damage are clearly resolved and identifiable while the corresponding X-band spectrum fails to distinguish any of the overlapping species. Orientation-specific hyperfine coupling has been observed in molecules relevant to biochemistry, solid-state, and fossil fuel research. Full g-matrix resolution, even for molecules with small g-anisotropy, enables complete characterization of the unpaired electron while opening the door to the study of previously unavailable motional regimes. Spin-trapped radicals will benefit as well and for some of the same reasons. VHF EPR spectroscopy should predictably reduce (sometimes eliminate) the need for fractionation and spectral deconvolution techniques. Finally, the better point sensitivity of VHF EPR has yet to be fully exploited for free radicals. Many systems that simply have been unapproachable by low-field techniques now lend themselves to analysis.

SPIN LABELS. Based on recent work I have seen, much of the spin-label research I performed in my early days needs to be redone. Some VHF researchers assert that this may well be true for nearly all spin-label work done to date. Small changes in environmental dielectric, poorly resolved or unnoticed at low-field, produces marked changes at VHF. Discrete orientations are spectroscopically isolated. Lineshapes become sensitive to motional types. These capabilities combine to produce a spectroscopy capable of simultaneously differentiating label populations while enabling full characterization of the motional/electronic characteristics. Sensitivity to motion is expanded to both smaller (fast motion) and longer (slow motion) correlation times. Lastly, improved point sensitivity opens the door to work with ever-decreasing amounts of labelled material.

METAL CENTERS. Metal atoms, particularly those demanding very low temperatures and wide field sweeps present considerable technical challenge. As a result, metal spectra are under-represented in VHF "notebooks" at this time. Nonetheless, the metal work that has been done at VHF appears promising indeed. Spectra for copper, iron, nickel, manganese and vanadyl ions, in some cases showing orientation-dependent hyperfine and super-hyperfine couplings, have been observed. Direct and full characterization of zero-field splittings has been made in others. Suppression of "forbidden" transitions greatly simplify analysis for yet other systems. While some of us anxiously await more work to be done on relevant systems, it is safe to say that VHF is an important and perhaps necessary tool for metal spectroscopy.

SUMMARY. The "proof of principle" work has been done: VHF EPR spectroscopy is the tool of choice for many areas of EPR research. At the same time it may well become that facet of EPR which lends itself to routine analytical procedures for certain types of atomic centers. VHF EPR allows us to revisit systems we've examined at low-fields, especially to clear up "loose ends" or ambiguous results. It also opens new arenas for study based on dramatic improvements in resolution and detectability. And VHF EPR is commercially available and more affordable than you may realize in the form of the HMF Series spectrometers from Res-Tech. Call us.

We shall be happy to pass along relevant references or product information at any time.

[1]Let me offer my sincere gratitude to those of you who have given freely of your time and expertise in designing the HMF. You represent talent, experience and insight seldom if ever seen in a commercial environment.

[2]For further information on either applications of instrumentation, please contact us at Resonance Technologies, Inc.; 207 Webster Street; PO Box 6125; Franklin, NH 03235-6125; USA. ☎: 603-934-5661; FAX: 603-934-7143.

THE COMPUTER CORNER

Edited by Philip D. Morse II, Keith P. Madden, and Richard Cammack

This column is a regular feature of the EPR Newsletter and covers all computer aspects of EPR. We solicit comments, suggestions, tips, and questions from our readers. Please send contributions to Reef Morse (E-mail:reef@xenon.che.ilstu.edu), Keith Madden (E-mail: keith.p.madden.1@nd.edu) or Dick Cammack (E-mail: udbc033@hazel.cc.kcl.ac.uk).

EPR List Server *(This is a shorter version of an article in Vol 5 #3 of the EPR Newsletter).*

Many times we have EPR-related questions to which we don't have the answer but have the vague feeling that "someone out there" does know the answer. There has been no way to ask such questions of the general EPR community, but this problem has now been solved. Reef Morse has established a list server on the main VAX computer at Illinois State University, Department of Chemistry.

You can get on the list by sending the single word SUBSCRIBE to the list administrator at epr-list-request@xenon.che.ilstu.edu and you will be automatically placed on the list. You will receive a response from the list processor, usually within one or two minutes.

Messages to the list are sent to the list itself at epr-list@xenon.che.ilstu.edu and your message will be sent to all the other subscribers on the list immediately. As the list is set up now, you will also receive a copy of your posting. This confirms that your posting has been sent out.

Currently there is no limitation on who may subscribe to the list, and there is no cost to subscribe.

Any topic of interest to the EPR community is appropriate. Example of such topics could be: requests for information about samples, formats for exchange of EPR data, information about spectrometer construction and repair, sample preparation, requests for post-doctoral or other staff positions, and the like.

If you have questions or comments regarding this list, send them directly to: reef@xenon.che.ilstu.edu. He is the person responsible for setting up and maintaining this list.

Finally... Please feel free to subscribe to and use this list. A list is only as useful as its subscribers want it to be.

EPR Software Database

The software database of programs on all topics relevant to EPR/ESR/ENDOR/ESEEM is being updated for 1994. It is a directory of user-written programs, commercial software, and some useful algorithms. It includes some references about the use of computers in EPR spectroscopy. The list is dependent on what users provide. We are always interested to receive information about new software or updates. These may be sent by electronic mail to Richard Cammack at udbc033@hazel.cc.kcl.ac.uk. He can also respond to requests for specific information, but a quicker way to obtain this information is to download the whole list (about 100 kbytes) by electronic mail through Anonymous FTP at the Illinois EPR Center (See Newsletter Vol. 4 #4). To obtain copies of the programs described in the database, contact the authors directly. The list explains the terms under which the programs are supplied. Much of the information about programs has been obtained through Software Sessions at various EPR meetings, the latest being at the meeting of the ESR Group of the Royal Society of Chemistry in Cardiff, March 21-25, 1994. As part of the poster session, several computers were available for programmers to demonstrate their software. We also hope to have a Software demonstration at the Rocky Mountain Conference in Denver, July 31-August 5, 1994. So come along, and bring a floppy disk!

Richard Cammack
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Request for Assistance

In 1978, Gerard van VEEN in the Netherlands published an article on the simulation of EPR spectra of

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powders in the Journal of Magnetic Resonance (Vol. 30, pp. 91 sqq.). I would be very grateful for the computer program mentioned in his article. Edgar Soulie', Service de Chimie Mole'culaire, Centre d'Etudes de Saclay, 91191 Gif-sur-Yvette Cedex, FRANCE; FAX: 33-1-69-08-79-63; e-mail: spectro@violette.saclay.cea.fr.

TIPS & TECHNIQUES

WINDING COILS FOR THE BRUKER ENDOR CAVITY PART 2: IMPEDANCE MATCHING WITH TRANSFORMERS

Chris Bender
NIH Biotechnology Resource for Pulsed EPR
Albert Einstein College of Medicine
1300 Morris Park Avenue
Bronx, NY 10461

In general, ENDOR coils have characteristic impedances considerably less than the 50Ω standard of transmission line cables and components. As I mentioned in the previous note on this topic[1], the typical impedance of an 18 turn silver wire (0.01" dia.) is about 12Ω, and the mismatch affects the power delivery from the amplifier to the coil. The latter can often be observed as the fluctuation of rf power while the frequency is swept. For many applications, one can live with these mismatch power losses, depending on the nuclei and frequency range of the transitions one wants to observe. The power fluctuations become problematic; however, when one wants to detect transitions that occur below 5 MHz in the rf spectrum (e.g. most weakly coupled nuclei other than ^{1}H and ^{19}F), or when attempting to quantify nuclei from the intensity of the Triple resonance line (see paper by Möbius[2] on this aspect of the technique). When the coil is not matched at low frequencies (usually below 5 MHz) power is not delivered to the coil efficiently and the resultant H_2 magnetic field is inadequate to drive the spins of low gyromagnetic ratio. Furthermore, the mismatch at low frequency may lead to severe baseline distortions; usually observed as a rapid rise that may or may not be monotonic.

As with the coil, one has to be willing to make adjustments in matching strategies depending on the nature of the experiment. I have used broadband transformers and variants of a Pi-network to match the Bruker ENDOR accessory. For the most part, the transformers are based on the design of Ruthroff[3], although a second design developed by Guanella[4] is also suitable. In the description of their ENDOR/Triple spectrometer, Forrer, Schweiger, and Günthard[5] include a transformer that is commonly used to match high power antenna (Figure 1), and it is used to match the rf_2 parallel posts (the rf_1 coil is servo tuned).

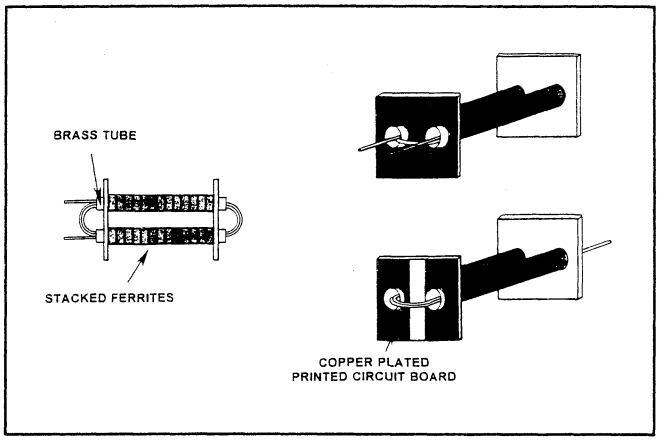

FIGURE 1: Broadband impedance matching transformer (Adapted from ref. 7). The darkened regions on the PC board are for electrical contact. Leads are attached to the split face and connected to the low impedance circuit.

The transformer depicted in Figure 1 is of the design that is generally familiar. It can be readily identified as being constructed of coupled windings of disparate number of turns. The brass tube and the plated printed circuit board at the end constitute a single turn, whereas the wire threaded through the brass tube consists of four turns (each loop is a turn). The primary and secondary are therefore easily identifiable. Transmission line transformers of the type designed by Ruthroff[3] and Guanella[4] tend to be a bit more inscrutable and operate on the principle of summing voltage with a delayed voltage. The transmission line analysis[3] indicates that power transfer between lines is most efficient when Z_1/Z_2 is 4, hence the adoption of the circuit as an impedance matching transformer. The design and construction of transmission line transformers is relatively straightforward; however, it does help to understand some of the terminology and conventions.

The 50Ω standard for transmission line impedance is used because it represents a design compromise between two properties of high frequency transmission lines. The power carrying capacity of transmission lines peaks at 30Ω, whereas attenuation losses are minimal at 75Ω[6]. Another concerns the definition of transformer type. Rf circuit components are often designated balanced or unbalanced, and therefore transformers are often designated by the types of components they match in addition to the impedance ratio. The only definition of balanced vs. unbalanced circuit elements that I could find simply stated that a balanced device is ". . .

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constructed symmetrically with respect to the feed point.[7]" An unbalanced device is apparently not so constructed. The way one determines the category into which a given device falls is by drawing the transmission line representation (two port, parallel line) of the circuit element and basing the classification on whether the signal travels down one or both of the parallel lines. For example, a section of 50Ω coax cable is unbalanced because the signal radiates down the center conductor only; conversely, a dipole antenna is balanced because both arms radiate. It follows that an ENDOR coil is an unbalanced element, therefore a 12Ω coil should be matched by a 4:1 unbalanced-to-unbalanced (unun) transformer. Lastly, a ferrite transformer is designated tightly wound if all the turns touch; wire configurations are denoted as twisted pair or parallel (see Figure 2).

In a given circuit the transformer can be imagined as having two functions: it acts as a load to the source and as a source to the low impedance load. The ENDOR circuit

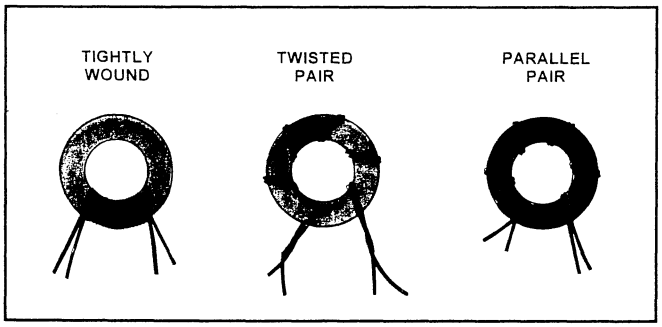

FIGURE 2: Winding strategies for toroidal transformers (left to right: tightly wound; twisted pair; parallel winding).

requires a pair of transformers to separately match the coil/cavity to the power amplifier and the 50Ω termination (and any rf monitoring circuits). In general, the transformer operates by reactive coupling and behaves as a bandpass filter. An ideal transformer has a flat response over a broad frequency range (Figure 3).

A 4:1 Ruthroff unun transformer and its typical application are illustrated in Figure 4. The "4" designates the high impedance side of the transformer; ratios different from 4:1 can be prepared by tapping, mismatching wire dimensions, or stacking 4:1 transformers. The wire is typically wound onto a ferrite core, which can be a rod or toroid, and the wire pair can be tightly wound, twisted, or simply paired. Construction details are schematically outlined in the lower portion of Figure 4. Design considerations are relatively simple. Principal concerns are the matching ratio, power handling capability, and characteristic impedance (of the transformer itself). Ruthroff demonstrated that the

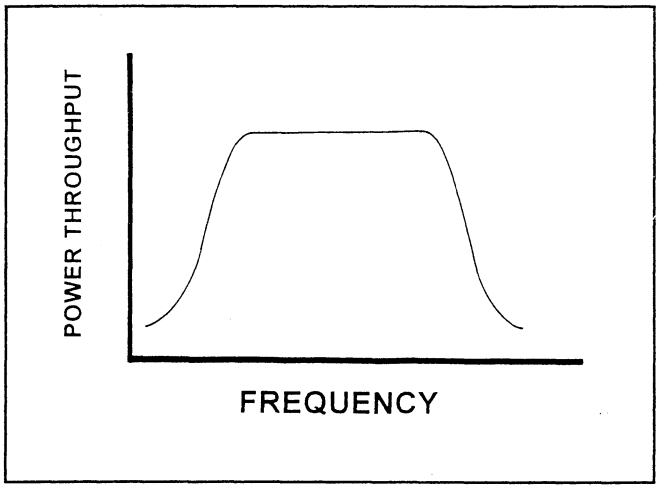

FIGURE 3: Idealized power transforming profile of a broadband transformer.

optimal performance of a transformer is obtained when its characteristic impedance is the geometric mean of the operating input and output impedances, plus or minus 10-20%; that is, 25Ω for the 50:12Ω matching transformer. The characteristic impedance is adjusted by trial and error based on experimental trends that follow from the physical dimensions of the wire, the ferrite core, etc. (see ref. 6).

The power handling capabilities of the transformer are dependent upon the size (diameter and cross-sectional) of the

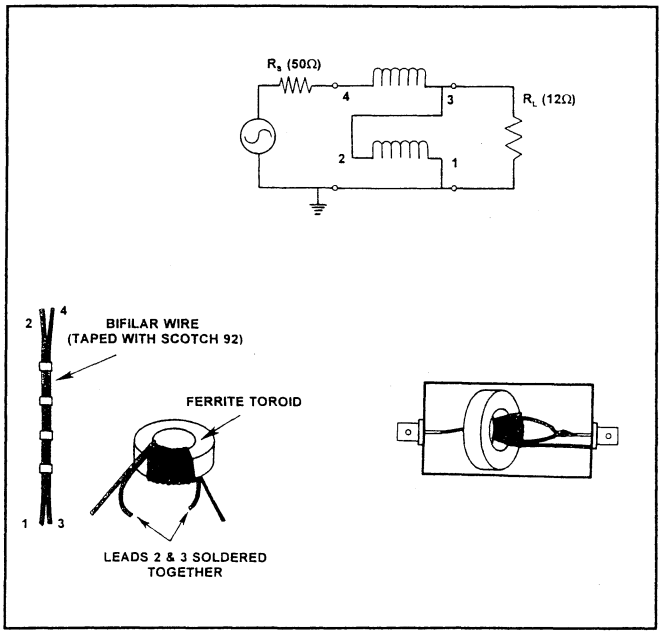

FIGURE 4: Schematic diagram of Ruthroff 4:1 unun transformer and stages of construction. Circuit representation shows a 50 source (leftmost), transformer (center, 4-port device), and a load to be matched (right).

ferrite and its permeability, both of which determine the heat dissipation ability of the coil. A short book by Sevick[8] provides the culminated data of many trial and error studies; in short, the lower permeability (less than 300) ferrites better handle high powers. The trade-off by going to low permeability is that one needs more turns in the toroid. The upshot of Sevick's studies is that a 1" diameter ferrite of permeability less than 300 is adequate for power handling at the 200W level; 1kW power requires a toroid with minimal diameter of 1.5". Interestingly, the way to test the transformer is by the so-called "soak" test (Sevick's term), which entails the application of 1kW rf for a period of time and checking to see if the thing heats up (I am reminded of a cartoon from childhood that featured a character testing for duds on a bomb assembly line by hitting each with a mallet).

Other design considerations are described by Sevick in his text[8]. Variations in the optimal frequency range can be obtained by altering the characteristic impedance of the transformer with low impedance windings. DeMaw describes transmission line transformers wound with 25Ω coax instead of 14-18 gauge wire[9]; however, stripline taped together also works well. Improved high frequency performance is attained with a trifilar version of the Ruthroff transformer. Twisting the wire pair apparently has little effect on the performance of large (o.d. ≥ 1 inch) toroidal transformers[10]. The rationale behind twisting the wire is that one obtains improved coupling between the lines, but the benefits of this technique seem to be significant only for very thin wire (40 gauge and up).

For the most part, I've used Ruthroff transformers constructed by using 4-5 turns of a twisted pair of 14 gauge wire. Originally, I worked with 0.7" diameter toroids of low permeability (Micrometals, Anaheim, CA), and this arrangement worked well at low frequencies with the 100 and 300W ENI amplifiers at Michigan State. More recently, I have experimented with other designs, in particular trifilar and stripline versions of the Ruthroff and Guanella transformer. The trifilar design works better at frequencies above 30 MHz than the bifilar transformer; the stripline offers, as promised by Sevick in his text[8], slightly better low frequency performance because of better approximation to the optimal characteristic impedance.

As I mentioned in the opening paragraphs, I build application-specific transformers. In part, this is because I use a variety of different coils; however, even with a single coil it is best to have more than one transformer type. The reason pertains to the inherent impedance behavior of reactive circuit elements. An ideal inductor (or capacitor) will exhibit a linear variation of its impedance as the frequency of the rf voltage is changed[10]. It is possible, in principle, on very broad spectroscopic sweeps to find that the match ratio (e.g. 4:1) is not correct at some point. Bench tests with my coils indicate that the slope of these plots is not steep, and a specific turns ratio is adequate for sweeps 30 MHz wide (although I prefer to use a more conservative 10 MHz sweep and piece together broadband spectra).

The transformers are typically built into Pomona (or equivalent) "black boxes." Ordinarily one would use BNC or some other type of connector to make the transformer convenient to use; however, there is a subtle design factor that needs to be considered. Most connectors that one buys are designed for 50Ω operation, so attaching a standard connector to the 12Ω end of a transformer should be avoided. I have discussed this with application engineers from two manufacturers of connectors and they agreed with this assessment[11]; I have not actually tested transformers with 50Ω connectors to see if the disparity actually matters to performance. What I have chosen to do with these transformers is put standard BNCs (or type N) on the high impedance (50Ω) side and put nonconstant impedance UHF connectors on the 12Ω side. Most of the commercial UHF connectors work well up to 500 MHz, so there is no problem of rf leakage. The most familiar UHF connector is the large diameter single conductor plug with the serrated edge on the female unit; there is also a smaller BNC-like unit that is made by Amphenol. I frankly cannot say whether switching to UHF connectors over standard item 50Ω connectors is worth the inconvenience of redesigning or modifying the commercial set-up; my own work with the redesign of system components grew out of

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the implementation of our spin echo ENDOR apparatus, which is home-built down to the cavities.

Finally, I must confess that I do not as yet match our ESE-ENDOR coils. The reason is that design limitations are inherent to the cryostat system that we use. Our spectrometer operates with an immersion dewar, and the coil is connected to 50Ω stainless steel coaxial cables that run down the waveguide sections into the dewar. Due to the construction, I would have to put the transformer on the side of the cavity and in the helium bath, which precludes ferrite cores (one can make air coil Ruthroff transformers; however, omitting the ferrite compromises the operating frequency range). I am experimenting with making a low impedance coaxial transmission line that matches the rf coil and which can then be transformer matched to the amplifier on the dewar exterior (a quick fix can be had using the commercial 25Ω coax available from Oxford Instruments and Lake Shore Cryogenic[13], although the 25Ω impedance is a little too high).

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10. According to Bowick, the number of turns per inch determines the characteristic impedance of the transformer; however, his book (ref. 11) describes toroids of very fine wire.
11. Bowick, C. RF Circuit Design, Howard Sams, Indianapolis, IN 1982. Chapter 1.
12. Neither application engineer gave definitive answers; while both said it probably would be better to match properly, one said he did not feel it was necessary to match for operating frequencies below 500 MHz; judging from their hobbyist magazines and books, radio amateurs seem to be fanatical about matching, which may reflect FCC licensing regulations.
13. Lake Shore Cryogenics, 64 East Walnut St., Westerville, OH 43081, USA. Ph: 1-614-891-2243.

ACOUSTIC MAGNETIC RESONANCE SPECTROMETER— DESIGN AND APPLICATIONS, II

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In a previous note to the Newsletter[1], I described features of the acoustic microscope that might be used to ameliorate the practice of acoustic magnetic resonance (AMR). The most significant problem associated with AMR has always been the coupling and propagation of the acoustic wave to the sample, and therefore most of the published work in this branch of magnetic resonance pertains to studies of crystals, metals, and thin films. The information that one can, in principle, obtain from the acoustic experiment provides motivation for finding improved methods of coupling so that less "pristine" materials be examined.

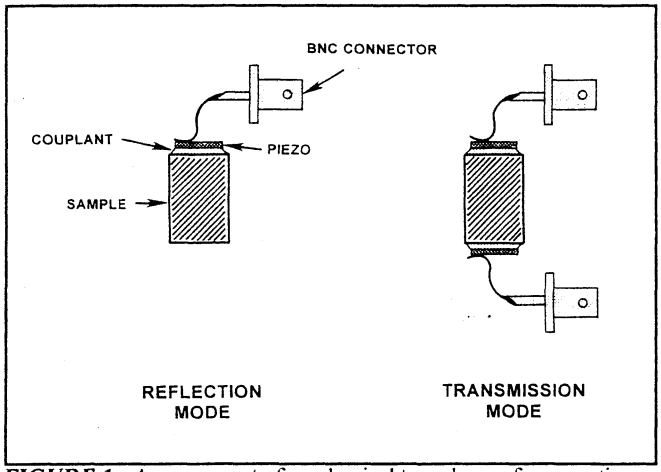

FIGURE 1: Arrangement of mechanical transducers for acoustic magnetic resonance. Piezoelectric material (e.g. quartz crystal) is bonded to polished sample.

The most commonly used method of ultrasonic excitation of a sample for magnetic resonance is the mechanical coupling to a piezoelectric material, as first introduced by Bolef[2] (Figure 1). One can use a quartz crystal or, preferably, thin films of either cadmium sulfate or zinc oxide that are deposited onto the sample. Some ceramic materials, such as barium titanate, are used when an unusual shape is required (e.g. for focusing the ultrasonic beam). The physical contact between the piezoelectric material and the sample is made (exclusive of

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the vapor deposited CdS and ZnO) by using a low freezing point solvent (e.g. 1-pentene) as a bonding agent. The acoustic microscope, as described in the previous note[1], uses a thin film of water between a ceramic "objective lens" and the sample.

The mechanical mode of acoustic coupling imposes serious constraints upon the sample for optimal study. The technique is not typically one of high sensitivity, and the signal can be further degraded by interference among the acoustic waves. In order to avoid destructive interference one must ensure that the sample have optically flat and parallel faces. The practical rule of thumb is that surface roughness be very much less than the acoustic wavelength and that the opposing faces of the sample be parallel to less than a wavelength. These stringent criteria for sample preparation have ensured that AMR remain an esoteric technique for the study of very restricted sample types.

Examples of mechanical acoustic coupling to amorphous materials have been reported[3]; however, further development is needed before the technique can be generally applied. Detection of changes in the magnetization of the sample can be made by using SQUID technology[4], and the idea that underlies the use of the SQUID detector is valid for both excitation and detection; one can couple to acoustic modes of a sample via an electromagnetic field.

The concept of electromagnetic coupling to acoustic modes can be understood from a simple example based on the solenoid. We know from basic electronics that a current carrying wire coil produces a magnetic field that will couple to a ferrite core. The reverse is also true; the current "senses" any fluctuations in the magnetic field that occur as a result of mechanical changes in the core. If the ferrite is vibrated at acoustic frequencies, the magnetic coupling to the coil will influence the current, which can be used as a detection mode. Conversely, imposed oscillations in the current can be used to drive vibrations in the ferrite. Phenomena of this type are what we as spectroscopists ordinarily try to eliminate as microphonic noise.

In the late nineteenth century it was discovered that the pressure of gases could be modulated by an interrupted light source that was directed on the cell. This optico-acoustic effect can be attributed to three mechanisms of origin that may or may not contribute to the observed effect at any given time. Depending upon the intensity of the radiation, the phase (thermodynamic) of the material, the optico-acoustic effect can be attributed to thermal excitation of the media, a localized change of aggregation state of the media, or electrostriction.

The three excitation mechanisms can be readily understood on the basis of familiar physico-chemical concepts. Thermal excitation pertains to irradiation of a vibrational stretching mode (e.g. O-H) in a small region of the sample. The modulated excitation will propagate via non-radiative mechanisms and thereby generate the acoustic wave. When a very intense laser beam is used the energy is not disposed rapidly enough and localized changes of the aggregation state (e.g. a phase transformation) will occur and generate a mechanical shock wave that can be modulated. The third mechanism of optico-acoustic interaction is

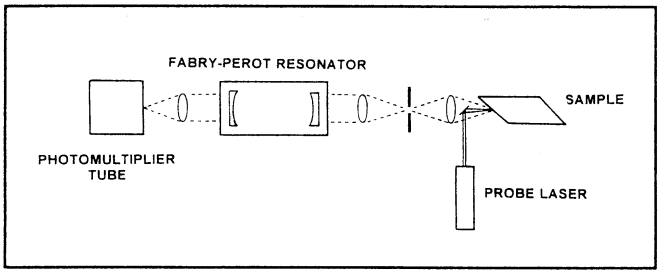

FIGURE 2: Experimental set-up for Brillouin scattering and phonon spectroscopy. Depending on incident radiation and angle of scattered light, phonon frequencies up to 34 GHz can be detected.

electrostriction, which denotes the mechanical deformation of materials in an electric field. Electrostriction tends to be the smallest of the three; however, it is important for the Brillouin scattering phenomenon (see Figure 2).

An acoustic microscope uses laser excitation in a manner analogous to the mechanical transmission and reflection transducers that were described in the previous note. The principal design difference between optical and mechanical acoustic microscopes lies in the design of the transducers, which for the former are designed only to focus light and should not be excitable. There are slight differences among the mechanisms of acoustic wave generation when one compares solid and liquid sample media. For example, there is a lack of surface and shear waves in liquids, and anisotropy in ordered media affects acoustic propagation. Regardless of the modes excited, however, the method of acoustic wave generation entails modulation of laser radiation incident upon

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the sample. This is accomplished by using high frequency pulse trains. A typical case is 100ps pulses that are delivered at 7ns intervals during an experimental time interval of 200ns.

Optico-acoustic excitation could be used with a SQUID magnetometer detector for magnetic resonance experiments; however, the SQUID has its limitations in the sense that it is tied to cryogenic technique. A more general experiment can be designed on the optical effects of acoustic waves. Diffraction of the incident laser beam by an acoustically modulated medium provides a photometric method of detection. This follows from the fact that acoustic waves act as a diffraction grating and, because the incident light intensity is divided equally among diffracted rays, changes in the transmitted light intensity (at a given point in space) can be used as a detection scheme.

A preferred experimental technique would eliminate the need for separate excitation and detection technologies, and this can be achieved by a scattering method analogous to Raman[5,6]. Brillouin scattering is identical to Raman in the sense that scattering is produced by polarization of atoms in the radiation field and the resultant emission of dipole radiation; the difference is the type of coupled modes (i.e. phonon in the Brillouin experiment). Like Raman, the scattered radiation is frequency shifted; however, the frequency shifts by phonons ($\Delta\omega \lfloor 0.1$ cm^{-1}) are much smaller than those observed in a Raman experiment and one needs a Fabry-Perot interferometer in place of the customary monochromator (see Figure 2).

The experimental concepts outlined above are feasible and are being explored for application to magnetic resonance studies. It is possible that they may prove to be impractical. On the other hand, a modest first step towards a biological application of AMR (albeit mechanically coupled) may best be an experiment analogous to the electron spin echo detection of ENDOR. Early AMR experiments were performed indirectly, and acoustic resonance was detected by its effect (amplitude modulation) on an NMR or EPR line[2]. Both cw- and pulsed ENDOR are essentially the same type of indirect detection experiment, and it seems natural to consider the plausibility of performing an acoustic double resonance experiment. The rationale for performing the acoustic variant of ENDOR is the sensitivity of quadrupole interactions to the type of mechanical deformations that would be incited by an acoustic wave. The quadrupole moment is dependent upon the electric field gradient, which, in turn, can be modulated by lattice distortions (driven by acoustic waves).

Our electron spin echo studies of certain biological iron complexes have demonstrated that certain classes of metal centers yield uncharacteristically shallow echo modulation by ^{14}N nuclei associated with ligand molecules. Typical examples are the mixed-valence binuclear non-heme iron centers of hemerythrin-like proteins. The paramagnetic species consists of an antiferromagnetically coupled (effective) Fe(II)/Fe(III) pair. The key point here is the antiferromagnetism; antiferromagnetically coupled centers are typified by strong coupling to acoustic modes. It follows that it might be advantageous to exploit this property of antiferromagnetism that otherwise is deleterious to recording electron spin echo or ENDOR data. In short, the aim is to perform an experimental test of whether one can drive quadrupole transitions acoustically while monitoring the electron spin echo amplitude or saturated EPR signal.

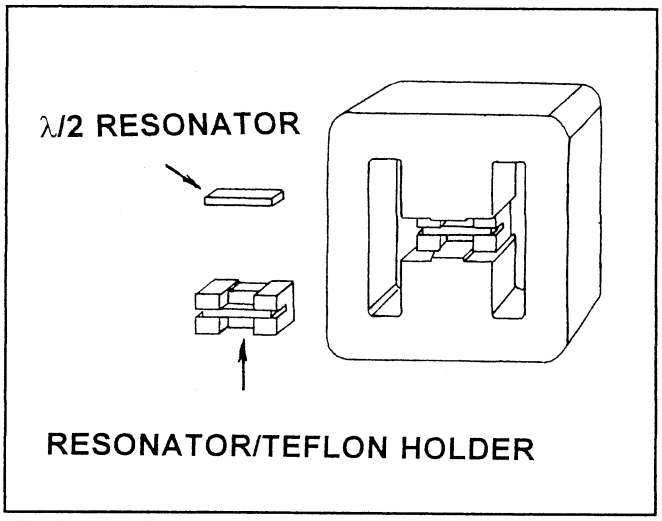

FIGURE 3: Mims transmission cavity for pulsed EPR. λ/2 strip serves as a resonator and support for perturbation experiments (LEFE, ENDOR).

A drawing board sketch of a resonator for acoustic modulated spin echo experiments is depicted in Figure 3 and is based on mechanical coupling using the "Mims cavity." To those not familiar with the cavity, it operates in transmission mode; a λ/2 strip serves as the resonant element. The sample is put into teflon wells adjacent to the strip; typically, there is 150-250 μl of sample of thickness 80-100 mil (acoustic attenuation in the sample should not be problematic with this dimension at cryogenic temperatures). Ordinarily, the resonant strip serves as a support for the ENDOR coil or as a high-voltage electrode for linear electric field (Stark Effect) studies, and the question at hand is whether the strip also can be used as an acoustic transducer. The two factors being explored are: determining a way to make the strip function as both a resonator and acoustic transducer (i.e. can we put a CdS layer on the dipole and how thick should this layer be)

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and, secondly, assessing whether one can reliably form glasses (i.e. the frozen sample) free of microscopic cracks.

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AN EPR SAMPLE CELL SUITABLE FOR SKIN TISSUE USE

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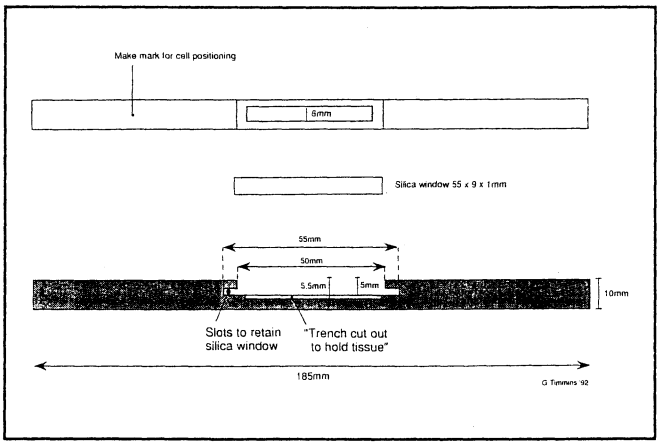
York YO1 5DD, UK

Recently we have been using EPR techniques to study radical production in skin tumour promotion (Carcinogenesis **14**: 1499-1503, 1993) and would like to share details of the construction and use of this sample cell. The cell is constructed from 10mm diameter PTFE rod, machined as in the accompanying figure, together with a silica window. Tissue samples (3-5 skin biopsies up to 5mm in diameter) are placed dermis down in the "trench" of the cell, any treatments applied, and the window slid into place above the tissue (it is important to remove subcutaneous fat or the samples may be dislodged due to their thickness). The assembly is then placed into the cavity, with the skin parallel to its front, and spectra recorded; the cell works well in a Bruker TE_{102} cavity, and also in a JEOL cylindrical cavity, although tuning can be difficult in the latter. Whilst the cell has only been used for skin samples thus far, it may prove suitable for other tissues. Should further information be required, the authors may be contacted at the above address.



TIPS FOR VARIAN EPR USERS

James R. Anderson, Research Specialties

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☎\fax: 312-728-6570

1. Out-of-production critical parts Varian no longer supplies replacement parts, but sometimes a special production run is possible by organization of a group purchase. For example, I have arranged to commission production of some Varian klystrons and some field-scan potentiometers, as described on p. 28 in the Equipment and Supplies Exchange.

2. The Varian oscilloscope module This module sits idle during most of the EPR experiment with use mainly during tune-up at the beginning, during sample changes and occasional spectra displays. The life of the CRT and high-voltage power supply can be extended by partially switching off the CRT and high voltage during these long idle periods.

One appropriate method for this is to switch in a 47.5 ohm resistor in series with the -20 volt invertor supply lead. This will reduce the filament voltage and the high voltage to the CRT. The reduced voltage produces a filament temperature that is just visible and which will prolong the life of the cathode. Reduced cathode emission appears to be the most frequent failure mode, followed by high voltage failures. Keeping the filament partially on reduces the thermal shock experienced during turn-on and allows for faster turn-on times. The reduced high voltage reduces stress and heating of the high voltage components, adding to their longevity.

This resistor can be switched out by a switch on the front panel just below the CRT. There is room for a chassis-mounted power resistor as well. (50 watt Dale showed no signs of heating). Warm-up time is about 15 sec. after initial turn-on, so that in use the resistor is switched out (shorted) to observe the display and switched in during idle times.

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CONFERENCE REPORTS

ROUNDTABLE DISCUSSION OF QUANTITATIVE EPR

June 12, 1993, Sofia, Bulgaria

Participants: The conferees were L. Antov, A. Christova, R. Clarkson, K. Dyrek, G. Gochev, M. Ivanova, M. Iwaizumi, V. Nagy, Y. Ohba, N. Patev, G. Rist, J. A. Weil, N. D. Yordanov, M. Zdravkova.

Main Topic Areas: The principal topics for discussion were Chemical Specimen, Instrumentation, Analysis of Spectral Data, Quantum Mechanical Aspects.

1. Chemical Systems for calibration (and for standard materials)
   a) Gases (O_2) - Isotropic lineshapes. Problems with sensitivity, spectral intensity distribution over rotational levels
   b) Liquids - May have isotropic lineshapes. Problems of chemical stability. Good candidates for primary standard reference materials include DTBN, DPPH, TEMPOL. Need to calibrate the concentrations of these radicals (need analytical methods for radical concentration)
   c) Solids - allow wide temperature range (as desired)
      1) Single crystals - problems with anisotropy and forbidden line intensities
      2) Amorphous samples
      3) Powders - packing problems. Ideally, one should have the packing density of a powder sample and reference material as identical as possible. Any dilutant used should not be hygroscopic and should allow the preparation of a homogeneous mixture.

Sample geometry (point, line, etc.), packing density, grinding, and particle size are important factors that should influence the experimental design of quantitative work.

Accurate work requires several analytical methods (EPR and others). An accuracy of ±1% in the analysis of the primary reference materials would be a good goal to aim at. Practically, a reproducible precision of ±2% may be possible in quantitative EPR work.

Multiple reference materials for samples containing different transition metal ions may be necessary. Quantitation of transition metal ions seems quite challenging, with issues of anisotropic transition probabilities, forbidden transitions, etc., to complicate the analysis.

Standards for pulsed EPR are a new and important need that will not be discussed at this time.

2. Instrumental details
   a) Sample tubes - Many difficulties arise from irregular wall thickness, irregular thicknesses at sealed tube ends, and differing tube materials. There are definite advantages in not having tubes sealed at the ends. There may be problems in some very dilute systems with samples adsorbing on tube walls (dilute DPPH, for example).
   b) The effect of tube materials and samples producing and augmentation or reduction in microwave power is important for all systems, no matter whether a single or dual sample cavity is used. E- and B-field inhomogeneities produced by different dielectric properties of sample and reference, for example, cannot be eliminated by even very careful corrections.
   c) Resonators - Several good modes for quantitative work include TE104, TE011, LGR, BLGR. The use of rods instead of coils for the production of field modulation may lead to more homogeneous modulation amplitude across a sample. Modulation frequency must be carefully chosen (with respect to sample T_{1e}) so that no passage effects are produced. VHF-EPR presents an entirely new set of problems. A reference material situated in the resonator to normalize signal amplitudes seems almost a necessity!
   d) Temperature - It is desirable to have reference materials stable over a range of at least 15 to 30□C.
3. Data Collection and processing
   a) Gaussian lines need a field sweep width of 20× the peak-to-peak linewidth in order that the integrated intensity include 98% of the sample. Knowledge of the lineshape is essential in determining the proper parameters for accurate work. Spectral simulation, in order to determine the key factors influencing signal amplitudes in the sample, seems essential before accurate quantitative work can be accomplished.
   b) Baseline problems are thorny. It may be possible to avoid some of these problems by:
      1) simulation of spectra
      2) numerical baseline correction
      3) digital subtraction of baseline
      4) Fourier transformation of data and elimination of low-frequency component

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ELECTRON SPIN RESONANCE OF RADICALS AND METAL COMPLEXES, 1st INTERNATIONAL CONFERENCE OF THE POLISH ESR GROUP, ZAKOPANE, POLAND, May 31-June 4, 1993. The 1st International Conference of the Polish ESR Group "Electron Spin Resonance of Radicals and Metal Complexes," organised by the Institute of Nuclear Chemistry and Technology, Dorodna 16, 03-195 Warsaw, Poland, (Organising Committee: Andrzej Chmielewski, Hanna B. Ambroz, Zbigniew Zimek) was held in Zakopane situated in the Tatra Mountains National Park.

56 scientists from 6 countries (Germany, Great Britain, Italy, Poland, Sweden) attended the Conference and presented their works on ESR of biochemistry, organic chemistry, inorganic chemistry, metal complexes and on modern development of magnetic resonance techniques.

The book of abstracts had been edited and was presented to the participants upon arrival. The Conference Proceedings will be published in a special edition of the Journal Radiation Physics and Chemistry.

The plenary lectures were delivered by J. Stankowski - EPR in Fullerenes; J. Kroh - Electron Interaction with Stabilizing Matrix; S.K. Hoffmann - Electron Spin-Echo Studies of Spin-Spin Relaxation Processes; B.C. Gilbert - Studies of the Generations and Reactions of Free Radicals in Chemical and Biochemical Systems; M.C.R. Symons -ESR Studies of Radiation Damage to DNA and Proteins; H. Kurreck - Mimicking Primary Processes in Photosynthesis--Covalently Linked Porphyrin Quinones; A. Charlesby - Pulsed NMR Studies, T_2 Relaxation and Physical Properties of Macromolecules; M. Brustolon - Molecular Dynamics of Radicals in the Solid State--ESR, ENDOR, and PULSED ESR Studies; A. Plonka - Dispersive Kinetics of Radiation-induced Species in Condensed Media; and W. Froncisz - Multiquantum ESR Spectroscopy.

Two competitions were conducted in the course of the Conference - for the most active participant in discussions and for the best poster. The Jury, Prof. Gilbert, Prof. Michalik, and Dr. Krzyminiewski, awarded two first prizes (ex equo) to Prof. Martyn Symons and Prof. Harry Kurreck for the most active participation in the discussions, and to Anna Zalewska, Dr. Iwona Wawer, and Prof. Zbigniew Kecki for the best poster, "Effect of Gallotannins on DPPH Radicals."

Due to our eminent scientist participants, all the lectures were very interesting and the poster session was busy and successful.

The social programme was comprised of an excursion to the Morskie Oko (Eye of Sea) lake, a remnant of the Ice Age, surrounded by Mieguszowieckie Peaks, and the conference dinner with a performance by the local Tatra Mountain Highlander Music and Dance Group.

The picturesque surroundings of the conference site, friendly spirit and organisation have gained the good opinion of our foreign and home guests, as we conclude from the many letters we have received since the Conference.

Professor Hanna Ambroz
Warszawa, Poland

WORKSHOP ON *IN VIVO* EPR AND EPR STUDIES OF VIABLE BIOLOGICAL SYSTEMS at DARTMOUTH MEDICAL SCHOOL, HANOVER, NEW HAMPSHIRE, USA, October 17-21, 1993

Theme and attendees

This report attempts to summarize some of the predominant themes and conclusions of the workshop. Copies of the complete program, list of attendees, and abstracts can be obtained for the cost of reproduction and mailing ($10) from H. Swartz, HB 7252, Strasenburgh Hall, Dartmouth Medical School, Hanover, NH, 03755, USA. The overall theme was the special opportunities and the special problems associated with carrying out EPR studies in functional biological systems. The meeting was held at Dartmouth Medical School, Hanover, NH, USA on October 17-22, 1993 under the sponsorship of the IERC (supported by NIH) and Dartmouth Medical School (Department of Radiology). Bruker provided additional financial support. There were approximately 70 attendees from 15 countries. Most or all of the laboratories with major programs in *in vivo* EPR were represented, including groups from NIH, U. of Chicago, Yamagata Technopolis, Johns Hopkins, Ohio State U., Showa U., U. of L'Aquila, Dartmouth/U. Illinois, and U. of Surrey.

Studies on Intact Animals

The studies on intact animals followed several different themes. The key variables in the approaches that were discussed included spectroscopy vs. imaging, localized vs. non-localized spectroscopy, frequency of the EPR spectrometer, the use of continuous wave vs. pulsed techniques, and the type of biological parameters and endpoints that were addressed.

Continuous wave vs. pulsed EPR Laboratories from NIH and the University of Surrey (UK) reported on early results using pulsed EPR techniques at low frequencies (250-280 MHz). While the early results have been promising, considerable technical problems have been encountered because of the short relaxation times of the nitroxides and implementation of this approach for biological problems will be dependent on overcoming these technical problems.

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Alternative approaches to *in vivo* EPR Results also were presented (Aberdeen U. and URA du CNRS, Strasbourg) on the progress of related techniques which seek to use double resonance involving nitroxides to measure phenomena *in vivo*. The detection is via NMR, which provides potential means to exploit the instrumentation developed for NMR imaging to reflect the EPR transitions. Potentially these approaches could be used to measure local concentrations of nitroxides and oxygen. While impressive progress continues to be made with this approach, additional technical developments are needed to attain the sensitivity needed for most biological applications.

Frequency of the EPR spectrometer Most of the results dealing with measurements that led to data applicable to specific biomedical problems were done with continuous wave, low frequency EPR (1 GHz) and the results are described below. Several laboratories (U. of Chicago, L'Aquila University, Ohio State University) are focusing on the use of continuous wave, very low frequency EPR (about 150-300 MHz) for *in vivo* studies because of the greater depth of penetration of the electromagnetic fields at these frequencies. The ability to go to these depths (several cm) would greatly facilitate applications to larger animals including, potentially, use in clinical medicine. The results of these approaches are promising although to date they principally have produced results on feasibility rather than solutions to biological problems. These efforts have been augmented by some very clever approaches to obtain maximally useful paramagnetic materials (see paragraph on oxygen sensitive paramagnetic materials).

Spectroscopy vs. imaging The initial goal of many of the instrumental developments focused on imaging and while this remains an important part of many programs, to date most of the biologically relevant results have been accomplished with localized spectroscopy. Some impressive results were reported on feasibility studies of imaging, especially for the concentration of nitroxides and of oxygen in the heart (Johns Hopkins) and the whole animal (U. of Chicago) and the distribution of nitroxides in animals or model systems (U. L'Aquila, Ohio State U., Yamagata Technopolis, Showa U.). At this time, however, the use of localized spectroscopy clearly dominated in reports which presented results that added significantly to the understanding of important biomedical problems. The advantage of this approach, at this time, is the ability to get a good signal/noise ratio and, often, sufficient spectral resolution to utilize the full amount of information that potentially is available in EPR spectra. Several different methods of localization where employed, with the predominant methods being localization on the basis of the sensitive volume of the detector and localization on the basis of the position in the tissues of particulate paramagnetic materials. The particulate paramagnetics also can be exploited to provide data simultaneously from several locations, using several particles and one dimensional magnetic field gradients. The biomedical results from spectroscopy are described below.

Results of potential biomedical importance There was an impressive number of reports in which results were presented that demonstrated that *in vivo* EPR techniques have come of age in terms of immediate applicability to important problems. The parameters that were measured most frequently were the concentration of oxygen and the concentration of nitroxides.

Measurements of the concentration of oxygen These types of measurements appear to be the ones that are the most immediately applicable to solve critical problems in biomedicine. This is due to the need for making such measurements *in vivo* and the lack of other means that can make these measurements with the accuracy, sensitivity, and repeatability achievable with EPR. Three of the laboratories (Dartmouth, U. of Chicago, and Johns Hopkins) have been especially active in this area (perhaps non-coincidentally all three are headed by physicians and are aiming towards clinical applications where this approach may be especially important). Results were presented in which the concentration of oxygen was measured in liver, brain, heart, joints, skeletal muscle, kidneys, and tumors (Dartmouth/Illinois); whole body and tumors (U. of Chicago); and heart (Johns Hopkins). In each of these systems there are critical physiological, pathophysiological, and therapeutic phenomena which are dependent on the concentration of oxygen and which now may be addressed directly using EPR methods.

One of the keys to the development of EPR as a leading method to measure the concentration of oxygen has been the development of paramagnetic materials that have high sensitivities to the concentration of oxygen. Nitroxides have been used for these types of measurements for many years and continue to be very effective, as demonstrated by the Johns Hopkins group. The University of Chicago group has developed an isotopically substituted nitroxide which, in combination with appropriate computer manipulations of the EPR spectra, can provide both enhanced sensitivity to the concentration of oxygen and the concentration of the nitroxide. The latter measurement is very important because it provides a means to overcome a potential major limitation of the uses of nitroxides to measure the concentration of oxygen *in vivo:* the effects on the spectra of the nitroxide concentration changes which occur because of bioreduction.

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The development of particulate paramagnetic materials that are very sensitive to oxygen and also very stable appears to offer the most sensitive and versatile approaches to the measurement of the concentration of oxygen and have been the basis of the first EPR study in a living human (Dartmouth group, using India ink). Several particulate materials have been developed/introduced by the Dartmouth/Illinois groups including lithium phthalocyanine, fusinite (a type of coal), chars (especially from carbohydrate precursors), and India ink (based on carbon black). The latter is being considered as the basis for the introduction of an EPR apparatus for the measurement of the concentration of oxygen in patients.

Measurements of the concentration of nitroxides. There also were a number of reports in which *in vivo* EPR was used to obtain very useful data linked to the concentration of nitroxides. These included monitoring the conversion of a drug (nitrosobenzene) to a nitroxide (Ohio State U.), following the reduction of nitroxides (L'Aquila U., Showa U.), measuring antioxidant activity using ascorbate (Showa U.), and monitoring the release of pH sensitive nitroxides (Humboldt U. Berlin/Dartmouth).

Studies in model systems and *in vitro*

The versatility and applicability of EPR techniques for the study of biological systems at these levels of organization were well illustrated by a series of presentations that included: the use of EPR to measure the concentration of oxygen in cellular systems (U. of Illinois, Dartmouth); measuring radiation doses using teeth (Moscow); following changes in the motion of membranes in living cells and model systems (Harvard, U. of Indiana-Purdue, Einstein Col. Med., U. Ljubljana); imaging of small pieces of tissues or cellular aggregates at X-Band (J. Stefan Institute) or higher frequencies (U. of Illinois/Moscow Inst. of Chem. Phys.); following generation of free radicals during differentiation (Tech. U., Berlin); following metabolic processes by reduction of nitroxides (Meiji Col. Pharm, Humboldt U. Berlin, Dartmouth) or reactions with ascorbate (Cambridge U.); following the concentrations and ligands of metal ions (Dartmouth, Humboldt U. Berlin); measuring the amounts of SH-containing materials in cells (Weizmann Institute); and the development of contrast agents for MRI (U. Louvain).

Studies of nitric oxide and other reactive intermediates

This is an area of very rapid development, especially in regard to the measurement of nitric oxide, the "molecule of the year". A variety of innovative and effective new means to detect and perhaps quantify such intermediates were described by investigators from Medical College of Wisconsin, NIEHS, University of Oklahoma, U. of Illinois, and Dartmouth. The complex nature of the measurements were discussed very well and it was apparent that with sufficient expertise and care this approach can be extremely valuable, while less sophisticated users are very likely to be mislead by the apparent simplicity of the technique.

Report by Prof. Harold M. Swartz
Dartmouth Medical School

BOOKS & PROCEEDINGS

Proceedings of The Polish-American Workshop on EPR Spectroscopy & Imaging in Biology & Medicine

Most of the papers presented during the Workshop (organized by the Polish Biophysical Society and held on November 30 through December 5, 1992, at the Jagiellonian University, Krakow, Poland) will be published as a special EPR issue of Current Topics in Biophysics. The Workshop purpose was to summarize the results of collaborative research done so far by the participating scientists, and to discuss its future, as well as to consider new joint projects. It was supported by the State Committee for Scientific Research in Warsaw.

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This two-volume issue is 100 pages and can be ordered for $2.50 US ($1.00 for the volume - $1.50 for surface rate mailing cost anywhere in the world), which would have to be transferred to the account number 47513-131935-132 in PKO BP. I.O. Lodz, belonging to the Polish Biophysical Society. U.S. readers may find it more convenient and less expensive to mail a check for $2.50 to: Polonia Travel Agency, Inc., 1130 West Lincoln Ave., Milwaukee, WI 53215. Please make check payable to "Current Topics," account #01522200, Lincoln State Bank, Milwaukee. Remember to enclose with your check the address to which the special issue is to be sent; allow at least 2 months for surface mail delivery after the issue is in print. Note that the regular individual subscription rate is $4.00 US per issue (without postage), whereas institutional rate is $8.00 US. The amount of $1.00 US per issue means that a significant (75%) promotional reduction in price is offered to anybody on the mailing list of the International EPR(ESR) Society. Readers of the EPR Newsletter who need more information about payment from other countries may contact Mrs. M. Elas, Jagiellonian University, Laboratory of Radiospectroscopy of Cancer, Institute of Molecular Biology, Al. Micklewicza 3, Krakow 31-120, Poland, ☎: 48-12-341-422; FAX: 48-12-336-907; E-mail: martyna@mol.ul.edu.pl, TELEX: 032-22-97 UJ PL.

The meeting of 50 participants, mainly from Poland, addressed the following topics: *In vivo* EPR spectroscopy (Swartz, USA), *In vivo* EPR spectroscopy and imaging of free radicals in the heart (Zweier, USA), Photoreactivity of retinal pigments (Sarna, Pol.), Metal-binding properties of neuromelanins (Korytowski, Pol), EPR criteria of tumor-host interactions (Plonka, Kaminska, Lukiewicz, Pol.), Evaluation of implant-recipient interaction by EPR spectroscopy (P. & B. Plonka, Lukiewicz, Pol.), Using very low-frequency EPR to define bulk characteristics of pharmacologic compartments of specific tissues in vivo (Halpern, USA), Whole-body S-band *in vivo* ESR studies on bioreduction of nitroxides in new-born mice (Cleszka, Elas, Wojcik, Dubis, Pajak, Lukiewicz, Pol.), Site-directed spin labelling studies on protein structure and dynamics (Hubbell, USA), ESR measurements in the presence of external electric fields (Froncisz, Pol.), Measurements of the concentration of oxygen under biologically pertinent conditions (Swartz, USA), Spin- label oximetry in dense cell suspension: problems in closed- and open-chamber methods (Ligeza, Swartz, Subczynski, Pol.-USA), Changes in the redox properties of normal and neoplasic cells during cell cycle (Panz, Pol), Bacterial mutant strains unable to reduce nitroxides (Lukiewicz, Nealson, Saffarini, Pol-USA).

Information reported by S. J. Lukiewicz

Principles of Electron Spin Resonance, a new title in the **Ellis Horwood Series in Physical Chemistry** (*Series Editor: T.J. Kemp, Dept. of Chemistry, Univ. of Warwick*), is available from Simon & Schuster. Appr 400 pages, Hardback isbn: 0-13-721762-5, approx. £75, or $127.00. Published June 1992. Ellis Horwood Ltd., Market Cross House, Cooper Street, Chichester, West Sussex, PO19 1EB, UK. *Address orders to: International Book Distributors, 66 Wood Lane End, Hemel Hempstead, HP2 4RG, UK.*

NOTICES OF MEETINGS

INTERNATIONAL CONFERENCE on BIORADICALS DETECTED by ESR SPECTROSCOPY, Institute for Life Support Technology, Yamagata, Japan, June 12-16, 1994.

The organizers are Hitoshi Kamada, Yamagata Technopolis Foundation (YTF), president, and Hiroaki Ohya-Nishiguchi (YTF), general secretary.

The conference will treat an aspect of life-support technology with special attention to ESR spectroscopy including new technology, technology transfer, ESR imaging, spin trapping and labeling, metalloproteins, medical applications, antioxidants and food sciences, and characterization of bio-materials. The conference program will include opening lecture, plenary lectures, session lectures, invited reports, original research contributions, and poster session.

YTF is now organizing a world-wide research center for investigating bioradicals based on ESR spectroscopy, *Institute for Life Support Technology (LIST)*. The research center was opened in April, 1993. Thus the conference has yet another meaning–namely, celebrating inauguration of the kernel of its researches on bioradicals.

The organizing committee will try to do their best in involving you in the warm and friendly atmosphere of Yamagata, offering the nature and natural foods most famous in Japan, *the other side of Japan.*

Scientific scope of the Conference: The conference will treat all aspects of bioradicals with special attention to ESR spectroscopy. Sessions planned: 1) New technology and technology transfer; 2) ESR imaging; 3) Spin trapping; 4) Spin labels and oximetry; 5) Metal complexes and metalloproteins; 6) Biomedical applications; 7) Antioxidants and food sciences; 8) Tissues, cells and biomaterials; 9) Others.

The Organizing Committee consists of: H. Kamada (YTF), *Chairman*; H.Ohya-Nishiguchi (YTF)*, *General Secretary*; M. Hiramatsu (YTF), *Secretary*; T. Akatsuka (Yamagata Univ.); N. Hirota (Kyoto Univ.)*; M. Inoue (Osaka City Univ.)*; Y. Ikegami (Tohoku Univ.); M. Iwaizumi (Tohoku Univ.); K. Kuwata (Osaka Univ.); A. Mori (Okayama Univ.); H. Nakazawa (Tokai Univ.)*; E. Niki

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(Univ. of Tokyo); T. Ogata (Yamagata Univ.); K. Ohno (Univ. Industrial Technology)*; H. Sakurai (Kyoto Pharm. Univ.)*; T. Shiga (Osaka Univ.), J. Sohma (Kanagawa Univ.)*, H. Utsumi (Showa Univ.)*; T. Watanabe (Tokyo Univ. Marine Science)*; T. Yoshikawa (Kyoto Pref. Univ. of Medicine). (**program committee*)

The International Advisory Board is E.G. Janzen (USA), E. Niki (Japan), L. Packer (USA), H.M. Swartz (USA), M.C.R. Symons (UK). For information, contact Dr. Midori Hiramatsu, Institute for Life Support Technology, Yamagata Technopolis Foundation, 683 Kurumanomae, Numagi, Yamagata 990, Japan, 81-236-44-8088; fax: 81-236-44-9640.

SEVENTEENTH INTERNATIONAL EPR SYMPOSIUM at the 36th Annual Rocky Mountain Conference, Denver, CO, USA, July 31-August 4, 1994.

To be held at the Hyatt Hotel and cover all aspects of EPR spectroscopy. As 1994 is the 50th anniversary of Zavoisky's discovery of EPR in Kazan, we plan a special celebration in cooperation with the Zavoisky Institute. Representatives from the Zavoisky Institute at Kazan are expected to participate in the Denver conference. In addition to our traditional sessions on new EPR techniques and applications, there will be talks by early workers in the field and a celebratory banquet at the Denver Phipps Conference Center. Lectures will highlight the contributions of EPR studies in many disciplines including EPR in biology, organized by Harold Swartz, and a joint NMR/EPR session, organized by Hans Thomann. The recipients of Gold and Silver Medal awards from the International EPR Society will present the lectures: Jack Freed, Keith A. McLauchlan, Harold M. Swartz, and Wojciech Froncisz. Time for posters will be expended to include an evening poster session with refreshments. An open house Sunday evening at the University of Denver will highlight the Bruker ESP380 and German beer. The preliminary program was assembled prior to mailing this Newsletter, but posters can still be added. If you have not yet received a meeting notice, contact Profs. Gareth R. Eaton or Sandra S. Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208, USA. ☎: 303-871-2980 or 303-871-3102; FAX: 303-871-2254; E-mail: seaton@ducair.bitnet.

THIRTEENTH ANNUAL SCIENTIFIC MEETING AND EXHIBITION OF THE SOCIETY OF MAGNETIC RESONANCE , San Francisco, CA, August 6-12, 1994

Site: San Francisco Hilton Hotel. *Advance registration deadline*: July 6, 1994. *Contact*: Society of Magnetic Resonance, 1918 University Avenue Suite 3C, Berkeley, CA, USA. ☎: 1-510-841-1899; FAX: 1-510-841-2340.

XVIth INTERNATIONAL CONFERENCE ON MAGNETIC RESONANCE IN BIOLOGICAL SYSTEMS, "De Koningshof," Veldhoven, the Netherlands, August 14-19, 1994.

The *Scientific Program* will consist of plenary sessions, symposia in parallel sessions, special interest lectures and poster sessions. The official language of the ICMRBS is English; no simultaneous translation will be arranged. The ICMRBS is a biennial event. The last three conferences were organized in Madison (USA), Warwick (UK) and Jeruzalem (ISRAEL). Because the XVIth ICMRBS marks the 30th year for this conference series, a special historical session will be organized in cooperation with M. Cohn, O. Jardetzky and R.G. Shulman. The scientific programme will furthermore include topics in the following areas:

- Proteins, structure and function
- Protein structure determination
- Protein dynamics and folding
- Nucleic acids, structure and dynamics
- Protein-nucleic acid interactions
- Protein-peptide interaction
- Structural and dynamic aspects of biological membranes
- Glycoconjugates, structure and dynamics
- Solid state NMR of biological systems
- Approaches to magnetic resonance *in vivo*
- Aspects of functional imaging
- NMR studies of cells and tissues
- Advances in magnetic resonance imaging and microscopy
- Macroscopic localized spectroscopy for metabolic processes
- New developments in biological applications of EPR
- NMR of quadrupolar nuclei in biological systems
- Metalloproteins
- New experimental methods
- Photosynthesis

Deadlines: abstracts - June 15; final registration - June 15. For scientific and general information, contact: Secretariat XVIth

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ICMRBS, Bijvoet Center for Biomolecular Research, Padualaan 8, NL-3584 CH Utrecht, the Netherlands; ☎: 31-30-53-2652/2184/3801; FAX: 31-30-53-7623/54 0980.

INTERNATIONAL CONFERENCE ON RADICAL IONS, Dalhousie University, Halifax, Nova Scotia, Canada, August 21-26, 1994.

The *Scientific Program* will include plenary lectures, invited talks, and poster presentations. The conference will cover a wide spectrum of topics involving radical ions in chemistry, possibly including: spectroscopy of radical ions; gas phase studies; ultrafast studies; organic reactions and mechanisms; low temperature matrix studies; theory, structure and dynamics; ET in photosynthesis; and solvation effects.

Organizing Committee: D.R. Arnold (Dalhousie Univ.), P.H. Kasai (IBM-Almaden), J.A. Pincock (Dalhousie Univ.), and A.D. Trifunac (Argonne Natl. Lab.). *Registration fee*: $250 (Canadian), to cover the cost of the reception, conference dinner, etc. *Accommodations* in the Dalhousie University dormitories have been arranged. Halifax is easily accessible from major travel hubs in both Canada and the United States.

The conference will begin with a reception on Sunday, August 21, 1994, and end at 1:00 pm on Friday, August 26, 1994. For those arriving early, a Sunday outing is planned; accommodations on Saturday evening will be available.

For information, write to: A.D. Trifunac, Argonne Natl. Laboratory, Chemistry Div., 9700 S. Cass Ave., Argonne, IL 60439, USA FAX: 1-708-252-4995; e-mail: bowers@anlchm. The 2d circular will be mailed to all respondents in early 1994.

XXVII CONGRESS AMPÈRE ON MAGNETIC RESONANCE, Kazan, Russia, August 21-27, 1994.

The scientific program will include plenary and invited lectures, symposia, and poster sessions covering the latest achievements in current research, and new developments, trends, and applications in the field of magnetic resonance. Special attention will be given to the following subjects:

- EPR, NMR and NQR Microimaging and Material Science
- Glasses, Liquid Crystals, Polymers
- Low Dimensional Systems
- Magnetic Resonance in Very High Fields
- Magnetic Resonance of Intermediates
- Modern Developments in Solid State NMR
- Multiple Resonance and Multi-Dimensional Spectroscopy
- New Materials (High - Tc, Cn, etc.)
- New Methods and Techniques
- Non-Equilibrium Processes and Non-Linear Phenomena
- Phase Transitions
- Spin and Molecular Dynamics
- Spin Polarization Phenomena
- Systems with Orbital Degeneracy
- Time Domain EPR.

Invited speakers include: A. Angerhofer (Stuttgart), B. Bleaney (Oxford), B. Bluemich (Aachen), G. Bodenhausen (Lausanne), M. Bowman (Richland), M. Brustolon (Padova), L.C. Brunel (Grenoble), R. Ernst (Zürich), M. Goldman (Paris), U. Haeberlen (Heidelberg), R. Kaptein (Utrecht), B.I. Kochelaev (Kazan), Yu. V. Yablokov (Kazan), Ya. S. Lebedev (Moscow), M. Mehring (Stuttgart), K. Möbius (Berlin), J. Schmidt (Leiden), J.U. von Schuetz (Stuttgart), A. Schweiger (Zürich), H. Spiess (Mainz), J. Stankovski (Poznan).

The official language at the Congress is English. Young scientists and students are strongly encouraged to participate. Students will pay significantly reduced registration and accommodation fees. The Congress will take place in the Cultural Centre of Kazan State University (founded 1804); it has modern, well-equipped facilities for scientific meetings. At the Congress, the 1994 Zavoisky Award will be presented. Previous Zavoisky Awardees are Dr. W. Mims and Prof. B. Bleaney.

Organizing Committee: Prof. Kev M. Salikhov, Chairman and Dr. Nail M. Suleimanov, Scientific Secretary. ***Program Committee:*** Prof. A.V. Aganov (Kazan), Prof. V.A. Atsarkin (Moscow), Prof. E. Hahn (Berkeley), Prof. B.I. Kochelaev (Kazan), Prof. E.T. Lippmaa (Tallinn), Prof. Yu. N. Molin (Novosibirsk), Prof. I.V. Ovtchinnikov (Kazan), Prof. K. M. Salikhov (Kazan), Prof. D. Stehlik (Berlin). ***Executive Committee:*** I.A. Aksenov, V.A. Khramov, R.B. Malikova, Dr. R.Sh. Safin, Prof. M.S. Tagirov, E.A. Turiyansky.

Please indicate your intent to participate as soon as possible. Registration ends May 31, 1994. Send your name, address, phone, FAX, and E-mail to Dr. N. Suleimanov, Zavoisky Physical-Technical Institute, Sibirsky trakt 10/7, Kazan, 420029, Tatarstan, Russian Federation. ☎: 7-84-32-760503; FAX: 7-84-32-765075; TELEX 224 864 PTB SU: E-mail: aplmr@adonis.iasnet.com. The organizers are thankful to our magnetic resonance colleagues from the Free University of Berlin for support and encouragement.

EUROPEAN ESR MEETING ON RECENT ADVANCES AND APPLICATIONS TO ORGANIC AND BIOORGANIC MATERIALS, Paris, September 5-9, 1994.

Organized by the European Federation of ESR Groups presently consisting of: ESR Group of the Royal Society of Chemistry (UK), Gruppo Italiano di Resonanza di Spin Elettronico (I), Nederlandese EPR Discussie Groep (NL), Polish ESR Group (PL), Bulgarian ESR Group (Bul), and Groupe d'Application de la Résonance Paramagnétique Electronique (F). *Organizing committee*: Pr. J. Raffi (CEA/Univ. Marseille), Dr. B. Catoire (ENSAM - Paris), Dr. A.M. Riquet (INRA - Jouy-enb-Josas), Dr. J.M. di Meglie (Coll. France), Dr. J. Viret (CRSSA - La Tronche), Dr. C. Giannotti (ICSN-CNRS - Gif-sur-Yvette), Dr. Soulié (CEA - Saclay), Pr. A. Rassat (ENS - Paris), and Pr. J. Verdu (ENSAM - Paris). *Steering & Scientific Program Committee*: Pr. Klaus Möbius, *Chairman*, (Freie Univ. Berlin), Dr. B. Catoire (ENSAM Paris), Pr. J. Raffi (CEA/Univ. Marseille), Dr. A. Alberti (ICOCEA-CNR Bologna), Pr. M. Brustolon (Univ. Padova), Dr. D. Beckert (Max Planck Group Leipzig), Pr. H. Kurreck (Fr. Univ. Berlin), Pr. A.G. Davies (Univ. London), Dr. C.C. Rowlands (Univ. Cardiff), Pr. H. Ambros (Ins. Nucl. Chem. Lodz), Pr. A. Hoff (Univ. Leiden), Pr. E. de Boer (Univ. Nijmegen), and Pr. N.D. Yordanov (Bulg. Acad. Sci.). *Secretariat*: Dr. Bernard Catoire, GARPE,

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ENSAM, 151 Boulevard de l'hôpital, 75013 Paris, FRANCE. ☎: 33-1-24-62-99; FAX: 33-1-44-24-63-82. The European Symposium will be held at the Ministére de l'Enseignement et de la Recherche, 1 rue Descartes, 75005 Paris "Carré des Sciences"; the entrance to the lecture Hall "Poincaré" is 25 rue de la Montagne-Sainte Geneviève, 75005 Paris. The registration will be open on Monday morning September 5th at 8:30 am and the meeting will close on Friday the 9th. The accommodations will be in hotels in the city and can be chosen from a number of hotels of various categories. A limited number of individual rooms in the Cité Universitaire de Paris, 19 Boulevard Jourdan, close to the Parc de Montsouris, will be available.

Contact: GARPE - Dr. Bernard Catoire - ENSAM - 151, blvd. de l'Hôpital - 75013 Paris, FRANCE. ☎: 33-1-44-24-62-99; FAX: 33-1-44-24-63-82. (A second circular with the scientific program will be sent in July 1994.)

III INTERNATIONAL SYMPOSIUM ON MAGNETIC FIELD AND SPIN EFFECTS IN CHEMISTRY AND RELATED PHENOMENA, Chicago, Illinois, USA, September 25-30, 1994.

Scope of the conference: Spin chemistry and magnetokinetics originated in the late sixties with the discoveries of the radical pair mechanisms of CIDNP (chemical induced dynamic nuclear spin polarization) and CIDEP (chemical induced dynamic electron spin polarization). Currently spin chemistry covers a diverse scope of subjects ranging from natural photosynthesis to artificial photosynthesis, from magnetobiology to isotope separation. The subjects of CIDNP and CIDEP are now powerful spectroscopies for the unraveling of chemical reaction mechanisms and are based on an advanced understanding of spin chemistry. That small to large magnetic fields can affect the outcome of chemical reactions remains a fascinating topic today and is pursued by workers worlwide.

Topics to be covered:

- Magnetic Field Dependent Processes: in Solution, in the Gas Phase, in Solid State, on Surfaces, in Micellar Systems, in Supramolecular Aggregates, in Photosynthesis, in Enzymatic Reactions
- Magnetic Isotope Effects and Separation
- Spectroscopic Applications: Novel Developments in: CIDNP, CIDEP, RF and MW Stimulated CIDNP, RYDMR, ParaHydrogen Spin Labeling
- Magnetokinetic Theory
- Spin Chemistry and Magnetobiology
- Nuclear Spin Statistics Chemistry.

To receive further information regarding this meeting, please contact Dr. James R. Norris, Argonne National Laboratory, Chemistry Div., Argonne, IL 60439, USA; ☎: 1-708-252-3544; FAX: 1-708-252-9289; E-mail norris@anlchm.chm.anl.gov

INTERNATIONAL SOCIETY FOR FREE RADICAL RESEARCH, 7th BIENNIAL SCIENTIFIC MEETING, Sydney, Australia, November 7-11, 1994.

The conference will be held at the spectacular new Sydney Convention Centre, overlooking Sydney Harbour and adjacent to Sydney's central business district.

. The Scientific programme will include the application of free radical research in chemistry, biology, nutrition and medicine as well as environmental issues. Leading international and local experts will address such topics as cardiovascular diseases, cancer, aging, arthritis, vitamins and many other subjects in which the relevance of free radicals is being increasingly recognised. Chemistry of radical reactions, biochemistry, physiology and pathology and new topics not previously covered by SFRR meetings will be discussed, both in lectures and workshops held on each section.

For further information, contact Margaret Blackwell, ISFRR '94 Secretariat, Abacus Management Pty Limited, Box 77 PO, Pymble NSW 2073, AUSTRALIA; ☎: 61-2-983-9330; FAX: 61-2-983-9307.

EMARDIS-95, Sofia, Bulgaria, June, 1995.

The aim of the workshop is to cover all aspects of recent development in the theory, methodology, experimentation, instrumentation, etc. of the qualitative and quantitative aspects of Electron Magnetic Resonance (EPR, ENDOR, ESE) spectroscopy of disordered systems through lectures, posters and round-table discussions. Participants will be limited to about 40 persons. The official language of the workshop will be English.

For information, contact: N. D. Yordanov (Convener) or M. Zdravkova (Sci. Secretary), Institute of Kinetics and Catalysis, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria; ☎: 35-92-724-917 or 35-92-713-2546 (Yordanov) or 35-92-713-3917 (Zdravkova); FAX: 35-92-756-116 or 35-92-720-038; telex 22729 echban; E-mail: banchem@bgearn. A first circular of the EMARDIS workshop will be distributed in September of 1994.

ISMAR-95, TWELFTH CONFERENCE OF THE INTERNATIONAL SOCIETY OF MAGNETIC RESONANCE, Sydney, Australia, July 16-21, 1995.

This international conference will have sessions covering all major areas of magnetic resonance, including:

- Advances in imaging and microscopy
- Inorganic and multinuclear NMR
- Chemical applications of NMR
- EPR and applications
- Proteins and nucleic acids: structure and dynamics
- Developments in multidimensional spectroscopy
- *In vivo* spectroscopy and clinical applications
- Solid state NMR
- Membranes and liquid crystals
- New technology and experimental methods
- Advances in theory and computational methods

Presentations will be via plenary lectures, invited lectures, colloquia and poster sessions, with special invited lectures from some of the pioneers of NMR to commemorate the 50th anniversary of its discovery. A comprehensive trade exhibition will be held in conjunction with the conference. Companies wishing to display magnetic resonance hardware, software or accessories should contact the conference chairman. The social program will give delegates and their companions opportunities to meet informally and to get to know this magnificent harbourside city. We will be suggesting pre- and post-conference tours for those who wish to travel more extensively around

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Sydney or to other parts of Australia.

For more information, contact Dr. L.D. Field, Chairman ISMAR-95, Department of Organic Chemistry, University of Sydney, Sydney NSW 2006 AUSTRALIA, ☎:61-2-692-2060; FAX: 61-2-692-3329; E-mail: ISMAR-95@biochem.su.02.au

VII INTERNATIONAL SYMPOSIUM ON MAGNETIC RESONANCE IN COLLOID AND INTERFACE SCIENCE (ISMRCIS VII), Madrid, Spain, September 11-15, 1995 (*Preliminary*).

This Symposium, to be held at the central premises of the Consejo Superior de Investigaciones Cientificas (CSIC) in Madrid, Spain, September 11-15, 1995, is a continuation of the previous triennial conferences on the same subject started in San Francisco, USA (1976) and followed on in Menton, France (1979), Torun, Poland (1983), Muenster, Germany (1986), Newark, Delaware, USA (1989) and Firenze, Italy (1992). These symposia have become a major event whose aim is to provide a forum for physicists, chemists, and biologists at which to present and discuss their recent research in the field. The program will include plenary and invited lectures as well as oral and poster presentations. The official language is English. The proceedings will be published as full articles in an archival scientific journal.

Topics: Among the topics to be covered are:

- ●Adsorption, Catalysis and Surface Chemistry
- ●Interfacial Coordination Chemistry
- ●Molecular Sieves, Zeolites and Silicate Surfaces
- ●Intercalation Compounds
- ●Advanced Materials, Ceramics and Composites
- ●Surfaces, Interfaces and Nanostructures of Magnetic and Electronic Materials
- ●Dispersed Systems (including colloids, polymers and gels)
- ●Ordered Systems (including liquid crystals, self-assembling materials and micelles)
- ●Biological Systems, Membranes and Interfaces
- ●New Magnetic Resonance Techniques
- ●Other topics to be included depend upon the response.

Accommodations: The scientific activities will be held on the Campus of the CSIC located close to downtown Madrid. Information on accommodations and social programs will be published later.

Deadlines: Call for papers will be distributed by November 1994, with details about work presentation and relevant deadlines. If you are interested in attending this symposium and receiving next circulars, please supply the following preliminary-registration information, before July 15, 1994, to Dr. José Conesa, Inst. de CCatal. y Petroleoquimica, CSIC, Campus Univ. de Cantoblanco, 28149 Madrid, Spain; Fax 34-1-5854760; E-mail mrcis@icp.csic.es: *Name, Title, Affiliation, Address, Telephone, Fax, E-mail, Telex, Field(s) of interest, Suggestions for specific Conference topics, Tentative title of paper if you plan to submit one.*

Organizing and Program Committee Officers: Javier Soria, Chairman, CSIC; José L. De Segovia, Co-Chairman, CSIC; José C. Conesa, Secretary, CSIC.

POSITIONS WANTED

EPR and NMR Spectroscopist Seeks an Academic or Industrial Position. Biophysicist-solid state physicist, Ph.D. '87, research/teaching experience. Now research worker/teacher at Department of Physical Chemistry, Faculty of Chemical Technology, Slovak Technical University. Research experience: A) liquid- and solid-state EPR spectroscopy of biological, organic and inorganic materials (Bruker 200D SRC NMR Spectrometer with Aspect 2000 Computer). Special research experience: membrane biophysics, drugs-membrane interaction, spin-label EPR spectroscopy (International Training Course, Hungarian Academy of Sciences, Szeged, Hungary). Also sol-gel or glass solid-state EPR spectroscopy; transition-metal spin labels. B) liquid- and solid-state NMR spectroscopy of biological, organic, and inorganic materials (Varian 300 MHz VXR spectrometer). Special research experience: 1D, 2D, and pseudo-3D multinuclear NMR spectroscopy of bioploymers, using Varian Unity 500 MHz spectrometer (postdoctoral fellowship at McGill University, Pulp and Paper Research Center, Montreal, Canada). Also sol-gel or glass multinuclear NMR spectroscopy. Wanted: faculty or research post, or opportunity to teach basic principles of resonance spectroscopy or biophysics. Please contact:

Dr. Milan Mazur, Department of Physical Chemistry
Faculty of Chemical Technology,
Slovak Technical University
Radlinskeho 9, CS-812 37 Bratislava, SLOVAKIA
FAX: 42-7-493-198

EPR Spectroscopist seeks a Postdoctoral Fellowship Position. Semiconductor physicist, 32 years old, Ph.D. '88, research worker of the Institute of Semiconductor Physics (Novosibirsk, Russia). Research experience: EPR of defects in irradiated semiconductors, spin-dependent transport in semiconductors, EPR of paramagnetic centers in quantum size semiconductor structures. Please contact:

Dr. A.A. Karanovich
Inst. Semiconductor Phys.
Russian Acad. Sci., Siberian Branch
pr.Lavrenteva 13, 630090 Novosibirsk, RUSSIA
☎: 38-32-354255;
FAX: 38-32-354265; Telex: 133243 FONON SU;
email: lab24@isph.nsk.su

POSITION OPEN

Postdoctoral Research Position available beginning immediately in organic EPR spectroscopy in solution. Studies in EPR Spin trapping experiments exploring capabilities of new spin traps and new spin trapping methods will be the major emphasis. Also, collaborative work with off campus EPR users will be necessary. Minimum qualifications include a recent Ph.D. in chemistry, biochemistry, or biophysics and experience in EPR spectroscopy.

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Please send a resumé and three letters of recommendation to:
Dr. Edward G. Janzen, Director **or**
Dr. Yashige Kotake, Associate Director
Nat'l Biomedical Cntr for Spin Trapping and Free Radicals
Free Radical Biology and Aging
Oklahoma Medical Research Foundation
825 N.E. 13th Street
Oklahoma City, OK 73104 USA
FAX: 1-405-271-3980 Please, no calls or e-mail.

NATIONAL INSTITUTES OF HEALTH POSTDOCTORAL POSITION available October 1, 1994 to study nitric oxide in a variety of biological systems using ESR. Applicant must have a Ph.D. in chemistry, biochemistry, or biophysics with a strong background in spectral simulation. Candidates must have less than five years postdoctoral experience. Stipends range from $25,000 to $32,000 per year depending on experience. NIEHS is an Equal Opportnity Employer. Send resumé and three letters of recommendation to:
Dr. Ronald P. Mason
National Institutes of Health
National Institute of Environmental Health Sciences
P.O. Box 12233, MD 10-03
Research Triangle Park, NC 27709 USA

EQUIPMENT & SUPPLIES EXCHANGE

FOR OWNERS OF VARIAN EPR SPECTROMETERS:
(1) FIELD SCAN POTENTIOMETERS
(2) REPLACEMENT KLYSTRONS

(1) Varian E-3, E-4 and E-9 and early E-109 users: I have arranged for a custom group order of replacement field scan potentiometers using Varian's specifications and the original vendor part number. These Model #3406 are 30 ohm, 0.06% linearity 3,0 turn pots with a center tap and have infinite resolution. This replacement can solve field stability problems arising from a noisy wiper. If you would like to participate and make this opportunity possible, please contact me regarding your interest. The price would be $723.00 each with a $35.00 handling fee per order plus shipping charges (we need to get 25 to get this price). They have a long shelf life. A purchase order would be required. The expected delivery time is about 160 days. There can be no returns on this order, but a vendor's 1-year warranty would apply.

I can also rebuild these parts, but the turn-around time would be long due to batch requirements. So I recommend an order of at least one new pot, which will allow the old one to be recycled at some later date at a price of around $525.00 depending on the batch size at that time (I would expect most pots are suitable for rebuilding). Please indicate your interest.

(2) Varian V-4500, E-3, E-4, E-9, E-104, and E-109 users: I am also arranging with Varian one large order for replacement Varian X-Band Klystrons. If we have a sufficient quantity, Varian will supply us with possible volume pricing. So I need to know your needs and that you would be willing to commit to a purchase order (at a later date). The pricing would probably be in the $6000 range, and I would extract a $100.00 handling fee per klystron; shipping/ insurance costs are additional. Varian would warranty these for 3 years from purchase date. Delivery times may be long term (~6 months). If you need Q-Band klystrons, let me know, as I expect that these also can be supplied. Prompt response will help in determining the Varian's pricing.

Contact: James R. Anderson at Research Specialties, 5629 N. Maplewood, Chicago, IL, USA 60659.
☎/FAX: 1-312-728-6570.

WANTED: HALL EFFECT SENSOR

We are seeking a Hall effect sensor for the Varian V-4500 EPR (V-2100 B power supply).

Please contact: Eliane Wajnberg, Centro Brasileiro de Pesquisas Fisicas, R Xavier Sigaud 150, 22290-180 Rio de Janeiro Brazil.E-mail: ElianeW@brlncc.bitnet.

WANTED: HALL PROBE

We urgently need a Varian E-4 magnet Hall Probe - P/N - 908742-05 and an E-112 magnet Hall Probe - P/N - 929279-02B. If available, please contact or send to Prof. P.T. Manoharan, RSIC, IIT, Madras - 600 036, INDIA.

REQUEST FOR ASSISTANCE - MANUAL OR TECHNICAL INFORMATION NEEDED FOR HILGER-WATTS SPECTROSPIN.

Our Department of Physics has received a Hilger-Watts Microspin Spectrometer through the generosity of Louvain University. We have Microspin Amplifier and Detector Type FA 206, Nr. 008, Microspin X Band Generator Type W 903, Nr. 960 H and Newport Pagnoll, England, Electromagnet Type D. We did not receive a technical manual for the spectrometer and urgently need one to complete the setup (we also received no resonance cavity or connection guides). If anyone, please, help us to obtain copies of the proper manuals for the above items? Please contact Prof. Dr. Ioan Inţa, Department of Physics, Transilvania University, Str. Colina Universităţii, Braşov 2200, ROMANIA.

AVAILABLE: VARIAN V 4500 MODULES.

Modules for the Varian V4502 EPR spectrometer are available from G. R. or S. S. Eaton at the University of Denver. E-Maii. geaton@ducair.bitnet.

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AVAILABLE: BOXCAR AVERAGER

An inexpensive boxcar averager designed for use in ESE spectrometers is available from the University of Denver. At slow repetition rates it gives about two orders of magnitude better S/N than the well-known PAR 162/164 boxcar. Contact: Richard Quine at the University of Denver, Denver, CO 80208 USA E-mail: rquine@diana.cair.du.edu. ☎: 1-303-871-2419.

OFFERED: HELP IN THE DESIGN AND CONSTRUCTION OF EPR ELECTRONICS

The University of Denver is able to provide design and construction services for EPR-related electronics such as low noise signal pre-amplifiers, timing systems for pulsed EPR, or complete microwave bridges. Contact: Richard Quine at the University of Denver, Denver, CO 80208 USA. E-mail: rquine@diana.cair.du.edu ☎: 1-303-871-2419.

WANTED TO BUY: USED EPR SPECTROMETER

A unit such as a Varian E-4 or E-9 would be ok. Electromagnet (or cavity) is not necessary. If you know of an available unit please contact Mark Rubinstein, Naval Research Laboratory, Washington, DC, 20375, USA; ☎: 202-747-4207.

FIELD SCAN CARDS AVAILABLE FOR COMPUTER CONTROL OF VARIAN FIELD CONTROLLERS

Any Varian magnetic field controller can be modified to permit control of the magnetic field by a computer. An improved scan card design with better documentation at a lower cost is available from the University of Denver. Contact Richard Quine at the University of Denver, Denver, CO 80208 USA; e-mail: rquine@diana.cair.du.edu; ☎: 1-303-871-2419.

ANNOUNCEMENT

INTERNATIONAL OPPORTUNITIES FOR SCIENTISTS AND ENGINEERS

The Division of International Programs of the National Science Foundation (NSF), USA provides support for the following type of international activities:

1. Research Collaboration between U.S. and Foreign Scientists and Engineers:
   - Cooperative research
   - Planning visits
   - Joint seminars and workshops
2. International Research Experiences for Junior Scientists and Engineers:
   - Postdoctoral & Junior Investigator Research Fellowships
   - Dissertation Enhancement Awards
   - Summer Institutes for Graduate Students (in Japan only)

This division of NSF does **not** fund travel to conferences, but other NSF divisions do consider such proposals.

Information on any of the above may be requested by contacting NSF, Forms and Publications Unit, Washington, DC 20550; phone 1-703-306-1130. By bitnet: pubs@nsf; Internet: pubs@nsf.gov. On-line information that you may access by computer is available through their Science & Technology Information System (STIS) - ☎: 1-703-306-0214; E-mail: stisserv@nsf.gov or pubs@nsf.bitnet
(Extracted from NSF publication #91-10 – Revised 10/25/92.)

CORRECTED & NEW ENTRIES FOR THE ADDRESS DIRECTORY (Published for IES Members in Volume 5, No. 2, Summer, 1993)

(A NEW LIST WIL BE DISTRIBUTED TO IES MEMBERS LATER IN 1994.)

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Faniculli, Dr. Marco; Aarhus Univ., Inst. Phys. & Astron., DK-8000 Aarhus C, DENMARK

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Maresch, Dr. Gunter G.; Bruker Analyt. Messt. GMBH, Am Silberstreifen, D-76287 Rheinstetten, GERMANY

Nagy, Dr. Vitaly Yu.; Russian Acad. Sci., Vernadsky Inst. Geochem. & Analyt. Chem., 19 Kosygin Str., Moscow 117975 RUSSIA. ☎:7-95-939-70-35; Fax: 7-95-938-20-54; e-mail: nagy@geochem.msk.su

Sentjurc, Dr. Marjeta; Correct ☎: 386-61-1259-199; Fax: 386-61-273-677

Shvachko, Yuri (not Shvachiko); Correct Address: Kovalevskaya Str. 18 GSP 170; ☎: 7-343-2-444-482; Fax: 7-343-2-445-244; Telex: 721524SIFM SU; additional e-mail: elph@ifm.e-burg.su

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